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BOOK OF ABSTRACTS

in alphabetical order by first author

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

Boron isotopic analysis of Oceanic deposits as a recorder of Continental emergence in the Archean

Avishai Abbo, Horst Marschall, Axel Gerdes

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The onset of plate tectonics on Earth brought about rapid accumulation of continental crust, and the transition of continental crust from being mostly submarine to mostly subaerial. Tracking the timing and rate of continental emergence has broad implications on the onset of plate tectonics and to our understanding of its operation in its early days. Different approaches to study and trace continental emergence address the continental crust itself, whether in specific localities or in compilation of large datasets. Such approaches may be challenged as such that either represent local activity rather than the global regime, or that they might suffer from various kinds of biases. We attempt to overcome some of these shortcomings by utilizing Boron isotopic analysis of Archean and Proterozoic Oceanic sediments. Boron is a continental element that is concentrated in the continental crust over time. The Oceanic Boron budget is mostly controlled by the balance between influx from continental weathering carried by rivers and the out-flux during alteration of Oceanic crust. The onset of widespread continental emergence means the largest Boron influx into the Ocean begins to operate, thus greatly affecting the Oceanic B concentration and isotopic budget. We analyzed samples of Archean and Proterozoic Chert and Iron Formations for B isotopes using in-situ LA-MC-ICP-MS in order to construct the Oceanic Boron isotopic record from that time. Considering the fractionation between seawater and silica/Fe-oxides we observe that Archean seawater was 10-20‰ lighter than modern seawater, indicating a lower volume of emerged continental crust.

Lecture*Topic:* 1.7 Experimental Petrology and Geochemistry**Experimentally determined NH₄⁺ - K⁺ exchange coefficient between phengite and fluids at 700°C/4.0GPa****Nada Abdel-Hak^{1,2}, Axel Kitte³, Jens Kallmeyer³, Monika Koch-Müller^{1,2}, Bernd Wunder¹**¹Section 3.6. Chemistry and Physics of Earth Materials, Deutsches GeoForschungsZentrum (GFZ), Potsdam, 14473, Germany;²Institute of Applied Geosciences, Technische Universität Berlin (TUB), Berlin, 10623, Germany; ³Section 3.7. Geomicrobiology, Deutsches GeoForschungsZentrum (GFZ), Potsdam, 14473, Germany

Phengite is the main nitrogen (N) carrier in high-P/T metamorphosed rocks in subduction zones (e.g. **Halama et al., 2017; Abdel-Hak et al., 2020**). N is incorporated as ammonium (NH₄⁺) substituting for K⁺. The significant amounts of NH₄⁺ observed in natural phengite from the high-P metasediments of the Dora Maira Massif (**Busigny et al., 2003**) suggest that N can be retained during subduction and recycled into the deep mantle. Understanding the pathways of N during subduction, however, requires an understanding of the partitioning behavior of N within the hosting phases (**Mikhail et al., 2017**). Accordingly, we studied the exchange of NH₄⁺ between phengite and fluid experimentally.

Piston-cylinder experiments using the "synthesis exchange technique" (**Zimmermann et al., 1997**) were performed at 700°C, 4.0 GPa for the synthesis of K-NH₄-phengites solid solutions. Starting materials were solid oxide mixtures and chloridic solutions.

After the experiments, solid run products were examined by X-ray powder diffraction with Rietveld analysis, and infrared spectroscopy. Cations in the product fluids were analyzed by ion chromatography.

Resulting coefficients (K_D) for the K- NH₄ exchange range from 0.77±0.13 to 1.42±0.18. Results show that at these P-T conditions, NH₄⁺ partitions equally between phengite and coexisting fluid. **Pöter et al. (2004)** performed partitioning experiments between tobelite (an NH₄⁺-muscovite mineral) and fluid at lower pressures (0.4 & 1.5 GPa). Here, contrary to our results, NH₄⁺ shows preferential partitioning into the fluid phase. This pressure-induced change in the partitioning behavior highlights the significance of high pressures in increasing the extent to which N can be recycled during subduction.

Lecture

Topic: 2.2 From dust to planets

INSIGHTS INTO THE GENESIS OF APOLLO LUNAR SOILS FROM CADMIUM STABLE ISOTOPES

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We present Cd isotope data on Apollo 12 (A12) mare soils and Apollo 16 (A16) highland soils to understand the volatile element distribution and processes of mass-dependent stable isotope fractionation at the lunar surface. Further, thermal neutron capture (*n.c.*) effects, reflected by an enrichment in ¹¹⁴Cd due to neutron absorption by ¹¹³Cd, record the history of near-surface exposure to galactic cosmic rays.

Our results show that Cd concentrations are on average lower in A12 than A16 soils. Covariations between $\epsilon^{112/110}\text{Cd}$ and the maturity index are observed for A12 soils but not for A16 soils. Likewise, the positive covariation between *n.c.* effects and maturity index of A12 soils is lacking for A16 soils. In $\epsilon^{112/110}\text{Cd}$ -Cd space, A12 and A16 soils define distinct negative correlations indicative of a Cd isotope dichotomy. These correlations reflect either Rayleigh fractionation due to evaporative Cd loss or binary mixing between mare basalt, highland feldspathic crust and Procellarum KREEP components. The Apollo 12 correlation intersects the BSE value corresponding also to the composition of the immature and KREEP-rich soil 12033. The $\epsilon^{112/110}\text{Cd}$ -*n.c.* effect correlation in A12 soils constrains further the compositions of the KREEP and mare components to be, respectively, isotopically light and heavy. A corollary of a KREEP composition comparable to the bulk Earth value is that the Moon and Earth share a similar Cd isotope signature. This, in turn, would imply Moon formation from a well-mixed vapor disk without significant isotope fractionation imparted by volatile loss during and following the giant impact.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Petrography and Geochemistry of the Kohistan Batholith Granitoids from the Central Kohistan Magmatic Arc, Northern Swat, Pakistan

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The E-W trending Kohistan magmatic arc developed as an intra-oceanic island arc during the Cretaceous and became an Andean-type margin during Early Tertiary after collision with Karakoram plate. The Kohistan batholith constitutes the major unit of the arc and comprises a range of granitoids, and minor gabbro-diorite and metamorphosed volcanic and sedimentary rocks. This research focuses on the petrologic evolution of the rocks of plutonic association from west central part of the batholith in northernmost Swat to elucidate their geodynamic setting and relationship to crustal growth processes over time. The area was geologically and structurally remapped to obtain new field, petrographic and whole rock major and trace element data.

The studied area contains stock-size to batholithic bodies of granitoids, subordinate migmatites, stocks and plugs of gabbro-norite, doleritic dykes and a small intrusion of a diorite containing spectacular orbicules. The granitoids show textural and mineralogical variation, with some being strongly gneissose and or porphyritic. Amphibole and biotite are common to most rocks. Based on petrographic and geochemical data, the investigated granitoids cover a range of compositions, i.e., granite, granodiorite, tonalite, quartz monzonite, and (quartz) diorite which stretches for 70 km up to eastern Afghanistan. They are calc alkaline, metaluminous to peraluminous, calcic to alkalic, and dominantly magnesian in composition, except a few more fractionated granites which fall in the ferroan field. Our new data suggests, that the different granitoids were emplaced as independent plutons over a considerable length of time.

Poster

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Considering the potential chromite resources of Mirdita (Albania), Troodos (Cyprus) and Muğla (Turkey) ophiolites

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Chromitites are economically relevant sources for chromium, and platinum-group elements (PGE). Since chromium is resistant to corrosion and abrasion, it is a vital item in stainless (74%), alloy steel markets (19%) and refractory materials. The PGE are used in catalytic converters, auto-catalysts, chemical manufacture, electrical products, petroleum refining, and jewelry. The European Commission published the global chromite production in 2020, which amounts to 40 million tons. Currently, the primary chromite production stems from South Africa (46%), followed by Kazakhstan (16%), Turkey (11%), and India (10%). Albania (2%) is the third-largest producer of chromite in Europe after Turkey (11%) and Finland (4%). Although Cyprus has chromite resources, there is currently no economic mining activity in this country. However, Cyprus could be an additional important supplier since it belongs to the European Union and can thus advance as an essential production country for the European Union. Due to the limiting countries mining chromite and the limitation in the refining step, there is a risk that the chromium supply could lead to bottlenecks.

After studying the chromitites of three different places: Mirdita (Albania), Troodos (Cyprus) and Muğla (Turkey) ophiolites from point of Scanning Electron Microscope (SEM), Electron Prob Microanalyzer (EPM). Our preliminary data shows that the chromitites of the different deposits show similarities. However, our data sets also shows that the chromium concentrations in Cyprus are lower compared to the samples from Turkey and Albania. Further research on these samples sets is needed. Therefore, we will conduct Raman spectroscopy and carry out further geochemical and petrological studies to understand the genesis of the chromite deposits.

Lecture

Topic: 6.1 Earth surface processes in extremely water-limited environments

Application of U-Pb LA-ICP-MS dating to unravel climate evolution and surface processes

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Geochronological tools may play an important role in understanding the coupled evolution of biosphere and Earth surface processes. Intermittent wet periods in arid and hyper-arid environments drive mineral precipitation and mineral transformations, which have the potential to be dated with the U-Pb isotopic system.

With the knowledge and expertise gained in the last few years with the relatively new method of laser ablation U-Pb dating of carbonates, we are now embarked mainly, but not only, on the dating of sulfate phases.

We have successfully applied the method to gypsum-anhydrate nodules sampled at variable depths in soil pits. These nodules are formed by repeated hydration-dehydration events of the soil, which is formed by atmospheric deposition of sulfate. By dating them, we are able to track periods of water availability in arid to hyper-arid environments, such as the Atacama Desert. Other samples that were successfully dated to some extent, which are also linked to water supply, are calcretes and silcretes, gypsum wedges, and minerals formed in supergene Cu enrichment processes. Zircon extracted from volcanic ash layers have also been dated to constrain the timing of lake formation.

Poster

Topic: 11.3 Young Scientist Session

The Distribution of Geogenic and Anthropogenic Rare Earth Elements and Yttrium in Major European Rivers: The PANORAMA River Monitoring

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Rare earth elements and yttrium (REY) are vital components in numerous high-technology products and processes. Consequently, they are continuously released into the environment from various point and diffuse sources and have become emerging micro-contaminants in natural waters. The presence of anthropogenic Gd due to the release of Gd-based MRI contrast agents via the effluents from waste water treatment plants is well-documented from all continents except Antarctica. Contamination with anthropogenic La has been reported for the lower reaches of the Rhine River in Germany. However, in spite of these observations of anthropogenic REY in the environment, a systematic overview on the distribution of all naturally occurring geogenic and anthropogenic REY in major European rivers and lakes is still lacking. To fill this gap, waters and organisms (with a focus on mussels) from rivers and lakes in the European Union are studied as part of the EU-ITN "PANORAMA".

We will report first results from recent sampling campaigns, including samples from the Danube River and its major tributaries between its headwaters in southwestern Germany and just downstream of Belgrade, Serbia, from the Seine River in the vicinity of Paris, France, and for major rivers of the Iberian Peninsula in Portugal and southern Spain. These will be compared to data for rivers in the North German Basin (Ems, Weser, Elbe, Havel), the Rhine River and its tributaries between Lake Constance and the German-Dutch border, and several major rivers on the Fennoscandian Shield in Sweden and Norway.

Lecture

Topic: 11.3 Young Scientist Session

The Late Paleogene remnant sea to foreland basin sedimentation along the western margin of the Himalayas, an insight into early Himalayan evolution

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The well preserved late Paleogene sedimentary record of the north Sulaiman Range offers a unique record of the early Himalayan evolution along its western margin. This study is focused on the provenance, biostratigraphy and sedimentary facies analysis of this important sedimentary archive. The petrographic and geochemical analysis of the late Paleogene sandstone units reveals their derivation dominantly from a recycled orogenic and suture belt zone of the nascent Himalayas in the north with some contributions from Indian fore bulge and or cratonic areas in the east-northeast. The source rocks for these sandstones are acidic igneous and low to medium grade metamorphic and uplifted fold and thrust belt sedimentary rocks within a semi humid to humid tropical settings. The biostratigraphic and sedimentary facies analysis shows that epicontinental marine sedimentation took place in inner to outer shelf settings in middle Lutetian to Priabonian times, the deposition in the lower Oligocene time occurred in mid to high tidal flat settings prior to subsequent filling of the north Sulaiman basin in upper Oligocene and Miocene time with fluvial sediments in response to the uplift associated with India-Asia collision.

Poster

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Transtensional fault segments and fluid migration in the Upper Rhine Graben

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The Upper Rhine Graben is utilized for geothermal- and hydrocarbon exploration, and considered for lithium mining from brines. Subsurface exploration requires an understanding of reservoir- and fault properties, the geomechanical response of faults, and associated fluid migration. Slip- and dilation tendency analysis is conducted to identify fault segments in the stratigraphy, which might potentially act as fluid migration pathways.

Fluid migration is reflected by upward hydrocarbon migration of different oil types sourced from the Posidonia shales along fault zones and locally from the Lower Pechelbronn Beds (eg. Bruss 2000). For example, the reservoir quality of the previously explored and hydrocarbon producing Cenozoic Meletta beds is highly variable, decreasing with depth, ranging from 4.5 to 26.3% porosity and 0.09 to 150 mD permeability at ambient conditions (Bruss 2000, Sauer 1981, Schad 1964).

Published stress field and structural data indicated the considered N-S trending fault section of the generally NNE-SSW oriented Leopoldshafen fault 7 km north of Karlsruhe to have a transtensional character enabling fluid migration. High slip and moderate dilation tendencies indicate this fault segment to be favourably oriented within the present-day stress field to slip or creep, depending on rock strength and SGR fault properties.

Lecture

Topic: 11.3 Young Scientist Session

Influence of Quaternary glaciations on subsurface temperatures, pore pressures, rock properties and petroleum systems in the onshore northeastern Netherlands

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Pleistocene ice ages had a profound influence on the subsurface, in parts, until the present day. Ice masses during glacial advances partly covered onshore Netherlands during two glacial periods, the Elsterian and Saalian stages. This study presents a 3D basin and petroleum systems model of the northeastern Netherlands with implemented glacial stages to address the influence of low surface temperatures and the mechanical loading of ice sheets on the subsurface. Two ice sheet thickness scenarios were used to constrain results based on published ice sheet thickness estimates.

Overall, Quaternary glacial stages substantially impact the temperature and pressure distribution in the subsurface. Subsurface temperatures are significantly reduced during glacial stages, leading to lowered present-day temperatures and a low geothermal gradient in the shallow subsurface. In deeply buried sedimentary formations, pressures build up with every glacial advance resulting in overpressures at the present day. Glacial stages do not directly influence the petroleum generation of petroleum source rocks in the area, but high pressures during loading might have impacted petroleum expulsion of the early mature Coevorden Formation. Hydrocarbon accumulations in the Lower Saxony Basin were simulated to investigate the possible effects of mechanical ice loading and unloading on hydrocarbon migration. A loss of Coevorden Formation-sourced hydrocarbons to the surface was calculated in the Lower Saxony Basin during the glacial stages, indicating an influence of glacial loading on the Mesozoic petroleum system.

Lecture

Topic: 7.3 Assessment of the Earth System through Micropaleontology

The Paleocene -Eocene Thermal Maximum indications based on Planktic and large foraminiferal Turnover across the Kurdistan Foreland Basin (N. Iraq)

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The evidence for warming comes from a variety of sources, the most compelling of which is the diversification, extinctions and evolutions of the planktic and benthic forams across the Paleocene -Eocene Thermal Maximum (**PETM**). In Kurdistan foreland basin the PETM event is characterized by the late Paleocene planktic foraminifera biozone (*Morozovella velascoensis*- **P.5**) that is turnover to the by the first appearance and radiations of the shallow benthic foraminifera, (*Alveolina aramaea* Zone.**SBZ.5**, *Alveolina pasticillata* -*Nummulites frassi*-*Nummulites deserti* Zone. SBZ.6). The late Paleocene (Thanetian) predominated warm benthic foraminifera diversification and rapid evolution manifested by several species of the hyaline, porcelaneous walled foraminifera like (*Alveolina*, *Somalina*, *Orbitolites*, *Idalina*, *Nummulites frassi*, *Nummulites deserti*, *Rotalia trochidiformis*, *Lockhartia conditi* *Ranikothalia nuttalli*, *Assilina*). They are also marked by the rapid extinction of late Thanetian aged Ranikothalids, Glomalveolinids(at the upper most of Kolosh Formation) , and the rapid dominance of Alveolinids and Nummulitids in the early Ypresian carbonates (Sinjar Formation). In addition to first appearance and rapid diversifications of the dasycladacean green algae, coralline red algae, echinoids, and bryozoans. They are associated by the unusual morphologies of the giant gastropods and pelecypods as coquina band about 1.m thick. Moreover, all faunal lines of evidence point to rapid variations from cold to warm water condition, and from low CO towards more CO₂.

Lecture

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Quantifying microstructures of Earth materials: Reconstructing higher-order correlation functions using deep generative adversarial networks

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Key to most subsurface processes is to determine how structural and topological features at small length scales, i.e., the microstructure, control the effective and macroscopic properties of earth materials. Recent progress in imaging technology has enabled us to visualise and characterise microstructures at different length scales and dimensions. An approach to characterisation is the sampling of multi-point spatial correlation functions - known as statistical microstructural descriptors (SMDs) - from images. SMDs can then be used to generate statistically equivalent structures having different scales and additional dimensions – this process is known as *reconstruction*. We use higher-order SMDs (*n*-point polytope functions) to characterise two hydrothermally altered rocks as examples of quantifying varying degrees of geometric complexity in the Earth's lithosphere. Using a generative adversarial network (GAN), trained with Wasserstein-loss and gradient penalty, we subsequently reconstruct two-dimensional electron microscopy images of these rocks. In addition to improving the training stability of GANs, we show that our model is capable of reconstructing higher-order, spatially-correlated patterns of complex earth materials, capturing underlying structural and morphological properties. Our approach is critical to address a wide range of geoscientific challenges aiming at reconstructing morphology-dependent physical rock properties to, e.g.: i) increase the number of digital samples from limited real samples to, e.g., assess the variability of rock transport properties; ii) perform upscaling, i.e., generate representative domains from high-resolution images of small complex samples and couple microstructures to macroscopic phenomena; iii) reconstruct 3D microstructures when only 2D images are available.

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Trace metal mobility during magnetite to hematite transformation in iron ores

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Iron oxides are ubiquitous minerals in the earth's crust and earth scientist are utilizing their chemical complexity to characterize rock/ore forming conditions. Compared to magnetite, only few studies exist on hematite, although $\alpha\text{-Fe}_2\text{O}_3$ is an abundant alteration/weathering/metamorphic product in primarily magnetite-bearing rocks and ores – under certain conditions hematite represents the main iron oxide mineral. Hematitization of magnetite (including pseudomorphism after magnetite, i.e., martitization) take place by coupled dissolution-precipitation process (CDR) under redox and non-redox fluid-rock reactions in static or dynamic structural state. These mechanisms have impact on the iron oxide trace elemental budget. In order to understand better the chemistry of metamorphic- and alteration-induced hematitization in various ore settings (iron oxide apatite IOA, Fe-skarns, iron formation and related hematite ore), we report in-situ LA-ICP-MS data from hematite and precursor magnetite. The aims are to test the use of hematite in magnetite discrimination diagrams, and to define element proxies to characterize certain oxide transformation conditions.

Results show that hematitization significantly modify trace metal budgets in iron oxides. Metamorphic hematitization in various domains shows rather consistent depletion of low-valent and enrichment of high-valent elements. Alteration-induced martitization show contrasting mobility, allowing discrimination of hydrothermal from weathering-related condition, even within the same deposit. Elements commonly used in magnetite discrimination diagrams (particularly Al, Ti, Mn, Ni, Co, but also HFSE or REE) are variously modified by up to several orders of magnitudes, meaning that hematite analyses should be avoided in those diagrams. Further examination will aim to explain characteristic element mobility and “fingerprint” ore-forming/-altering processes, including fluid-rock ratios.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Reconstructing seasonal growth rate changes in fossil giant clams using sub-daily resolved LA-ICPMS

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Bivalves are important environmental archives that can provide past "climate snapshots" at high temporal resolution. The long-lived giant clam *Tridacna* builds large (< 1 m), dense aragonite shells in which seasonal to daily bands are recorded both structurally and chemically. Therefore, *Tridacna* have been key archives of seasonality and extreme weather events in (sub)tropical reefs since their appearance in the early Miocene. Detailed ontogenetic ages and growth rates can be assessed by counting the daily bands and measuring their intervals, which range from a few micrometres to tens of micrometres. However, in many areas of our late Miocene *Tridacna* shell, daily bands were not continuously countable. Continuous optical analyses of daily bands are also time-consuming in organisms that can live for up to a century. A more efficient approach is to utilize daily geochemical cycles, measured via ultrahigh-resolution Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICPMS). First, daily geochemical cycles were recognizable even in areas where we failed to identify daily bands optically. Second, through computational evaluation of the daily cycles' wavelengths (e.g., wavelet transform) we can develop daily growth rate models. Consequently, we can track the ontogenetic age and the growth-rate variability and compare it to the corresponding (sub)seasonal geochemical data ($\delta^{18}\text{O}$, E/Ca). This allows us to evaluate the relationships between geochemical signals, environmental parameters, and shell growth to tackle growth rate and ontogenetic effects as well as seasonal biases. Displaying geochemical data against time rather than shell distance further improves multi-annual and inter-organism comparisons of palaeoseasonality reconstructions.

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Spatial precipitation shifts in the Doce Basin (SE Brazil) during MIS 6-5

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Precipitation patterns in present-day southeastern Brazil are mainly regulated by the South American Summer Monsoon. The southeast Brazilian Doce Basin is expected to suffer from droughts and flooding as a result of future climate induced shifts in the monsoonal precipitation pattern. Data on past spatiotemporal precipitation shifts are scarce but valuable, especially for climate sensitive regions. We analysed X-ray diffraction-derived mineralogical data for the 150–70 ka period (marine isotope stage (MIS) 6 to MIS 5) on samples obtained from marine sediment core M125-55-7 close to the Doce river mouth (20°S). Within the river-derived fraction, we discriminated between two mineral assemblages with varying abundances between glacial and interglacial times and precession-forced variability only visible in MIS 5. The first assemblage has high contents of kaolinite and gibbsite and indicates intensified lowland erosion of mature tropical soils. The second one has higher contents of well-ordered illite, quartz and albite and points to intensified erosion of immature soils in the upper Doce Basin. Prevailing high kaolinite contents in late MIS 6 indicate pronounced lowland soil erosion and weak monsoonal activity. The dominance of the illite-rich mineral assemblage in MIS 5, particularly during times of high austral summer insolation, indicates strong monsoonal rainfall and physical erosion in the upper catchment. In times of lower insolation in MIS 5, the summer monsoon weakened, leading to decreased precipitation and runoff in the upper catchment and dominant lowland erosion as indicated by an increase in the abundance of the kaolinite-rich mineral assemblage.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

Non-classical crystallisation mechanisms in hyaline foraminifer biomineralisation

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Foraminifers are an ubiquitous group of marine unicellular organisms, which form shells (tests) made of CaCO₃. Since their tests can withstand dissolution and accumulate in the sedimentary record, foraminifers are a critical part of the global carbon cycle and provide one of the most important archives for paleoclimate research. Therefore, a confident link between environmental parameters and proxy signals recorded in their shells is essential, and a detailed mechanistic understanding of their biomineralisation is vital knowledge.

We have synthesised a diverse array of microscopic and diffraction-based methods to investigate hyaline foraminifer tests on a nanometre- to micrometre scale. We show that chamber walls exhibit a nanogranular fracture surfaces together with a crystallite domain size of approximately 100 nm, and that these nanocrystals are organised in crystallographically aligned micrometre sized units oriented towards the chamber surfaces. From this, we conclude that hyaline foraminifer tests are made of mesocrystals, which strongly indicates the presence of non-classical crystallisation mechanisms during foraminiferal biomineralisation (1).

Non-classical crystallisation pathways likely involve metastable carbonates, phase transitions to stable phases, and organic matter in diverse functions. Hence, they are expected to distinctly influence isotopic fractionation and trace element incorporation into the final biomineral, which are proxies for environmental conditions. This highlights the necessity to closely investigate non-classical processes in the organisms as well as in experimental models, to reduce uncertainties arising from vital effects and enable accurate and precise reconstructions.

(1) A. I. Arns *et al.*, accepted in *Geochemistry, Geophys. Geosystems* (2022), doi:10.1029/2022GC010445.

Topic: 11.3 Young Scientist Session

Maturation and migration processes in intact source rock micro plugs induced by chemical and thermal treatment: A new approach combining Rock-Eval pyrolysis and organic petrography

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This study proposes a new approach to investigate hydrocarbon generation and migration processes in petroleum source rocks under laboratory conditions. For the first time, programmed open-system pyrolysis using a Rock-Eval 6 instrument is applied on small, polished source rock plugs to induce changes in the type and distribution of solid bitumen, which is qualitatively investigated by means of organic petrography before and after treatments. This approach allows us to directly visualize the evidence of solid bitumen (SB) formation and distribution after the following treatments: (1) thermal extraction (300°C for 3 min), (2) chemical extraction of the surface using dichloromethane (DCM), and (3) artificial maturation up to 400 to 500°C. After each step, the surface of micro plugs was digitally scanned to allow a comparison of specific areas of interest before and after the treatments.

After thermal extraction, the volume of observed SB in the early- and moderately mature samples slightly increased, while most of the thermally mobilized bitumen from inside the plug was evaporated. The initial solid bitumen was not or hardly affected by thermal extraction at 300°C for 3 min, i.e. it was thermally stable at this temperature. After DCM treatment, SB in the early mature samples was almost completely dissolved. While some SB was dissolved in the moderately mature sample showing more mature and stable SB. After the artificial maturation, the volume of SB in early- as well as in moderately mature samples increased, indicating the presence of new SB due to bitumen migration from the plug.

Lecture

Topic: 10.1 Geoscience Communication and Education

GEOWiki@LMU – an online platform for university and school education in geosciences

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GEOWiki@LMU is a constantly growing open platform for the promotion of practical and research-oriented knowledge acquisition. Its major objective is to provide information on methodologies relevant to geosciences, with focus on field, preparation and analytical methods. GEOWiki@LMU offers students a quick overview including helpful practical tips and references to relevant literature where these methods are taught. In addition, there are online tutorials for students, e.g. polarization microscopy. In the so-called GExikOn, articles are currently being created on the topics of rocks, minerals and soils. The subsection GEOWiki@School, which is currently under construction, is aimed primarily at pupils, students and teachers, providing geoscientific topics for school teaching.

GEOWiki@LMU is elaborated by and for students of earth sciences. The contents are developed by students in courses or on their own initiative in interdisciplinary teams. All topics are discussed in weekly editorial online-meetings and revised in close collaboration with lecturers and scientists. The students' own initiative is essential for the development of GEOWiki. They give decisive impulses for the selection and structure of the topics, write the articles and are involved in acquisition of funding. All graphics, icons and videos are created by the students. The website is also programmed by students, according to the motto: what doesn't fit is made to fit. The content is optimized for mobile devices, so information can be accessed spontaneously in the field, laboratory or comfortably on the couch.

Lecture

Topic: 10.1 Geoscience Communication and Education

GEOWiki@Schule – eine geowissenschaftliche Online-Lernplattform für den Schulunterricht

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Das GEOWiki@Schule ist ein Teilbereich der frei zugänglichen Online-Lernplattform GEOWiki@LMU, das derzeit auf Initiative von Lehramtsstudent:innen entsteht. Ziel ist es Schüler:innen und Lehrer:innen für die faszinierende Welt der Geowissenschaften zu begeistern und sie mit den geowissenschaftlichen Methoden vertraut zu machen. Hierfür sollen geowissenschaftliche Themen und Konzepte so aufbereitet werden, dass sie für Laien und Jugendliche unterschiedlicher Altersklassen nachvollziehbar sind und problemlos im Schulunterricht eingesetzt werden können. Leider ist das Fach „Geowissenschaften“ als Unterrichtsfach nicht in allen Bundesländern vertreten. In den Lehrplänen der MINT-Fächer, speziell in den Fächern Chemie, Physik, Mathematik und Biologie gibt es aber neben dem Fach Geographie viele Anknüpfungspunkte für geowissenschaftliche Fragestellungen. Der Fokus des GEOWiki@Schule liegt hierbei vor allem in der Ausarbeitung und Bereitstellung praktischer Lehreinheiten, die je nach Fragestellung im Gelände, im Labor oder auch im Klassenzimmer durchgeführt werden können. Zur Steigerung des naturwissenschaftlichen Interesses und der Motivation der Schüler:innen ist eigenständiges Experimentieren und Forschen an Alltagsphänomenen ein hilfreiches Mittel. Da Lehrkräften im Unterrichtsalltag erfahrungsgemäß oft die Zeit und die Ressourcen fehlen um neue Konzepte zu entwickeln und auszuarbeiten, haben die Lehramtsstudierenden des GEOWiki-Teams diese Sache selbst in die Hand genommen: Sie haben bei StudForschung@GEO Mittel für ein eigenes Forschungsprojekt beantragt, bei dem sie Experimente und praktische Lehreinheiten im Feld und Labor entwickeln, dokumentieren und didaktisch ausarbeiten. Die Ergebnisse werden in Form von Artikeln und Videos gemeinsam mit praktischen Tipps für Lehrkräfte und Hintergrundwissen für die jeweilige Altersklasse aufbereitet und in der Rubrik „GEO Erleben“ im GEOWiki@Schule veröffentlicht.

Lecture

Topic: Frontiers in Mineralogy Talk

Earth's mantle: probing a hidden heavy-weight

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Earth's mantle comprises the vast region between the crust and core, some 84% by volume and 67% by mass – a real heavyweight. The superposition of key events – all ultimately rooted in the mantle – conditioned the evolution of the whole Earth system that produced our hospitable and resource-rich, yet fragile habitat. These include magma ocean crystallisation during Earth's tumultuous beginnings, the formation of first atmospheres and oceans, the emplacement and emergence of weatherable crust, the transition to plate tectonics, and volcanism at and away from plate margins that continues today.

The mantle is poorly exposed on the ocean floor and as tectonically exhumed rocks, and sampled by sparsely distributed mantle-derived magmas carrying small fragments plucked from their wallrocks. Much of what we know relies on applying the petrologist's ever-growing toolbox to these direct and indirect mantle samples. This is complemented by high-pressure experiments and computational models, which establish the phase relations and dynamic behaviour of mantle rocks, and the physical properties of its minerals.

Many mantle mysteries remain, reflecting the dearth of samples from deep Earth and deep time. Among these are the origin, size, locus and persistence of different mantle reservoirs recognised in mantle magmas of various ages, as reflections of mantle structure and convective vigour. Other key questions concern the mantle's temperature and redox evolution, affecting its dynamic behaviour and melting relations through time, and the origin and cycling of its volatile element inventory, the partial degassing of which contributes to the air we breathe today.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Isotope fractionation mechanisms involved in carbonate formation revealed by high-precision triple oxygen isotope analyses

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The oxygen ($\delta^{18}\text{O}$) and clumped (Δ_{47}) isotope composition of carbonates are widely used proxies for palaeotemperature. However, Earth surface carbonates are rarely formed in isotope equilibrium but often show oxygen and clumped isotope compositions that do not accurately reflect their crystallisation temperature. Isotopic disequilibrium commonly observed in biogenic carbonates and speleothems is inherited from the dissolved inorganic carbon pool of their parent solutions. A combination of isotope systems, e.g., $\Delta_{47}-\delta^{18}\text{O}$, $\Delta_{47}-\Delta_{48}$, can uncover and correct for such kinetic effects [1].

The analysis of the $^{17}\text{O}/^{16}\text{O}$ ratio to the more commonly investigated $^{18}\text{O}/^{16}\text{O}$ ratio in carbonates — referred to as the triple oxygen isotope method — expands the traditional oxygen isotope scheme by another dimension and; thereby, allows the identification of fractionation processes involved in carbonate formation. In addition, the triple oxygen isotope method can give insight into the diagenetic history of ancient carbonates and offers the possibility of reconstructing the primary isotope compositions of altered samples [2].

Here, we report triple oxygen isotope ratios ($\Delta^{17}\text{O}$) of various altered and unaltered biogenic (e.g., brachiopods, belemnites) and abiogenic (e.g., speleothems, laboratory precipitates) carbonates. The high-precision measurements were performed on CO_2 gas from acid digestion, using tunable infrared laser differential absorption spectrometry (TILDAS) [3]. Based on the results, we will discuss what combination of kinetic isotope fractionation and diagenetic processes could have played a part in the formation of the investigated carbonates.

[1] Bajnai et al., 2020, Nat Comms; [2] Wostbrock et al., 2020, GCA; [3] Pack et al., this conference.

Poster*Topic:* 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology**Timing and metamorphism of the root of a magmatic arc on the West Gondwana margin: a case study of the Socorro Nappe and São Roque Domain in south-eastern Brazil****Mikaella Balis¹, Bernhard Schulz¹, Mario da Costa Campos Neto²**¹TU Bergakademie Freiberg, Germany; ²University of São Paulo, Brazil

The assembly of West Gondwana resulted in a high-grade nappe system of south-eastern Brazil that comprises a magmatic arc remnant (Socorro-Guaxupé Nappe). The UHT metamorphism is product of the collision between the Paranapanema block (active margin) and the São Francisco craton (passive margin) and decompression, but also related to a pre-collisional stage (Rocha et al., 2017; Tedeschi et al., 2018). The U-Pb ID-TIMS and U-Th-Pb_T EPMA monazite peak metamorphic ages systematically decrease towards the lower nappes describing an orogenic front migration from ca. 630-570 Ma (Campos Neto et al., 2011; Westin et al., 2021). The southernmost segment (Socorro Nappe) comprises gneisses with varied degrees of migmatization that unveil UHT-HT conditions, e.g., spinel + quartz and melt (quartz + K-feldspar) inclusions in garnet, neosomes with garnet + orthopyroxene and garnet + cordierite that are associated with amphibole ± pyroxene-bearing mesocratic gneisses. The paragneisses host a peak assemblage of garnet + sillimanite (needle trail inclusions) whereas biotite + sillimanite in the foliation are potentially retrograde. SEM-MLA and BSE imaging of monazite reveal complex microstructures. Monazite from the paragneisses displays homogeneous, moderate zonation and/or cloudy internal structures. A spinel-cordierite-garnet leucosome hosts peritectic garnet in which monazite inclusions are cloudy and weakly zoned. EPMA core-to-rim profiles of garnet show Fe-Mg zonation in a paragneiss whereas none in the neosomes. The overall composition is almandine and pyrope (X_{Alm} 55-70%; X_{Prp} 25-37%) and low Ca. We combine geothermobarometry and petrochronology of monazite to understand the metamorphic transition from lower to upper crustal rocks in the Neoproterozoic orogen.

Lecture

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Case studies on the role of orbital forcing in Cretaceous greenhouse climates

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The Cretaceous was characterised by a greenhouse climate with high sea levels, resulting in its famous carbonate-rich strata which often present a remarkable rhythmicity. Orbitally-forced cyclic sedimentation patterns have been used to obtain stage durations and to refine the Geologic Time Scale. Despite the common application of cyclostratigraphic techniques, the exact origin of rhythmic banding patterns often remains unknown, as well as the role of orbital forcing in climatic extremes such as the Oceanic Anoxic Events (OAEs).

This contribution will explore the role of orbital forcing in the nature of rhythmic sedimentation and in the timing of carbon cycle perturbations in selected intervals of the Cretaceous. The 405-kyr cycle of eccentricity exerts a strong influence on bulk carbonate carbon isotope records and likely controls the timing of climatic events immediately preceding and postdating the Cretaceous/Paleogene Boundary. In the mid-Cretaceous, the timing of some OAEs may be linked to the grand eccentricity cycle (~2.4 Myr). In both time intervals, the orbital configuration is likely not the cause of environmental change, but may rather exacerbate the effects of other forcing mechanisms, such as large scale volcanism, by temporarily enhancing seasonal extremes. Elucidating the role of orbital forcing in past greenhouse climates of the Cretaceous crucially depends on the integration of climate sensitive records with independent age control from radio-isotopic dating and integrated bio-, magneto- and chemostratigraphy.

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Using Novel Geochemical Proxies to Correlate the Volcanic Atmospheric Input of the North Atlantic Igneous Province (NAIP) at the Paleocene – Eocene Thermal Maximum (PETM)

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Large Igneous Provinces (LIPs) have caused significant environmental perturbations, including global warming and oceanic anoxia. At least five mass extinction events throughout Earth's history temporally coincide with the occurrence of LIPs. Geochemical proxies for volcanism in sediments deposited at the time of LIP events can potentially link the volcanic record with the record of environmental change and extinction at <10 ky timescales. Previous studies have used mercury (Hg) enrichments in sediments as a proxy for past volcanism. However, mercury concentrations are sensitive to alteration, the presence of organic matter, and can be enriched in detrital minerals, e.g. pyrite.

We present ICP-MS trace element data from the Fur section in Denmark, where ash layers related to NAIP volcanism are interbedded with sediments deposited immediately after the PETM carbon isotope excursion. Systematic differences in trace element concentrations between ash layers and sediments indicate the potential value of arsenic (As), antimony (Sb), tellurium (Te), rhenium (Re), and thallium (Tl) as volcanic proxies. These elements are enriched in the sediment layers compared to the ashes and correlate with Hg/TOC. In particular, we observe elevated concentrations in Te (up to 600 ppb), compared to the average continental crustal value of about 3 ppb. Leaching of samples with dilute acid suggests that ash particles have degassed Te during eruption, whereas the sediments which were deposited more slowly, incorporate Te in a loosely bound form consistent with an atmospheric origin. We conclude that these trace elements are valuable proxies for the reconstruction of past volcanism.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Origin of highly siderophile element fractionation and excess ^{187}Os in rocks from the CM-1 core of the Oman Drilling Project (Oman ophiolite)

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The southern massifs of the Oman ophiolite were often considered as a model for the structure and composition of crust at fast-spreading ocean ridges. However, the influence of late-stage convergent plate margin magmatism on the evolution of lower crustal and upper mantle rocks in the ophiolite is still poorly understood. Here, we report new constraints from highly siderophile and other chalcophile element abundances and $^{187}\text{Os}/^{188}\text{Os}$ on samples from the CM-1 drill core of the Oman Drilling Project. Main results are: (1) Abundances of most elements in this study were not affected by low-temperature alteration. (2) In harzburgites and dunites from the top of the mantle section, chalcophile elements predominantly are controlled by traces of sulfides, precipitated from sulfide-saturated, incompatible element-depleted magmas. (3) The overlying dunite-rich crust-mantle transition zone (CMTZ) is extremely depleted in Pd, Se and Re, indicating that parent magmas were sulfide-undersaturated. (4) The mafic unit on top shows local sulfide saturation. (5) Ru/Ir and Os/Ir in CMTZ dunite are suprachondritic, whereas values in the overlying mafic unit are subchondritic. Hence, rocks of the mafic unit are products of magmas that initially crystallized cumulate olivine and a laurite-ehrllichmannite phase in CMTZ. (6) Suprachondritic initial $^{187}\text{Os}/^{188}\text{Os}$ of CMTZ, the mafic unit and other lower crustal gabbros suggest that most of the lower crust was affected by magmas that contained excess radiogenic ^{187}Os , presumably a result of slab-derived inputs during the short-lived subduction zone stage.

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

PySILLS, a newly developed Python-based open source tool for a modern data reduction of LA-ICP-MS experiments

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Laser ablation – inductively coupled plasma – mass spectrometry (LA-ICP-MS) is a sensitive, efficient and cost-effective method for analyzing the major, minor and trace element compositions of minerals as well as of fluid and melt inclusions. Due to the high spatial resolution, low detection limits and multi-element capabilities of the LA-ICP-MS technique, it is ideally suited for rapid in situ chemical analysis of geological materials with minimal sample preparation requirements. Because of the wide use of LA-ICP-MS in geosciences, materials sciences and life sciences, there is a considerable need for modern data reduction tools that combine an intuitive and efficient workflow, a comprehensive statistical analysis and the strengths of open source software development. The new LA-ICP-MS data analysis tool PySILLS is completely written in Python, a popular, high-level and general-purpose programming language. A key design concept of PySILLS is to keep the code simple, in order to make the development of plugins, for example novel quantification methods for the analysis of fluid or melt inclusions, as user-friendly as possible. Another key concept is to keep the workflow and the possible settings efficient and flexible. PySILLS was initially developed in the context of a MSc thesis project and has been brought to the level that the widely used SILLS tool offers, and features already a number of important improvements. Further extensions, for example the implementation of user-developed plugins such as a fluid inclusion quantification method that combines LA-ICP-MS and microthermometric data with thermodynamic modeling, can be expected in the near future.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Structural control on magma composition in northern Iceland and the southern Kolbeinsey Ridge

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Geochemically enriched plume sources interacting with depleted, adiabatically upwelling mid-ocean ridge mantle allow for the tracing of processes of melting and melt transport through the mantle and crust. New major, trace element and Sr-Nd-Pb isotope data from glasses along the Southern Kolbeinsey Ridge and Tjörnes Fracture Zone, along with published data from the northern Iceland Theistareykir, Krafla and Askja volcanoes. We combine these with new whole rock and glass data from the early-Holocene Sveinar-Randarhólar fissure, which is located 60 km North from Askja volcano and 30 km east off-axis of the Northern Volcanic Zone rift. In the case of the recent plume-ridge interaction between the Kolbeinsey Ridge and the Northern Volcanic Zone, the preservation of the geochemical mantle heterogeneity is the result of a preferential extraction along existing structural weaknesses. The mixing of plume and mid-ocean ridge sources prior to melting is preserved because of limited crustal interaction of the melts. In contrast, the Sveinar-Randarhólar fissure displays a remarkable major, trace element and petrological homogeneity over a total length of ~75 km indicating limited fractionation, and interaction with the neighbouring country rocks. We can show that the magmas were transported from a reservoir underneath Askja volcano at sub-surface levels for ~60 kms likely due to remnant ice coverage in the region before reaching surface levels. We conclude that the efficient transport of off-axis magmas is the result of a strong, pre-existing structural domain opening extensive pathways for magma transport over lateral distances of 10-100's of kilometres.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Unusual IOA deposit associated with carbonatite in South Morocco: Mineralogy, geochemistry and REE-Nb-Ta mineralization

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Iron oxide-apatite (IOA) deposits are known to be closely associated with silicate igneous rocks. However, a recent study in the Oulad Dlim massif (South Morocco) revealed the first occurrence of massive IOA deposits hosted by Paleoproterozoic dolomite carbonatite in the Gleibat Lafhouda area. In addition, significant REE-Nb-Ta enrichments seem to be unique to this IOA occurrence. Preliminary results have indicated an exploration tonnage target of ~49 million tons with mean compositions at 0.4% Nb₂O₅, 265 ppm Ta₂O₅, 508 ppm U₃O₈, 0.2% REE, and 35% Fe₂O₃. Columbite-(Fe) is the main Nb-mineral and occurs closely associated with Fe-phases, whereas microlite and Ta-rich pyrochlore are mainly associated with coarse-grained apatites hosted by Fe-oxides and silica breccia. Significant REE contents are hosted by monazite-(Ce), which is usually associated with large apatite crystals. The processes leading to this mineralization with direct links to carbonatite are still poorly understood. However, geochemical characteristics and textural relationship suggest that they are genetically linked to the carbonatite and intensively remobilized by late hydrothermal fluids at multiple stages. This study aims to provide new mineralogical and geochemical insights on the petrogenesis of the IOAs and their associated ore mineralization. Understanding new occurrence types of the IOAs will significantly advance our understanding of their formation and will provide important information on the magmatic/hydrothermal evolution of this unusual IOA occurrence and its significant REE, Nb, and Ta mineralization.

Poster

Topic: 11.3 Young Scientist Session

“Heat In Place” assessments for Berlin/Brandenburg’s deep geothermal potential

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Geologically located in the Northeast German Basin, Berlin and most parts of Brandenburg are known to be potentially suitable for deep geothermal energy usage. This source of energy is not yet well-established in the area. However, regarding Germany’s transition towards climate-friendly and regional energy solutions, the energy demand from renewables is rapidly increasing. Thus, geothermal exploration and assessing geothermal potential is significant. We assess “Heat In Place” (HIP) as quintessential part of the geothermal potential for a series of litho-stratigraphic units for Berlin and Brandenburg.

Geothermal potential is defined as considering characteristics of a specific geothermal plant and/or the geological reservoir. We concentrate on the latter geological aspects and take a 3D geological and two different 3D thermal models of Brandenburg as basis for the HIP calculations. This HIP approach corresponds to a volumetric quantification of contained energy within 16 litho-stratigraphic units, each taking variable thickness, mean temperature, porosity, density, and specific heat capacity into account. This results in a series of new geothermal potential maps derived from different thermal models: Firstly, conductive heat transport, and secondly, coupled thermal-hydraulic simulations. We aim at deepening the understanding of HIP maps for geothermal power plant site decision making by showing how the calculated heat varies between those two modelling approaches, and different parameter estimates.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Assessing the role of microbes and the chemical conditions necessary for the formation of microbialites

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Microbialites are organosedimentary deposits formed by benthic microbial communities that mediate mineral precipitation. They have received particular attention since they are found throughout the geological record up to 3.43 billion years ago and are considered as among the oldest traces of life on Earth. It has been known for several decades that the abundance of microbialites has varied over geological time with an overall decline during the Phanerozoic. Yet, the question of what between biological and/or physico-chemical variations may have changed the abundance of microbialites over geological times remains debated. This calls for a better appraisal of the conditions necessary for the formation of modern microbialites. Here, I will first review (omics) studies about the importance of specific microorganisms in microbialite formation (e.g., Iniesto et al., 2020 & 2021). Then, I will present a recent database listing the physico-chemical parameters of more than a hundred aqueous environments where modern microbialites form. The analysis of this dataset highlights that specific chemical conditions in seem to be always met, thus appearing as necessary for microbialite formation. Moreover, the comparison of this database with existing databases listing close to 8000 continental freshwater systems allows further insight on the potential of modern environment for microbialite formation. Overall, I will discuss how this suggests that the change of the chemical composition of the ocean might be a primary driver of the decline of microbialite abundance over geological times. I will conclude by tentative speculations about the fate of microbialites on an evolving planet.

Lecture

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

U-Pb in garnet by LA-ICPMS: dating extremely U-poor minerals

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Traditionally, “laser-ablation-geochronologist” have taken advantage of the developments in analytical techniques; trying to improve the spatial resolution in their analysis; i.e. reducing the spot size as much as possible. On the other hand, those advances in instrumentation have opened not only the possibility of analysing smaller sample volumes but also lower concentrations. Minerals with low U (and Pb) contents (< 1 µg/g) like garnet have become the target of in-situ U-Pb geochronology since it has been demonstrated that isochrons can be potentially obtained. In this contribution, we explored the current limits of in-situ U-Pb geochronology: what are the minimum Uranium concentrations from which an accurate and precise U-Pb age can be obtained?

For that purpose, we have analysed garnets from different localities that were unsuccessfully analysed in the past using single-collector instruments. These garnets have been re-measured using a Neptune Plus MC-ICP-MS coupled to a RESOLUTION-LR ArF Excimer laser. The analyses were performed in static mode measuring the masses ²⁰⁶Pb and ²⁰⁷Pb with Secondary Electron Multiplier (SEM) and ²⁰²Hg, ²⁰⁴Pb and ²³⁸U with the Multiple Ion Counters (MIC). The analysed garnets have typically U contents below 10 ng/g, which taking into account the spots sizes used, results in a Uranium amount ca. 3,000 times less than compared to conventional LA-ICPMS zircon analysis. About 15–30 spots are sufficient for a regression line in the Tera-Wasserburg diagram, yielding a precision of typically <3 % for the lower intercept age. The analysed. Challenges and details of the method will be discussed.

Poster

Topic: 5.6 Natural archives as recorders of past climate and environmental conditions – processes, methods and applications

A terrestrial archive of marine environmental conditions in Antarctica - evidence from snow petrel stomach oil deposits

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In the Southern Ocean microfossil records from marine sediments indicate large shifts in species assemblages and nutrient cycling in response to changing climatic conditions and sea-ice extent during the Late Pleistocene and Holocene. While the northern latitudes of the Southern Ocean are relatively well covered by sedimentary records, little is known about past changes in sea-ice coverage and the abundance and activity of polynyas, and associated ecological changes in near coastal areas off East Antarctica. In that regard, deposits of fossil stomach oil of snow petrels (*Pagodroma nivea*) (also termed Antarctic mumiyo) are unique records that can be found in un-glaciated terrestrial areas of Antarctica. The stomach oil is of dietary origin and contains information on the composition of snow petrel food, which is linked to environmental conditions in the marine foraging range of the birds, such as summer sea-ice variability and productivity in the coastal ocean. Our geochemical data (lipids, stable isotopes, inorganic composition) suggests that this information is preserved to some extent in the fossil stomach oil deposits. Radiocarbon analysis shows that the material comprises records of hundreds to thousands of years, with the oldest deposits being older than 50 thousand years. Stratigraphic analysis combined with geochemical data and correlation with coastal sediment records, makes the deposits a novel archive of past marine environmental conditions, biogeochemical cycling, and food web structure.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Tin and bronze in prehistoric Central Asia, or: how a slag sheds new light on an old question – Results from a multidisciplinary approach

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Central Asia is considered one of the key regions as a potential supplier of Bronze Age tin and thus – at least part of – the answer to the question of the "tin mystery". Large tin ore deposits are known from Afghanistan, Uzbekistan, Tajikistan as well as Kazakhstan, and compared to other tin-bearing provinces such as Cornwall/Devon, the Erzgebirge or the Iberian Peninsula, mining archaeological evidence for ancient tin ore mining is abundant. This is certainly due to the fact that underground mining was common, whereas in the other regions mining of alluvial deposits may have been predominant. However, what was lacking until recently was archaeological evidence of ore smelting and, moreover, analytical evidence of how the ores impacted on local and supra-regional bronze metallurgy. Here we present the results of the study of a unique bronze slag from near the Mušiston tin-copper deposit in Tajikistan with microscopic, mineralogical, chemical and isotopic analysis. According to the results, the slag has unusual mineralogical characteristics and can be clearly associated with the nearby deposit on the basis of chemistry and isotopy. This is thus the first time that a slag from a tin smelting process can be used to trace the tin/bronze metal produced back to its ore source. Building on this important result, we also present first data of bronze artefacts from Central Asia to provide a preliminary assessment of the importance of the Mušiston ores for bronze metallurgy.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Geowissenschaftliches Prozessverständnis in Bergsenkungsgebieten

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Rohstoffgewinnung geht mit einer mehr oder minder massiven Veränderung der Landschaft und den natürlichen Verhältnissen einher. Die für unseren Alltag notwendige Entnahme von Ressourcen beeinflusst nahezu alle Aspekte des Naturhaushaltes: Wasser, Boden, Flora und Fauna. Aus geowissenschaftlicher und geoökologischer Sicht betrifft das insbesondere die sogenannten Polder im Ruhrgebiet; Areale, die durch den Steinkohleabbau erhebliche Bergsenkungen erfahren haben und heute kontinuierlich entwässert werden müssen.

Im Projekt „MuSE - Multisensor-Geomonitoring zur Optimierung der nachbergbaulichen Wasserhaltung“ sollen für solche Gebiete Konzepte entwickelt werden, nach denen die Wasserhaltung möglicherweise optimiert werden kann. Ziel ist es, Ideen zu entwickeln, das Polderwasser bspw. in Dürreperioden sinnvoll in Land- und Forstwirtschaft zu nutzen oder den Polder bei Starkregenereignissen vielleicht sogar als Pufferspeicher einsetzen zu können, um zu erwartende Schäden zu verhindern.

Um ein Prozessverständnis aufzubauen, gehen die Geowissenschaftler:innen des FZN dreistufig vor: Neben den klassischen geowissenschaftlichen Ansätzen über die Geologie, den Boden, die Vegetation und Wetterparameter (in situ-Komponente) sollen letztlich Bewertungen auf Basis von Satellitendaten (Sentinel 1 und 2) eine flächenhafte Aussage erlauben. Zur besseren Interpretation dieser Daten werden hochauflösende Multispektraldrohnen eingesetzt, um mögliche Wasser- und Vegetationsindizes abbilden und mit dem Satellitensegment vergleichen zu können. Beispielhaft stellt der Vortrag die kombinierten Ansätze einer Sensordatenfusion aus In situ-Messkomponenten, einer Ground Truthing-Ebene aus UAV-gestützten Sensoren und (bislang noch eingeschränkt) dem Satellitensegment mit einer Konzentration auf die ersten Beiden Aspekte vor.

Lecture*Topic:* 1.7 Experimental Petrology and Geochemistry**High-pressure phase relations in the system Fe-Ni-Cu-S up to 14 GPa****Christopher Beyer¹, Thilo Bissbort^{1,2}, Rebecca Hartmann¹, Raul Fonseca¹**¹Ruhr-Universität Bochum; ²University of Delaware

Base metal sulfides (Fe-Ni-Cu-S) are ubiquitous phases in mantle and subduction-related lithologies. Depending on their Cu and Ni content, sulfides may melt incongruently, leaving a solid residue called monosulfide solid solution (mss), and a Cu-Ni-rich sulfide melt. However, the persistence of crystalline sulfide phases like mss in the Earth's mantle has long been up for debate, as the presence of both mss and sulfide melt in mantle rocks would lead to the fractionation of chalcophile elements during mantle melting. Recent studies have shown that the average mantle sulfide is fully molten at average mantle potential temperatures (1300–1400 °C) up to 8 GPa (ca. 240 km). However, sulfide inclusions found in diamonds show a broad compositional spectrum, ranging from Ni-poor and Fe-rich (eclogitic), to Ni-rich and Fe-poor sulfides (peridotitic), with their Cu contents being generally low. Results on the melting properties of average mantle sulfide are thus not applicable to the full compositional range shown sulfide compositions sampled by diamonds originating from greater depths. Here we present the results of an experimental study where the melting properties of typical sulfide compositions found in diamond inclusions associated with eclogites and peridotites have been determined. Experiments have been carried out between 0.1 MPa and 14 GPa, and between 850 and 1590 °C. Results show that solid mss in Fe-rich, Ni-poor sulfide inclusions associated with eclogites persist to higher pressures and temperatures compared to their more Ni-rich peridotitic counterparts. Our results have implications for the recycling of chalcophile elements during subduction-related processes.

Lecture

Topic: 3.2 Composition and evolution of deep planetary interiors

Insights into magmatic evolution in the southern Central European Volcanic Province: Petrology and Geochronology

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Based on U-Pb geochronology, strongly SiO₂-undersaturated foidites and melilitites in the southern Central European Volcanic Province (SW Germany, E France) were shown to have formed during two distinct periods in different regions. An Upper Cretaceous to Lower Eocene group (~72–47 Ma) is characterized by melilite-free nephelinites, nepheline basanites, and hauynites, whereas an Oligocene to Miocene group (27–9 Ma) is represented by olivine melilitites and melilite-bearing nephelinites. Both rock series were generated by extremely low degrees of partial melting of the metasomatically overprinted sub-lithospheric mantle, but exhibit a number of distinct mineralogical, mineral chemical, and whole-rock geochemical features. However, thermodynamic modelling did not reveal significant differences for melt temperature, oxygen fugacity, and silica activity. Accordingly, the foiditic and melilititic melts formed at temperatures of 1100–1350 °C and their polybaric crystallization started at ~14 kbar. The silica activities vary for both age cohorts between ~0.4 and 0.9 with a Δ FMQ of +1 to +4. Thus, it is likely that the differences between the rock series reflect a temporally and spatially heterogeneous sub-lithospheric mantle source beneath central Europe and are coupled to different depths of melt formation, various initial melt compositions, and/or different degrees of partial melting. Besides, an influence of crustal contamination and fractionation cannot be completely excluded. Magmatism in both periods is associated with asthenospheric doming and surface uplift causing erosion and isostatic compensation in the Alpine foreland. These processes indicate decompression and are interrupted by a period of subsidence resulting in a ~20 Myr volcanic hiatus.

Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

River evolution in the Atacama Desert: comparisons of cosmogenic nuclide and molecular clock dating approaches

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The Atacama Desert in northern Chile is considered to be the driest, oldest desert on Earth. None-the-less, even the hyperarid core of this desert is host to several deeply incised, fluvially active river canyons. The history of these drainages is tied to the tectonic and climatic evolution of the region, however, the timing and hence the mechanisms driving canyon formation are poorly constrained.

We have used cosmogenic ¹⁰Be exposure ages to define the Quaternary incision history for the southern tributary of the Tiliviche River, which exits to the Pacific approximately 19.5°S. Ages from flights of fluvial fill-cut terraces at two separate locations are consistent and suggest this branch of the river formed shortly after 2 Myr ago by relatively slow fluvial incision. This slow incision persisted until around 300–400 kyr ago, whereupon rates of downcutting increased by around an order of magnitude.

In this contribution, we discuss how the timing of the Tiliviche River incision rate increase may relate to tectonic mechanisms, both local faulting and with regards to proposed increases in regional scale crustal uplift. We include exposure ages from several proximal sites and suggest linkages between these events and the Tiliviche River evolution. Lastly, our project aims to compare the results from cosmogenic nuclide dating with fluvial histories derived from the timing of amphipod speciation. Our initial results show that there is much potential in combining cosmogenic nuclide approaches with molecular clock dating and implies river evolution in this area is controlled by a common, regional-scale process.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

AN INTERDISCIPLINARY APPROACH FOR CHARACTERIZING ANCIENT MATERIALS: BUILDING MATERIALS FROM THE HELLENISTIC-ROMAN CITY OF SOLUNTO (SICILY) AS A CASE OF STUDY

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This presentation gives an overview of the advantages combining thin-section optical petrography with X-ray microdiffractometry (μ -XRD²) and scanning electron microscopy with energy dispersive spectroscopy (SEM-EDS) for the analysis of well contextualised archaeological materials.

The Hellenistic-Roman city of Solunto (Sicily) offers an ideal case of study as the houses, in which typically lime based mortars and plasters are used, are well studied from a building history point of view.

To characterize this type of building materials in detail optical thin section petrography is a well-established tool not only regarding the minerals, but more important for determining textural and compositional features. However, optical microscopy has its limitations to characterize opaque phases or minerals below the optical resolution. This can be overcome using μ -XRD², allowing non-destructive and local highly resolved structural analysis of the uncovered thin sections, where an identification of minerals with optical microscopy is not possible.

Pairing these two methods with SEM-EDS, results in a comprehensive study of the microstructural characteristics and chemical composition. This makes it possible to analyze not only the aggregates and inclusions but also the typically fine crystalline binder within this type of building material.

Our results, in combination with the analysis of the archaeological context, provide new insights into technology transfer in general, but also a better understanding of the different and interconnected strategies of selecting and processing local resources and the adaption of the used mortars to various architectural features.

Lecture

Topic: 10.2 Geoethics – fostering ethical perspectives in Geosciences

Geoethics, applied philosophies of geoSTEM

Martin Bohle

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The geoSTEM disciplines (Geosciences, *Erdwissenschaften*, *Sciences de la Terre*) are relevant to Planet Earth's stewardship in times of anthropogenic global change. Research into 'responsible geosciences' recently led geoscientists to amalgamate insights into societal and geoscientific features of the World and Earth. The outcome is a set of geo-philosophical frameworks. As a particular philosophical framework, Geoethics emerged a decade ago as "*research and reflection on the values which underpin appropriate behaviours and practices, wherever human activities interact with the Earth system*" [1; p. 30].

Experiences show that ethically sound operational practices depend on environmental, social and cultural settings. The composite design of geo-philosophical frameworks enables context-depending practices, hence, a pluralism of socially rational ethical choices; favourable of 'comparative justice' [2].

Various epistemic-moral geo-philosophical frameworks (geoethics) can be assembled. For example, Kohlberg's, Jonas', and Bunge's political philosophies about the level of cooperation of agents, the responsibility of agents of change, and the individual balance of agent's well-being and duty, respectively, offer a geoethics that proposes a realist-materialist understanding of societal fabrics [3]. Consequently, geoethics are multiple, although based on a common epistemic foundation in geoSTEM expertise.

1. Peppoloni S, Bilham N, Di Capua G (2019) Contemporary Geoethics Within the Geosciences. In: Exploring Geoethics. Springer International Publishing, Cham, pp 25–70

2. Sen A (2010) The idea of Justice. Penguin Books, London, UK

3. Bohle M, Marone E (2022) Phronesis at the Human-Earth Nexus: Managed Retreat. *Front Polit Sci* 4:1–13. <https://doi.org/10.3389/fpos.2022.819930>

Poster

Topic: 10.2 Geoethics – fostering ethical perspectives in Geosciences

A critical look into the past – The hidden colonial heritage in mineralogical museums

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Mineralogical Museum at the University of Bonn, Germany

The provenance of objects –in terms of chronology of ownerships – in museums and collections is a cutting-edge topic discussed especially among art historians, historians and ethnologists. Until now, the emphasis is on works of art and cultural objects linked to either Nazi-confiscated art or to objects linked to a colonial context. Discussions about restitutions to legal successors or societies of origin engage scientific communities, feuilletons as well as the public. In geoscientific museums, the provenance of objects usually refers to the exact location of finding. Here, a broader, more critical approach is overdue as many geoscientific objects might have a similar critical background as the above-mentioned groups of objects. As mineralogical museum with several historical collections dating from the end of the 19th and beginning of the 20th century, we shed light on objects with a potentially colonial background. To begin with, we focus on minerals originating from the former German colonies in Africa. Like other museums worldwide, we host hundreds of specimens from Tsumeb in Namibia. The mine got established under German rule in the late 19th century. It did not only supply the German Empire with tons of ores, but also private collectors and museums worldwide with minerals for their collections. We began to review our inventory regarding the number of specimens, historical (previous ownerships) and chronological (moment of exploitation) background. We take a critical look into the past of our 200 years old institution and hence contribute to public and scientific discussions related to the provenance of objects in museums.

Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

1. Halogens as tracers for mineralizing fluids in the Sn-W-Cu province of the Cornubian batholith, SW England

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Despite their well-known economic potential, the genesis of deposits associated with magmatic-hydrothermal fluids derived from granitic plutons is still not fully understood. The Cornubian batholith (SW England) represents an example of those: it was intensely mined for Sn and Cu, but also hosts W mineralizations and Li-rich granitic rocks.

This study explores the use of halogens as tracers for the formation of such critical element enrichments, across the transition from magmatic to hydrothermal conditions in this well-studied natural laboratory of a Variscan S-type system. Given the high incompatibility of heavy halogens (Cl, Br, I) in most minerals, they are reliable indicators of fluid provenance and evolution and readily discern geofluid reservoirs, but questions remain as to halogen behaviour during crucial ore-forming processes such as fluid exsolution or phase separation.

In situ LA-ICP-MS analysis of fluid inclusions and whole-rock combustion ion-chromatography will provide a detailed assessment of halogen behaviour across the magmatic-hydrothermal transition in samples ranging from granites and pegmatites, to greisens and mineralized Sn-W-Cu hydrothermal veins.

Preliminary results show a progressive dilution of fluids with magmatic Br/Cl - I/Cl signatures and elevated concentrations of Cu, Sn and W as the main factor controlling mineralization.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Insight into formation of hydrothermal ore deposits using a hydrothermal autoclave and X-ray absorption spectroscopy

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Hydrothermal fluids play an important role during the formation of most economically explored ore deposits. While cycling through the crust these supercritical fluids efficiently dissolve and transport metals from the source rocks; metal-rich minerals precipitate on their way towards the Earth's surface. In general, compositions of hydrothermal ore fluids are well known, e.g., by analyzing fluid inclusions in ore minerals. However, because sources and physiochemical characteristics of hydrothermal fluids vary widely, complexation and speciation of metals in the fluid and precipitation mechanisms of ore minerals are still matter of controversial debates. Conclusions on metal complexation and speciation in the fluids are usually based on analysis of quench experiments that do not consider the probably non-quenchable nature of hydrothermal metal complexes e.g., as previously reported for gold (Pokrovski et al., 2015). Thus, reliable information on metal complexation and speciation during ore deposit formation can only be obtained using in-situ data.

Here, we present an autoclave dedicated to in-situ characterization of hydrothermal fluids at high pressures and temperatures at Deutsches Elektronen-Synchrotron (Klemme et al., 2021). Besides discussing details of the experimental set-up we will also focus on results of two ongoing projects dedicated to formation of W and Sn hydrothermal ore deposits.

G. Pokrovski et al., PNAS 112 (44), 2015; Klemme et al., Rev Sci Instr. 92, 2021

Funding: Bundesministerium für Bildung und Forschung (BMBF) grant FKZ 05K16PMA, DESY Center for Molecular Water Science - Early Science Project.

Poster

Topic: 7.3 Assessment of the Earth System through Micropaleontology

Neogene palaeoceanographic changes off northern-central Chile based on benthic foraminifera from the Bahía Inglesa Formation

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The modern oceanographic setting off northern-central Chile is characterized by highly productive waters and an extensive Oxygen Minimum Zone (OMZ), both resultant from coastal upwelling induced by the Humboldt Current System. However, oscillations of upwelling and OMZ properties during the Neogene are still poorly understood. Here, we assess palaeoceanographic conditions based on benthic foraminifera assemblage data of marine sediments from the Bahía Inglesa Formation (Upper Miocene-Pliocene), recovered from the Quebrada Tiburón outcrop (27°42' S, 70°59' W). Quantitative paleoenvironmental analyses of benthic Foraminifera >250 µm from 6 samples are currently conducted. Preliminary results show shifts in both, the diversity and abundance of hyaline species over the studied interval. High abundances of planospiral (predominantly epifaunal) morphotypes in sandy, heavily bioturbated parts of the studied section alternate with diatom-rich sediments bearing predominantly serial (infaunal) taxa such as *Bolivina aenariensis* and *Uvigerina peregrina/striata*. The observed changes in assemblage composition imply significant changes in biological productivity, bottom-water oxygenation, and ultimately, coastal upwelling off Chile in the Neogene. Further refinements of the stratigraphic model for the studied section will clarify the timing of the here described preliminary observations of paleoenvironmental fluctuations. This study contributes to project A4 “**Land-ocean coupling between the Humboldt Current System and Atacama palaeoclimate in the Neogene**” of CRC 1211 “**Earth-evolution at the dry limit**”.

Lecture

Topic: 2.2 From dust to planets

Building Earth

Audrey Bouvier

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Studies of meteorites and samples returned from space missions bear the chemical and physical records of planetary formation processes. Mass-independent isotopic anomalies measured in planetary materials indicate two separate accretion reservoirs corresponding to a more volatile-rich region (carbonaceous) in the outer solar system and a more volatile-depleted one (non-carbonaceous), the inner and terrestrial planet formation region [1].

Unequilibrated enstatite chondrites are within 10 parts per million from the Earth's mantle $^{142}\text{Nd}/^{144}\text{Nd}$ composition [2-4]. This difference between the Earth and chondrites may either have been produced by early Sm/Nd fractionation from chondritic materials or was already present within the disk. The isotopic anomalies in ^{145}Nd and ^{148}Nd measured in non-carbonaceous chondrites and achondrites also indicate that a change of the inner disk composition occurred within the first 1.5 million years of solar system formation [5]. On the other hand, major (e.g. Mg/Si) and siderophile elements suggest that enstatite chondrites can neither be the main component forming Earth nor the late accreted materials [6, 7]. Elemental and isotopic fingerprints indicate that the Earth may be primarily built from unsampled materials formed closer to the Sun (e.g. [5]), while volatiles indicate variable sources. Dynamical modeling provides additional constraints on these complex physical, chemical, and isotopic records of Earth and terrestrial planet formation.

[1] Kruijer et al. (2020). [2] Bouvier et al. (2016). [3] Burkhardt et al. (2016). [4] Boyet et al. (2018). [5] Frossard et al. (2021). [6] Fischer-Gödde et al. (2020). [7] Budde et al. (2019).

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Constraining the mantle sources of Italian magmatism through high field strength elements and $^{176}\text{Hf}/^{177}\text{Hf}$

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High Field Strength Elements (HFSE) are a powerful proxy to investigate specific processes occurring in complex magmatic settings. Being only little released by slab derived fluids/melts, HFSE are not easily overprinted by subduction processes and are also sensitive to peculiar metasomatic processes such as carbonatite infiltrations. We report high-precision HFSE isotope dilution concentration and $^{176}\text{Hf}/^{177}\text{Hf}$ data from representative magmas of the Neogene to Quaternary Italian volcanism (i.e., Vesuvius and other Central Italy volcanoes, Tyrrhenian seafloor, Etna, and Pantelleria).

Etna and Vulture volcanic rocks show Nb/Ta ratios much higher than OIB and MORB. The high Nb/Ta cannot be explained by an influence of the Ionian subduction and may reflect carbonatite metasomatism in the mantle. A C-rich metasomatic event explains the large CO₂ degassing of Etna and it is consistent with a mantle flow that erodes the bottom portions of the SCLM.

Other Italian volcanoes do not show an anomalously high Nb/Ta with the exception of leucite-bearing rocks from Mid Latin Valley (Central Italy). Hafnium isotopes are partially decoupled from Nd isotopes. Vulture, Vesuvius, and leucite-free magmas from Mid Latin Valley show variations in $^{143}\text{Nd}/^{144}\text{Nd}$, but rather constant $^{176}\text{Hf}/^{177}\text{Hf}$. Given the lower mobility of Hf (with respect to Nd) during subduction processes, the constant $^{176}\text{Hf}/^{177}\text{Hf}$ could reflect a common asthenospheric component. Since the Tyrrhenian seafloor and intraplate volcanoes of the region (e.g., Pantelleria and Etna) show more radiogenic Hf, the signature of Vesuvius, Vulture, and leucite-free rocks of the Mid Latin Valley could reflect a less depleted asthenospheric mantle source.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Magmatic controls on the ore-forming potential at the submarine Brothers volcano, Kermadec arc

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The submarine Brothers arc volcano ~350 km NE of New Zealand is a unique site for studying active magmatic-hydrothermal ore formation. In 2018, IODP Expedition 376 cored the subsurface to provide insights into the third dimension and the evolution of the volcano and associated ore-forming system. We present new petrological and geochemical data on unaltered volcanic rocks from Brothers as well as from two adjacent volcanic ridges. Lavas erupted at these ridges represent potential mafic analogues to the dacites at Brothers. The volcano is located at the arc frontal end of a cross-arc volcanic chain that extends into the backarc. This cross-arc chain is assumed to be the surface expression of an anomalously warm zone in the mantle wedge and the devolatilization of the partially subducted Hikurangi Plateau enhance slab input. This increased flux facilitates the transfer of metals to the wedge and is efficiently liberating metals from residual sulfides in the mantle wedge. As a result, magmas erupted at Brothers volcano and the adjacent volcanic ridges are enriched in ore metals and metalloids. Whereas sulfide saturation is initially suppressed by a high melt oxidation state ($\Delta \log fO_2$ of +1.5 FMQ), the dacitic lavas of Brothers volcano are depleted in chalcophile elements (e.g., Cu, Au), which limits its porphyry ore potential. This is due to late-stage sulfide segregation during magmatic differentiation. However, other metals and metalloids (e.g., Mo, As, Sb) are progressively enriched and ultimately transferred into the epithermal-hydrothermal system by fluids exsolving from the cooling magma.

Poster

Topic: 8.1 Geosciences and Waste Management

Computational Investigation on the Adsorption and Photodegradation of Glyphosate in its zwitterionic form on a Rutile (110) Titanium Dioxide Surface

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In times of steadily increasing demand for food due to the continuous growth of the world population, herbicides like glyphosate are heavily used to ensure the supply of crops all around the world [C. Benbrook, *Environ. Sci. Eur.* **28**, **2016**, 3.]. Therefore, the leaching of these chemicals into ground and surface waters has become an increasingly troubling issue since several ways of exposure to humans are possible [Singh *et al.* *Environ. Chem. Lett.* **18**, **2020**, 663.].

The investigation of possibilities for adsorption and degradation of pollutants like glyphosate can be approached from a computational point of view to provide insight while being less expensive than experimental studies. Earlier studies using DFT and higher-level wave function methods have proven to give valuable results and show the ability of TiO₂ to fixate and degrade the glyphosate dianion [L. Gerhards, PhD thesis, Carl-von-Ossietzky-Universität Oldenburg, **2021**; Balzaretti *et al.* *ChemRxiv*, **2021**, DOI 10.26434/chemrxiv.14465436.v1].

In this work the adsorption, photoexcitation and degradation of zwitterionic glyphosate on a rutile (110) surface is considered and different adsorption geometries and degradation pathways are evaluated using DFT methods. Additionally, the effect of an acidic environment on the surface and the adsorption is investigated. The calculations have shown that the adsorbed zwitterion is hardly affected by electronic excitation of the system, furthermore several degradation pathways have been evaluated, showing that the zwitterion tends to behave and degrade differently from the dianion on the surface, being in agreement with experimental data [Muneer *et al.* *Int. J. Photoenergy*, *2008*, **2008**, 1.].

Lecture

Topic: 2.2 From dust to planets

Moderately volatile element fractionation in chondrites constrained by isotope dilution and Cd and Zn isotopes

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Volatile elements in chondrites are usually depleted relative to CI chondrites. To disentangle the processes that affected volatile elements in the protoplanetary disk and on parent bodies, we present high-precision isotope dilution concentration data for S, Cu, Zn, Ga, Se, Ag, Cd, In, Sn, Te and Tl as well as Cd and Zn stable isotope compositions for carbonaceous, ordinary, enstatite and Rumuruti chondrites.

In carbonaceous chondrites, volatile elements with 50% condensation temperatures (T_c) between 1040 and 800 K show a progressive depletion with decreasing T_c , while volatile elements with $800\text{ K} > T_c > 500\text{ K}$ are almost unfractionated, exhibiting a “hockey-stick” depletion pattern that represents the primary volatile element signature of carbonaceous chondrites.

Ordinary and Rumuruti chondrites show a similar pattern of volatile element depletion, but only for Cu, Ga, Ag, Zn, Te and Sn. The covariation of Zn, Te and Sn abundances with matrix abundances in ordinary and Rumuruti chondrites suggests that they contain a primitive CI-like matrix component just like the carbonaceous chondrites. Sulfur and Se are less depleted in ordinary and Rumuruti chondrites, indicating different physicochemical conditions in their formation regions. The unsystematic behavior of the most volatile elements Cd, In and Tl along with Cd and Zn (only ordinary chondrites) stable isotope fractionation suggest secondary redistribution processes on the respective parent bodies due to open system thermal metamorphism.

Enstatite chondrites show no such systematic volatile element abundance patterns with T_c . Notably, their depletion pattern reveal similarities with those of evaporation experiments using carbonaceous chondrite powders under reduced conditions.

Lecture

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

UHT granulites from the Kaapvaal craton – garnet U-Pb ages record a long period of extreme temperatures in the lower crust in the Archean

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Ultrahigh temperature granulite xenoliths are reported from four cretaceous kimberlites on the Kaapvaal craton that are aligned along the NNE axis of the Witwatersrand basin. The granulites consist of garnet, sillimanite, sapphirine, orthopyroxene, plagioclase and quartz in various proportions. Peak metamorphic conditions were estimated from garnet+sapphirine+quartz to lie above 1050°C and pressures between 0.9 – 1.2 GPa (Dawson et al., 1997). Zircons gave ages around 2.72 Ga (Schmitz and Bowring, 2003), the same age as the voluminous Ventersdorp flood basalts.

We determined U-Pb ages and trace element contents simultaneously on garnets by split stream LA ICP MS. Sixteen ages fell between 2.9 and 3.1 Ga (± 0.06 Ga) and two overlap with the zircons. We interpret the data such that the main age group records a prolonged period of UHT metamorphism of ca. 200 Ma. Such an extended duration can be attributed to a thickened crust, high contents of radioactive elements and high thermal advection from the mantle in the Archean (Harley, 2016). Witnesses of high temperature processes during that period are the 3.1 Ga granulite metamorphism at mid-crust level of the Vredefort dome, voluminous K-accentuated granitoid intrusions (3.14 -3.04 Ga), the continuous infilling of the Witwatersrand basin between 2.96 and 2.78 Ga with basaltic magmas at its base and intercalated between its sediments and the final collision of the Kaapvaal East and West Blocks at around 2.9 Ga. The two youngest garnet and the zircon ages may reflect a reestablishment of UHT conditions by the Ventersdorp magmatism.

Lecture

Topic: Frontiers in Mineralogy Talk

Critical mineral resources related to the rise and fall of a supercontinent

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The European Variscides host significant resources of energy and technology critical raw materials (ETRs) associated to various types of hydrothermal systems. Hydrothermal mineralization in central and western Europe is mainly related to the i) amalgamation and ii) the breakup of the supercontinent Pangea during the Late-Paleozoic and Mesozoic, respectively. These mega tectonic events also facilitated the formation of mineral deposits in northern Africa and eastern North America. Late-Paleozoic magmatic-hydrothermal activity was associated with the formation of greisen, skarn and epithermal vein systems that host valuable Li, Sn, W, Ag, Zn, Sb Cu and In. Conversely, Mesozoic rift-related hydrothermal activity resulted in the formation of unconformity-related vein type mineralization, which host significant resources of Co, Ni, Bi, Ag, Zn and fluorite.

This talk provides a brief overview on the different deposit types and associated ETRs in central Europe and discusses ore-forming mechanisms in two distinctly different geological environments (orogenic vs. rift-related). After discussing ore-forming mechanisms on the deposit scale, the findings are complemented by a large amount of recent geochronological data (mainly in-situ LA-ICP-MS U-Pb) that constrain the age of individual ore deposits and mineral occurrences in the context of the larger tectonic framework of central Europe. These results are integrated into preliminary continental-scale geological models for Late-Paleozoic and Mesozoic hydrothermal systems in central and western Europe. The preliminary models convincingly demonstrate that individual ore deposits are local expressions of geological processes that occur on a mega tectonic scale – driven by the rise and fall of the supercontinent Pangea.

Lecture

Topic: 2.2 From dust to planets

Nucleosynthetic Zn isotope anomalies reveal the heritage of Earth's volatiles

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Determining the provenance of volatile elements in Earth is key for understanding the processes that led to its habitability. Based on volatile element abundances and H and N isotope data it has been argued that Earth's volatile element inventory largely stems from the addition of volatile-rich outer solar system (CC) material to a volatile-poor protoEarth made of inner solar system (NC) material [1-2]. However, recent work has shown that an inner or outer solar system origin of Earth's volatiles cannot be distinguished by these approaches [3]. Nucleosynthetic isotope anomalies might offer a direct way of identifying the origin of the volatile materials accreted by Earth [4], however, until now, no such anomalies have been identified for volatile elements. Here, we report the detection of isotope anomalies for the moderately volatile element Zn. Using a comprehensive set of meteorites we show that Zn exhibits the same fundamental isotopic dichotomy between NC and CC materials as non-volatile elements. Terrestrial Zn has an isotopic composition between NC and CC bodies, demonstrating that Earth accreted Zn from both, the inner and outer Solar System. Extending this finding to other volatile elements, and combining the Zn data with anomalies in non-volatile elements yields a coherent picture of the fraction and nature of CC materials in Earth, and thus their relevance for its habitability.

[1] Braukmüller et al., 2019 Nat. Geosci. 12 [2] Marty, 2012 EPSL 313–314 [3] Piani et al., 2020 Science 369 [4] Burkhardt et al., 2021 Sci. Adv. 7

Poster

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Reconstruction of paleoredox conditions in the Upper Jurassic - Lower Cretaceous Bazhenov Sea (West Siberian Basin, Russia)

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The Bazhenov Sea covered around 2 million km² of the Mesozoic West Siberian Basin (WSB) during Volgian to Early Berrasian times, resulting in the deposition of highly organic-rich black shales as part of the stratigraphic unit "Bazhenov Horizon". As black shales are excellent archives for past large- to small-scale sedimentary systems, the study's objective is to develop a detailed depositional model reconstructing the transgression-regression cyclicity, paleoredox conditions, paleosulfidicity and -bioproductivity that prevailed during the black shales' sedimentation, and to infer insights into the primary forces and mechanisms favouring enhanced organic matter preservation and accumulation.

For this, elemental analysis, Rock-Eval pyrolysis and petrographic observations were carried out on a large number of core samples from seven well sections from the south-western WSB (Frolov region). Systematic inorganic and organic composition patterns reveal sequential and regional variations of sedimentary and diagenetic conditions in the study area.

The obtained data show that the sediments were deposited in a marine environment with significant contribution of authigenic minerals and subordinate detrital influence. The enrichment of redox-sensitive inorganic and organic compounds indicates reducing and periodically sulfidic conditions in the bottom and uppermost pore water columns during deposition. Sections that show evidence of anoxia or euxinic conditions simultaneously have the lowest terrigenous influence, suggesting that anoxia is closely linked to sea-level fluctuations in the course of eustatic transgression-regression cycles. The correlation of organic matter and redox proxy enrichments suggests that organic matter accumulation and preservation are mainly controlled by these paleoredox condition variations linked to regression-transgression cyclicity.

Lecture

Topic: 6.1 Earth surface processes in extremely water-limited environments

The Martian subsurface structure at the InSight landing site revealed by marsquakes

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We analyzed the seismological data collected by the InSight mission, which landed on Mars in November 2018, in order to reveal the first tens of meters of the subsurface structure underneath the landing site. Here, we performed horizontal-to-vertical analysis (H/V) for different wind-dependent noise periods and for martian seismic events data (marsquakes). The final H/V curve presents a characteristic trough at 2.4 Hz and a strong peak at 8 Hz. We inverted this H/V curve for the 1D shear-wave velocity structure at the InSight landing site. Based on our inversion results, we propose a strong site effect at the InSight site to be due to the presence of a shallow high-velocity layer (SHVL) over low-velocity units. The SHVL is likely placed below a layer of coarse blocky ejecta and can be associated with Early Amazonian basaltic lava flows. The units below the SHVL have lower velocities, possibly related to a Late Hesperian or Early Amazonian epoch with a different magmatic regime and/or a greater impact rate and more extensive weathering. An extremely weak buried low-velocity layer (bLVL) between these lava flows explains the data around the 2.4 Hz trough, whereas a more competent bLVL would not generate this latter feature. These subsurface models are in good agreement with results from hammering experiments and compliance measurements at the InSight landing site. Finally, this site effect is revealed only by seismic events data and it explains the larger horizontal than vertical ground motion recorded for some marsquakes.

Poster

Topic: 11.3 Young Scientist Session

Neogene-Quaternary evolution of the La Baja Guajira Basin, Colombia: burial and thermal history with implications on petroleum systems

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The La Baja Guajira Basin is the primary gas-producing region of Colombia. This study analyses regional 2D-seismic reflection and borehole data to better understand the Neogene-Quaternary events controlling the basin.

The basement's configuration controlled the sedimentation, and its structural depressions formed the main depocenter (Tayrona Sub-basin). The basement is a pre-rift sequence that displays an abrupt westward deepening of its top from 0.8 km to 12 km depth over 30 km.

Two phases of rifting occurred during the Early Miocene: 1) half-graben formation along onshore and proximal offshore areas, and 2) extension migrated westward and formed the necking domain along the distal offshore area.

From the latest Early Miocene to the Early Pliocene, subduction of the Caribbean Plate underneath South American Plate influenced the basin's offshore area by compressional deformation associated with inverted reactivation of larger normal basement-rooted faults.

During the Middle Miocene, the extension had ceased, sediments filled significant residual accommodation space, and the proximal area remained quieter favouring the deposition of clinoforms that prograded westward until the Quaternary.

Two exhumation pulses (Middle Miocene and Early Pliocene) of adjacent areas resulted in increased subsidence and sedimentation rates, which led the rocks to reach maximum temperature peaks and burial depths. In the Late Miocene, a period of erosion affected the northern proximal areas.

From Late Pliocene to Pleistocene, sea-level changes dominated over tectonism. Ongoing hydrocarbon generation can be expected in the south. High sedimentation rates calculated can lead to microbial gas generation and favour the preservation of biogenic gas accumulations.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

On the genesis of post-subduction porphyry copper magmas

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For subduction-related porphyry Cu deposits, it is generally agreed that the ore-forming magmas fractionate from mafic magmas produced by slab fluid±melt-fluxed melting of the asthenospheric mantle wedge. This model, however, is not able to explain post-subduction porphyry Cu deposits that formed after the termination of slab subduction. Popular models suggest that post-subduction porphyry Cu magmas are partial melts of former lower crustal sulfide-rich arc cumulates with or without minor contribution from potassic mafic magmas. Here we re-appraise this model via a combined approach of natural sample studies and piston-cylinder experiments. The Sanjiang region of SW China is a typical post-subduction porphyry Cu metallogenic belt that formed during the India-Asia continental collision. Based on a detailed petrographic study, we investigated whole-rock elemental and Nd-Sr-Pb isotopic compositions of variously evolved magmatic rocks and garnet-bearing xenoliths throughout the southern Sanjiang region. The results demonstrate that the continental collision-related porphyry Cu magmas formed solely by fractionation of potassic mafic magmas, and that the lower crustal partial melting model built upon wrong radiogenic isotopic compositions of the investigated garnet-bearing xenoliths. The potassic mafic magma fractionation model is further supported by crystallization experiments using a basaltic trachyandesite sample as starting material. The experimental run products reproduce not only the mineral crystallization sequence of magmatic rocks in the southern Sanjiang region but also the liquid line of descent defined by the whole-rock data. Hence, we suggest that the role of pre-existing lower crustal arc cumulates in forming post-subduction porphyry Cu magmas has been greatly overestimated.

Poster

Topic: 6.3 Fractionation of metal(loid) stable isotopes during low-temperature Earth surface processes

Clay dissolution/re-precipitation drives extreme Li isotope fractionation during tropical weathering

Maria Chapela Lara¹, Heather L. Buss², Michael J. Henehan¹, Jan A. Schuessler¹, William H. McDowell³

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Lithium isotopes are the best tracers of weathering intensity, but little is known about the processes that fractionate them in highly weathered settings, where secondary minerals play a dominant role in weathering reactions. To help fill this gap in our knowledge of Li isotope systematics, we investigated Li isotope fractionation at an andesitic catchment in Puerto Rico*, where the highest rates of silicate weathering on Earth have been documented. We found the lowest $\delta^7\text{Li}$ values published to date for porewater (-27‰) and bulk regolith (-38‰), representing apparent fractionations relative to parent rock of -31‰ and -42‰ , respectively. We also found $\delta^7\text{Li}$ values that are lower in the exchangeable fraction (-49‰) than in the bulk regolith or porewater, the opposite than expected from secondary mineral precipitation. We interpret these large isotopic offsets and the unusual relationships between Li pools as resulting from two distinct weathering processes at different depths in the regolith. At the bedrock-regolith transition (9.3–8.5 m depth), secondary mineral precipitation preferentially retains the lighter ^6Li isotope. These minerals then dissolve further up the profile, leaching ^6Li from the bulk solid, with a total variation of about $+50\text{‰}$ *within* the profile, attributable primarily to clay dissolution. Importantly, stream water $\delta^7\text{Li}$ (about $+35\text{‰}$) is divorced entirely from these regolith weathering processes, instead reflecting deeper weathering reactions (>9.3 m). Our work thus shows that the $\delta^7\text{Li}$ of waters draining highly weathered catchments may reflect bedrock mineralogy and hydrology, rather than weathering intensity in the regolith covering the catchment.

*Chapela_Lara_et_al., 2022, JGR-ES.

Poster*Topic:* 1.3 Bridging length and time scales in the modelling of geomaterials**Speciation of Rare Earth Elements (REEs) in hydrothermal systems****Rajorshi Chattopadhyay, Sandro Jahn**

Institute for Geology and Mineralogy, University of Cologne, Germany

The Rare Earth Elements (REEs) are an important group of elements both geologically as well as economically. REEs find important applications in the fields of green energy, electric vehicles and electronics. They are also important tracers for geological processes under hydrothermal /high grade metamorphic conditions. The ability of fluids to mobilise the REEs depend on the chemical composition and the presence of suitable ligands like chloride, fluoride. Ab initio molecular dynamics simulations (AIMD) have been used to predict stability constants of various REE complexes and REE speciation under hydrothermal conditions (Stefanski and Jahn, 2020; Guan et al, 2020). However, AIMD simulations often suffer from significant finite time and size effects. Classical potentials on the other hand solve the problems of AIMD to some extent but they often oversimplify the description of atomic interactions. Several interesting phenomena like formation and breaking of bonds are not captured by classical potentials. Hence a good compromise would be to use ReaxFF (Duin et al. 2001). Another potential drawback of simple pairwise additive classical potentials is their implicit description of multipolar effects which play a significant role in solvation of ions in aqueous solvents. These multi-body effects become essential when dealing with multivalent ions, in concentrated solutions and in interfacial environments (Tazi et al, 2012). Here, we discuss results from preliminary simulations with classical potentials (Migliorati et al. 2017). We demonstrate the finite size and finite time effects associated with AIMD and how classical potentials can be potentially used to overcome them.

Plenary Lecture

What (probably) controls the size of mineral deposits

Cyril Chelle-Michou

ETH Zürich, Switzerland

Theoretical, conceptual, technical, and analytical advances over the last century have allowed not only to develop and refine models for the formation of mineral deposits, but also to develop cost-effective exploration methods to identify new deposits. However, once a new orebody is identified, it requires extensive drilling campaigns and massive investments to quantify its metal content. This is associated with increasing economic risks and social and environmental impacts, that are magnified by the current need to search for increasingly deeper orebodies (under cover). In order to mitigate such risks, it would be advantageous to be able to determine (even coarsely) the size of the newly discovered deposit as early as possible during exploration.

While commonly advocated magmatic, hydrothermal and geochemical processes and their associated fertility indicators may indeed pinpoint toward the formation of a deposit, they fall short in explaining their ranges in metal endowment which typically cover over four to five orders of magnitude in each deposit type (e.g. porphyry copper deposits, MVT deposits). Here we discuss how understudied physical factors in porphyry copper and MVT deposits (such as fluid flow duration, magma intrusive flux and timescales in tandem with the thermo-mechanical conditioning of the crust) contribute to the fertility of such systems. Further we will explore possible ways to assess this 'physical fertility' from the rock record by combining cutting edge analytical methods and advanced numerical models.

Lecture

Topic: 1.6 Probing (bio)geochemical reactions at mineral interfaces using micro- to nanoscale techniques

The influence of phospholipids on the structure and composition of ferrihydrite colloids

Zhengzheng Chen^{1,2}, Jeffrey Paulo H. Perez¹, Roberts Blukis¹, Glen J. Smales³, Brian R. Pauw³, Jessica A. Stammeier¹, Jörg Radnik³, Liane G. Benning^{1,2}

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Organophosphates (OP) are important nutrient components in soils and they readily interact with abundant iron phases. Ferrihydrite (FHY), a ubiquitous iron phase in soils, plays a major role in iron-mediated carbon storage. However, the influence of OP on FHY formation, transformation or stabilization is poorly understood. Here we investigated the effects that glycerol phosphate (GP; model organophosphate compound) has on the structure and properties of synthetic FHY. FHY-GP was synthesized by coprecipitation using variable initial molar P/Fe ratios (0.01 to 0.5). The solids displayed typical 2-line FHY X-ray diffraction pattern and chemical analyses showed that they all had a final P/Fe ratio of no more than 0.2. With increasing initial P/Fe ratio, we observed a sharp decrease in specific surface area from 290 to 3 m² g⁻¹ with an associated reduction in porosity. Analyses of solid products by small angle X-ray scattering revealed that the at high initial P/Fe ratios the solids formed were cluster with diameters of ~ 1.2 nm. Local structural and bonding environment analysis derived from infrared spectroscopy and Fe K-edge X-ray absorption spectroscopy, showed that with increasing P loading, the bonding configuration gradually transitioned from the initial binary binuclear to monodentate mononuclear geometry, while the average coordination number of edge-shared Fe polyhedral decreased from 3.2 to 1.3 and the corner-shared Fe polyhedral disappeared. These results indicated that during the formation of the FHY-GP, the Fe(III) polymerization was likely impeded by the GP, with an increasing P/Fe ratio strongly affecting the resulting FHY-GP structure.

Lecture

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Out-of-plane permittivity of nanoconfined geofluids: a molecular dynamics study

Alireza Chogani, Oliver Plümper

Utrecht University, The Netherlands

In fluid-driven mineral replacement reactions, reaction-induced porosity generation is one of the most important mechanisms that provide fluid pathways into the reaction front. Our multi-scale electron microscopic imaging techniques show that majority of these generated pores are at the nanometer scale. Due to the large surface-to-volume ratios, fluids confined in this nanoporous rock network demonstrate new properties. For example, the permittivity of nanoconfined water is no longer a scalar quantity like bulk and shows a tensorial behavior because of the anisotropy of the system perpendicular to the wall direction. In the present study, we used molecular dynamics (MD) simulations to investigate the out-of-plane permittivity of water confined between two mineral slabs at elevated pressures and temperatures. We explored the rock material effect by simulating calcite, brucite, and quartz as confining minerals. In all cases, with the reduction of the width of the nanochannel the out-of-plane permittivity of water declines. Thus, in smaller nanopores ($\varphi < 10$ nm) there is a significant difference between the permittivity of nanoconfined and bulk water that can have a profound impact on mineral solubility, aqueous speciation, and fluid transport properties in nanoporous metamorphic rocks. Although a rise in the out-of-plane permittivity is seen through the decreasing temperature or increasing pressure, its value in all cases is much lower than the bulk water dielectric constant in similar conditions.

Lecture

Topic: 11.3 Young Scientist Session

Earth's lower mantle may be harder than expected: Al, Si diffusion in bridgmanite

Laura Czekay, Nobuyoshi Miyajima, Catherine McCammon, Daniel Frost

Bayrisches Geoinstitut, Germany

Diffusion of atoms in crystalline solids at high temperatures and pressures influences dynamic processes in Earth's lower mantle. This study aims to better understand the physical behaviour of Earth's most abundant mineral with implications for lower mantle viscosity. Previous studies that measured Si-self diffusion coefficients in bridgmanite (Brg) showed a value at 25 ± 1 GPa and 1800 °C of $\text{Log}_{10}(D_{\text{Si}}) = -18 \pm 0.5$ (based on units of m^2/s). Our study revealed a significant slower diffusion coefficient that may challenge previous calculations of lower mantle viscosity. We investigated Al, Si interdiffusion in Brg experimentally at 24 GPa and 1750 to 2000 °C using a multianvil apparatus using diffusion couples composed of bridgmanites that were pre-synthesised from 0-5 mol.% Al_2O_3 -bearing MgSiO_3 enstatite. The Al diffusion profiles were analysed across the diffusion interface in the recovered samples using a scanning transmission electron microscope equipped with an energy-dispersive X-ray spectrometer. The obtained diffusion coefficient for interdiffusion (volume diffusion) at 24 GPa and 1800 °C was $\text{Log}_{10}(D_{\text{Al,Si}}) = -20.1 \pm 0.7$. The resulting data can be used to estimate deformational strain rates of Brg in the lower mantle based on different creep mechanisms controlling the viscosity.

Poster*Topic:* 1.2 Methods in Geochemistry and Mineralogy**Al, Si interdiffusion in Al-bearing bridgmanite under lower mantle conditions: Analytical TEM study****Laura Czekay, Nobuyoshi Miyajima, Catherine McCammon, Daniel Frost**

Bayrisches Geoinstitut, Germany

Diffusion studies in minerals are a fundamental tool for understanding the rheological properties of Earth's mantle. Previous theoretical studies on deformational strain rates show that the key mechanism for deformation in bridgmanite (Brg) is diffusion-controlled creep of the slowest element, Si. The Al, Si interdiffusion rate in Brg is thus essential for understanding mantle dynamics. Brg diffusion couples were synthesised from 0-5 mol.% Al₂O₃-bearing MgSiO₃ enstatite at 24 GPa and 2073 K using a conventional multianvil apparatus. A scanning transmission electron microscope (STEM) can provide a resolution down to the nanometre scale and is therefore ideal for studying slow diffusion, such as in this study. To achieve reliable results from STEM analysis, it is necessary to carry out sample preparation carefully. In this study, a focused ion beam was used for (S)TEM sample preparation. The Al substitution mechanisms in Al-bearing Brg diffusion couples in the recovered samples were analysed using an energy-dispersive X-ray spectrometer. The measured diffusion coefficient for Al, Si interdiffusion at 24 GPa and 2073K was $\text{Log}_{10}(D) = -20.1 \pm 0.7$ (based on units of m²/s). The result is two to three orders of magnitude slower compared to the previously reported Si self-diffusion coefficient $\text{Log}_{10}(D_{\text{Si}}) = -18 \pm 0.5$ at 25 GPa and 2073 K. The slower diffusion rate places limits on deformational strain rates of Brg in the lower mantle.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

The dual-clumped isotope thermometer as a tool to identify and correct for isotopic disequilibrium in the clumped isotope composition of biogenic carbonate

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The clumped isotope composition (Δ_{47}) of marine biogenic carbonates is an increasingly applied proxy for temperature reconstruction. The clumped isotope measurement is particularly valuable as Δ_{47} is independent of the $\delta^{18}\text{O}$ of seawater. However, kinetic effects during biomineralization can impact the Δ_{47} of some marine archives, impeding accurate paleotemperature reconstruction.

Dual carbonate clumped isotope thermometry (i.e., simultaneous Δ_{47} and Δ_{48} measurements on a single carbonate) has the potential to identify kinetically driven isotopic disequilibrium in biogenic carbonate and facilitate the reconstruction of carbonate formation temperature independent of kinetic biases. We present the dual-clumped isotope compositions of several key marine archives, historically used to reconstruct changes in sea surface temperature and $\delta^{18}\text{O}$ across the Phanerozoic. These include brachiopods, cold and warm-water corals, and belemnites.

Corals and brachiopods exhibit disequilibrium Δ_{47} and Δ_{48} , corresponding kinetic effects relating to mixing of an equilibrium DIC pool with kinetically derived HCO_3^- produced by hydration and hydroxylation of CO_2 . We demonstrate how measurement of the dual clumped isotope composition of corals and brachiopods can be used to correct for kinetic bias in Δ_{47} , yielding more accurate temperature reconstructions ($<\pm 3^\circ\text{C}$ at the 95% confidence interval). Dual clumped isotope thermometry, therefore, (re-)opens brachiopod and coral archives for reconstruction of shallow and intermediate water mass temperatures on geological timescales. Furthermore, we confirm that belemnites precipitate calcite in dual-clumped isotope equilibrium yielding precise growth temperatures, thus belemnite Δ_{47} may be reliably used as a proxy for Mesozoic sea surface temperatures ($<\pm 2.5^\circ\text{C}$ at the 95% confidence interval).

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

Optimized sequential extraction for chromium from laterite deposits

Ruth Esther G. Delina^{1,2}, Jeffrey Paulo H. Perez¹, Jessica A. Stammeier¹, Roberts Blukis¹, Liane G. Benning^{1,2}

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Chromium is naturally enriched in nickel laterite deposits, the world's main source of nickel. Both of its main redox species (III and VI) are important, but Cr(VI) is the more mobile, toxic and carcinogenic pollutant species. It is often leached from nickel laterites, potentially contaminating ground- and drinking waters. Thus, it is crucial to quantify the partitioning for chromium in the laterite host phases because these associations dictate the potential mobility, bioavailability and toxicity of chromium. Although such assessments are usually evaluated through sequential extraction procedures (SEP), so far, no SEP has been designed, tested and validated for chromium partitioning from laterites that are typically dominated by iron (oxyhydr)oxides.

Here we evaluated existing SEPs and optimized and validated a new scheme. For our optimized SEP, we tested the efficiency of various extractants on Cr- and Fe-bearing phases (e.g., goethite, chromite) commonly present in nickel laterites. We then applied our SEP on nickel laterites from the Philippines. Our results revealed that Cr recovery was up to 10x higher compared to non-Ni laterite optimized standard SEPs. The developed SEP efficiently dissolved crystalline Fe phases recovering 25-34% of the total chromium. Existing SEP schemes only recovered 2-18% because they only partially dissolved the host goethite and hematite. Our SEP also prevented the overestimation of organic matter bound Cr. It could also quantify strongly adsorbed chromium oxyanions. These improvements provide a better quantification of different chromium hosts and thus improve our understanding of the potential environmental impacts of chromium in mining-impacted lateritic areas.

Lecture

Topic: 6.1 Earth surface processes in extremely water-limited environments

$^{87}\text{Sr}/^{86}\text{Sr}$ ratios as tracer for gypsum sources and redistribution processes

Katharina Deußen, Carsten Münker, Michael Staubwasser

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Gypsum group minerals in the Atacama Desert occur in pedogenic profiles or as primary lacustrine sediments and are subject to complex redistribution processes. The $^{87}\text{Sr}/^{86}\text{Sr}$ composition of gypsum is a useful tool to trace the source of the gypsum deposits. A sequential digestion method was developed to analyze gypsum and its inherent detrital silicate components separately. Samples were taken from the Central Depression and the Western Cordillera, including Miocene - Pleistocene lacustrine deposits and some pedogenic gypsum.

The $^{87}\text{Sr}/^{86}\text{Sr}$ compositions measured in gypsum range from 0.7065 to 0.7074, and are in most cases similar to that of the detrital components, indicating that the gypsum composition is influenced by the underlying bedrock through parental water-rock interaction. Interestingly, most samples yield lower $^{87}\text{Sr}/^{86}\text{Sr}$ ratios than present day waters from the Atacama Desert. The $^{87}\text{Sr}/^{86}\text{Sr}$ ratio varies strongly between the different samples, reflecting the highly variable bedrock composition in the Atacama Desert that was often neglected in previous studies. There are some outliers with strongly enriched $^{87}\text{Sr}/^{86}\text{Sr}$ values up to 0.7128 in the detrital components. This mismatch can be explained by various sources of gypsum and detritus, which can be achieved through processes like aeolian redeposition of gypsum into a basin with a bedrock carrying a distinct Sr signal or by dissolution and reprecipitation of the gypsum by waters with different Sr signals. Also, in some cases, the parental brine may reflect the bedrock composition of the water catchment rather than the bedrock composition of the basin, where lacustrine gypsum precipitates.

Lecture

Topic: 4.5 Tectonic Systems (TSK Open Session)

Force-balance changes at the subduction-to-collision transition and implications for mountain building

Armin Dielforder, Andrea Hampel

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The elevation of mountain belts increases at the subduction-to-collision transition in response to crustal thickening and processes like slab breakoff, but the main parameters controlling how much mountain height increases remain poorly understood. Based on analytical and finite-element force-balance models, we show that the increase in mountain height depends mainly on the magnitude of the shear force along the plate boundary fault (megathrust) and the reduction of submarine margin relief. During oceanic subduction, the megathrust shear force is balanced by the gravitational effect of the margin relief and the deviatoric stresses in the upper plate are low. When the submarine margin relief is reduced during the closure of the ocean basin, the effect of the gravitational force decreases and the upper plate experiences enhanced deviatoric compression, which allows the mountain height to increase until the deviatoric stresses beneath the high mountains are low again. If the increase in mountain height cannot keep pace with the submarine relief reduction, the compression of the upper plate increases by a few tens of MPa, which promotes tectonic shortening and mountain building. Our findings indicate that mountain height can increase by hundreds of meters to a few kilometers during continental collision, depending primarily on the trench depth during the subduction stage and possible syncollisional changes of the megathrust shear force.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

A new tool to decipher the past silica cycle? The Si isotope signatures of radiolarians: taxa-specific isotope difference and their potential for studying past biogeochemistry

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Dissolved silica (DSi) is an essential nutrient for marine silicifiers, and its cycling is closely linked to the biological pump and carbon cycle. The biological uptake of DSi and subsequent formation of biogenic opal (BSi) discriminate against heavier ^{30}Si isotopes, resulting in BSi with lighter isotope compositions than surrounding seawater. The resulting stable isotope compositions ($\delta^{30}\text{Si}$) of BSi have proven reliable tools to reconstruct the DSi concentrations of bottom waters (sponges) or surface ocean nutrient utilization (diatoms). However, crucial information from the subsurface and intermediate waters is missing to fully reconstruct silica cycling.

A new tool to close this gap is the $\delta^{30}\text{Si}$ of radiolarians ($\delta^{30}\text{Si}_{\text{rad}}$), marine zooplankton dwelling in shallow to deep depths. Radiolarian $\delta^{30}\text{Si}$ is thought to reflect DSi concentrations of the surrounding seawater, but estimations of a fractionation factor indicating how radiolarians discriminate against the ^{30}Si are difficult due to the inability to culture radiolarians: Accordingly, estimates are limited to analyses to comparisons of radiolarians from surface sediment and DSi concentrations from their habitat depths. So far, only two studies have estimated an apparent fractionation factor ($\Delta^{30}\text{Si} = \delta^{30}\text{Si}_{\text{rad}} - \delta^{30}\text{Si}_{\text{DSi}}$) for radiolarians, ranging between -0.0‰ and -1.2‰. The differences in $\Delta^{30}\text{Si}$ could now be attributed to different radiolarian taxa, likely caused by taxa-specific Si isotope fractionation during DSi uptake.

Significant inverse relationships have also shown the assumed relationship between $\delta^{30}\text{Si}_{\text{rad}}$ and DSi concentrations. However, these relationships still have large uncertainties, and $\delta^{30}\text{Si}_{\text{rad}}$ cannot identify changes below 10 to 15 μM DSi, highlighting the need for more investigations.

Poster

Topic: 6.4 Landslides – detecting, monitoring, modeling, assessing hazards, and coping with risks

A Review and Database of Landslide Induced Tsunamis

Katrin Dohmen, Anika Braun, Tomás Manuel Fernandez-Steeger

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Landslide induced tsunamis are a well-known phenomenon and have been reported many times in the international literature. The research has focused so far on the investigation of individual case studies and on modelling of tsunami waves but up to now there is no overview of all documented landslide tsunamis that happened in the past and what might be learned from those events.

The objective of this study is a review and comparison of the known case studies. A database of parameters that are relevant for the tsunami generation and propagation is established. Those include the properties of the landslide, the waterbody geometry and tsunami properties.

Particularly high waves can be triggered when slopes collapse and fall into waterbodies with little water volume like rivers, lakes or narrow bays that are widely isolated from the open sea. Catastrophic landslide tsunamis occur frequently in fjord landscapes with elongated and narrow waterbody geometries with steep and - due to deglaciation processes - instable slopes. Also, in seismically active regions where earthquakes can trigger landslides, many landslide tsunamis have been reported. A third scenario with an especially high potential for landslide tsunamis are reservoir lakes, where seasonal water level variations may cause slope instabilities.

The findings of this work will contribute to a better understanding of the generation of landslide tsunamis. They can be used in a next step to identify potentially endangered areas and to take preventive measures regionally, for example to set up monitoring systems on slopes at risk.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Microbial iron cycling during deposition and diagenesis of Banded Iron Formations

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Banded Iron Formations (BIFs) are marine sediments consisting of alternating iron (Fe)-rich and silica (Si)-rich layers which were deposited between 3.8 to 1.85 Ga during the Precambrian era. BIFs represent important proxies for the geochemical composition of Precambrian seawater and provide evidence for early microbial life. Iron present in BIFs was likely precipitated in the form of Fe(III) minerals, such as ferrihydrite ($\text{Fe}(\text{OH})_3$), either by anoxygenic photoautotrophic Fe(II)-oxidizing bacteria (photoferrotrophs), by microaerophilic Fe(II)-oxidizing bacteria, or by the abiotic oxidation of dissolved Fe(II) (i.e. Fe^{2+}) by O_2 produced by cyanobacteria. However, the mineralogy found in BIFs today shows not only oxidized minerals like hematite but also (partially) reduced minerals like magnetite and siderite. This might be due to the presence of ancient dissimilatory Fe(III)-reducing microbes, which were able to reduce parts of the Fe in the primary precipitated Fe(III) minerals back to Fe(II). In our current work, we combine both oxidative and reductive Fe transformation processes in cycling experiment by co-culturing marine Fe(II)-oxidizing (oxygen-producing cyanobacteria *Synechococcus* PCC 7002) and Fe(III)-reducing bacteria (*Shewanella colwelliana*) in the presence of different iron and silica concentrations to investigate the microbial impact on Fe mineral formation. These experiments and the resulting data will allow to discern processes occurring during the deposition and diagenesis of BIFs and better interpret early Earth conditions. Here, we show first results from the cycling experiments, which reveal the mineral assemblages that can be formed under such conditions that mimic processes in marine sediments of the early Earth.

Lecture

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Aridification in the terrestrial record: A case study from the Nullarbor Plain of southern Australia

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The Nullarbor Plain in southern Australia is an extensive treeless area (ca. 200,000 km²), almost devoid of surface water, reflecting the modern expression of Plio-Pleistocene aridification. The rapid climatic shift from the humid late Pliocene to arid early Pleistocene drove the Nullarbor Plains development as an important biogeographic barrier, facilitating distinct diversification of numerous taxa to the east and west. Despite the significance of this environmental change, absolute age constraints on terrestrial aridification are rare. To improve understanding on the timing of aridification in the Nullarbor Plain, we combine petrographic, mineralogical, chemical, and (U-Th)/He thermochronological data from ferruginous indurations that overprinted middle-upper Eocene Ooldea Sands in the eastern Nullarbor Plain. Integrated analyses reveal (i) secondary pedogenetic relic features hosted in marine siliciclastic sediments, (ii) later geochemical transformation of pedogenetic features, and (iii) subsequent growth of polycrystalline iron oxides in response to an inferred groundwater decline. Thermochronological results tie the latest stage of this polyphase genesis (i.e., the ferruginization) to the Plio-Pleistocene transition. Review of other local and regional climate proxies shows profound temporal correlations with the formation of ferruginous indurations. These dates constrain a turning point in southern Australia's landscape evolution, associated with the initiation of a vast arid landscape separating mesic environments, with implications for habitat fragmentation and species diversity.

Poster

Topic: 4.3 The role of fluids in metamorphic and metasomatic reactions

C-O-H-S fluids released by subducted serpentinite and the implications for arc-magma oxidation

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Serpentinites are able to carry H₂O, ferric iron, carbon and sulfur into subduction zones, where they stepwise released fluid during dehydration. These C-O-H-S fluids are intimately linked to magma oxidation and ore formation within magmatic arcs. However, the mechanism of the transfers of carbon, sulfur and ferric iron into fluids is poorly known. It is also controversially discussed if C-O-H-S fluids can oxidize arc magmas. Our new thermodynamic models focus on the species produced by C-O-H-S fluids during subduction. Closed system modeling provides molar concentrations of such species under different P-T conditions, showing that reducing species generally have high solubilities at low P-T conditions. Oxidizing species mainly remain in the fluid after increasing P-T conditions. Open system fluid fractionation shows that only 5-14% of carbon is transported to the mantle wedge, while the amount of sulfur loss is as high as 55-100% at sub-arc depths. Almost all lost carbon and sulfur are released as oxidizing species. The redox properties of the fluids are controlled by sulfur, resulting in an oxygen fugacity of the fluids being 0.6-0.95 log units higher than that of the HM buffer. Sulfur loss is a function of the whole-rock compositions and the subduction geothermal gradient, demonstrating elevated sulfur fluxes to be released from serpentinite in cold subduction zones compared to warm ones. Our modeling results are consistent with petrological observations and global-arc-basalt oxygen fugacity calculations and highlight that the C-O-H-S fluids released from the subducted slab can considerably contribute to the composition of arc magmas.

Lecture

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

In situ-produced cosmogenic krypton in zircon: its potential for Earth surface applications

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Analysis of cosmogenic nuclides produced in surface rocks and sediments is a valuable tool for assessing the rates of processes and the timing of events that shaped the Earth surface. The various nuclides that are used have specific advantages and limitations that depend on the time range over which they are useful, the type of material they are produced in and not least the feasibility of the analytical effort. Anticipating novel applications in Earth surface sciences, we develop in situ-produced terrestrial cosmogenic krypton (Krit) as a new tool, the motivation being the availability of six stable and one radioactive isotope (⁸¹Kr, half-life 229 kyr) and of an extremely weathering-resistant target mineral (zircon). We provide proof of principle that terrestrial Krit can be quantified and used to unravel Earth surface processes.

Lecture

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Extreme As partitioning into pyrite during hydrothermal siderite replacement in As poor fluids

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Pyrite is among the most abundant sulphide minerals in the Earth's crust and an important sink for As and valuable elements like Au and Te (1, 2). Hence, arsenian pyrite is of potential economic interest, but also an environmental hazard if As is released to ground- and surface waters. Knowing the limits and mechanisms of As incorporation in pyrite is therefore required to better understand the formation of high-grade ore deposits and to assess the contribution of As to contamination sites. It is suggested that As either substitutes for S or Fe in the bulk crystal or forms localized high-As domains within the pyrite lattice. In various studies, partition coefficients (D_{As}) were determined that range from $D_{As} = 300 - 1600$, with D_{As} being the ratio of the As concentration in pyrite relative to the corresponding fluid (3). However, previous studies focused on As-rich fluids (1 – 200 ppm), whereas the partitioning behaviour in low-As fluids (<1 ppm) has not been studied to date. We synthesized pyrite under Carlin-style, hydrothermal conditions (200°C, pH 5) by replacing siderite in H₂S-rich fluids containing As concentrations between 1 ppb and 10 ppm. Quantitative fluid analysis and high-resolution LA-ICP-MS mappings indicate an order of magnitude stronger partitioning of arsenic from As-poor fluids (1 ppb, $D_{As} = 15000$), leading to unexpectedly high enrichment of As in pyrite. This observation suggests a highly efficient mechanism of As fixation into pyrite from As-poor fluids at moderate temperature conditions.

References:

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- [2] Kusebauch et al.(2019). DOI:[10.1126/sciadv.aav5891](https://doi.org/10.1126/sciadv.aav5891).
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Lecture

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Magnetic mineralogy of sediments and its geological implications: advances and challenges

Ramon Egli

ZAMG, Austria

Magnetic iron minerals are almost ubiquitous in rocks and sediments and convey important information about geological processes and past variations of the Earth's magnetic field. The recent development of new magnetic measurement techniques at various scales, from bulk samples down to individual crystals, opens new opportunities for tackling interesting questions about planetary magnetic fields, the ancient Earth, the biogeochemical cycle, and transport processes in the atmosphere and the oceans. On the downside, magnetic characterization techniques are intrinsically non-unique and must be used in combination with micromagnetic modelling and other analytical tools. Once the magnetic fingerprint of specific magnetic mineral categories – such as silicate inclusions and authigenic magnetite in sediments – is determined, fast, non-destructive measurements can be used to trace the processes responsible for their variation in space and time.

Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

A new experimental approach for the determination of the diffusivity fractionations of water isotopes in air

Mohammed El-shenawy, Daniel Herwartz, Michael Satubwasser

University of Cologne, Germany

Water isotopes are key tools to understand the dynamics of the global hydrological cycle. A well constrained hydrological model requires a precise definition of isotopic diffusion and equilibrium fractionation factors (DIFF and EIFF, respectively) among water phases. Although there is a consensus on the EIFFs in the community, there is still a debate regarding the precise DIFF. Few experimental studies were performed to define the DIFFs of water in air, however, their data are scattered significantly. Most of these experiments were designed to gradually evaporate a small body of water forced by a stream of either dry nitrogen or air. This design induced several complications, including turbulence, surface cooling and isotopic heterogeneity in the water body, which required additional steps of corrections that may affect the final calculation of the DIFF.

In this study, we performed a passive approach using a hygroscopic salt (Anhydrous CaCl_2) to absorb water vapor from air (nitrogen) under controlled relative humidity at room temperature in a glove box. Once the CaCl_2 granules exposed to humid air, it progressively absorbed water vapor until it dissolved into the water forming a brine. At the early stage of the absorption the thin water film upon the surface of CaCl_2 reflects a pure isotopic diffusion of water vapor, while the final stage of absorption (i.e., brine) represents a pure isotopic equilibrium between water vapor and the brine. Hydrogen and oxygen isotope measurements of these two stages of absorption will be presented in the meeting.

Lecture

Topic: 1.3 Bridging length and time scales in the modelling of geomaterials

A model for the angle of repose of granular materials on planetary surfaces

Filip Elekes¹, Eric Josef Ribeiro Parteli²

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One of the most important observables characterizing the packing and flowability of particulate systems is the angle of repose, i.e., the angle between the horizontal and the sloping side of a heap of particles. Indeed, this angle provides an excellent proxy for particle size on planetary surfaces, because the smaller the particle is, the larger the impact of attractive van der Waals forces relative to particle weight. A mathematical expression for the angle of repose would thus provide a useful tool for bridging between the geomorphologic and particle scales, and would have implications in various industrial sectors as well. We have recently obtained such an expression from direct numerical simulations of particle-scale processes using Molecular Dynamics applied to granular physics [1]. Our simple expression reproduces the angle of repose observed in a very broad range of experiments, including particle sizes consistent with aerosols, sand and pebbles, and gravity values from 6% to 100 times the Earth's gravity. The future application of our equation might help to infer, for instance, on the size, surface energy and grain density of particles constituting granular surfaces on various celestial bodies of our solar system.

[1] Elekes, F.; Parteli, E. J. R. An expression for the angle of repose of dry cohesive granular materials on Earth and in planetary environments. *Proc. Natl. Acad. Sci. USA* 118 (38), e2107965118 (2021). doi:<https://doi.org/10.1073/pnas.2107965118>

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

Open Science – more than Open Access

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The Berlin Declaration from 2003 was the starting point for Open Access to scholarly publications. Today, however, we speak about Open Science that reaches far beyond Open Access and represents collaborative, transparent and accessible research that includes all kinds of research results: scholarly literature, research data, software, samples, instruments, etc. In addition, efforts such as the FAIR Principles and the Enabling FAIR Data Commitment Statement, combined with increasing demands for machine accessibility to data, have raised user expectations towards the capabilities of research data repositories and datacentres. These repositories are often key partners supporting researchers in fulfilling the new requirements. This presentation will draw the line from major statements and requirements of Open Science, delineate the role of research data repositories as well as major research infrastructures, like the fNFDI4Earth or EPOS (European Plate Observing System) are additional players in making research data accessible in harmonised form.

Poster

Topic: 4.5 Tectonic Systems (TSK Open Session)

Interim report about geological survey in the Monticiano-Roccastrada metamorphic core complex (MRMCC, S-Tuscany, Italy) with considerations about its stratigraphic and tectonic development

Hubert Engelbrecht

Environmental Geology, Germany

The study area is part of the Mid Tuscan Ridge: a linear belt of metamorphic core complexes, exhumed during M-L-Tertiary times. They separate the N-Appenninic main belt from the Tuscan metamorphic zone, which originated during the opening of the N-Tyrrhenian back arc basin. This resulted from postcollisional rollback of the steeply W-dipping Adriatic subduction zone: effecting the migration of eastbound, paired compressional-extensional deformation fronts and of magmatism in the overlying crust (literature data).

The central part of the MRMCC (Farma Valley) was chosen for revision of geological field work. The already accomplished map part including resulting stratigraphic and tectonic facts are displayed:

Results: Above a fragmented and extended uniform base - Devonian pelagites - different Carboniferous, coeval, predominantly siliciclastic depositional areas developed as highstand systems tract above a downlap surface. Their recent proximality trend is westbound and their sedimentary environments, separated by normal faults, represent the shelf, lower slope, base of slope and basin margin. Sediment input was triggered by tropical storms and/or seaquakes. The deposits of these environments are covered by regressive, littoral-deltaic siliciclastics (Permian).

During E-M-Tertiary subduction related tectonic burial, the Carboniferous normal faults were reactivated, so that mentioned slope and basin deposits were thrust onto inner shelf deposits. M-L-Tertiary unroofing caused exhumation from ca. 25 km depth. A megabreccia got exposed. It is arranged in subzones, characterised by distinctive metamorphism and deformation.

Farma Valley is probably geomorphological expression of an exhumed tear fault, part of the fracture system controlling the eastward migration of the Tuscan Magmatic Province.

Lecture

Topic: 1.3 Bridging length and time scales in the modelling of geomaterials

'Where to land the next Mars rover?' and 'How much drugs are in our soils?' - a computational study of natural sorptive materials

Valentina Erastova

University of Edinburgh, United Kingdom

'Where to land the next Mars rover?' and 'How much drugs are in our soils?' - to answer these questions, we must look at the fundamental processes at the mineral and material interface.

In this talk, I will discuss our approach to the development of molecular models of two important sorptive materials - black carbons and smectite clays - and show how the use of atomistic simulations provides us with information about the physicochemical processes at their interface.

Our goal is to facilitate the uptake of molecular modelling to assist in the development of environmental pollution remediation materials, understanding seasonal fluctuations of the pollutants in water bodies, constructing mineral-assisted origin of life hypotheses, and guiding our search for biosignatures in Space.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Gallium-Aluminium Ratios as a proxy for Archean seawater: First Insights from the 2.7 Ga old Temagami Banded-Iron Formation, Canada

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¹Jacobs University Bremen, Germany; ²Kiel University, Germany; ³Federal Institute for Geosciences and Natural Resources (BGR), Germany

Banded iron formations (BIFs) are robust geochemical archives used for the reconstruction of the evolution of the Precambrian hydrosphere-atmosphere system. Here, we present preliminary results on the gallium and aluminium concentrations in detritus-free samples from adjacent metachert and magnetite bands in the Neoarchean Algoma-type Temagami BIF, Canada. Gallium and Al are geochemical partners with rather coherent behaviour during magmatic and clastic sedimentary processes. However, Ga and Al fractionate in hydrous environments, leading to different Ga/Al ratios in soils, river water, seawater, and hydrothermal fluids. Therefore, the Ga/Al ratio may be used as a source proxy, similar to the better-constrained Ge-Si systematics in Precambrian BIF. Ga-Al systematics may yield information on the major sources to seawater during deposition of Fe oxide and metachert BIF bands.

Measurements of adjacent Temagami BIF bands with solid (i.e., laser-ablation) and solution (i.e., acid-digested sample) ICP-MS show distinct differences for metachert. Gallium is highly susceptible to interferences in mass spectrometric analyses, and thus high-resolution ICP-MS or QQQ-ICP-MS needs to be used. Our preliminary results suggest that, in marked contrast to Ge and Si, Ga and Al do not show large differences between magnetite and metachert bands in the Temagami BIF. However, our preliminary Ga/Al ratios for the Temagami BIF are generally lower than those of modern seawater, possibly indicating Ga-Al fractionation between BIFs and their seawater source and/or lower Ga/Al ratios in ambient Temagami seawater.

Poster

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Connection of sulfide species and sedimentary trace metal cycles in the Namibian shelf – implications for paleo-marine redox proxies

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The identification of redox-states and -cycling in the paleo-ocean is typically based on the application of geochemical proxies in the geological record. In particular total organic carbon (TOC) and total sulfur (TS) contents, trace metal (TM) enrichments, elemental ratios (e.g. TM/Al, Fe/Al) and stable isotope compositions (e.g. of sulfur and molybdenum) in siliciclastic sedimentary rocks are used to distinguish between anoxic-ferruginous and -sulfidic conditions of the past [e.g. 1]. For the understanding of depositional and diagenetic mechanisms that may affect these proxy signatures, their detailed calibration in modern marine environments is, however, required. Notably, the connection of TM accumulation, TOC content and sulfide production is still not fully understood. In this context, open-marine shelf sediments connected to upwelling regimes are of high importance given that high organic carbon burial fuels sulfate reduction and the accumulation of TMs in the sediment.

Here we investigate sediment cores from different redox-regimes along the Namibian shelf, which are controlled by the Benguela upwelling system. Sediments were deposited under anoxic-sulfidic to oxic conditions and show a correlation of TOC (average: 3.57 to 8.93 wt-%) and TS concentrations (average: 1.02 to 1.42 wt-%). In contrast, TM enrichments are mainly uncorrelated with TOC and TS contents. Indeed, the extraction of different sulfide species and their sulfur isotopic compositions reveal variabilities in the sulfur cycling between the investigated settings and an influence on the accumulation of TMs. We discuss the importance of different sulfur species on TM redox-proxies.

[1] Calvert and Pedersen (1993) Marine Geology 113, 67-88.

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

Timing and conditions for peak metamorphism in Isua (Western Greenland)

Benjamin Chaim Fievé Eskesen¹, Kathrin Fassmer², Carsten Münker³, Thomas Ulrich¹, Kristoffer Szilas⁴, Thorsten Nagel¹

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We present a Lu-Hf-garnet-amphibole-whole rock age of 2.59 ± 0.11 Ga for a carbonaceous garnet-hornblende-mica schist from the Isua supracrustal belt (western Greenland). Petrological data indicate prograde garnet growth towards regional peak-metamorphism at amphibolite-facies conditions. Mylonitic foliation in the sample formed at least partly during and after garnet growth. The sample does not show any hints of earlier metamorphism. These results cast doubt on the accepted concept that peak metamorphism and associated deformation in the Isua supracrustal belt are attributed to Eoarchean tectonics. This is remarkable as deformation style and metamorphism have been viewed as reflecting intense horizontal accretion or even subduction and are the one of pillars, on which models of early plate tectonics rest.

Lecture

Topic: 11.5 Open Session - Geology

Exploring the geothermal potential of North Rhine-Westphalia – insights into the intermediate and deeper subsurface

Sarah Esteban Lopez, Kim Roya Nokar, Martin Sattelberger, Vladimir Shipilin, Burcu Tasdemir, Immanuel Weber

Geological Survey of North Rhine-Westphalia, Germany

The rising demand for heating applications in North Rhine-Westphalia (NRW) based on regional, climate and environmentally friendly energy sources has prompted the federal state government to further evaluate the geothermal potential of NRW. Therefore, the Ministry of Economic Affairs, Innovation, Digitalisation and Energy and the Geological Survey of NRW have initiated two projects: “Geothermal Characterisation of the Lower Rhineland and northern margin of the Rhenish Mountains” and “Geothermal Characterisation of the Greater Münster area”. These projects investigate the intermediate to deep subsurface to foster the use of hydrothermal energy in NRW.

In the initial stage three regions were defined: the Lower Rhineland, the northern margin of the Rhenish Mountains and the central Münsterland. In these project areas, Cretaceous, Dinantian (Lower Carboniferous) and Middle to Upper Devonian carbonate rocks are of particular interest because they occur at depth levels down to several thousands of meters, and are expected to possess good fluid pathways.

The project’s work packages include the digitalisation and harmonisation of existing geodata, complementing our borehole database system, the implementation of geo- and petrophysical measurements, and the acquisition of 2D seismic data in the central Münsterland, and the central and eastern Lower Rhineland. A first key asset in the project was a c. 300 m deep drilling conducted in the Düsseldorf area.

The results of the projects are presented in a geothermal online portal which serves as a driving force for future geothermal project planning and will assist in taking a step towards a climate-friendly heat supply.

Lecture*Topic:* 11.3 Young Scientist Session**H₂O phase separation in FeO-free phonolitic melt****Dennis Eul, Anja Allabar, Patricia Petri, Marcus Nowak**

University of Tuebingen, Germany

Melt degassing is an important driving force for accelerated magma ascent from storage regions toward the surface and volcanic activity. Hence, the investigation of degassing processes of H₂O as the most abundant volatile in magmas is important. One of the key properties of eruptive products used in reconstructing volcanic degassing processes is the vesicle number density (*VND*) of volcanic glasses. The formation of such vesicles can be explained by nucleation in the metastable region of the melt-H₂O system (e.g. Hurwitz and Navon, 1994). The nucleation rate of vesicles in rhyolitic melts increases exponentially with increasing supersaturation and *VND* increases exponentially with decompression rate (*dP/dt*) (e.g. Hamada et al. 2010; Hajimirza et al. 2019). However, for phonolitic melt with 2.71 wt% FeO (Vesuvius white pumice, VAD79) independence of *VND* on *dP/dt* has been observed (Allabar and Nowak, 2018). Therefore, these authors proposed spinodal decomposition, a non-activated mechanism at the thermodynamic limit of stability, as a phase separation mechanism.

Aiming to derive a possible effect of FeO on the phase separation mechanism in phonolitic melt, we performed decompression experiments with iron-free hydrous VAD79 melt and decompression rates of 0.17, 1.7, and 5 MPa/s. Our first results suggest a dependence of *VND* on *dP/dt* which can be approximated by the *VND* – *dP/dt* relation of Toramaru (2006). This indicates that the FeO melt component substantially affects the type of phase separation mechanism of hydrous phonolitic melt.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Analysis of surface displacements caused by mine flooding for the project FloodRisk with SAR Interferometry

Markus Even, Malte Westerhaus, Hansjörg Kutterer

KIT, Germany

During the last decades, one hard coal mine in Germany after the other stopped production and entered the post-mining phase. The last pits that terminated active mining were Ibbenbüren and Prosper-Haniel in 2018. For reasons of cost efficiency, the pumping of mine water is reorganized in this phase and levels are allowed to rise up to a certain depth below the surface. This process goes along with pressure changes in the rock that may e.g. cause surface displacements, seismicity or increased leakage of soil gases. In order to gain a better understanding of its effects and their dependency on the geological situation, the interdisciplinary project FloodRisk funded by the German Federal Ministry of Education and Research (BMBF) started investigating the post-mining process from the perspectives of geology, geophysics and geodesy. The present paper takes the perspective of geodesy and uses Interferometric Synthetic Aperture Radar (InSAR) to investigate surface displacements at Ibbenbüren and in the eastern Ruhr area for the period January 2018 to March 2021.

Poster

Topic: 7.3 Assessment of the Earth System through Micropaleontology

Significance of millennial-scale coastal upwelling and Rio Loa variability for Atacama paleoclimate during MIS 2

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The Atacama Desert located in northern Chile is one of the driest places on earth. The factors determining recent hyperarid climate conditions are known and their interplay and variability on interannual and decadal time scales are generally understood. Evidence for wetter (yet arid) conditions in the Atacama's past is provided by episodic lacustrine and fluvial deposits. The main watercourse of the Atacama Desert is the Rio Loa sourced by rainfall in the Andean mountains. Information on changes of terrestrial supply to the ocean is recorded in marine sediments.

The sediment core SO-104-52KL has been collected on the upper continental slope (~340 m water depth, 21°S) off the *Rio Loa* during a cruise with RV Sonne. The preliminary age model based on ¹⁴C-dating constrains the top and base of the core to 16 and 42 ka, respectively. Very high average sedimentation rates will allow paleoceanographic and paleoclimatic studies of high resolution (millennial to centennial time scales) during the last glacial period. The location of the core on the continental slope off the Rio Loa mouth allows for the parallel evaluation of the Humboldt Current System and Andean rainfall as moisture sources for the Atacama Desert. Microfossils such as benthic foraminifera from this interval are abundant and well-preserved. Together with XRF-data, grain-size and lipid biomarker analyses, the expected proxy data will provide new insights into the dynamics of land-ocean coupling between the Atacama Desert and the eastern Pacific Ocean through characterization of coastal upwelling properties and Rio Loa runoff.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Fluid evolution and Re enrichment in the Maronia porphyry system, NE Greece: Insights from pyrite, molybdenite and quartz micro-analysis

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The monzonitic-granitic intrusion of Maronia in NE Greece hosts an anomalously Re-rich Cu-Mo ± Au porphyry system. The mineralization is dominated by pyrite, molybdenite, chalcopyrite, native Au, and rheniite (ReS₂) in quartz-bearing hydrothermal veins associated with potassic, sericitic, and advanced argillic alteration. To decipher the hydrothermal processes leading to the enrichment of Re, Mo, and Au, we used detailed imaging techniques such as BSE-SEM and CL-SEM combined with in-situ trace element analysis of pyrite, molybdenite, and quartz by EPMA and LA-ICP-MS, in-situ δ³⁴S analysis of pyrite by LA-ICP-MS and fluid inclusion microthermometry in quartz from different veins and miarolitic cavities.

Hydrothermal quartz CL intensity, textures and Al/Ti and Ge/Ti ratios are characteristic for each vein type and Ti-in-quartz thermometry indicates a temperature decrease from 600°C to 300°C during the porphyry-epithermal transition. Arsenic, Au, Ag, Te, Pb, Cd, and Se contents and ratios of As/Sb, Co/As, Se/Tl, Se/Te and Se/Ge in pyrite record changes in the physicochemical fluid conditions. Extreme Re enrichment in molybdenite at Maronia (̄=3922 ppm) compared to the global average from porphyry deposits (̄=779 ppm) is likely controlled by a district-wide Re-rich magmatic source, whereas the enrichment of Re in B-type (̄=5532 ppm) relative to D-type (̄=1954 ppm) veins seems to be related to changes in fluid temperature, salinity and fO₂. Our multi-mineral trace element approach allows us to constrain the framework of the physicochemical fluid parameters during the porphyry-epithermal transition favorable for the enrichment of Re and related precious elements like Au, Ag and Te at Maronia.

Lecture

Topic: 5.6 Natural archives as recorders of past climate and environmental conditions – processes, methods and applications

What beachrock can and can not do as a sea level indicator: setting out to refine the model of beachrock facies interpretation based on examples from Oman and South Africa

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Beachrocks are coastal sediments that are lithified through the precipitation of carbonate cements. It is widely acknowledged that lithofacies in beachrocks are variable and their interpretation is useful when using beachrock as a sea-level indicator. Surprisingly, the facies variability of beachrocks remains understudied as they are almost exclusively described as seaward dipping, sandy, slab-shaped outcrop forming in low energy dissipative beach environments. The Mission Rocks coastline of South Africa is in stark contrast. Here the coast comprises an up to 3 m thick platform of beachrock, where a variety of sedimentological facies are observed. The northeastern coastline of Oman is rich in unusually coarse beachrock conglomerates and also beachrocks showing a diverse ichnological community. In our studies we aim to use sedimentological facies analysis, petrography and SEM to unravel the deposition- and cementation processes of several beachrock facies. Beachrock lithofacies that can be linked to a certain sea-level are then utilised to refine the current model of beachrock facies interpretation used in sea-level research. However, some of the newly described facies raise questions about the accuracy of beachrock facies interpretation. In particular, an unusual beachrock breccia interposed amongst the breakdown remnants of the platform at Mission Rocks beach comes to mind. The breccia documents a cycle of simultaneous erosional breakdown and depositional build-up of the beachrock platform, a yet undescribed process for the development of beachrock, and inhibits a cement mineralogy indicative of marine phreatic cementation while forming in the supratidal zone.

Poster

Topic: 11.5 Open Session - Geology

Shards of glass: incorporation of trash in modern beachrock on Eleuthera Island, Bahamas, and its implications for in situ studies of fast carbonate cementation

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Beachrocks are bodies of beach sediment cemented with carbonate minerals. They are not only useful archives of coastal evolution, but are also investigated as means of protection from coastal erosion. Beachrock formation is known to permanently alter the morphodynamics of a coastline and lock sediment in place, while reflecting wave energy. The cementation occurs on a scale of years rather than millennia, but observations of very young beachrocks with well constrained ages are still rare. Furthermore, our understanding of the cementation process is limited, although crucial to the creation of artificial beachrocks for engineering purposes.

On the Bahamian island Eleuthera modern beachrocks have incorporated high amounts of trash such as glass, rubber and microplastics. While the inclusion of anthropogenic materials into the rock record raises questions on limestone nomenclature, it also provides chances for the study of beachrocks. The glass is of particular interest as it shows no signs of rounding, indicating very recent cementation. This facilitates an in situ observation of the cementation process over an extended period of time, uncovering possible links to environmental parameters like temperature, availability of freshwater, inundation and weather phenomena like storms. To unravel the structure of the microbial communities involved in cementation a combination of petrography, SEM and environmental DNA can be used on the cements.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Isotopically anomalous metabolic oxygen in marine vertebrates as physiology and atmospheric proxy

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Pack et al. (2013) showed that the triple oxygen isotope composition of bioapatite along with a mass balance model of land-living mammals can be used as proxy for the ¹⁷O anomaly of ambient air O₂ and hence pCO₂ in combination with the global primary productivity (GPP). Here, we present an analytic protocol for high-precision triple oxygen isotope analyses along with new data of tooth enamel of a set of marine vertebrates, including sharks, dolphins, and whales. The goal is to demonstrate whether traces of anomalous inhaled oxygen are also found in these species, whether differences are observed between sharks and marine mammals, and if the triple oxygen isotopes hence could provide information about marine vertebrate physiology, e.g., metabolic rate or drinking behavior.

Marine mammal data show a clear signature of isotopically anomalous metabolic oxygen in their bioapatite. This is related to a low flux ratio of isotopically normal drinking and food water to anomalous metabolic oxygen. Traces of anomalous metabolic oxygen are also observed in shark bioapatite. Sharks and mammals have overlapping ¹⁸O/¹⁶O ratios, but distinct ¹⁷O signatures. Our new data suggest that triple oxygen isotopes are a valuable new tracer to assess the physiology of extant and extinct marine vertebrates and may provide a new proxy for past atmospheric CO₂ mixing ratios and global primary biosphere production (Feng et al. 2022).

Feng et al. (2022) *Geochimica et Cosmochimica Acta* **328**, 85-102.

Pack et al. (2013) *Geochimica et Cosmochimica Acta* **102**, 306-317.

Lecture*Topic:* 7.3 Assessment of the Earth System through Micropaleontology**A 300,000 year record of cold-water coral mound build-up in the SE Alboran Sea (western Mediterranean): insights from benthic foraminifera****Robin Fentimen¹, Andres Rüggeberg¹, Eline Feenstra¹, Efraim Hall¹, Valentin Rime¹, Torsten Vennemann², Irka Hajdas³, Antonietta Rosso⁴, David Van Rooij⁵, Thierry Adatte², Hendrik Vogel⁶, Norbert Frank⁷, Anneleen Foubert¹**¹Department of Geosciences, University of Fribourg, Switzerland; ²Institute of Earth Surface Dynamics, University of Lausanne, Switzerland; ³Laboratory of Ion Beam Physics, ETH Zürich, Switzerland; ⁴Department of Biological, Geological and Environmental Sciences, University of Catania, Italy; ⁵Department of Geology, Ghent University, Belgium; ⁶Institute of Geological Sciences and Oeschger Centre for Climate Change Research, University of Bern, Switzerland; ⁷Institute of Environmental Physics, University of Heidelberg, Germany

Little is known about the build-up of Mediterranean cold-water coral mounds at the scale of multiple interglacial-glacial cycles. This study concentrates on the long-term development of coral mounds within the East Melilla Coral Province (Southeast Alboran Sea) and exposes how the distribution of benthic foraminiferal assemblages can provide key palaeoenvironmental information about the long-term processes driving coral mound development. The multiproxy investigation of core MD13-3462G reveals that mound build-up took place during both interglacial and glacial periods, at average aggradation rates ranging between 1 and 10 cm.kyr⁻¹. These observations imply that corals never thrived but rather developed under stressful environmental conditions. High abundances of infaunal benthic foraminifera (*Bulimina marginata*, *Bulimina striata* and *Uvigerina mediterranea*) suggest that weak seafloor oxygenation associated to important terrestrial organic matter input characterized interglacial periods, whilst the dominance of large epibenthic species (*Discanomalina coronata* and *Lobatula lobatula*) and Miliolids is probably linked to stronger Levantine Intermediate Water circulation and fresher organic matter input during glacial periods. Glacial periods are further characterized by peak abundances of the erect branching bryozoan species *Buskea dichotoma*. Moreover, planktonic (*Globigerina bulloides*) and benthic (*Lobatula lobatula*) $\delta^{18}\text{O}$ records show typical interglacial-glacial variations during the last two interglacial-glacial cycles. This is in contrast with $\delta^{18}\text{O}$ records generally recovered from coral mounds in the Atlantic and implies that the northern part of Brittlestar Ridge I experienced reduced albeit relatively continuous accretion.

Poster*Topic:* 1.3 Bridging length and time scales in the modelling of geomaterials**Adsorption of the drug molecule carbamazepine in zeolites: Studying host-guest and guest-guest interactions with DFT calculations****Michael Fischer**

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In the past two decades, pharmaceuticals and personal care products (PPCPs) have been identified as environmental contaminants of considerable concern due to their significant hazard potential. The anticonvulsant drug carbamazepine (CBZ, $C_{15}H_{12}N_2O$), widely prescribed in the treatment of epilepsy, is a particularly relevant PPCP contaminant: It is hardly removed by conventional wastewater treatment techniques, shows considerable persistence in environmental waters, and negatively affects different organisms. Currently, various technological options are being considered to remove CBZ and other PPCPs from wastewaters, including (photo)oxidation processes, membrane separations, and adsorption-based separations. Hydrophobic high-silica and all-silica zeolites have been identified as promising adsorbents for the removal of organic contaminants. In this contribution, the adsorption of CBZ in 11 all-silica zeolites having different pore sizes and connectivities was investigated using dispersion-corrected density functional theory (DFT) calculations (CP2K code, rev-vdW-DF2 functional). On the basis of calculations considering a single CBZ molecule per simulation cell, IFR- and AFI-type all-silica zeolites were identified as systems with the highest affinity towards CBZ. Both of these frameworks contain one-dimensional channels outlined by 12-membered rings of SiO_4 tetrahedra. An analysis of the lowest-energy configurations showed that a "good fit" of CBZ into the pores, which maximises van der Waals interactions, is critical to achieve a high affinity, whereas hydrogen bonds are only of minor importance. Further calculations investigating the adsorption of two CBZ molecules per simulation cell indicated that attractive guest-guest interactions are more significant in zeolites with larger pores.

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Lecture

Topic: 1.8 Minerals and Mineral Properties

The power of crystal optics

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It is demonstrated here that refractive-index measurements can be used to determine details of chemical compositions and physical properties of crystals. For example, the H₂O content of hydrous minerals can be determined from their mean refractive indices with high accuracy as shown for 157 zeolite-type minerals and compounds (Fischer et al., 2020). This is especially important when only small crystals are available not suitable for thermal analyses or for other reliable methods of measuring the amount of H₂O. The physical basis for these predictions is the additivity of electronic polarizabilities of cations and anions. If the chemical composition and the molar volume of a compound are known, the total electronic polarizability can be calculated from the sum of the individual polarizabilities of the elements. Using the Anderson-Eggleton equation, the mean refractive index can be calculated. Deviations between observed and calculated mean refractive indices can be used, e.g., to identify ion conductors showing unusually high discrepancies. We have evaluated more than 3000 datasets of minerals and compounds to determine the electronic polarizabilities of four anions and 76 cations in various coordinations. Based on these parameters, the mean refractive index for more than 2000 minerals and compounds could be calculated with an error <2%. Some groups of compounds are identified showing systematic deviations. The results are compared with the Gladstone-Dale approach after Mandarino (1976).

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Lecture

Topic: 2.2 From dust to planets

Mass dependent $\delta^{74/70}\text{Ge}$ variations within chondrites: Insights on inner–outer Solar System dichotomy**Guillaume Florin¹, Béatrice Luais², Damien Cividini²**¹Freie Universität Berlin, Germany; ²CRPG-CNRS, University of Lorraine, Nancy, France

The moderately siderophile and volatile elements are strong tracers of early solar nebula processes, including condensation and accretion-collision of meteorite parent bodies. Among them, the germanium ($T_{50\% \text{ condensation}}=825\text{K}$) shows significant isotopic fractionation between metal and silicate phases in undifferentiated chondrites and in differentiated planetesimal reservoirs (i.e. mantle–core) [1,2]. Additionally, germanium isotopic data ($\delta^{74/70}\text{Ge}\text{‰}$) correlate with oxygen anomalies ($\Delta^{17}\text{O}$) in ordinary chondrites [1], demonstrating its capacity to trace oxidizing processes during accretion as well as genetic links between parent bodies. Here we present new high precision $\delta^{74/70}\text{Ge}$ data obtained on bulk carbonaceous (CC) and ordinary (OC) chondrites, and an enhanced version of the $\delta^{74/70}\text{Ge}-\Delta^{17}\text{O}$ correlation to assess NC-CC dichotomy.

Bulk CC have positive $\delta^{74/70}\text{Ge}$ values, showing exceptional large variations of $\approx 1\text{‰}$, from CI (Orgueil) with the heaviest composition ($\delta^{74/70}\text{Ge}=+0.901\pm 0.060\text{‰}$) toward lighter composition in CV (Allende) ($\delta^{74/70}\text{Ge}=+0.096\pm 0.120\text{‰}$), whereas bulk ordinary chondrites display negative $\delta^{74/70}\text{Ge}$ [1]. The $\delta^{74/70}\text{Ge}$ values and matrix fraction (%) of OCs and CCs are positively correlated and describe a mixing line between CI composition and a [Ge]-depleted- $\delta^{74/70}\text{Ge}$ -light component. In addition, OC and CC type chondrites present fundamental stable $\delta^{74/70}\text{Ge}$ dichotomy that follow O, Ti, and Cr isotopic anomalies [3]. Within CC, the mass dependent $\delta^{74/70}\text{Ge}$ compositions are exceptionally well correlated with $\Delta^{17}\text{O}$, $e^{54}\text{Ti}$, and $e^{54}\text{Cr}$, questioning the origin and processes that lead to isotopic signature dichotomy between the inner and outer the Solar System.

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Lecture*Topic:* 1.8 Minerals and Mineral Properties**Tetravalent lead in nature****Laura Christina Folkers¹, Rainer Pöttgen²**¹STOE & Cie GmbH, Germany; ²Institut für Anorganische und Analytische Chemie, Universität Münster, Germany

Of the three industrially important lead oxides PbO, Pb₃O₄ and PbO₂ [1-4] the first two are readily accessible through chemical synthesis, whereas PbO₂ can only be reached through high pressure, electrochemical or strongly oxidizing synthesis routes [5-7].

In nature lead dioxide forms oxidatively during hydrothermal mineralization [8]. The respective β modification, named plattnerite is a rare mineral and has hitherto only been characterized by powder X-ray or neutron diffraction.

The samples studied originate from Mine du Pradet in Cap Garonne, France and from Mount Trevasco in Bergamo, Italy. Single crystal X-ray diffraction measurements show that β -PbO₂ crystallizes in the rutile-type structure with space group $P4_2/mnm$ without additional reflections or a sign for a structural transformation between room temperature and 90 K [9].

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Lecture

Topic: 7.1 Geo-Biosphere interactions through space and time: new analytical and experimental approaches to the fossil record

Resolving microbial carbonate mineralization in extreme environments: from diagenetic noise to environmental signal

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Microbial carbonates are unique deposits formed by the direct or indirect action of benthic microbial communities. They witness early life since Precambrian times, and occur in a wide variety of environments - from marine to continental settings. Although their deposition forms a continuum through geological time scales, microbial carbonates dominate geological records when extreme environmental conditions prevail. Many studies have focused on the characterization of microbial carbonate fabrics and processes of microbial mediated carbonate mineralization in recent environments, but the presence of organic compounds in ancient microbialites remains often questionable. Moreover, microbial carbonates witness high spatial fabric heterogeneity at micro- and nanoscale and often the functional role of specific organic compounds in carbonate mineralization is not yet resolved. Additionally, diagenesis occurs at different spatial and temporal scales but mostly starts in nano- to micro-environments immediately after initial precipitation. This renders detangling diagenetic and environmental signals in microbial carbonates often difficult.

This study highlights the importance of sedimentary petrography, multi-scaled X-ray computed tomography (3D-visualization) and Raman spectroscopy combined with geochemistry and experimental approaches to unravel precipitation mechanisms, environmental conditions and early diagenesis of microbial mediated Ca-Mg carbonates in extreme environments. The unique presence of Holocene and Pleistocene microbialites in the Danakil Depression (Afar, Ethiopia) at varying preservation states, evidences (1) the co-occurrence of both biotically mediated and abiotic driven mineralization processes through space and (2) a continuum between primary precipitation and early diagenetic modification through time.

Lecture

Topic: 5.6 Natural archives as recorders of past climate and environmental conditions – processes, methods and applications

New proxies in limnogeology to quantify Quaternary landscape change

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Up to 65% of ice-free landscapes are predicted to be directly affected by climate change until the end of the century, a number that increases to 80% if also accounting for land use. This places great pressure on one of our most important resources – soils – particularly in densely populated areas and agricultural hotspots. Additionally, landscapes play a significant role in the global carbon cycle, and, thus, in the global climate system.

A comprehensive new approach to simultaneously study climatic, environmental, and anthropogenic controls on Quaternary landscape evolution has been developed in recent years. The research systematically applies traditional palaeo-climatic and -ecological (pollen) proxies along with a novel method to infer catchment erosion to temporally highly resolved and continuous lake sediment sequences. The new method, predominately applied to fluvial deposits in the past, is based on uranium isotope analyses and provides estimates of the time fine grained detritus (<63 µm) spends between comminution in a weathering horizon and final deposition in a sedimentary sink.

The applicability of the novel proxy is tested by fundamental research and demonstrated by the application to a sediment record from south-eastern Australia. The research provides crucial insights into the understanding of the novel (uranium isotope) proxy's response to catchment and lake-internal geochemical processes and provides insights into a complex interplay between vegetation, climate, and catchment erosion in south-eastern Australia. It particularly highlights the need for research on Australia's role as global terrestrial atmospheric CO₂ sink in the geological past.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Anoxia – Driver of the Late Permian Mass Extinction in shallow marine basins?

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The Late Permian mass extinction (LPME) was the most catastrophic extinction of marine life during the Phanerozoic. Widespread marine deoxygenation associated with the eruption of the Siberian Traps is considered one of the main drivers of the drastic diversity decline seen in the fossil record. However, while evidence of photic zone euxinia has been reported for some regions, others appear to have, at least locally, oxic conditions during the LPME. Here we present redox sensitive metal concentrations (e.g. Mo & V) combined with other redox proxies (e.g. V/Cr) from shallow marine carbonate sections from the southern Alps to assess local marine redox during the LPME. Our results show an increase in Mo, V and U in the sediment just prior to the LPME, suggesting the development of local anoxia. However, the sedimentary V/Cr and Ni/Co ratios support consistently (dys-)oxic conditions before and throughout the LPME, with values generally <2 and <4.5, respectively. These seemingly contradictory observations are likely due to increased weathering following the eruption of the Siberian Traps, which could explain the increased concentrations in redox sensitive metals even under oxidizing conditions. This suggest that the LPME within the shallow marine sediment of the southern alps might not have been triggered by deoxygenation, but by other environmental changes, such as temperature rise or increased metal toxicity.

Lecture

Topic: 4.3 The role of fluids in metamorphic and metasomatic reactions

Metamorphic reaction kinetics at “dry” and “wet” conditions in the binary MgO-SiO₂ system

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Reaction rims contain a wealth of information that can be used to decipher the P-T-t-X history of metamorphic and metasomatic rocks. One of the most important parameters that controls reaction rim growth dynamics is the presence of volatiles, which can affect rim thicknesses, phase stabilities and the development of rim microstructures.

We performed reaction rim growth experiments to investigate net-transfer reactions in both “dry” and “wet” systems. Reaction rims were produced between single crystals of quartz and periclase in an internally heated pressure vessel (IHPV) at 0.3-0.4 GPa and 1100-1300 °C for 66 h to 168 h. In “wet” experiments, a ppm amount of water was introduced by pre-annealing periclase single crystals at water saturated conditions, which is gradually released during rim growth experiments.

First results indicate the formation of single enstatite or forsterite and double enstatite-forsterite reaction rims in the “dry” and “wet” systems respectively. When water-doped periclase is used as a reactant, reaction rim growth rates increase from $10^{-18.23 \pm 0.18}$ to $10^{-17.67 \pm 0.03}$ m²/s at 1100 °C and from $10^{-16.95 \pm 0.06}$ to $10^{-16.16 \pm 0.01}$ m²/s at 1200 °C. In experiments that were entirely anhydrous, no reaction rim formed at all. These observations suggest that water may act as a catalyst and that a certain fluid threshold is needed to initiate metamorphic re-equilibration.

These findings imply that reaction rims may be used to discriminate between kinetically “dry” and “wet” systems and have thus the potential to monitor the presence of extremely small amounts of water during metamorphic reactions in natural systems.

Poster

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Fossilization of Precambrian microfossils in the Volyn pegmatite, Ukraine

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The Volyn biota are a distinct and uncommon example of 3D-preservation of ~1.5 Ga old Precambrian fossils, recovered from cavities in pegmatites, which were the habitat for microorganisms in the deep biosphere. The Volyn pegmatite district is associated with the Paleoproterozoic Korosten Pluton, Ukraine. Breccias, formed during collapse of miarolitic cavities, contain decaying OM, which released NH_4^+ , responsible for the late-stage formation of buddingtonite and tobelite-rich muscovite. The age of the fossils can therefore be restricted to the time between the pegmatite formation, at ~1.760 Ga (zircon U-Pb), and the breccia formation at ~ 1.5 Ga (muscovite Ar-Ar).

The organic matter (OM) is characterized as (oxy)kerite. Microanalytical investigations show that fossilization likely occurred during a hydrothermal, post-pegmatitic event, by silicification dominantly in the outermost 1-2 μm of the microfossils. The hydrothermal fluid, derived from the pegmatitic environment, was enriched in SiF_4 , Al, Ca, Na, K, Cl, and S. The OM shows O enrichment where N and S content is low, indicating simultaneous N and S loss during anaerobic oxidation. Mineralization with Al-silicates starts at the rim of the microfossils, continues in its outer parts into identifiable encrustations and intergrowths of clay minerals, feldspar, Ca-sulfate, Ca-phosphate, Fe-sulfide, and fluorite. As geological environment for growth and fossilization of the microorganisms we assume a geyser system, in which the essential biological components C, N, S, and P were derived from microorganisms at the surface. Fossilization was induced by magmatic SiF_4 -rich fluids.

Lecture

Topic: 7.3 Assessment of the Earth System through Micropaleontology

The Precambrian Volyn biota, Ukraine – example for a continental micro-ecosystem of the deep biosphere

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The Volyn biota, a distinct example of 3D-preservation of ~1.5 Ga old Precambrian fossils from huge cavities in granitic rocks as a habitat for microorganisms in the deep biosphere, consist of several different types of organisms. Most common are filaments of variable diameter (10 µm-range to 100 µm-range) and length up to cm. Branching, segmentation, outgrowths, and a central channel are typical. Ends can be simple rounded, thinning out, or with outgrowths. Filaments grew on mineral substrate (?sessile organisms); filaments with two ends indicate growth in soft clay media or floating in water. Spherical objects in the size of tens of µm could represent spores or other types of seeds. For larger objects, some with conical shape, in the 100 µm-range, no recent analogue is obvious. Bi(S,Te) nm-minerals in filaments, either irregularly distributed or in rod-like arrangement, have an analogue in recent fungi, but also in other microorganisms. Objects with flaky to irregular shape are reminiscent of a former biofilm. Filaments are also partly covered with a sheath, interpreted as extracellular protein substance. $\delta^{13}\text{C}/^{12}\text{C}$ -isotope values of approximately -40 ‰ to -50 ‰, typical for methanogenic bacteria, and a range of $\delta^{15}\text{N}/^{14}\text{N}$ -isotope values of +2 ‰ to +9 ‰ also indicate different organisms.

The crucial fact for the excellent 3D-preservation of the microfossils is their occurrence in cavities of igneous rocks, which preserved them from further diagenetic-metamorphic overprint as common in sediments. These microfossils give an impressive insight into Precambrian life in the deep biosphere.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Alchemy in Mannheim? – Mineralogical and chemical analysis of 17th-18th century technical ceramics and lead glazed earthenware.

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This presentation focuses on technical ceramics from various early Modern dumping contexts ranging from a well to latrine and surface fills within in the former city walls of Mannheim.

Additionally domestic glazed earthenware from a latrine fill were analysed that exhibited alterations to surface texture and colour or were covered with residues which were hypothesised to be affiliated to *chymistry* practices during this period.

The analytics were performed using a combination of chemical analysis via micro-X-Ray Fluorescence (μ XRF) and/or Scanning Electron Microscope with Energy Dispersive Spectroscopy (SEM-EDS) as well as mineralogical analysis via micro-X-Ray diffraction (μ -XRD²), to determine the nature of pyrotechnological processes as well as the source of alterations and residues. Technical ceramics were further analysed via ceramic petrography to define their technological characteristics, including refractoriness and the pyrotechnological processes in which they were used.

Preliminary results suggest that while most of the glaze alterations seem to be caused by weathering processes during burial, some may be related to misfiring or refiring processes. Jarosite was identified at the surface of some domestic ceramic fragments and might be connected to separation processes in precious metal working but could be formed by weathering as well. However, iron and alkaline rich slags with specks of precious metal alloys further strengthen this interpretation. Other crucibles contained slags indicating pale ore assaying.

Lecture

Topic: 10.1 Geoscience Communication and Education

Geoscience transfer on guided tours into the Messel Pit UNESCO World Heritage Site, Hesse, Germany – A public outreach challenge

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Welterbe Grube Messel gGmbH, Germany

Public outreach to transfer geoscientific themes embraces a wide field of activities. University PR on geoscientific investigations, natural history museum exhibitions on e.g. Dinosaurs, the establishment of geo-trails with geoheritage interpretation, UNESCO Global Geopark formation with conferences, Geo-Film Festivals and access activities into the unique World Heritage Fossil Site (WHS) Messel Pit, Hesse, Germany are mosaic pieces of the picture ensemble. The bridge between geosciences and public outreach as serious measures is small. It is important to widen it to enthusiast population for Planet Earth. The Messel Pit WHS has picked up the challenge to develop it in direction of a motorway, giving access into this geosite by

- a) regularly offered, professionally realised guided tours,
- b) by staff and guides with an academic degree and
- c) developing a new frame on program offers into this terrestrial Eocene fossil site.

Limited by a fence around, a guided tour frame of public accessible, bookable tours of different tour duration and for different target groups, inclusive children, handicapped and adults was realized in a changing society. A certain time the focus was on visits into the geosite. From 2011 onwards a visitor center with various geo-themes became a complementary mosaic piece for the Messel Pit experience of visitors. Data on the length of offers, type of offers and type of groups visiting were examined and are presented. Regular activities on a variety of topics and of high quality, leading to quality of life in a fast changing society are the visitor's champions.

Lecture

Topic: 8.1 Geosciences and Waste Management

Asbestos detection in buildings to prevent contamination of the recycling material stream

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The BMBF-funded research project “RECBest” aims at developing reliable methods for the detection and removal of hazardous building materials before demolition and at enhancing the resulting recycling material (RCM) through specialised processes. This presentation discusses select findings of the first year of research focusing on the detection of asbestos in buildings.

In September of 2021 the VDI 6202-3 was published, giving a statistical approach to the exploration and assessment of asbestos in buildings. Therefore, five condemned buildings that had previously been inspected for asbestos not using the VDI 6202-3 were again examined according to the VDI 6202-3. Comparing the results of both approaches showed that the standardised VDI method led to more reliable and detailed results. However, the common limitation remains the surveyors conducting the inspection as they have to correctly identify possible asbestos-containing materials beforehand.

A common problem during the inspection of condemned buildings for asbestos are concealed materials such as rebar spacers made of asbestos concrete. Thus, a non-invasive method of detecting rebar spacers using radiography was tested on a block of reinforced concrete. The resulting two-dimensional pictures clearly showed the locations of the rebar within the concrete block. Although the rebar spacers themselves could not be observed, the wires used to hold the spacers in place were visible and can therefore indicate where core drilling samples should be obtained.

Lecture

Topic: 2.2 From dust to planets

Effect of shock pressure on the Verwey transition in magnetite: Modelling of the magnetic susceptibility with various distributions of transition temperatures

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Magnetite occurs as an accessory mineral in many rocks. It shows a strong ferrimagnetic behavior with a phase transition at about 120 K (Verwey transition temperature), which causes a strong increase in magnetic susceptibility by warming through the transition. The transition temperature shows a complex dependence on chemical composition, oxidation and internal stresses and was suggested as an indicator of shock pressures in terrestrial impact structures [e.g., 1].

Here, susceptibility curves were modelled between 80 and 200 K assuming probabilistically distributed transition temperatures representing variations in local stress fields. An improved version of a previously presented model was used [2]. The model was applied to susceptibility curves of magnetite-rich iron ore shocked at 5, 10, 20 and 30 GPa in laboratory experiments with subsequent heat treatment [3,4]. The results show a clear change from a sharp normal distribution of transition temperatures in unstressed ore towards a broad heavy-tailed Lorentz distribution in highly stressed samples. This behavior can be related to shock-induced dislocations. The distribution of transition temperatures in stressed ore indicates interactions between magnetic domains and could be useful e.g. for the distinction between stress and oxidation effects on the Verwey transition of rocks.

[1] Carporzen et al. (2006), *Earth Planet Sci Lett* 251, 305-317; [2] Fuchs et al. (2019), AGU Fall Meeting 2019, GP23B-0790; [3] Reznik et al. (2016), *Geochem Geophys Geosyst* 17, 2374-2393; [4] Kontny et al. (2018), *Geochem Geophys Geosyst* 19, 921-931.

Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Fluid inclusion triple halogen (Cl-Br-I) systematics as tracers of fluid provenance in metamorphic and magmatic systems

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Heavy halogens are exceptional tracers of fluid provenance due to their largely conservative behaviour during most fluid-rock interaction processes. In particular, Br/Cl ratios have long since been established as a tracer of fluid origin in certain geological settings (e.g. unconformity-related ore systems), where they have significantly contributed to our understanding of ore forming processes. However, mounting evidence suggests that similar Br/Cl signatures can, in fact, be produced by very different geological processes, significantly impacting the applicability of Br/Cl as a fluid source tracer to other crustal environments. Iodine provides an additional proxy and constraint that makes it possible to discern between these different processes and is thus crucial in utilizing the full potential of halogens as fluid provenance tracers. The generally low concentrations of iodine in crustal fluids have posed significant analytical challenges, and iodine analysis was until very recently only possible using bulk analytical techniques.

Recent advances in halogen fluid inclusion microanalysis have made it possible to determine Cl-Br-I systematics in individual fluid inclusions, providing novel opportunities for the study of complex ore forming systems with protracted and complex overprinting fluid signatures. We present a comprehensive triple-halogen fluid inclusion LA-ICP-MS dataset of various magmatic and metamorphic systems, showcasing the power of Cl-Br-I systematics in identifying and characterizing fluid sources, reconstructing processes such as fluid mixing, and the – rather surprising – temporal changes in metamorphic halogen signatures between the Archean and the Phanerozoic.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Magma evolution and epithermal ore formation at Conical Seamount, Papua New Guinea

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The Tabar-Lihir-Tanga-Feni (TLTF) island chain in northeastern Papua New Guinea hosts the world-class Ladolam gold deposit on Lihir island as well as several other Au prospects. Several young seamounts are located around Lihir and were studied in detail by three RV Sonne cruises in 1994, 1998 and 2002. While most of these seamounts are considered barren, Conical Seamount, located southeast of Lihir island, shows evidence for epithermal-style mineralization and has been interpreted as a submarine analogue to the Ladolam deposit. It offers a rare opportunity to study a porphyry-epithermal ore system at a juvenile stage and compare it to a mature system nearby.

In the first phase of our research project, we focus on the igneous system underlying the epithermal ore-forming system at Conical. We study the lavas as well as minerals and glass inclusions to reconstruct melting processes, magma evolution and ore fertility using detailed petrology, *in situ* geochemistry and thermobaric modelling. Special emphasis is given to volatile as well as trace metal and metalloid contents in bulk rocks, glasses and glass inclusions. Mineral zonation and the compositional diversity of pyroxene-hosted glass inclusions point towards repeated magma recharge and the potential existence of multiple magma stagnation levels. While the high melt oxidation state ($\Delta \log fO_2$ of +0.5 to +2 relative to FMQ) at Conical is advantageous for the enrichment of chalcophile elements in the evolving melt, high volatile contents may promote early fluid exsolution and the transfer of metals and metalloids into the epithermal system.

Lecture*Topic:* 6.2 Rates and Dates of Earth Surface processes: Methods & Applications**Denudation rates from meteoric $^{10}\text{Be}/^9\text{Be}$ in lithologically heterogeneous catchments****Nestor Gaviria-Lugo¹, Charlotte Lauchli², Anne Bernhardt², Patrick Frings¹, Dirk Sachse¹, Hella Wittmann¹**¹GFZ German Research Center for Geosciences, Germany; ²Institute of Geological Sciences, Freie Universitat Berlin, Germany

Accurate determination of denudation rates is crucial for the quantification of Earth surface processes like soil formation and the consumption of CO_2 during silicate weathering. *In situ* ^{10}Be is the most widely used proxy to quantify denudation rates over millennial timescales, but this system is severely limited in settings where quartz is absent. In contrast, the meteoric cosmogenic $^{10}\text{Be}/^9\text{Be}$ ratio is independent of quartz presence, but one important parameter that must be known is the ^9Be concentration ($[\text{}^9\text{Be}]$) of the underlying parental bedrock. In lithologically homogenous catchments, an average upper continental crust ^9Be value is commonly assumed.

However, this approach may not be appropriate in the lithologically heterogeneous catchments that we encountered along a N-S (26°S to 38°S latitude) gradient in Chile. By sampling ~ 100 hand-sized pebbles per catchment from the riverbed near the catchment mouth, we investigated the variability in $[\text{}^9\text{Be}]$ of different rock types from each catchment, and calculated area-weighted mean parental $[\text{}^9\text{Be}]$ via a combination with the distribution of lithologies in the catchments. We assessed the consistency of denudation rates calculated from the meteoric $^{10}\text{Be}/^9\text{Be}$ (D_{met}) against denudation rates derived from the *in situ* technique (D_{insitu}).

Current data from 7 catchments shows that D_{met} are in very good agreement with previously published D_{insitu} along Chile: a peak in D of around 0.25 mm/yr at 34°S latitude, and consistent decreases to $<0.1\text{ mm/yr}$ in N and S directions was reproduced. This supports the versatility of the meteoric $^{10}\text{Be}/^9\text{Be}$ proxy and encourages its application in catchments containing multiple lithologies.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

On the trail of oxygenic photosynthesis in ancestral Cyanobacteria on early Earth

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While oxygenation of the atmosphere on early Earth is attributed to cyanobacterial oxygenic photosynthesis, the limitations on their expansion is not well understood. Our work is focussed on assessing the impact of early Earth conditions on ancestral lineages of Cyanobacteria.

Iron is essential for photosynthetic pigment biosynthesis, however the high availability of iron on early Earth contrasts the present-day scenario. We have recently investigated the evolution of iron uptake receptors across the Cyanobacteria and found phylogenetic evidence of commonly occurring uptake mechanisms in the Proterozoic but not the Archaean. The release of oxygen not only alters the redox balance of the environment, it also induces stress on cellular biochemistry by generating oxygen free radicals. We demonstrate that, in a simulated marine environment, deep branching Cyanobacteria undergo less oxidative stress under an anoxic atmosphere than today. Additionally, we demonstrate increased O₂ accumulation for aquatic cultures of Cyanobacteria under a 24-hour diurnal cycle compared to a 12-hour cycle. Finally, we show that nitrogen fixation is not restricted under the anoxic, elevated CO₂ rich atmosphere of the Archaean.

In summary, our research to date suggests that reduced iron acquisition efficiencies may have limited the spread of Cyanobacteria on early Earth, while oxidative stress, does not appear to have been a limiting factor for filamentous strains. Further investigations into the role heterotrophic siderophore iron acquisition within a benthic or free-living community will further elucidate the conundrum of iron limitation in a ferruginous world.

Ramdohr-Poster

Topic: 8.1 Geosciences and Waste Management

The story of Sc in bauxite residues and its journey from ore to waste to value

Marie C. Gentzmann^{1,2,3}, Christian Adam¹

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Bauxite residue (BR) is a massive waste stream generated worldwide from Alumina production that is intensely studied for its potential reuse and as a secondary resource for various metals. More recently the recovery of the technology metal Scandium (Sc), which can be enriched in BRs, has attracted the interest of research and industry. Sc enrichment in BR was discovered more than 25 years ago, however there is a lack of comprehensive knowledge about its association and distribution. Geochemical and mineralogical insights that provide a connection between the Sc occurrence in the primary bauxite ore and the BR are scarce.

In this study, we present the results of detailed mineralogical investigations on BRs of different geological backgrounds and on the Sc behavior during the recovery process by leaching. The results were determined by combining wet chemical, microtextural and structural analyses with statistical design of experiments. They provide an understanding of how the Sc association changes from ore to waste depending on the primary bauxite and the chosen leaching conditions. The primary bauxite and the atmospheric conditions during bauxitization determine how Sc is distributed in the BR. BRs derived from karstic bauxites formed under partly reducing conditions are hence more prone to contain higher mass fractions of easily leachable Sc than BRs derived from lateritic bauxites. The recovery achieved by leaching therefore depends on the Sc distribution and will furthermore determine the viability of Sc recovery from BR. The research was funded by the EU's H2020 SCALE program under GA No. 730105.

Lecture

Topic: 8.1 Geosciences and Waste Management

The importance of mineralogy for a circular economy of the construction sector - examples from the ReMin funding initiative

Marie C. Gentzmann¹, Sören Henning¹, Michael Szurlies¹, Thilo Brämer², Andre Bertram³

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One of the challenges on the way towards a more sustainable future is the transition from linear to circular economy (CE). The need to conserve and substitute primary raw materials wherever possible has driven research and development to study the potential of wastes and residues as important resources. The construction sector, in particular, has great potential to reduce parts of its high primary raw material demand by using mineral residues from various sources.

In the presented funding initiative “ReMin” (“Ressourceneffiziente Kreislaufwirtschaft – Bauen und mineralische Stoffkreisläufe“) 16 research projects deal with resource efficient CE approaches. They aim to use construction and demolition wastes, metallurgical slags, incineration bottom ashes (IBA), mine tailings and other residues for the development of new construction materials. In this context, the investigation of the mineralogy and chemistry of the materials and processes is fundamentally important. Geoscientific aspects within the projects include e.g. the understanding of cement-clinker formation from thermally treated slags, the efficient separation of metallic and non-metallic particles in the fine fractions of IBA or mine tailings and the species and chemical bonding and behavior of heavy metals in waste streams. Other topics are the safe detection and separation of asbestos in mixed construction wastes and the investigation of the recycling potential of e.g. alternative gypsum sources. The accompanying research project “TReMin” with partners from CUTEK, Fraunhofer IWKS and BGR aims to support those research actions by networking and transfer of the results within and beyond ReMin and on a national and European level.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Take a walk on the clay-site - tracing raw materials through experimental archaeometry

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Suitable raw material is the basis for every ceramic object. In order to study the artisanal choices and factors associated with the selection of clays for Bronze Age ceramic production a raw-material survey has been carried out near the excavation site of *Grutt'i Acqua* on the peninsula of Sant'Antioco (Sardinia). This project is characterized by a transdisciplinary combination of experimental archaeology and mineralogical material science analysis - carried out in a cooperation between ArchaeoLytics and the Institute for Archaeological Studies of the Ruhr-University Bochum.

Nineteen clay-rich sediments have been collected and processed to examine their suitability to produce pottery according to local Bronze Age techniques and diagnostic vessel shapes. Based on standardized test-tiles the dry- and fire-shrinkage as well as the color-variations have been recorded for firing-experiments at 600 and 900°C. Ten samples out of this series have been selected for further investigations including polarizing microscopy, XRD and XRF. Preliminary comparisons with local Bronze Age shards show clear distinguishing features, allowing a solid provenance study. In addition, our field experiences, the in-situ processing of raw materials and the X-Ray data provide us with a more profound and broader understanding of the local Bronze Age pottery in the area of *Grutt'i Acqua*.

Lecture

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

No unique temperature of equilibration for mantle peridotites - Thermal histories told by differently diffusing cations based on novel calibrations

Vasileios Giatros¹, Dimitrios Kostopoulos¹, Panagiotis Pomonis¹, Evangelos Moulas²

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We generated novel thermometric formulae for cation exchange reactions between mantle minerals involving species of different diffusivities (FeMg orthopyroxene-spinel; CrAl & CaMg clinopyroxene-orthopyroxene) and used them in conjunction with published expressions (FeMg olivine-spinel; CaMgFe clinopyroxene-orthopyroxene) to decipher the thermal history of peridotites from diverse tectonic settings. When tested on abyssal peridotites, $T_{CrAl\text{-}opx\text{-}cpx}$ vs. $T_{CaMg\text{-}cpx\text{-}opx}$ form tight trends with $T_{CrAl\text{-}opx\text{-}cpx} \geq T_{CaMg\text{-}cpx\text{-}opx}$ at $T < 1060^\circ\text{C}$ and $T_{CrAl\text{-}opx\text{-}cpx} \leq T_{CaMg\text{-}cpx\text{-}opx}$ at $T > 1060^\circ\text{C}$ in accordance with crossing diffusivities of Cr_{opx} and CaMg_{cpx} at about that temperature, with the latter becoming smaller at higher temperatures and blocking higher as the peridotites are quickly emplaced and cooling at the ridge. Both $T_{CrAl\text{-}opx\text{-}cpx}$ and $T_{CaMg\text{-}cpx\text{-}opx}$ are higher than the widely used $T_{CaFeMg\text{-}cpx\text{-}opx}$ in abyssal peridotites by $\sim 100^\circ\text{C}$ on average. On a $T_{CrAl\text{-}opx\text{-}cpx}$ vs. $T_{FeMg\text{-}opx\text{-}sp}$ plot there is clear-cut distinction between peridotite massifs (major ocean basins, oceanic forearcs, oceanic backarcs, ophiolites, ocean-continent transitions, Alpine-type) from peridotite xenoliths (cratons, intracontinental rifts, continental backarcs, active continental margins, oceanic within-plate) with $T_{CrAl\text{-}opx\text{-}cpx}$ being invariably larger than $T_{FeMg\text{-}opx\text{-}sp}$ for the peridotite massifs reflecting the blocking of the slower-diffusing cations at higher temperatures upon cooling. The higher $T_{FeMg\text{-}opx\text{-}sp}$ exhibited by the xenoliths are ascribed to some, probably magmatic, heating event at a time prior to their transport to the surface. The Alpine-type peridotites of Beni Bousera, Morocco, that were exhumed in the footwall of a lithosphere-scale extensional shear zone display increasing $T_{CrAl\text{-}opx\text{-}cpx}$ and $T_{CaMg\text{-}cpx\text{-}opx}$ towards the shear zone but flat $T_{CaFeMg\text{-}cpx\text{-}opx}$, $T_{FeMg\text{-}opx\text{-}sp}$ and $T_{FeMg\text{-}ol\text{-}sp}$ profiles demonstrating the memory of the slower-diffusing cations.

Poster

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

No unique temperature of equilibration for mantle peridotites - Thermal histories told by differently diffusing cations based on novel calibrations

Vasileios Giatros¹, Dimitrios Kostopoulos¹, Panagiotis Pomonis¹, Evangelos Moulas²

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Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

Crustal growth and reworking in the early Archean Narryer Terrane: new evidence from strontium isotopes in apatite inclusions

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The limited preservation of ancient crustal material poses a challenge for understanding the composition of Earth's early crust. As a result of poor preservation and near-ubiquitous overprinting by later geological events, deciphering the early evolution of our planet often relies on the isotopic composition of resistive minerals, such as zircon. Although the isotopic information recorded by zircon grains has proved an invaluable asset to workers seeking to understand the geological evolution of the Earth, it is limited by the range of elements easily incorporated into the structure of the mineral.

One way to overcome these limitations is by analysing inclusions of other minerals that were trapped within the zircon during crystallisation. Apatite has great potential in this respect, as it is commonly found as inclusions in magmatic zircon and records a variety of useful isotopic information. Here we present an approach for investigating igneous petrogenesis and crustal evolution by combining ⁸⁷Sr/⁸⁶Sr measurements of apatite inclusions with U–Pb and Hf isotope analysis of their host zircon crystal. The Sr isotope information contained in the apatite can be accessed by applying a novel SIMS technique we developed for this purpose.

A case study applying this new approach to Eoarchean igneous rocks of the Narryer Terrane in the northern Yilgarn Craton of Western Australia demonstrates how this can be used to understand the evolution of this key locality, with implications for both regional geology and the growth of the continental crust.

Lecture

Topic: 2.2 From dust to planets

Siderophile volatile element inventory in lunar magmatic rocks and mantle sources

Philipp Gleißner, Julie Salme, Harry Becker

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The volatile element inventory of the Moon and the processes of volatile loss and/or gain (e.g., degassing and late accretion) are key aspects for our understanding of the Earth-Moon system. Elevated concentrations of volatile elements and water in lunar rocks have recently invigorated the discussion on the volatile content of the lunar interior and on the extent to which the volatile element inventory of lunar magmatic rocks is controlled by degassing. Here we report mass fractions of the siderophile volatile elements Cu, Se, Ag, S, Te, Cd, In, and Tl in lunar magmatic rocks, analyzed isotope dilution ICP-MS techniques. Similar mass fractions of Cu, S, Se, and Ag and fractional crystallization trends in mare basalts and magnesian suite norites indicate that these elements are less prone to magmatic degassing than proposed previously. Disturbed fractional crystallization trends of more volatile elements (e.g., Tl, Cd) and enrichments of the latter in brecciated ferroan anorthosites indicate their redistribution and vapor deposition. Differences in element ratios between lunar magmatic rock suites suggest a predominant control of S, Se, Cu, and Ag by mantle source compositions. New estimates of mantle source compositions of low-Ti mare basalt suites reveal low mass fractions of Cu, S, Se, and Ag and element ratios in the lunar mantle that are significantly different from the terrestrial mantle. Our new data support the hypothesis of volatile loss prior to formation of the lunar mantle sources and indicate limited degassing of mare basalts.

Poster*Topic:* 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment**Towards coupled geodynamic and hydrothermal numerical rift models of sediment-hosted Copper and Zinc deposits****Anne Glerum¹, Philipp Weis^{1,2}, Joseph Magnall¹, Sarah Gleeson^{1,3}, Sascha Brune^{1,2}**¹GFZ German Research Centre for Geosciences, Potsdam, Germany, Germany; ²University of Potsdam, Potsdam, Germany;³Freie Universität, Berlin, Germany

Many large sediment-hosted base metal deposits occur in failed continental rifts and the passive margins of successful rifts, e.g., in the MacArthur Basin, Australia, and the Selwyn Basin in Canada. Continental rifts and their margins provide a specific mix of elevated temperatures and heat flows, fault networks to facilitate fluid flow, sediment supply from the rift shoulders, and ocean water contributing pelagic sediments and sulfate. The large-scale geodynamics thus provide the necessary ingredients for metal leaching and deposition to occur on a variety of spatial and temporal scales. To understand the geodynamic controls on ore formation, we are therefore coupling the geodynamic code ASPECT^{1,2} (coupled to the landscape evolution model FastScape^{3,4}) with the hydrothermal fluid flow code CSMP++^{5,6} to include realistic pressure, temperature, and heat flow conditions, as well as permeability and sediment distributions, for fluid flow and metal leaching/deposition. This coupled workflow crosses temporal scales of millions of years to years and spatial scales of hundreds of kilometers to meters. We present preliminary results from geodynamic modelling of large-scale continental rifting and hydrothermal simulations at specific snapshots of the upper 10 km of crust of this large-scale geodynamic evolution, showing the effect of rift duration, adjacent craton thickness, and erosion efficiency on sediment-hosted Cu and Zn deposits.

¹Kronbichler et al. (2012). GJI191(1), 12–29.²Heister et al. (2017). GJI, 210(2), 833–851.³Neuharth et al. (2022). Geology, 50(3), 361–365.⁴Braun & Willett (2013). Geomorphology, 180-181, 170-179.⁵Weis et al. (2014). Geofluids, 14(3), 347–371.⁶Rodríguez et al. (2021). GCubed, 22(6).

Lecture

Topic: 7.3 Assessment of the Earth System through Micropaleontology

Metabolic adaptations of foraminifera to oxygen depletion and their role in marine nutrient cycling

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Benthic foraminifera are ubiquitous marine protists that inhabit environments from the deepest part of the ocean to saltmarsh meadows slightly above sea-level. Various species of foraminifera have highly specific adaptations to the environmental conditions in their ecological niche. Their high abundances in oxygen depleted environments and their metabolic adaptations to anaerobic conditions make them key players in marine nutrient cycling.

Here I will review the recent advances in understanding those adaptations. Benthic foraminifera from oxygen depleted environments are a rare example of eukaryotes that are able to denitrify and thus an important sink for reactive nitrogen in the oceans. Several species even show a metabolic preference of nitrate over oxygen as an electron acceptor. Several enzymes that are involved in foraminiferal denitrification are transcribed by eukaryotic RNA. These denitrification steps are thus executed by the foraminifers themselves and use enzyme homologues that are known from bacterial denitrification. Still, the foraminiferal denitrification pathway is incomplete. Recent studies indicate that previously undescribed enzymes as well as bacterial symbionts might be responsible for the missing steps in the foraminiferal denitrification pathway.

Furthermore, there is a widespread occurrence of intracellular phosphate storage in benthic foraminifera, which encode genes required for both a creatine phosphate and a polyphosphate metabolism. Both dephosphorylation of creatine phosphate and hydrolysis of polyphosphates are likely also adaptations to oxygen depletion. The high intracellular phosphate storage in foraminifera has previously been overlooked in benthic phosphorous cycling. It constitutes an important mobile reservoir in benthic ecosystems and facilitates phosphogenesis in some environments.

Lecture

Topic: 1.7 Experimental Petrology and Geochemistry

Chemical interdiffusion in Na-rich alkaline melts: insights from tephrite-phonolite couple experiments

Diego González-García, Florian Pohl, Stepan P. Krasheninnikov, Philipp Beckmann, Harald Behrens, François Holtz

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Although alkaline melts represent an important fraction of the magmatism in ocean islands, there is a lack of chemical diffusion data in such compositions. We present here the result of a series of interdiffusion experiments using natural tephritic and phonolitic melts from the Canary Islands as endmembers. Experiments were run in two internally heated pressure vessels at a pressure of 300 MPa, temperatures from 1150 to 1300°C, oxygen fugacity from NNO to approx. NNO+3, and water contents between 0.3 and 3.3 wt.%. Major element concentration-distance profiles were measured by electron microprobe and effective binary diffusion coefficients (D) were obtained by a modified Boltzmann-Matano analysis.

Results show a wide range of diffusivities for different cations, following the sequence Na >> Al > K Mg = Fe = Ca > Si > Ti. Na diffusivities are the fastest and are consistently 1 log unit above those of Si for a given experiment. Al diffusion is remarkably fast, falling ca. 0.4 log units above Si, an effect not observed before in diffusion studies. The relationships between log D and H₂O content in melt for all cations are strongly non-linear and can be fitted by using an exponential function, with an apparent convergence in diffusion coefficients towards the water-rich end. Our results provide new data on chemical interdiffusion in Na-rich, highly alkaline melts and allow to test chemical controls of magma mixing in Tenerife, where banded pumices are common in several bimodal ignimbritic units.

Lecture

Topic: 4.3 The role of fluids in metamorphic and metasomatic reactions

Hidden in plain sight: using Atom Probe Tomography to understand the formation of invisible gold deposits

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Carlin-type gold (CTG) mineralization is one the best studied, yet poorly understood gold mineralization styles in the world. These deposits occur predominantly along NW-SE trends in central Nevada and are characterized by invisible gold thought to be hosted in sulfide minerals (Cline et al., 2005). CTG accounts for 9% of worldwide gold production, with all of it currently coming from five mining districts in northern and central Nevada. The discoveries of new CTG deposits in the Yukon Territory, China, and Kyrgyzstan as well as the presence of significant CTG-like-gold in already known deposits in Europe will drastically increase the importance of these deposits in the upcoming years.

Despite the vast resource that CTG deposits entail, surprisingly little is known about their formation mechanisms, fluid source, or even the manner in which the gold is hosted. We know that the gold tends to occur as trace elements within micro-to-nano-scale domains within pyrite. With the recent application of atom probe tomography to geologic materials we now have the nano-analytical techniques to truly understand these cryptic and globally important deposits.

We combine high-resolution electron probe microanalysis (EPMA) and laser ablation inductively coupled mass spectrometry (LA-ICP-MS) with atom probe tomography (APT) to better understand the composition and isotopic signature of the ore fluids, how gold is hosted in these deposits, and why sulfide minerals make such great hosts for gold and other critical metals.

Lecture

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Cosmogenic $^{10}\text{Be}/^9\text{Be}$ in speleothem as a proxy for paleo-weathering rate

Darryl Edward Granger¹, Adrian A. Singleton¹, Anton Vaks², Philip Pogge von Strandmann³

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Meteoric ^{10}Be is introduced to the ground surface as fallout from cosmic-ray production in the atmosphere, while ^9Be is a trace element released by mineral weathering. The $^{10}\text{Be}/^9\text{Be}$ ratio in soil and sediment is therefore used to infer the rate of primary mineral weathering over the timescale of ^{10}Be accumulation, typically 10^3 - 10^5 y. Although beryllium is retentive in soils, a small fraction is released to groundwater.

In carbonate landscapes, groundwater beryllium accumulates in cave speleothem, and can be used to track changes in soil $^{10}\text{Be}/^9\text{Be}$ over time. Independently dated speleothem offer a novel way to monitor weathering rate at a single site over glacial-interglacial timescales. Here, we present a $^{10}\text{Be}/^9\text{Be}$ record from Soreq Cave, Israel, which we interpret as a weathering history of beryllium-bearing silicates (primarily feldspar) in the overlying terra rossa soil derived from loess. Results show that silicate weathering rates vary 2-fold with temperature over the past ~175 ky, from a low of $2\text{-}3 \text{ t km}^{-2} \text{ y}^{-1}$ during cool glacials to a high of $5\text{-}6 \text{ t km}^{-2} \text{ y}^{-1}$ during warm interglacials. Considered as an Arrhenius relationship, the weathering rate indicates an activation energy of $97 \pm 16 \text{ kJ/mol}$, similar to other field-based estimates for feldspar weathering.

Although the beryllium isotopic record in speleothem is likely to be complicated by factors such as changing vegetation and soil depth, our initial work shows promise as a proxy for local soil weathering rates through time, offering a new method for quantifying relationships between climate, soils, and landscape evolution.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Coupling heat conductivity, lithofacies and reservoir quality of the coal-bearing Upper Carboniferous in the eastern Ruhr Basin, NW Germany

Jonas Greve^{1,2}, Benjamin Busch², Dennis Quandt², Mathias Knaak¹, Christoph Hilgers²

¹Geological Survey of North Rhine-Westfalia, Germany; ²Applied Geosciences – Structural Geology & Tectonics, Karlsruhe Institute of Technology (KIT), Germany

The Ruhr Basin in Germany is one of the most extensively studied 3D rock volumes due to decades of subsurface coal mining. Mine flooding associated with the closure of the coalfields may lead to local stress perturbation but also may enable post-mining geothermal applications. However, important geothermal parameters of the Upper Carboniferous clastics are poorly constrained with respect to flow and thermal properties. To improve the understanding of the subsurface heat flux, a dataset of petrophysical parameters is presented for three drill cores of the Westphalian A and B. The studied core material shows fourth order sequences of coarsening/fining upwards cycles in an overall shallowing upward trend. Up to 17 m thick sandstones are associated with a delta front, mudstones and siltstones with a lower delta plain with up to 4 m thick coal seams with a lower delta plain (wetlands) environment. Low compressional wave velocities of 2886 m/s in sandstones are related to higher porosities of up to 15.6%. Likewise, porosity is a major control of thermal conductivity with up to 5.3 W/(m*K) in sandstones. In less porous samples thermal conductivity depends rather on the mineralogy. The low thermal conductivity (mean 3.0 W/(m*K)) of mud and silt-dominated deposits is due to the presence of organic matter or sheet silicates. Generally, low porosity (mean 5.6%) and permeability (mean 0.1 mD) of the rock matrix indicate that fluid flow during mine flooding and potential future geothermal applications will primarily rely galleries and on permeable faults and fracture systems.

Poster

Topic: 10.1 Geoscience Communication and Education

Digital educational tools – smart solutions for heavy stuff

Edouard Grigowski¹, Anne Zacke¹, Fides Friedeberg¹, Gösta Hoffmann²

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Although geoscientific topics (e. g. climate change, natural hazards, geoheritage) engage public, media and politicians, the visibility of geosciences as subject labs behind. Classic ways of public relations are still relevant, but we need additional, complementing communication instruments to transport geoscientific topics. Such instruments are digital offerings. They are very attractive for younger people and technophile persons in general. They are easily accessible and a very useful medium to address our topics to the public. Additionally, they are up-to-date educational tools and can help to explain complicated geoscientific contexts in an understandable, modern and brisk way. As geoscientific museum we naturally use classic ways of communication – our exhibitions – but we also work on digital solutions to reach a wider audience and get people attracted. The granted project is a cooperation with the mobile database of OutcropWizard and the project 30 Geotope³ – Germany's most beautiful geosites in 3D, both developed at the Institute of Geosciences at the University of Bonn. We develop a tailor-made museum app that goes beyond the function of conventional applications. They usually give additional information about objects, provide short movies, audio sequences, etc. We develop the app to link exclusive objects in our showcases with their place of origin, guiding our visitors digitally from the museum into the field. Our guests will get the opportunity to explore different exciting geological sites across the country and to get in touch with the wide variety of geoscientific topics. We achieve this by implementing photogrammetric and laser-scanned 3D models of outstanding locations.

Lecture

Topic: 4.5 Tectonic Systems (TSK Open Session)

Cenozoic fault development in the central segment of the Upper Rhine Graben: Constraints from 3D-seismic data north of Karlsruhe (SW-Germany)

Jens Carsten Grimmer, Florian Bauer, Lars Houbert, Thomas Hertweck, Eva Schill

Karlsruhe Institute of Technology (KIT), Germany

The Cenozoic graben filling is currently investigated for heat storage potentials (DeepStor-project). The structural model based on 3D-seismic and borehole data constrains the geometry and sedimentary thicknesses of potential reservoirs of the DeepStor area north of Karlsruhe. Beside these site specific addressed questions the structural model was used to improve understanding of the development of structures and sedimentary units during Upper Rhine Graben development. The c. 44 km² 3D-seismic area is dominated by two major (N)NE-(S)SW-striking, W-dipping Leopoldshafen and Stutensee growth faults showing normal displacements of several hundred meters, most likely displacing crystalline basement rocks. Fault shadowing effects reduce imaging quality, identification and resolution of seismic reflectors with increasing depth mainly in the footwall. Footwall strata of the Leopoldshafen dip at very shallow angles to the E. Major growth strata along the Leopoldshafen fault comprise the early Miocene Hydrobia beds implying major fault activity during early Miocene times. Fault growth strata display migration of fault activity towards rift interior with time. NNW-striking en echelon normal faults, linked with relay ramps and antithetic faults, are limited to Cenozoic strata unconformably overlaying middle Jurassic rocks. Fault length – displacement analysis of individual faults indicate complex concomitant major and minor faulting activity, tip migration and subsequent fault linkage of minor fault segments that have evolved during progressive transtension.

Lecture

Topic: 8.1 Geosciences and Waste Management

Sustainable metal (Fe) recovery using stamp press bricks made of dusts and sludges from iron and steel making processes

Lars Gronen¹, Carsten Gondorf², Thomas Willms², David Algermissen¹, Lorenz Mild², Thomas Echterhof², Herbert Pfeifer²

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In 2020 approximately 1.5 million tons of dusts and sludges were produced in German steel plants along the integrated steel route via blast furnace and LD converter. These residues from steel making still contain considerable amounts of Fe-oxides as wustite, magnetite and hematite. Thereby, these residues are undergoing intense internal recycling for Fe recovery. However, the fine particle size and the high moisture often hampers the direct recycling in the blast furnace. Thus, the materials are today sintered together with primary resources in the sinter plant or being agglomerated with cement in brick plants.

With the ongoing decarbonization of the European steel industry blast furnaces as well as sinter plants being replaced by DRI furnaces and smelter aggregates like electric-arc furnaces, which producing comparable amounts of dusts and filter sludges. Therefore, the internal recycling of dust and sludge must find other methods within steel making. In the presented study, agglomerate bricks produced by a stamp press are investigated for their potential of dust and sludge recycling in electric-arc and shaft furnaces. Due to oxidic Fe-minerals present in the residues, the bricks need to have self-reducing properties which can be achieved by the addition of reducing agents needed for mineralogical modification. Satisfactory self-reduction properties were proven by high grades of metallization for the tested sample materials with limited coke content. By the application of wheat and potato starch as alternative binder and reduction agent, CO₂ emission can be decreased tremendously as demonstrated by larger scale furnace experiments.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

Big Data in Geoscience – How to approach our largest challenge of today?

Jürgen Grötsch

Energy Transition Centre Amsterdam, The Netherlands

In the past decades, the amount of digital subsurface and geoscience data has grown exponentially, and many companies and government organizations are dealing nowadays with Petabyte-scales of data, still growing fast. On the other hand, hardware, storage solutions, technical applications and data management utilities have not kept up with such rapid developments. This resulted in a big gap and hampers the use of AI and data-driven workflows in complex subsurface projects, be it in hydrocarbon exploration and development, geothermal energy projects, CCS, H₂-storage and the search for nuclear waste sites, but also integrated scientific research programs.

The Open Subsurface Data Universe (OSDU) project is aiming at addressing this challenge and has already resulted in a fundamental change the energy industry approaches data management. OSDU is a consortium with now some 228 companies with geoscience, software technology, data center and service industry backgrounds pooling their efforts to address above challenges via a common open-source, cloud-agnostic data platform, ie OSDU. Also, government organizations and universities are participating in the project.

Georeferencing, data security and accessibility via API layers in the cloud are key features in making data searchable, secure, sharable, and easily retrievable. The project managed by the Open Group Organization has generated not only a fully scalable geoscience data platform but also a new application ecosystem for geoscientists and engineers with many more use cases to come resulting in a revolutionary change on how we can deal with geoscience data and workflows.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Constraining the interplay of magmatic and hydrothermal processes during ore formation with numerical models

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Magmatic-hydrothermal ore deposits form our largest resources of Cu, Mo, Sn and W and are formed by fluids released from magmatic intrusions into a hydrothermal system within the country rock. The potential to form world-class deposits critically depends on cross-boundary fluid fluxes at this magmatic-hydrothermal interface, which is one of the key unknowns in our current understanding of these deposits. Capturing the dynamics of these interface processes with numerical models requires to resolve mass and energy fluxes as a continuum that extends beyond the roots of hydrothermal systems and bridges the gaps between fluid flow and magma dynamics. Magma is mobile during intrusion events and can convect until it reaches a crystal lockup due to cooling and crystallization. During this process, the magma reservoir reaches fluid saturation and exsolves metal-bearing magmatic volatiles to the host rock. This magma solidification behavior depends on its chemical composition, which can be constrained by geochemical analyses of field samples. We have developed a consistent formulation for fluid generation and transport in a coupled model for viscous flow according to the Navier-Stokes Equations and porous flow with Darcy's Law. Our simulation results suggest that the interplay of magma emplacement, magma convection and fluid release during crystallization exerts a strong control on the ore-forming potential. This contribution will present preliminary results from our coupled magmatic-hydrothermal model.

Lecture

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

Expanding the U-series disequilibrium dating to minerals beyond Zircon by LA-ICP-MS

Marcel Guillong¹, Jörn-Frederik Wotzlaw¹, Franziska Keller¹, Francesca Forni², Razvan-Gabriel Popa¹, Olivier Bachmann¹

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In situ U-Th disequilibrium dating is applicable to Uranium bearing minerals crystallizing the past 300 ka and has long been the domain of ion microprobes. We introduced analytical protocols employing laser ablation inductively coupled plasma mass spectroscopy (LA-ICP-MS) to date igneous zircons in 2016. Using a high sensitivity sector field ICP-MS and applying corrections for interferences yields zircon U-Th isotope data comparable in precision to SIMS data.

When zircon is not available, other minerals may be used for U-Th geochronology. Thanks to the unmatched versatility of LA to vary the ablated amount by increased crater sizes and repetition rate, we showed that this technique is suitable for dating minerals with less than ~1 ppm U. A general approach to date new minerals is established and used successfully on garnet, ilmenite and vesuvianite. Details and challenges using the method, including an unexpected interference from contamination and some results from a quadrupole ICP-MS are discussed.

Examples of ilmenite ages are obtained on samples from the Aso-4 caldera-forming eruption and Nisyros. Magmatic garnets from eruptions at Somma-Vesuvius has been recently proven to give important insights into the lifetime and dynamics of phonolitic magma chambers. Additionally, U-Th disequilibrium dating of vesuvianite in the skarn lithic clasts from the same deposits provides additional information about the timing of interaction of the alkaline magmas from Vesuvius with the carbonate country rocks. The versatility of this technique opens a variety of new avenues for quantifying the timing of earth processes.

Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Debunking the myth of Germany being a country poorly endowed in high technology raw materials

Jens Gutzmer

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For several decades, there has been a widely accepted paradigm that „Germany is rich in poor ore deposits“. This paradigm was communicated with conviction especially by experts, i.e. geoscientists active in the raw materials sector. And, indeed, this paradigm appeared well justified as the known endowment of Germany in bulk commodities such as iron, manganese or copper was small in resource tonnage and of too low grade in comparison to world-class deposits in countries such as Australia, South Africa or Chile. Yet, from today's perspective there are some sound arguments why this paradigm may be outdated. Tangible reasons include (a) a marked shift in the portfolio of mineral commodities that are in the focus of a global raw materials industry that needs to generate the supply needed to meet the ambitious goals of the energy transition *sensu lato*; (b) the almost complete lack of modern mineral exploration across most of Germany for more than 30 years – and thus a sincere lack of knowledge about mineral endowment in the subsurface environment; (c) the well-recognised need to render global mineral exploration and production more sustainable. These arguments, combined with the well-known exceptional mineral endowment of regions such as the Erzgebirge or the Kupferschiefer basin across central and south-eastern Germany provide motivation to revise the widely held paradigm. Germans should, indeed, today be regarded as a highly prospective and attractive exploration frontier located in the heart of Europe.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

The Alkaline Complex of Iivaara (Finland): Shallow Intrusive Setting and Fluid Separation

Fahmi Hakim, Dennis Obwocha Achoki, Tobias Fusswinkel, Sven Sindern

RWTH Aachen University, Germany

This study presents the petrogenesis of intrusive rocks of the Iivaara alkaline complex (Finland) and associated enrichment of elements, which are mostly carried by titanite and apatite. Comprehensive mineralogical and textural observations were made and mineral chemical analyses were performed on apatite, titanite, clinopyroxene, and feldspathoid group minerals using EPMA and LA-ICP-MS.

Intrusive rocks exposed in the Iivaara alkaline complex are mainly composed of ijolite group rocks, nepheline syenite, and pyroxenites. They generally show low mineralogical variability but large textural variety. Several textures indicate magmatic formation conditions, including special textures of mingling, schlieren, and Unidirectional Solidification Texture (UST). Some others show fluid-derived formation conditions like replacement texture of primary minerals, breccia as well as veins.

The marked textural heterogeneity present at the margin of the magmatic intrusion and the innermost zone of the fenite aureole, reveals that the current erosion level of the Iivaara exposes the roof zone of an alkaline silicate intrusion. It is characterized by fast cooling, steep temperature gradients, association of small magma batches crystallizing at different conditions, and by expulsion of fluids.

The high abundance of secondary feldspathoid group minerals, apatite, and titanite attests to the significant enrichment of halogens (F, Cl), CO₂, SO₄, P, and Ti in these rocks crystallized from melts or fluids, which in part have agpaitic character.

Mineral chemical data reflect two main stages of fluid expulsion, a syn-magmatic Ca-dominated fluid causing marked fenitization of the wall rocks and a syn- to post- magmatic fluid forming feldspathoid minerals.

Poster

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Magnetic polarity and enviromagnetic stratigraphy of Early Pleistocene terrace deposits of the Lower Moselle: towards a robust chronology of the Main Terraces Complex (MTC) of the Rhenish Massif (RM)

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Controlled solely by the Earth's core, Earth's Magnetic Field reverses its polarity aperiodically on time scales of 10^4 to 10^6 years. This process is recorded by magmatic rocks and by sediments of a wide range of depositional environments, providing a Magnetic Polarity Stratigraphy (MPS). In combination with climate sensitive magnetic and sedimentological parameters, MPS forms the backbone of Neogene magnetic time scales yielding a temporal resolution of c. 10^4 years. Here, we combine for the first time the methodologically independent approaches of MPS with cosmogenic depth profile and burial isochron dating in order to improve the chronology of the MTC of the Lower Moselle using up to date methods. Magnetic polarity data from terrace accumulations and their sandy-silty cover beds reveal clear polarity changes from reversed (old) to normal (young) accompanied by climate indicative magnetic and sedimentological characteristics. Taking into account relative terrace elevations and age constraints from cosmogenic dating, a chronostratigraphic assignment of the MTC to an age interval ranging from c. 1.3 to 0.78 Ma is proposed. This period is characterized by increasing uplift of the RM marking the end of the trough valley period and antedating the onset of the formation of the entrenched valleys. The palaeomagnetically dated increase in subsidence of the Upper Rhine Graben at about 1 to 1.2 Ma ago (Scheidt et al., 2015) coincides with the magnetic dating of the end of the trough valley period in the RM suggesting a common cause of a fundamental change in western European crustal stress fields.

Lecture

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Experimental and isotopic insights into mineral-fluid interactions at Earth's surface in natural and engineered systems

Anna L. Harrison¹, Vasileios Mavromatis¹, Jacques Schott¹, Cameron Wood², Avni Patel³, Eric Oelkers¹, Katharine Maher⁴, Siobhan A. Wilson³, Maija Raudsepp³, Jon Golla⁵

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Mineral-fluid interactions underpin element cycles, mobility of hazardous and valuable metals, and removal of CO₂ from the atmosphere. The fractionation of isotopes provides insights into the processes controlling mineral-fluid reactions in both natural and human-influenced environments. Similarly, the isotopic compositions of minerals reflect the environmental conditions, such as temperature and fluid composition, at the time of mineral formation. Interpreting environmental conditions of the Earth's past and designing strategies for remediation of pollutants and greenhouse gases requires an understanding of the mechanisms of mineral-fluid interaction. We use experimental approaches and analysis of stable isotopes (Mg, C, O, Ca, Si) to investigate processes controlling mineral-fluid interactions and the isotopic composition of minerals at Earth's surface conditions, with a focus on the weathering reactions that remove CO₂ from the atmosphere. Our experiments demonstrate that element exchange between carbonate minerals and fluids continues at bulk mineral-fluid equilibrium potentially resulting in alteration of isotopic signatures and immobilization/remobilization of metals. Similarly, isotope fractionation during non-stoichiometric wollastonite [CaSiO₃] dissolution suggests mass exchanged is not unidirectional even far from chemical equilibrium. On the other hand, mineral dissolution-precipitation reactions are revealed to be dependent on water activity, controlled by relative humidity, with reactions effectively arrested below a threshold relative humidity. Together, our research explores the processes controlling mineral-fluid interactions at the mineral-surface scale, with implications for the global scale element cycles operating over geologic timescales.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

Mapping radiation-damage annealing in zircon

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Radiation damage accumulates in the zircon lattice due to α -disintegration of trace levels of U, Th, and their α -emitting daughters. Upon heating, the lattice damage anneals in two stages by elimination of point defects and crystallization of amorphous domains. Raman spectroscopy is the method of choice to track lattice repair over the two stages due to changes in Raman positions and bandwidths (FWHM) of different bands during annealing. In annealing experiments with controlled time and temperature conditions, the process is usually monitored by Raman measurements after each experimental run. Raman mapping of partially annealed zircon proves to be even more effective than point measurements: (1) the zoning in actinide concentrations enables the comparison of annealing in zones with different initial damage; (2) spatial effects of annealing such as the fading of zoning can be taken into account; (3) tracking changes in the Raman signal from each spot in the map enables to acquire a large amount of annealing data.

While earlier studies produced Raman maps of zircon annealed at high temperatures, we focused on low-temperature stage I annealing. We carried out isothermal annealing experiments on four polished Plešovice zircon grains (1.5 – 2 mm diameter), at temperatures between 300 and 610 °C, with durations between 5 minutes and 70 days, mapping out four Raman bands after each annealing run. Our results show the progressive evolution of the Raman parameters with annealing time and temperature and allow the comparison to natural samples that underwent annealing during their geological history.

Lecture

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

Zircon Raman thermochronology in practice: first results and implications

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Zircon Raman dating rests on measurements of (1) self-irradiation damage in the zircon lattice from the Raman bandwidth (FWHM), and (2) the U and Th concentrations in the same volume. Ages are calculated from the ratio of the dose-equivalent damage estimate and the effective uranium content (eU). As the lattice damage anneals at high temperatures, zircon Raman dating is a thermochronological method, whose results are interpreted in terms of the thermal history of a zircon with respect to the method's closure temperature (T_c). T_c estimates based on laboratory annealing experiments span a range from 260 to 370 °C for various Raman bands and kinetic models.

We dated zircon samples from igneous and metamorphic rocks with a known thermal history, combining Raman spectroscopy with SIMS and EPMA, to test (1) the general applicability of zircon Raman dating, and (2) whether the experimental estimates of the closure temperature match the closure temperature determined on natural samples.

Lecture*Topic:* 2.1 Changes of solid Earth's processes through deep time**Temporal evolution of ^{142}Nd signatures in SW Greenland – new insights from high precision MC-ICP-MS measurements****Eric Hasenstab¹, Jonas Tusch¹, J. Elis Hoffmann², Mario Fischer-Gödde¹, Kristoffer Szilas³, Carsten Münker¹**¹Universität zu Köln, Germany; ²Freie Universität Berlin, Germany; ³University of Copenhagen, Denmark

The short-lived ^{146}Sm - ^{142}Nd decay system is a powerful tool to investigate early geodynamic processes. Here, we introduce a new analytical protocol that allows measuring $^{142}\text{Nd}/^{144}\text{Nd}$ isotope compositions at the lowest ppm-level by MC ICP-MS. This new method is applied to various Archean to Proterozoic rock types (TTGs, boninites, tholeiites, dikes) from the Isua region, SW Greenland. While our results are consistent with previously reported elevated $^{142}\text{Nd}/^{144}\text{Nd}$ compositions^[1,2], our study is the first to statistically resolve small $^{142}\text{Nd}/^{144}\text{Nd}$ isotope differences between rocks from the 3.7 Ga and the 3.8 Ga units of the Isua supracrustal belt. Further, we generally observe a strong decrease of ^{142}Nd anomalies between 3.8 Ga and 3.4 Ga, likely linked to the progressive admixture of unfractionated bulk silicate Earth material that progressively replenished the mantle beneath the Isua region. Such a geodynamic model is also in accord with observational constraints from trace elements and long- and short-lived radiogenic isotopes. The recurrence of elevated $^{142}\text{Nd}/^{144}\text{Nd}$ compositions in younger Mesoarchean rocks (~2.97-3.08 Ga) and one Proterozoic dike (~2.0 Ga) can be explained by mantle sources that were influenced by older Eoarchean recycled components or crustal contamination, respectively. This is also consistent with unradiogenic initial $\epsilon^{176}\text{Hf}$ and $\epsilon^{143}\text{Nd}$ values and enriched incompatible trace element patterns that have been reported for some of these rocks^[3].

[1] Caro et al. (2006), GCA, 70, 164-191. [2] Saji et al. (2018), GPL, 7, 43-48. [3] Szilas et al. (2015), MM, 79, 857-876.

Poster

Topic: 1.7 Experimental Petrology and Geochemistry

Challenges in the determination of highly accurate experimental mineral-melt partition coefficients

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Partition coefficients (D) depend on temperature, pressure, redox conditions, and on the chemical composition of solid and liquid. Trace element modeling of evolution of the Lunar Magma Ocean (LMO) rely on modeled and experimentally determined D's. However, most of these D's have large uncertainties, due to the *in-situ* analytical methods commonly used. Our aim is to develop an improved technique to obtain more accurate trace element partition coefficients from experimental samples. Since clinopyroxene (Cpx) is the most important carrier of trace elements in the crystallizing LMO, we currently focus on Cpx/melt partitioning.

We conducted 1-atm experiments with lunar compositions based on previous studies in gas-mixing furnaces. Starting material compositions contain a variety of trace elements including REE, transition metals, large ion lithophile and high field strength elements. Using the Re-wire loop technique, the experiments cover fO_2 relevant for the Moon (i.e., IW to IW-2).

We measured mineral separates and glasses using isotope dilution ICP-MS methods. The separation of Cpx and glass from the experimental mounts is a key challenge. We compare mechanical separation by drilling using a Micro-Mill 2.0 (Element Scientific Lasers) with separation by hand-picking and *in-situ* LA-ICP-MS measurements to assess which method yields the most accurate D's.

Our new partition coefficients of key trace elements in the LMO will improve models for its evolution.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Linking atmospheric and marine redox evolution during the Great Oxidation Event — Isotopic insights from the Duitschland and Rooihogte formations (South Africa)

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The correlative Duitschland and Rooihogte formations (Transvaal Basin) record a critical juncture in Earth's history since both formations archive a pronounced shift from mass-independent fractionation of sulfur (MIF-S) to mass-dependant fractionation of sulfur, indicative of a slightly oxygenated atmosphere. Surprisingly, however, while multiple sulphur isotope systematics has fundamentally shaped our understanding of atmospheric oxygenation, the evolution experienced within the marine realm has received comparatively little attention. Here we present geochemical transects of four drill-cores intersecting the two formations, affording a three-dimensional, yet somewhat counterintuitive, insight into marine response to atmospheric oxygenation. For instance, rather than signalling more oxygenated conditions, redox-sensitive trace elements disclose persistently suboxic–oxic marine conditions that, in fact, appear to worsen up-section. Interestingly, succeeding the loss of S-MIF, preliminary Mo-isotope data document a c.1‰ shift toward heavier $\delta^{98}\text{Mo}_{\text{NIST}+0.25\text{‰}}$ values. This additionally correlates with a negative shift in $\delta^{34}\text{S}$ to approximately -25‰, a range common for sulfate reducing bacteria, along with an overall increase in both sulfur content and Fe/Mn. This stratigraphic evolution reconciles with a deterioration of local redox conditions by Fe-rich (Mn-poor) sedimentation and/or microbially induced H₂S production, which would lower the Mo isotopic offset between $\delta^{98}\text{Mo}$ in shales and its seawater precursor. The marine redox potential is thus lowered from somewhere between oxic-suboxic to suboxic-anoxic conditions after the loss of MIF-S. Assimilated, at least within the Transvaal Basin, our data expose a geobiological feedback-driven causality between the earliest oxygenation of the atmosphere and a decreased redox potential of the marine realm.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

Exploring meteorite collections via non-destructive micro X-ray fluorescence analysis

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Meteorites offer a unique view on the formation and evolution of our solar system. Thousands of such samples exist in meteorite collections all over the world; however, this resource is by far not fully explored. One reason, among others, is that some rare meteorites, particularly those of historic importance, are usually museum objects. The sampling of such material should be avoided or significantly reduced, for example, by using non-destructive analytical tools. For this, spatially resolved X-ray fluorescence (micro-XRF) is an ideal technique. Several micro-XRF instruments that are currently available allow studying samples in the size range of meters to sub-millimeters with high spatial resolutions in the low μm range. There are several major advantages in micro-XRF with respect to other conventional micro-analytical instruments (e.g., SEM) including (1) the capability to handle large samples; (2) low detection limits (usually below those of SEM EDX systems), and (3) high analysis speed allowing to cover large areas in relative short time. We explore the analytical capacity of two different micro-XRF instruments. The first is an open beam system (M6 JETSTREAM) and the second (M4 TORNADO Plus) is an instrument with a vacuum chamber and several options for improving the light-element sensitivity. Here, we present several case studies from chondrites and achondrites with sample sizes up to 16×20 cm. We evaluate quantification of chemical compositions (whole rock, fragments and mineral components) by standard-free and standard-based methods and discuss possible micro-XRF-based classification of meteorites based on established criteria.

Lecture

Topic: 3.2 Composition and evolution of deep planetary interiors

Sheared peridotites from the cratonic mantle beneath Lesotho (Kaatvaal craton): Investigating deformation and related metasomatic processes from mid-lithospheric depth to the LAB.

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Sheared peridotites give direct evidence for deformation processes in the subcratonic mantle shortly before their transport to the surface by kimberlites. We studied 12 sheared peridotites (11 garnet-peridotites, one spinel-bearing) from three localities in Lesotho, which were entrained in the Late Cretaceous (90Ma). The peridotites exhibit different degrees of depletion from more fertile ($X_{\text{Fe}} \approx 91$) to depleted ($X_{\text{Fe}} \approx 93$). Typical for sheared peridotites, textures reveal a bimodal grain size with mm-size porphyroclasts, which are surrounded by 10s – 100s μm neoblasts. Our suite can be split into two groups: (i) low-T (<1250°C) and (ii) high-T (1400 ± 50 °C). The low-T sheared peridotites derive from various depths (3.5 – 5.5 GPa) in the lithospheric mantle whereas the high-T sheared peridotites equilibrated at high pressures (6 ± 0.5 GPa), corresponding to the lithosphere asthenosphere boundary (LAB) beneath the Kaapvaal craton.

Crystallographic preferred orientations of olivine verify the presence of metasomatic agents during deformation in both groups and reveal various types: B-, C-, E-, AG- and bimodal CPOs. Increasing Ti-contents in olivine and orthopyroxene neoblasts, accompanied with an increase in temperature in the low-T group, reveal a connection between metasomatism and deformation during interaction with (failed) kimberlites. In contrast, the porphyroclasts and neoblasts of all phases in the high-T peridotites have homogeneous major and trace element contents, implying (re-)equilibration (during deformation?). Trace element signatures in garnet, clinopyroxene and orthopyroxene indicate that metasomatism at the LAB caused either enrichments or depletions in the high-T sheared peridotites.

Poster

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Weathering geochronology of a deep (> 120 m) lateritic profile in northern Brazil

Beatrix Heller^{1,2}, Thierry Allard², Caroline Sanchez¹, Guilherme Taitson Bueno³, Jean-Yves Roig⁴, Cécile Gautheron¹
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Tropical weathering leads to the formation of deep weathering profiles called laterites. The Guiana shield has been tectonically stable and in tropical latitudes supposedly since the Cretaceous, allowing the formation of very deep (> 100 m) and old (tens of Ma) lateritic profiles.

In this contribution we present a coupled data set of kaolinite electron paramagnetic resonance (EPR) ages and (U-Th)/He ages of supergene hematite and goethite from a deep (> 120 m) weathering profile exposed in an open pit gold mine in the northern Brazilian state of Amapá. Coupling of the two methods which target different components of the lateritic profile allows us to reconstruct the formation and evolution of the presented profile throughout the entire Cenozoic. While (U-Th)/He ages on supergene hematite and goethite from the ferruginous duricrusts on the top of the profile record three discrete weathering events during the Late Cretaceous/Early Paleocene, Oligocene and Middle Miocene, kaolinite ages allow an insight into the vertical evolution of the profile. The oldest kaolinites, which are very well-ordered, are preserved in the saprolitic part of the profile whereas the kaolinites in the top of the profile show very recent (< 5Ma) rejuvenation. Disordered kaolinite captured in the lateritic duricrust was protected from this rejuvenation.

Lecture

Topic: 5.6 Natural archives as recorders of past climate and environmental conditions – processes, methods and applications

Reading the climate signals hidden in lateritic iron duricrusts

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Laterites are deep weathering profiles which develop under tropical and subtropical climatic conditions. Their geochemical and mineralogical composition is strongly influenced by the climatic condition under which they form, whereas the composition of the parental material plays a subordinate role. Due to their long-term stability throughout the intertropical zone, they are archives of past (sub)tropical climates. As different climatic signals are potentially superposed in old and constantly exposed laterites, disentangling of the paleoclimatic information preserved in these archives is a complex task. Hematite and goethite, which are the main components of the ferruginous duricrust that is present in most lateritic profiles, can be dated using the (U-Th)/He method allowing important geochronological constraints.

In this contribution we present how paleoclimatic information can be extracted from lateritic iron duricrusts by combining geochemical, mineralogical and geochronological methods. Our coupled data from the northeastern Guiana shield reveal the existence of important weathering events during the Oligocene and Middle Miocene related to ferruginous lateritic weathering conditions representative of contrasted tropical monsoonal climate. A significant change towards bauxitic weathering conditions, characteristic of more humid tropical monsoonal climate, happened during the Late Neogene as indicated by an increase in Th concentration, Al-substitution in goethite and precipitation of gibbsite.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Geochemistry and Petrology of Ultramafic Rocks from the Troodos Ophiolite, Cyprus: New Perspectives on the Evolution of Boninitic Melts

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The Troodos Ophiolite Complex in Cyprus consists of Neotethyan oceanic crust that formed above a subduction zone in a so-called suprasubduction zone setting (SSZ). In this geological environment, fluids from the subducting slab induce melting and metasomatism within the mantle wedge. Such processes are required for the formation of characteristic lithologies like boninites that are often associated with back-arc lavas.

Because of the low incompatible element abundances of SSZ mantle rocks and the associated analytical difficulties, previous geochemical analyses mainly focused on igneous rock suites of these ophiolites. Here, we used quadrupole ICP-MS to provide a complete trace element dataset for mantle harzburgites and pyroxenites from the western part of the Troodos mantle section. It confirms that the harzburgites are highly depleted up to 30 times more depleted than the primitive mantle. Both harzburgites and pyroxenites display U-shaped trace element patterns typical for SSZ settings, caused by the refertilization of depleted mantle with fluid mobile elements. Our data confirm previous assumptions about the highly refractory nature of the above-mentioned mantle region, which likely represents the mantle source for the Troodos boninite melts. Additionally, mineral microanalyses by EPMA reveal a link between ultramafic cumulates that precipitated from boninitic melts (Shen et al. (2020), Lithos) and pyroxenite veins in the sampled mantle section. We therefore propose a multi-stage model for the boninitic melts that includes 1) reactions of the percolating melt with the mantle peridotite, 2) the formation of ultramafic cumulates near the MOHO and 3) the eruption of the boninitic lavas.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

RNA trapping in 3D Hadean hydrothermal submarine vent models

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The question on how life emerged on Earth remains one of the biggest mysteries of mankind. Alkaline hydrothermal vents (AHVs) might have played a key role during the transition from pre-biotic chemistry to an RNA-world during the Hadean. Two major theories regarding the emergence of life on Earth are the hydrothermal vent metabolism-first (AHVs) and the information-first (RNA world) theories. It is unknown, whether these theories are mutually exclusive. This PhD project will use controlled laboratory experiments to investigate plausible scenarios, in which RNA is accumulated within the mineral matrix, that forms in AHV models under simulated Hadean ocean conditions.

AHVs are “chemical gardens” with steep eH-pH and T gradients, that would have provided potential energy for proto-life. They contain reactive mineral surfaces like Fe-sulfide and Fe-hydroxide and have a complex internal network of micropockets and channels, that might have concentrated nucleic acids.

We simulate AHVs in an anaerobic chamber containing a N₂-atmosphere. The experiment mimics Hadean conditions without oxygen. The setup contains a glass vial filled with the Fe-rich, salty and mildly acidic (pH ~5.5) „ocean“. A syringe injects the alkaline hydrothermal fluid (pH 9 to 12). Chemistry, flow-rate and temperature of the fluid can be varied. As the alkaline fluid mixes with the acidic iron “ocean“, changes in pH cause iron minerals to come out of their stability fields and precipitate forming chimney structures. Different types of RNA added to the „ocean“ before the injection might accumulate inside the hydrothermal chimney.

Poster

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Carbon Cycling at the Dawn of the Cenozoic

Michael J. Henehan¹, James Barnett², Borianna Calderon-Asael³, Volkan Özen⁴, Pincelli Hull³, Noah Planavsky³, Andy Ridgwell⁵, James Rae², James Witts⁶, Kate Littler⁷, Sarah Greene⁸, Ellen Thomas³, Mathis Hain⁹, Friedhelm von Blanckenburg¹

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The Paleocene – the first epoch of the Cenozoic (66–56 Ma) – spans numerous notable climatic and biogeochemical phenomena. In the oceans, the Paleocene saw the drawn-out recovery of calcifying plankton communities after severe extinction at the K-Pg, followed by one of the largest excursions in benthic foraminiferal $\delta^{13}\text{C}$ values of the last 100 Myr¹. On land, an as-yet-unexplained extreme step-change in global weathering regime is indicated by marine carbonate $\delta^7\text{Li}$ values². More generally, although benthic foraminiferal $\delta^{18}\text{O}$ suggests a greenhouse climate much warmer than today³, proxy estimates of atmospheric CO_2 in the Paleocene mostly indicate CO_2 levels similar to those of the relatively colder late Neogene⁴.

Here, I will show some new benthic and planktic foraminiferal boron and lithium isotope data that address outstanding puzzles in geochemical cycling and ocean chemistry at the dawn of the Cenozoic.

1. Friedrich, O., Norris, R. D. & Erbacher, J. Evolution of middle to Late Cretaceous oceans--A 55 m.y. record of Earth's temperature and carbon cycle. *Geology* **40**, 107–110 (2012).
2. Misra, S. & Froelich, P. N. Lithium Isotope History of Cenozoic Seawater: Changes in Silicate Weathering and Reverse Weathering. *Science* **335**, 818–823 (2012).
3. Westerhold, T. *et al.* An astronomically dated record of Earth's climate and its predictability over the last 66 million years. *Science* **369**, 1383–1387 (2020).
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Plenary / Goldschmidt Lecture

Beyond isotope proxies: employing triple oxygen isotope systematics in the water cycle and in chemical sediments as quantitative tool

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Carbonate classic and clumped isotope ratios ($\delta^{18}\text{O}$ and Δ_{47}) are used to reconstruct paleotemperature. However, kinetic isotope effects (KIE) induce a bias on absolute temperature reconstructions. High precision $\delta^{17}\text{O}$ measurements provide a refinement proxy to identify the direction and magnitude of KIEs in carbonates. Progress on this new proxy will be discussed.

The basic concept is similar to the combination of conventional oxygen and hydrogen isotope analyses in water. Combined $\delta^{18}\text{O}$ and $\delta^2\text{H}$ analyses are commonly used to approximate the magnitude of KIEs during evaporation. Triple oxygen isotope measurements in water are now used in a similar fashion. The simultaneous utilization of both trajectories provides a powerful approach to reconstruct quantitative paleoclimate information. We applied this approach to extracted water from ancient gypsum formed in the Atacama Desert and in Cyprus during the Messinian Salinity Crisis. Quantitative information on paleo-humidity and palaeohydrology are obtained. Effectively, this information is derived by quantifying KIE.

In this example, the KIE is related to diffusion of water molecules through air. Other examples of KIE include the breaking of chemical bonds, molecular mixing effects or steady states. Triple oxygen isotope trajectories allow to distinguish between such fundamental processes. Respective concepts will be explained using examples from chert and phosphate triple oxygen isotope systematics.

Lecture

Topic: 11.2 Latest Achievements in Scientific Ocean and Continental Drilling

Geologic framework and first results from ICDP BASE drilling in the Moodies Group (~3.22 Ga), Barberton Greenstone Belt, South Africa

Christoph Heubeck¹, Nic Beukes², BASE onsite geoscience team¹

¹Friedrich-Schiller-University Jena, Germany; ²University of Johannesburg, South Africa

The up to 3.5 km thick Moodies Group (ca. 3.22 Ga) of the Barberton Greenstone Belt, South Africa and Eswatini, exposes some of the oldest well-preserved sedimentary strata on Earth. Strata were deposited within only a few million years in prodeltaic to alluvial settings, with a dominance of tidal deltas and coastal plains; they provide a very-high-resolution record of Early Archean surface conditions. Widespread microbial mats, early diagenetic vadose-alteration zones and tidal rhythmites are common. Moodies strata provide a unique opportunity to investigate the conditions under which bacterial life spread and thrived on early Earth.

We show preliminary cross sections, overall core photographs and representative lithologic descriptions from the eight boreholes, each ca. 350-400 m in length, which were drilled November 2021 to May 2022 within the framework of the ICDP *Barberton Archean Surface Environments* (BASE) Project.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Eight ICDP boreholes and three tunnels through 3.7 km of Paleoproterozoic shallow-water strata probe the setting of early life

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The up to 3.7 km-thick Moodies Group (~3.22 Ga) of the Barberton Greenstone Belt, South Africa and Eswatini, comprises some of the oldest well-preserved sedimentary strata on Earth, deposited within only a few million years in prodeltaic to alluvial settings, with a dominance of tidal deltas and coastal plains. Moodies Group strata consist of polymict conglomerates, widespread quartzose, lithic and arkosic sandstones, siltstones, shales, and rare BIFs and jaspilites, all interbedded with tuffs and several lavas. They preserve abundant sedimentary structures and represent a very-high-resolution record of Paleoproterozoic surface conditions and processes. Widespread microbial mats, early-diagenetic vadose alteration zones and tidal rhythmites allow to investigate the environmental conditions under which bacterial life spread on early Earth. The ICDP Barberton Archean Surface Environments (BASE) Project drilled November 2021 to June 2022 eight inclined boreholes of 300-450 m length each through steeply inclined or overturned Moodies Group strata; the unweathered and continuous core record was complemented by sampling in three several-km-long tunnels and by detailed surface mapping. Two to three rigs operated concurrently, delivering twenty to sixty m of high-quality core daily, processed in a large, publicly accessible hall adjacent to the museum in downtown Barberton. An exhibition provided background explanations for visitors and related this fundamental geoscience research project to the recently established Barberton-Makhonjwa Mountains World Heritage Site.

Poster

Topic: 2.1 Changes of solid Earth's processes through deep time

The Malolotsha Klippe: Large-scale subhorizontal tectonics along the southern margin of the Archean Barberton Greenstone Belt, Eswatini

Christoph Heubeck¹, Benjamin Heredia², Tonny Thomsen², Armin Zeh³, Philipp Balling¹

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Whether Archean tectonics were horizontally or vertically dominated is debated because arguments bear on the kinematics and thermal state of the Archean mantle and constrain the formation of the earliest continental crust. Deformed strata of greenstone belts figure prominently in this debate because they record long periods and multiple deformation phases. Among the best-preserved belts counts the Barberton Greenstone Belt (BGB) of southern Africa. Geological mapping of its southern part in Eswatini (Swaziland), combined with U-Pb zircon dating, show that the region preserves a tightly re-folded imbricate thrust stack in which metavolcanic and -volcaniclastic strata of the Onverwacht Group, deposited at 3.34-3.29 Ga, have been thrust on top of ca. 3.22 Ga siliciclastic strata of the Moodies Group. The structurally highest element, the Malolotsha Syncline, forms a tectonic klippe of substantial size and is >1450 m thick. Forward modelling of a balanced cross section indicates that this thrust stack was part of a northwestward-verging orogen along the southern margin of the BGB and records a minimum horizontal displacement of 33 km perpendicular to its present-day faulted, ductily strained and multiply metamorphosed margin. Because conglomerate clasts indicate a significantly higher degree of prolate strain which extends further into the BGB than at its northern margin, the late-stage tectonic architecture of the BGB may be highly asymmetrical. Our study documents that the BGB, and perhaps other Archean greenstone belts, preserves a complex array of both vertically- and horizontally-dominated deformation styles that interfered with each other at small regional and short temporal scales.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

Towards a single Cosmochemical Database: MetBase and the Astromaterials Data System (AstroMat) started a common future

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MetBase is since more than 20 years one of the world's largest database for meteorite compositions [1], currently hosted in Germany. Recently, the Astromaterials Data System (AstroMat) has been developed as a data infrastructure to store, curate, and provide access to cosmochemical laboratory data. Astromat and MetBase have a shared goal: advancing the reuse of lab analytical data from astromaterials samples to maximise their value and impact for science, and therefore agreed to merge in two distinct steps:

1. With a pilot project funded by the NFDI4Earth [2] we will make MetBase data fully FAIR (findable, accessible, interoperable and reusable [3]), by adapting the recently established Astromat database schema [4], which is based on the EarthChem data model.
2. In a separate step, MetBase will be transferred and integrated into the Astromaterials system, a much higher level of integration, in which both databases will become one, making working with both entirely seamless.

The current MetBase graphical user interface will be modernised as part of the NFDI4Earth pilot project, then maintained at the GU Frankfurt, and become a general tool to access, visualise and work with cosmochemical and geochemical databases. Both MetBase and Astromat participate in the OneGeochemistry initiative, to contribute to community endorsed and governed standards for FAIR analytical data that will allow seamless data exchange and integration.

References: [1] <http://www.metbase.org>. [2] <http://nfdi4earth.de> [3] Stall et al. 2019. Nature 570(7759): 27-29. [4] <https://www.astromat.org>

Lecture

Topic: 10.2 Geoethics – fostering ethical perspectives in Geosciences

Is there an interdisciplinarity crisis in the Geosciences?

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Modern Geosciences profit substantially from interdisciplinary collaboration across the natural sciences and even beyond. Some recent advances have only become possible through these efforts. Consequently, interdisciplinarity is particularly relevant for the implementation of new research directions and the appointment of professors at Geoscience departments. However, it is common that positions are filled with mathematicians, computer scientists, chemists, physicists or biologists, which use their own methods to solve Geoscience problems. There is no question that this might lead to fruitful collaboration, but in practice this situation often results in severe problems in Geoscience teaching.

First, these scientists are usually hardly able to teach fundamentals of Geosciences or field courses as they were not trained in these areas themselves. Second, highly specialized courses are offered that are often way more appealing to students outside the Geosciences because they heavily rely on concepts and methodology from other natural sciences. Third, the methods used and taught by these scientists are commonly strongly focused on quantitative data, which tends to increase a general development towards generating large data sets without applying a deeper geoscientific thinking for their meaningful interpretation (see also Şengör, 2021).

The core competence of geoscientists – solving complex multi-scale spatio-temporal problems – is unique and not replaceable. Becoming more aware of our key expertise as Geoscientists paves the way for balanced and constructive – truly interdisciplinary – interactions in teaching and research. This will significantly strengthen the role of Geosciences in taking responsibility for solving major societal challenges in the 21st century.

Poster

Topic: 10.1 Geoscience Communication and Education

International Earth Science Olympiad (IESO) 2022: German National Team Field Investigation at the Leibniz Institute for Baltic Sea Research (IOW)

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The International Earth Science Olympiad (IESO) is an annual competition for secondary school students. It provides them to compete not only individually, but also in team quests, such as Earth Systems Projects (ESP) and International Team Field Investigation (ITFI). In 2022, the ITFI was carried out on a national level, and presented online by the national teams. Nir Orion (Weizmann Institute for Science Education, Israel), member of the IESO Examination Board about the task:

“A Field Investigation is a mini-study pertaining to a concrete Earth system phenomenon in a field site that combines limited and short field and laboratory studies. The study should relate to a focused research question, in terms of time and scope, that can be answered in a mini-study of 1-3 days of field observation, data collection and laboratory analysis. Criteria for the selection of the studied phenomena:

- Relate to a real and relevant environmental Earth system-based phenomenon.
- Data collection includes the use of up to date field instruments and lab measurements.
- A long-term data set may be provided to students following the one-time measurements at the field site.”

The success secret depends on the ability and possibility of mentors to collaborate with an academic research lab. The IOW invited the German national team to work on Glyphosat, which due to a newly invented analytical method, was detected in the Baltic Sea. We will describe chances and challenges, that a geoscience research institutes faces associated with the organisation of a Team Field Investigation project for school students.

Lecture

Topic: 3.1 Novel isotopic insights into high-temperature geochemical processes

Isotopic fractionation during planetary-scale processes

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Mass-dependent fractionation of isotopes has rapidly grown as a tool to study a large variety of geological/-chemical processes since the advent of mass spectrometry. Traditionally, the isotopes of relatively low mass elements such as hydrogen, oxygen and carbon were used to study dominantly low-temperature processes. Improvements in measurement precision have, however, enabled us to resolve fractionation occurring in the isotopes of nearly all elements in the periodic table during low- or high-temperature processes.

Isotopic fractionation can take place under two extreme conditions. Unidirectional, or kinetic, fractionation is typically relatively large and roughly proportional to the square-root of the mass ratio of the isotopes. Under chemical equilibrium, fractionation is typically smaller and decreases with the square of temperature as differences in zero-point vibrational energies control the isotopic fractionation between phases. These two scenarios are just one of the complexities that need to be unravelled when analysing isotopic fractionation, particularly when isotopic variations are small, as is often the case for relatively high-mass elements and when attempting to study high-temperature processes.

I will present a case where careful sample selection and analysis combined with theoretically or experimentally constrained isotopic fractionation factors and multiple chemical proxies allow isotopic fractionation to be a valuable tool to understand large-scale, planetary formation/differentiation processes.

Lecture

Topic: 10.1 Geoscience Communication and Education

Networking for more Geoscience in School Education – The Geoscience Education Field Officer Initiative

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In 2019, the European Geosciences Union (EGU) began a new initiative to appoint Geoscience Education Field Officers and train them to provide professional development to school teachers who have elements of geoscience in their teaching curriculum.

Today, officers are installed in 11 European countries and even more beyond Europe. Between the officers all type of educational expertise is represented, there are school teachers, university lecturers, geopark rangers as well as teacher trainers.

The officers are to liaise with a small group of EGU recognised supporters in their own country. In order to initiate this process in Germany, the initiative will be explained and potential modes of action discussed.

Lecture*Topic:* 2.1 Changes of solid Earth's processes through deep time**Deciphering the mechanisms of crustal formation in the Early Earth: Insights from Ti isotopes****Liam Hoare¹, Laura Rzehak-Wissink¹, Sebastian Kommescher^{1,2}, Moritz Jansen³, Elis Hoffmann⁴, Raúl Fonseca¹**¹Institut für Geologie, Mineralogie und Geophysik, Ruhr-Universität Bochum, Germany; ²Institut für Mineralogie, Leibniz Universität Hannover, Germany; ³Deutsche Bergbau Museum, Bochum, Germany; ⁴Institut für Geologische Wissenschaften, Freie Universität Berlin, Germany

Archean tonalite-trondjemite-granodiorite (TTG) plutonic rocks provide a unique, yet imperfectly understood record of crustal formation. Due to the incomplete nature of this record, there are varying interpretations on the prevailing tectonic regime responsible for the formation of juvenile continental crust. Thus, robust geochemical proxies are required to understand the (non-unique) processes of TTG formation. Ti isotopes have recently been utilised to investigate magma evolution in modern tectonic settings. Ti isotope fractionation is driven by the preferential sequestration of light isotopes in Ti-rich minerals (e.g., Fe-Ti oxides, amphibole). Consequently, melts in equilibrium with these phases are enriched in heavy isotopes. Ti isotopes are an ideal tool for tracing the formation of juvenile continental crust due to their sensitivity to amphibole, rutile and (to a lesser extent) garnet crystallization – major phases involved in TTG petrogenesis via dehydration melting of basaltic protoliths.

Preliminary Ti isotope measurements of amphibolites from the 3.7-3.8 Ga Isu Supracrustal Belt (ISB) in SW-Greenland, display $d^{49/47}\text{Ti}$ values comparable to mid-oceanic ridge basalts. Ti isotope compositions during TTG generation were modelled by combining this data and constraints from amphibolite partial melting experiments with mineral-melt Ti isotope fractionation factors. Low pressure melting with amphibole as the main Ti-bearing phase produce melts with $d^{49/47}\text{Ti} \leq \sim +0.2\%$, whereas models using higher pressure/high H₂O experiments containing rutile+amphibole produce melts with $d^{49/47}\text{Ti} \leq \sim +0.3\%$ and higher $d^{49/47}\text{Ti}$ at a given SiO₂. This suggests different source mineralogy/composition, pressure, and H₂O contents can influence $d^{49/47}\text{Ti}$ values during partial melting and that TTG formation processes are non-unique.

Lecture

Topic: 3.2 Composition and evolution of deep planetary interiors

Fe³⁺ in garnet and the V/Cr redox proxy: Two methods, one result. Oxygen fugacity of Paleoproterozoic ky/cor eclogites from the Kaapvaal craton - subducted equivalents of former troctolites

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The Earth's mantle was at metal saturation shortly after accretion ($\Delta\text{FMQ} \sim -4.5$; Frost and McCammon, 2004). This supposedly changed very rapidly to $\Delta\text{FMQ} \sim 0$ (= today's oxidation state of the MORB mantle) due to the disproportionation of Fe^{2+} in bridgmanite to $\text{Fe}^{3+} + \text{Fe}^0$. The latter was transferred to the core leaving an oxidized residue behind. Magmas from the mantle should therefore indicate the same oxygen fugacity through time. This is tested here with 3.2 Ga old kyanite and corundum eclogite xenoliths from the Bellsbank diamond mine on the Kaapvaal craton, i.e. metamorphosed troctolites (= olivine-plagioclase cumulates; Shu et al. 2016).

One method to estimate the oxygen fugacity of troctolites is based on the V/Cr ratio of the accumulating olivine (Mallmann and O'Neill, 2009). Modern day troctolites from the Pacific and the Atlantic form a correlation of V and Cr with a slope corresponding to $\Delta\text{FMQ} \sim 0$. The ky/cor eclogites yield a steeper slope corresponding to $\Delta\text{FMQ} \sim -2$ meaning that the Fe^{3+} content of the garnets should be close to zero. Our second method, the determination of $\text{Fe}^{3+}/\Sigma\text{Fe}$ in garnet with the flank method by EPMA (Hoefner and Brey 2007), gave $\text{Fe}^{3+}/\Sigma\text{Fe} < 0.03$ that yielded a mean ΔFMQ value of -1.6 as calculated with the oxybarometer of Vasilyev (2016). This indicates a gradual increase of oxygen fugacity in the mantle after core formation (see also Aulbach and Stagno 2016) and confirms that the oxidation state of Fe can be preserved in eclogites since the Archean.

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

Contrasting messages from sulfur and oxygen isotopes on the origin of Eoarchean crust

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Mantle-like oxygen isotope compositions in zircons from Eo- and Paleoeoarchean tonalite-trondhjemite-granodiorites (TTG) suites have been taken as evidence for the formation of early continental crust from juvenile hydrated basalts that formed in a plateau-like setting [1,2]. Other studies found elevated oxygen isotopes in zircons from >3.6 Ga TTGs in line with recycled crustal components in the sources (e.g., 3). Recent studies have shown that Eoarchean TTGs, amphibolites and mantle peridotites from the Itsaq Gneiss Complex (IGC) of SW Greenland bear small but significant mass independent sulfur isotope (MIF-S) anomalies in cap^{33}S and cap^{36}S (e.g., 4). These can only be explained by the incorporation of surface-derived sulfur of Archean age into the mantle and crustal sources. For the same suite of samples, oxygen isotope compositions in zircon and olivine overlap with mantle values, providing no indication for recycled material in the sources and therefore no evidence of early subduction processes. MIF-S anomalies have been observed in almost all Eoarchean magmatic rocks analyzed so far, which is a strong indication of a wide distribution of subduction processes in operation in the IGC. We argue that the oxygen isotope composition of zircon in TTGs may represent a mixed signal from different mafic source rocks and may not have the same resolution for surface-derived material compared to sulfur isotopes.

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Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Fully quantitative trace element mapping of microbial carbonates by LA-ICP-TOF-MS: Background, results and perspectives

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Trace element compositions of carbonate microbialites are valuable proxies to reconstruct shallow water microbial environments through Earth's history. Most of the published trace element data of microbial carbonates are obtained from bulk digestion or carbonate leaching of sample powders retrieved from microdrilling or via in situ laser ablation analysis calibrated to external reference materials such as NIST glasses. However, due to the complex formation mechanism of microbial carbonates, huge compositional differences are associated with spatial and lithological sample heterogeneities that cannot be fully resolved with the current analytical methodologies.

Here, we describe a new method using a high-frequency laser ablation (LA) system (NWR Image GEO193) coupled to inductively coupled plasma time-of-flight mass spectrometry (ICP-TOF-MS) and internal calibration via matrix-matching nanopowder carbonate reference materials to obtain rapid high-resolution quantitative trace element maps.

Our mapping results reveal that detrital elements such as, aluminium (Al), thorium (Th), bioactive elements such as cadmium (Cd) iron (Fe) barium (Ba) and nickel (Ni), and particle-reactive elements such as rare earth elements (REE) have concentrations distributions that correspond with the intrinsic bio-sedimentary layering in microbialite samples.

Here we present fully quantitative LA-ICP-TOF-MS trace element maps of a variety of microbialites from the Phanerozoic to the Archean. Our promising new method for rapidly obtaining spatial geochemical characteristics of microbialites that build the groundwork for follow-up research such as in situ U-Pb dating on truly authigenic carbonate phases or stable novel metal isotope analyses on individual layers to study bio-essential metal uptake in diverse microbial communities through deep time.

Lecture

Topic: Plenary Lecture

Andean uplift and consequences for species evolution in the Amazon drainage basin

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The Neogene uplift of the Andes strongly influenced environments, geography, and climate through time. In combination with global climate, sea level change and dynamic topography, this process (re)shaped the biogeography of the Amazon drainage basin. The western Amazon, was formed by a vast wetland that was controlled by orbital forcing and episodic marine influence, with dispersal of coastal flora and fauna into the Amazon heartlands. As uplift accelerated, the effects extended across the continent, leading to the birth of the Amazon River and sediment transport across continent and into the Atlantic. The river formed a bridge and a barrier for biotic dispersal but also affected the coastal environment. Here I will review recent geological and paleobiological data to illustrate the effects of geological change on neotropical biogeography.

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Lecture

Topic: 1.6 Probing (bio)geochemical reactions at mineral interfaces using micro- to nanoscale techniques

New opportunities to unravel the microarchitecture of mineral and organo-mineral associations by NanoSIMS using the upgraded O source

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NanoSIMS (nanoscale secondary ion mass spectrometry) allows unique elemental and isotopic analyses at nanometer spatial resolution and provided challenging insights into the architecture of soil organo-mineral constituents and valuable knowledge of crucial processes taking place at the microscale.

The NanoSIMS instrument is equipped with two ion sources: the Cesium source (Cs^+) convenient to detect ions related to organic matter distribution and the Oxygen source (O^-) favourable to provide information on mineral phases or metals in samples.

In this contribution a diverse range of case studies will be presented highlighting analytical and experimental applications of the NanoSIMS upgraded with an improved RF plasma O-source as recently installed at the TUM. With a spatial resolution down to 50nm and high stability, the upgraded O^- source is now best suitable for probing elemental and isotopic composition of minerals at the microscale, which provides ample opportunities for novel experimental applications.

Furthermore, extended analyses of soil organo-mineral associations are possible with both Cs^+ and O^- sources at similar resolution. This enables novel combinations of C, N, P and Si distributions depicted by the Cs^+ source with the distribution of e.g. Na, Mg, K, Ca and advanced measurement of Fe and Al as revealed by the O^- source. Post-processing tools for unsupervised clustering and supervised segmentation facilitate the comparison and quantitative analysis of the spatial architecture within intact soil structures.

These recently developed techniques provide an innovative platform to extend our understanding of biogeochemical processes taking place at organo-mineral and mineral-mineral interfaces at the microscale.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Fingerprinting fluid evolution and metal distribution in the Skouries porphyry Au-Cu deposit (NE Greece) by mineral micro-analysis

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The Skouries deposit in NE Greece is a platinum-group element enriched ($\varnothing=149$ ppb Pd, $\varnothing=30$ ppb Pt) Au-Cu porphyry system hosted by monzonite-syenite intrusions. The porphyry stockwork consists of quartz-rich A- and B-type veins associated with potassic alteration, followed by massive sulfide-bearing veins related to chlorite-sericite alteration, and D-type veins associated with sericitic alteration. The mineralization is dominated by chalcopyrite, pyrite, bornite, and magnetite associated with native gold and Bi-Pd-rich telluride inclusions. The mineral chemistry (EPMA and LA-ICP-MS) of chalcopyrite, pyrite, magnetite, and hydrothermal quartz was used to track the physicochemical fluid evolution, and to define mechanisms enhancing metal enrichment at Skouries.

Textural differences of hydrothermal quartz generations, as reflected by distinct CL-SEM intensities, were linked to Ti-in-quartz-thermometry and quartz trace element ratios, such as Ge/Ti, Sb/Ti and Al/Ti. These ratios record temperatures around 600°C for the A-type veins, suggest a reopening of veins by a second, hotter fluid pulse (>600°C), which was followed by a decrease in temperature below 600°C for the later B-type veins. Furthermore, the sulfide mineralization is characterized by systematic variations in trace element concentrations (e.g., As, Ag, Au) and ratios (e.g., Au/Cu, Co/Ti, Se/Te, As/Sb) fingerprinting physicochemical changes in the hydrothermal fluid system. Therefore, sulfide and quartz micro-analysis can help decipher small-scale processes within the porphyry system and allow to establish mechanisms controlling the metal endowment of porphyry deposits on a larger scale.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Four eruption cycles feeding the most voluminous Deccan Eruptions

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Large Igneous Provinces (LIPs) are unusual volcanic events in which massive amounts of melt ($\sim 10^6$ km³) erupt in relatively short time periods ($< 10^6$ yrs). Many LIPs were emplaced at the former positions of currently active hot spots and are thought to have formed due to extensive decompression melting of anomalous hot mantle triggered by an initiating mantle plume. Most LIP magmas have interacted extensively with the continental crust, however the location and dimensions of the crustal magmatic plumbing systems and the processes triggering eruptions are debated. Here we present new major and trace element and radiogenic isotope data for 43 individual lava flows from a continuous 1200 m thick stratigraphic profile through the upper, most voluminous part of the Deccan LIP (Bushe to Mahalabaleshwar Formations). Eruption rates for this section are constrained by published paleomagnetic directions and absolute U-Pb ages for zircons from weathered flow tops exposed in the profile. We find four magmatic cycles each lasting $\sim 10^4$ to $\sim 10^5$ yrs during which major and trace element compositions change systematically, which are best explained by repeated sequences of recharge, fractional crystallization and eruption. The lavas at the beginning of each cycle generally have the highest MgO contents, but are the most contaminated (lowest Ce/Pb and Nb/Th), inconsistent with the combined assimilation-fractional crystallization trends usually associated with single magma bodies. Rapid changes of isotopically different contaminants suggest that the magmatic cycles were fed by several different magma reservoirs at different levels in the crust, rather than a single large reservoir.

Poster

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

The lithium isotopic composition of Late Cretaceous seawater: Implications for a correlation between weathering, carbon cycle and climate

Sandra J. Huber^{1,2}, Vanessa Schlidt^{1,2}, Jorit F. Kniest^{1,2}, Linus Lenk¹, H.-Michael Seitz^{1,2}, Jacek Raddatz^{1,2}, Horst R. Marschall^{1,2}, Silke Voigt^{1,2}

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The cause and feedback mechanisms of Late Cretaceous climate cooling are not well understood to date. To evaluate the role of silicate weathering as a thermostat and sink for atmospheric CO₂, we generated a lithium isotopic record ($\delta^7\text{Li}$) of Late Cretaceous seawater using chalk as an archive.

The Late Cretaceous $\delta^7\text{Li}$ record (91–66 Ma) shows an overall increase by 3.5%. Superimposed, five positive $\delta^7\text{Li}$ events occur during this period, which mostly correlate with $\delta^{13}\text{C}$ anomalies in the late Santonian, latest Campanian to earliest Maastrichtian and mid-Maastrichtian. In contrast, the $\delta^7\text{Li}$ event in the mid-Campanian shows no correlation with a $\delta^{13}\text{C}$ anomaly. The overall increase in $\delta^7\text{Li}$ correlates positively with the increase in seawater $^{87}\text{Sr}/^{86}\text{Sr}$. The general shape of the $\delta^7\text{Li}$ curve resembles the evolution of deep-sea temperatures based on benthic foraminiferal $\delta^{18}\text{O}$ suggesting a link among the weathering flux, lowered atmospheric CO₂ concentrations and climate cooling. The apparent covariation between $\delta^7\text{Li}$ and $\delta^{18}\text{O}$ indicates a strong connection between the congruency of silicate weathering and climate change on a multi-million-year time scale. In contrast, the five positive $\delta^7\text{Li}$ excursions correspond to periods of decreased rates of change in seawater $^{87}\text{Sr}/^{86}\text{Sr}$, typical for a decelerated continental weathering flux.

Here, we suggest that enhanced clay mineral formation in lowlands, increasingly exposed during sea level falls, promoted more incongruent weathering and strong lithium isotope fractionation. The relation between the positive $\delta^7\text{Li}$ and $\delta^{13}\text{C}$ events appears to be more complex and requires further investigation through box models.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Belemnites as an archive for the seawater lithium isotope composition: Evidence in the belemnite rostrum for large vital effects

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The lithium isotopic composition of the seawater ($\delta^7\text{Li}$) can be used as a proxy for silicate weathering. So far, different archives like planktonic foraminifera, brachiopods, mollusks and bulk carbonates have been tested. To date only one study has investigated the $\delta^7\text{Li}$ in belemnite rostra.

A Late Cretaceous belemnite (*Belemnitella mucronata*) from the Campanian succession of Lägerdorf, Germany was investigated. The lithium isotopic composition of the chalk matrix surrounding the specimen has a $\delta^7\text{Li}$ value of $+21.9 \pm 0.06\text{‰}$ (2σ). The section across the belemnite rostrum displays signs of diagenetic alteration in its center and at the outer margin. The bulk belemnite was drilled from the intermediate pristine part of the rostrum – the domain that is considered least altered. The data analyzed by solution MC ICP-MS (Multi Collector Inductively Coupled Plasma Mass Spectrometry) revealed a $\delta^7\text{Li}$ value of $+36.8 \pm 1.4\text{‰}$ (2σ , $n=2$). We also conducted spatially resolved Li-isotope analyses across the rostrum by laser ablation MC ICP-MS. $\delta^7\text{Li}$ varies between $+20.5$ and $+59.8\text{‰}$ with the highest values in the intermediate pristine part of the rostrum. In contrast, low values were detected in the milky domains, which are considered as altered by diagenesis.

The distinct positive isotopic offset between *B. mucronata* and surrounding chalk ($15\text{--}21\text{‰}$ for bulk solution chemistry data) exceeds the magnitude of modern mollusks, which are also enriched by $2\text{--}8\text{‰}$ relative to the lithium isotopic composition of modern seawater. This positive offset indicates a high influence of vital effects during the biomineralization process of this species.

Poster

Topic: 1.8 Minerals and Mineral Properties

Behavior of chemically zoned acicular mullite fibers annealed at high temperature

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The synthetic analogue of the rare mineral mullite (solid solution ${}^{\text{VI}}\text{Al}_2^{\text{IV}}[\text{Al}_{2+2x}\text{Si}_{2-2x}\text{O}_{10-x}]$) is widely used in ceramics as “3/2-mullite” ($x\sim 0.25$), whereas single crystals grown from melt are “2/1-mullites” ($x\sim 0.4$) [1].

The investigated acicular mullite ceramic consists of single-crystalline fibers with high-Al mullite (M1) in the core and low-Al mullite (M2) in the rim [2,3], appearing as two distinct mullite phases in powder XRD patterns [2]. On annealing the as-prepared sample at 1550°C (24, 96, 192 and 384 h) the two zones gradually merge into one homogeneous phase [2]. Here, we present the details of this merging, investigating cross sections of fibers via TEM.

Observed changes in a) width of the transition zone, b) relative lattice orientations of the two zones and c) lattice parameter a document progressive homogenization of the mullite, which is complete after 384h. Concurrently, we observed Si-rich, round to rectangular amorphous regions, probably from partial melting, most strikingly after 384 h. An increasing amount of Si-rich glass phase with annealing time would explain the overall increase of average Al-content in mullite which we observed in our XRD data [2].

We thank Prof. K.T. Faber (NW University, Evanston, IL/USA) for the samples, and the DFG for funding (Grant FI442/24-1).

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Poster

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Sm-Nd dating of fluorites from the Vergenoeg, Buffalo and Morgenzon 533 KQ deposits, Bushveld Igneous Complex, South Africa: Evidence for late hydrothermal fluorite formation

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We investigated three fluorite deposits associated with the Bushveld Igneous Complex in South Africa for their trace element characteristics (e.g., REE+Th+U): the two major and world-class Vergenoeg and Buffalo deposits, as well as the small Morgenzon deposit. Combined with published and unpublished data from the Vergenoeg deposit (host rock and mineral separates), which yield an age of 2050 ± 17 Ma (MSWD = 0.65), the new host rock and fluorite Sm-Nd isotope data confirms a primary magmatic origin for the Buffalo deposit as well. Whereas the host rock data for Morgenzon plot close to the 2050 Ma isochron, the Morgenzon fluorite data significantly diverge and plot along an errorchron corresponding to an age of 318 ± 59 Ma (MSWD = 7.4). The Morgenzon fluorites are also depleted in the abundances of REE+Th+U by almost a factor 100 compared to the Buffalo fluorites. Cathodoluminescence (CL) imaging reveals complex zoning patterns with a wide range in bluish CL colours for the Morgenzon fluorite. In contrast, fluorite from Buffalo is always very homogeneous (pale bluish CL colour), which indicates a single stage and likely primary magmatic formation process for the latter. Combined trace element and isotope data and CL evidence for the Morgenzon deposit suggest a late hydrothermal fluorite formation unrelated to the Bushveld igneous event.

Lecture*Topic:* 1.2 Methods in Geochemistry and Mineralogy**Insights into triple oxygen isotope variations in Precambrian carbonates from CO₂ – O₂ equilibration****Oliver Jäger¹, Jakub Surma^{2,1}, Fabian Zahnow¹, Katharina Schier³, Michael Bau³, Andreas Pack¹**¹Georg-August-Universität, Germany; ²Earth-Life Science Institute, Tokyo Institute of Technology, Japan; ³Jacobs University, Bremen, Germany

Small mass-dependent variations in ¹⁷O/¹⁶O and ¹⁸O/¹⁶O, expressed as $\Delta^{17}\text{O} (= \ln(\delta^{17}\text{O}+1) - \ln(\delta^{18}\text{O}+1) \cdot \lambda_{\text{ref}})$, in carbonates provide insight into temperature dependent carbonate-water equilibration. Uncertainties between 10-15 per meg are required to distinguish equilibrium conditions and post-depositional alteration of carbonates. Measuring ¹⁷O/¹⁶O with conventional methods is hampered by isobaric interferences of the higher abundant ¹³C¹⁶O₂. A new methodical approach based on equilibration of sample CO₂ and O₂ over hot platinum was developed, demonstrating external reproducibility of $\Delta^{17}\text{O}_{\text{CO}_2}$ smaller than 10 per meg [1]. Here we present a modified experimental setup of this method. We developed an automatized procedure to minimize external error sources and reproduce experimental conditions. We show that $\Delta^{17}\text{O}$ of the equilibrated O₂ is affected by a mass independent fractionation (MIF) during isotope exchange. The MIF is induced by a strong thermal gradient in the reactor and the order of magnitude is coupled to the equilibration temperature. We analyzed a set of platform carbonates from the Proterozoic-Archean transition from the Transvaal Supergroup, South Africa to examine the origin of the secular shift of $\delta^{18}\text{O}$ in carbonates towards higher values from the Archean to today. The carbonates plot below the curve defined by calcite in equilibrium with seawater, which neither supports hot oceans nor lower $\delta^{18}\text{O}$ of Precambrian seawater. Modelling diagenetic alteration suggests, that the pristine oxygen isotope composition of carbonates may have been modified after deposition or that the carbonates may last re-equilibrated with (sea)water with slightly higher $\delta^{18}\text{O}$ and lower $\Delta^{17}\text{O}$.

[1] Mahata et al. (2013), Anal. Chem., 85, 6894-6901

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

How greenstone belts deform: Tectonic style along the southern margin of the Barberton Greenstone Belt, Eswatini

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The Barberton Greenstone Belt (BGB) and many other orogenic belts in cratonic basements have been classically thought to be large, first-order synclinal structures, thus supporting vertically-dominated models of early Earth lithosphere formation. We here argue for a late phase of BGB deformation involving significant horizontal shortening along the long, polymetamorphosed linear southern margin of the BGB with the gneisses of the Ancient Gneiss Complex of central Eswatini by investigating the Ntaba Mhlope Syncline, a small, steeply doubly (inwardly) plunging, highly strained syncline of Moodies Group (ca. 3.21 Ga) strata, about 3 km long and 0.6 km wide. This structure represents the lone remnant of Moodies Group strata in the central segment of the southern BGB. Its subvertically dipping, upper-greenschist-facies-metamorphosed strata consist of (from base to top) conglomerates, quartzose sandstones and subordinate shales and siltstones a few hundred m thick. Age spectra of detrital zircons from sandstones suggest a depositional age of ca. 3232±36 (2σ) Ma, similar to Moodies depositional ages elsewhere in the BGB. Deformation of conglomerate clasts is markedly constrictional; plunge is uniform and steep throughout the tight syncline, suggesting that strain followed folding. Geologic setting, fold style and prolate strain suggest that deformation occurred during substantial north-northwestward-directed shortening by folding and thrusting in high-strain zones at elevated temperatures, perpendicular to the BGB margin. These findings are comparable with similar deformation patterns along strike in the Malolotsha region further south but contrast with observations of regionally dominant oblate strain along the entire northwestern margin of the BGB.

Poster

Topic: 1.7 Experimental Petrology and Geochemistry

Experimental investigation of tuite stability in peridotite bulk and its role in the Earth's phosphorus cycle

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Ca-phosphates play a vital role in the global phosphorus, halogen and incompatible trace element cycle. During subduction, apatite, which is the most abundant terrestrial Ca-phosphate, breaks down to form tuite [$\gamma\text{-Ca}_3(\text{PO}_4)_2$] at depths of ~220-270 km. Whereas previous studies have already explored the stability and phase relations of Ca-phosphates and their capacity to carry phosphorus and incompatible trace elements to depths of approx. 550 km, no such data are available so far for the P-T range corresponding to the upper-to-lower mantle transition.

In this study, multi-anvil experiments were performed at 15 to 25 GPa and 1600 to 2000 °C using a spinel lherzolite doped with 3wt% synthetic $\beta\text{-Ca}_3(\text{PO}_4)_2$, selected incompatible trace elements and halogens as starting material. In this bulk tuite breaks down at or near the solidus between 1750 and 1800°C at 15 GPa and between 1600 and 1700°C at 25 GPa, yielding a negative slope of the tuite-out reaction(s). This indicates that tuite can be stable to depths of at least ~750 km in subduction zone P-T regimes and along the ACMA, allowing a potential stability in convecting mantle. Phases coexisting with tuite include bridgmanite, Ca-perovskite, majoritic garnet, ringwoodite, forsterite, clinoenstatite, ferropericlase, and melt. In the absence of tuite at 20 GPa, the major phosphorus carriers are melt and majoritic garnet. Beyond the stability of majoritic garnet and tuite, and for a bulk P content of 5800 $\mu\text{g/g}$, Ca-perovskite and bridgmanite are the major mineral hosts for phosphorus that can incorporate ~1400 $\mu\text{g/g}$ and ~87-131 $\mu\text{g/g}$, respectively.

Lecture

Topic: 4.3 The role of fluids in metamorphic and metasomatic reactions

Metasomatic Overprint by Carbonatite derived CaO in Kaiserstuhl Phonolites, Germany

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Carbonatites and silica-undersaturated rocks are closely related and occur in rift-related volcanic provinces. The proposed driving mechanism linking both magmatic series is that they share a common source which is driven by fractionation into a two-liquid solvus (Brooker & Kjarsgaard, JPet 52:1281-1305). Carbonatites and phonolites are, in consequence, closely related to each other. However, the interaction of both magmatic series after their separation and the role fluids play in this process are not fully understood. One location characterized by these types of rocks is the Kaiserstuhl volcanic complex (KVC) in Germany.

For the KVC we use Sr-Nd-Hf isotope, major and trace element data from phonolites, wollastonite-phonolites, carbonaceous sedimentary rocks and carbonatites to disentangle the possible effect of crustal contamination from primary mantle signatures. We found that the magmatic products show an overall EM-like signature. Moreover, the phonolites are enriched in CaO reaching up to 9.5 wt.% in the wollastonite-bearing phonolite. Previously it was thought that wollastonite formed due to contamination by carbonaceous sedimentary rocks, but this would not lead to EM-like signatures. This suggests that phonolitic melt became contaminated by carbonatitic melt, leading to a decarbonization reaction that caused the CaO enrichment. We therefore show that metasomatic processes can lead to mineral assemblages that are otherwise typical for Skarns. Furthermore, the role of metasomatic overprint could have been overlooked in other carbonatite-related volcanic provinces as well. This emphasizes the influence of melt and fluid phases on the formation of carbonatitic-related volcanic provinces, providing a cogenetic link between both magmatic series.

Lecture

Topic: 10.1 Geoscience Communication and Education

Geoscience Education for the Young Generation: mileko - The Mineralogical Science Kit

Bastian Joachim-Mrosko¹, Maria Mrosko², Junge Malte³, Seybold Lina⁴, Hecht Lutz⁵, Mock Dominik⁶, Fischer Lennart A.⁷, Stalder Roland¹, Simon Gilla⁸

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Geosciences only play a minor role in today's German and Austrian school curricula, although being strongly related to important topics such as climate change or the sustainability of resources. The Mineralogical Science Kit (Mineralogischer Lehrkoffer "mileko") aims at bringing back geoscientific and mineralogical contents into STEAM-fields (science, technology, engineering, art, mathematics) by linking mineralogy to regular teaching subjects.

In 5 different modules, pupils can not only discover the world of rocks and minerals but also get an understanding of important principles and processes such as redox reactions by extracting copper from ore (chemistry), the density of rocks that can be linked to the structure of the Earth's interior (physics, geography), or how the inner structure of materials affects their outer appearance by exploring natural crystalline bodies and their geometry (chemistry, mathematics). Since 2014, about 650 boxes were produced and sent to schools and museums all over Germany.

This year marks the start of a new format in the "mileko" portfolio, which is the development of an online accessible video channel. This new digital format aims to expand the applicability of the Mineralogical Science Kit by making geoscientific contents directly accessible for a broad young target group, which not only complements former activities but will also allow us to attract the attention of a wider audience. In combination with activities such as workshops and school visits, we hope to enhance discussions between children, teachers and scientific experts resulting in knowledge transfer from the scientific community to the public.

Lecture

Topic: 2.3 Uniformitarianism of crustal processes

Archaean greenstone belts of the Singhbhum Craton, India—windows into early Earth

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Archaean greenstone belts offer the opportunity to study the dynamic conditions on early Earth. The Singhbhum Craton of India hosts several volcano-sedimentary greenstone sequences that preserve Archaean rocks locally exceeding 3.5 Ga. We present a compilation of field, petrographic, geochemical, and geochronological results from the following greenstone sequences: 1) Daitari Greenstone Belt, 2) Gorumahisani Greenstone Belt, and 3) Nausahi Greenstone Belt. Major similarities include the association of mafic-ultramafic sequences, felsic volcanic rocks, and sedimentary units. These greenstone belts host altered carbonated/silicified volcanic rocks and cherts; an assemblage typical for Palaeoarchaeal successions. The cherts include bedded orthochemical sediments, silicified shales, silicified volcanoclastic rocks, and hydrothermally derived vein cherts. In all greenstone belts, the cherts preserve carbonaceous matter, which provides evidence for microbial life as old as c. 3.5 Ga ago. Raman thermometry of carbonaceous matter indicates greenschist facies grade of metamorphism. The Daitari and Gorumahisani belts host economic ore deposits (e.g., iron and minor gold respectively). In contrast, despite their akin lithological assemblages the Nausahi belt is yet to be prospected for such economic deposits. Therefore, understanding the geologic evolution of these greenstone belts will be crucial to evaluate early Earth processes and related mineralization from the Archaean record of the Singhbhum Craton.

Lecture

Topic: 2.2 From dust to planets

Petrographic and geochemical analysis of meteorite NWA 12547 with inverse zoned chondrules

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The best researched planetary system is our solar system. But even here we know very little about chemistry and composition of the bodies. In order to really explore and understand them, it is helpful to take a close look at the formation and thus the origin of everything in our solar system. Some meteorites, so called chondrites, were formed during this time and give us insights into the processes. They are therefore an important tool to understand the formation of all other bodies. A chondrite is mainly made out of chondrules which are millimeter big silicate pellets with different appearance.

One of this chondrites is the Meteorite NWA 12547. It is an ordinary L3 chondrite and is formed out of three different fragments. One consists of so-called inverse zoned chondrules. Inverse zoned chondrules are chondrules that have a pyroxene core and are surrounded by an olivine shell. This not very known silicate pellets with an inverted crystallization row is believed to have arisen from rapid cooling first which formed the pyroxene core, and then subsequent heating resulting in an olivine shell. The second fragment consists mainly of porphyritic and bar-shaped chondrules. This piece was cooled slowly in a first phase and rapidly thereafter, forming first idiomorphic olivines and then small pyroxene needles in the glassy feldspar matrix. The last piece is a residual melt, with a glassy matrix which was finally cooled at about 1450 °C.

Poster

Topic: 10.1 Geoscience Communication and Education

Geoscientific education in schools: Four workshops to encourage children to learn more about rocks and minerals

Malte Junge^{1,2}, Melanie Kaliwoda^{1,2}, Omar Gianola¹, Julia Holzmueller¹, Felix Hentschel¹, Wolfgang W. Schmahl^{1,2}

¹Mineralogical State Collection Munich (SNSB-MSM), Germany; ²University Munich, Crystallography, Germany

The current global pandemic has hit children and young people particularly hard. The online lessons brought a lot of distance and some children lost the fun of school education. In the Museum Mineralogia Munich there are now special workshops so that children and young people can enjoy school again. Among other things, the participants learn why volcanoes erupt, what we can learn from meteorites, how rocks are formed, but also what minerals and rocks have to do with our smartphones. The courses are designed in such a way that children and teenager can do as much practical work as possible. Microscopes are used, rocks and minerals are determined, crystal models are recreated with 3D pens or handicraft sheets and the rock cycle is additionally explained by a gravel card game. A key goal is to create enthusiasm for geosciences and other STEM subjects such as biology, chemistry, physics and mathematics. The courses are designed for two major age groups (8 to 12 years) and (above 13 years). Additionally, courses are adapted to the pre-knowledge and interest of the children. The four described workshops are organized as individual and consecutive courses to ensure a better connection between children and the museum. Additional programs offer longer-term projects where children can design their own exhibitions. The courses are financially supported by the Federal Ministry of Education and Research and take place in the Museum Mineralogia Munich.

Lecture

Topic: 10.3 Geoscientific museums and collections in the area of responsibility between science and public relations

Raw materials need and supply presented in exhibitions and workshops of the Museum Mineralogia Munich

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The need of raw materials for our society and our everyday life steadily increased during the last decades. In particular, the technological development demands for a secure supply as well as increasingly more metals. Therefore, a secured supply of raw materials is crucial for the economy worldwide. The supply risks of metals due to limited availability from only few countries became a political debate during the last decade, .i.e. defining the term critical raw materials. One essential aspect of critical raw materials are mineralogical and geoscientific questions as minerals host the valuable metals that we need for our technology. Therefore, also a mineralogical museum should deal with education for children, teenagers and adults of mineral raw materials and there need for our everyday life. The important link is to demonstrate them what kind of metals are inside in a smartphone. Looking at a world map and explaining where the minerals in our smartphones come from and what are the mineralogical and geological reasons for the enrichment of certain minerals in specific areas worldwide can be explained during workshops. This also allows the link to political consideration by discussion how small scale mining of minerals is used to finance conflicts such as in the Democratic Republic of Congo. Additionally, regional raw materials are important to be included in this discussion. The aim is to increase the awareness of the large variety of metals installed in the technical development combined with environmental concerns.

Lecture

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Trace element mobilization in the monzogranite of Soultz-sous-Forêts

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In the context of combined raw material and energy production, public attention focusses increasingly on geothermal power plants. The Upper Rhine Graben (URG) in southwest Germany and eastern France is of special interest as it represents a possible geothermal reservoir with raw material potential.

From around 1300 different oil as well as geothermal wells and thermal water wells, knowledge can be acquired about the reservoir rocks of different depths. In the URG, the Triassic sandstones and Variscan crystalline rocks have the greatest geothermal potential. Furthermore, from these wells, the geochemical properties of the fluids can be studied and related to the reservoir rocks.

Up to now, only limited knowledge is available about the recent fluid-rock interactions releasing trace elements to the fluid. There are several hypotheses about the reaction kinetics and transport mechanisms of the elements and water. One of the hypotheses is that trace elements are released by the alteration of feldspars and mica of the Variscan crystalline basement. To corroborate the hypothesis, initial mineralogical and geochemical analyses were carried out on partially altered monzogranite core samples which were extracted from different depths while constructing the geothermal power plant in Soultz-sous-Forêts (France).

The first results of geochemical and mineralogical analysis revealed a need to concretize the hypothesis. Based on the direct comparison between the unaltered mineral and the alteration product, it was determined that trace elements are released but can also be fixed. Thus, the question arises whether these alteration processes lead to the present fluid composition.

Lecture*Topic:* 1.8 Minerals and Mineral Properties**Structural investigations on iron-ore sinter phases – crystallography meets applied mineralogy****Volker Kahlenberg, Hannes Krüger**

University of Innsbruck, Austria

Sinter plants are an integral part for the preparation of iron ores for the blast furnace process. In a series of complex reactions, semi-molten, centimeter-sized aggregates are formed containing ore particles cemented by a matrix of Ca-rich ferrites that contain some silica and alumina. For these compounds, the acronym SFCA (**S**ilico-**F**errites of **C**alcium and **A**luminum) was coined. The SFCA phases with general composition $A_{14+6n}O_{20+8n}$ (A: Ca, Mg, Fe^{2+} , Fe^{3+} , Al^{3+} , Si^{4+}) act as the binder that keeps the sinters intact in order to withstand the loads in a blast furnace.

Depending on the value of n in the chemical formula, four different SFCA-phases can be distinguished forming a polysomatic series. They can be described with a modular approach involving the stacking sequence of "P" and "S" modules that can be imagined as being cut from the well-known pyroxene and spinel structure-types. The representatives with $n = 0$ ($A_{14}O_{20}$) are related to the sapphirine supergroup of minerals.

Even though the SFCAs are critical for the production of iron-ore sinters, it is surprising that there are still many open questions regarding their composition, atomic structure, thermochemistry and stability. For any target-oriented improvement and optimization of ore-sintering as well as thermodynamic modeling of the sinters, a much more detailed understanding of these fundamental solid-state properties of the SFCAs is essential. The present contribution provides - for the first time - a detailed crystallographic analysis on the impact of chemical variations on these compounds that are of relevance for the field of applied mineralogy.

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

Raman spectroscopy as a powerful tool for estimating the chromium to aluminum content in a range of different chromites

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Raman spectroscopy has been applied to study a range of chromites with variable chromium to aluminum to iron contents to determine conclusions about possible correlations between the chromium concentration and the position of the main Raman peaks within this mineral. It was found that a negative correlation exists between the chromium number, calculated from electron microprobe data, and the Raman peak number. Chromite grains with high chromium number show a low Raman peak, whereas samples with low chromium numbers show a higher Raman peak. Therefore, it was possible to infer a relationship between the mineral composition and Raman bands for this type of mineral. The measurements have clearly shown that it is possible to draw conclusions about the chromium content of the mineral based on the Raman peak alone. This shows that in simple chemical compositions, such as in chromites and olivines, the peak positions can provide initial information about the compositions of the minerals. Thus, it is possible to use Raman spectroscopy as a simple and fast investigation method, which we could proof on very different materials. This outcome supports a possible application of portable Raman devices on Earth or in space, i.e. for asteroids and/or other planets. Raman spectroscopy has more over proven to be a quick and powerful method to identify minerals and a lot of other materials investigated in the mineralogical state collection Munich. Therefore, we have also created a new in house Raman database (MSM_RMD = Mineralogical-State-Collection-Munich_Raman-Mineral-Database) for minerals, plastic, ore minerals and other materials.

Poster

Topic: 10.3 Geoscientific museums and collections in the area of responsibility between science and public relations

Sahara Dust Event in Central Europe in March 2022: over 100 micron sized particles!

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In late winter 2022 massive Saharan dust clouds have moved from S Algeria / Morocco over Spain and France to Central Europe and one of these reached S Germany at march 15th afternoon. During late winter times such Sahara dust events can be observed in central Europe quite regularly. This time, however, historic amounts of desert sand have been transported, i.e. huge amounts of reddish/orange dusts over part of the Alps and S Germany. The "orange" cloud was accompanied by heavy rainfalls which washed out the reddish Fe-rich Sahara dust during the following hours. A series of Sahara dust samples could be collected with the help of special collectors at 15th of march S of Munich, so that any contamination could be avoided. Within the first 2-3 hours mainly coarse grained material was washed out, afterwards the fine grained dusts were deposited and collected. A large range of particle sizes and morphologies could be detected, maximum sizes reached over 100 microns. Taking into account the long-range transport (more than 2500 km from S Algeria / Morocco via Spain/Portugal and France to Central Europe) one would expect only much finer dusts [3, 4]. Raman spectroscopy revealed quartz, Ti-oxides (anatase) and feldspar as the dominating phases (fig. 1b). Further experiments by X-ray diffraction and SEM are in preparation in order to extend our knowledge concerning the Sahara dusts of the march 2022 event.

Poster*Topic:* 1.5 Fundamentals and applied aspects of nucleation and crystal growth**Crystallization and nucleation study of transition metal phosphates: M-phosphate octahydrate and M-struvite****Stephanos Karafiludis^{1,2}, Ana Guilherme Buzanich¹, Franziska Emmerling^{1,2}, Tomasz Maciej Stawski¹**¹BAM Berlin (Bundesanstalt für Materialforschung und -prüfung), Germany; ²Humboldt Universität zu Berlin, Germany

Industrial and agricultural waste streams (waste waters, sludges, tailings etc.) which contain high concentrations of NH_4^+ , PO_4^{3-} and transition metals are environmentally harmful and toxic pollutants. Typically, separate pathways have been considered to extract hazardous and transition metals or phosphate as critical raw materials, independently from each other. Here, we report the synthesis routes for transition metal phosphate (TMP) compounds ($\text{M}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$, $\text{NH}_4\text{MPO}_4 \cdot 6\text{H}_2\text{O}$, $\text{M} = \text{Ni}^{2+}$, Co^{2+} arupite/pakhomovsykite and Ni-/Co-struvite), which allow for P, ammonia and metal co-precipitation. The precipitation of arupite/pakhomovsykite and M-struvite from industrial waste waters could be a promising P-recovery route. Through adjusting the reaction conditions, the stability, crystallite size and morphology of the as-obtained TMP could be controlled. Detailed investigations of the precipitation process using ex- and in-situ techniques provided new insights into their non-classical crystallization mechanism/crystal engineering of these materials. These TMPs involve transitional colloidal nanophases which subsequently aggregate and condense to final crystals after extended reaction times. However, the reaction kinetics of the formation of a final crystalline product vary significantly depending on the metal cation involved in the precipitation process. Ni-struvite is stable in a wide reactant concentration range and at different metal/phosphorus (M/P)-ratios, whereas Co tends to form Co-struvite and/or Co-phosphate octahydrate depending on the (M/P)-ratio. The observed various degree of stability could be linked to the octahedral metal coordination environment. The achieved level of control over the precipitates, is highly desirable for 3d- and P-recovery methods. Under this paradigm, the crystals can be potentially upcycled as precursor materials for (electro)catalytical applications.

Lecture*Topic:* 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment**In-situ Sb isotope variations of the orogenic Sb-Au deposits at Pezinok (Slovakia)****Andreas B. Kaufmann^{1,2}, Marina Lazarov², Stefan Weyer², Juraj Majzlan¹**¹Institute of Geosciences, Friedrich Schiller University Jena, Germany; ²Institute of Mineralogy, Leibniz University Hannover, Germany

Orogenic Sb-Au ore bodies of deposits near Pezinok (Malé Karpaty Mts., Slovakia) are hosted in metamorphosed black shales in amphibolites. The ore bodies contain parageneses with various Sb sulfides, sulfoxides, and oxides. Given the variable mineral assemblages, the deposit serves as a model to understand the behaviour of Sb isotopes from initially reducing to an evolving oxidizing system at μm -scales. Here we determined the *stable* isotope composition ($\delta^{123}\text{Sb}$) of antimony minerals *in-situ* using a deep UV-femtosecond laser ablation system coupled with MC-ICP-MS [1]. The precision of analyses was $<0.1\text{‰}$ and all analysis were reported relative to NIST 3102a.

Polished sections, containing assemblages of successively precipitated antimony minerals, show an isotopic range from -0.2 to $+0.8\text{‰}$. Stibnite, which is the most abundant mineral, shows an isotopic variation of around 0.35‰ (median = -0.2‰) that is generally lighter than $\delta^{123}\text{Sb}$ of kermesite (0.1‰), valentinite-senarmontite ($\sim 0.5\text{‰}$), and schafarzikite ($\sim 0.8\text{‰}$). This isotopic relationship is consistent with textural and thermodynamic observations, indicating earlier formation of stibnite, followed by kermesite, valentinite-senarmontite, and schafarzikite formation during decreasing temperatures and increasing $f\text{O}_2$. The large isotopic variation within and between different minerals can be explained by a Rayleigh fractionation model with enrichment of ^{123}Sb in the residual fluid and in successively later formed minerals. Therefore, the results of this study suggest that *in-situ* $\delta^{123}\text{Sb}$ values could be a promising tool to understand the evolution of orogenic Sb-Au deposits in space and time.

[1] Kaufmann et al. (2021), *JAAS*, **36**, 1554-1567.

Ramdohr-Poster

Topic: 6.3 Fractionation of metal(loid) stable isotopes during low-temperature Earth surface processes

Stable antimony isotope fractionation during surface alteration of primary ores

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The orogenic Sb-Au deposits near Pezinok, located in the Malé Karpaty Mts. (Slovakia), were mined until 1992. Ores were extracted by flotation with low recovery rates, resulting in mining waste with large amounts of Sb. Exposed to surface conditions primary Sb(III) minerals got oxidized and formed secondary Sb(V) phases. This change in Sb oxidation state is associated with Sb isotope fractionation indicating oxidative weathering conditions during their formation. $\delta^{123}\text{Sb}$ values of weathering products and precursor minerals were determined *in-situ* using a deep UV-femtosecond laser ablation system coupled with MC-ICP-MS and are reported relative to NIST 3102a using a protocol as described in [1].

Supergene products occur in two forms at Pezinok with different precipitation kinetics. Brandholzite ($\text{MgSb}_2^{5+}(\text{OH})_{12}\cdot 6\text{H}_2\text{O}$), the occurrence of which is restricted to samples with massive stibnite, formed large crystals with abundant stibnite inclusions. Its textural close association with stibnite and their similar $\delta^{123}\text{Sb}$ (median = 0.31 ‰_{stibnite} vs. 0.25 ‰_{brandholzite}) indicates quantitative dissolution of stibnite and quantitative, likely rapid, precipitation as brandholzite. Contrary, tripuhyite ($\text{FeSb}^{5+}\text{O}_4$), that does not show a close association with potential precursors, displays a ~0.8 ‰ isotopic range and likely formed over decades in the mine tailings. This is consistent with Rayleigh fractionation in an open system, which depends strongly on (1) amount of leached stibnite and (2) redox changes during transport and formation. Thus, $\delta^{123}\text{Sb}$ could be used as tool to understand the evolution of antimony deposits from initially reduced to more oxidizing supergene conditions.

[1] Kaufmann et al. (2021), *JAAS*, **36**, 1554-1567.

Lecture*Topic:* 4.1 Magmas and Fluids in the Crust**Element partitioning and selective mobilisation at the magmatic-hydrothermal transition in shallow igneous systems****Anne Kaufmann, Thomas Pettke**

Universität Bern, Switzerland

Fluid-melt partition coefficients (K_D) quantify the distribution of elements at the magmatic-hydrothermal transition and describe the potential for selective mobilisation and transport of elements from a solidifying magma into the overlying crust, where – in case of metals – it can ultimately result in the formation of magmatic-hydrothermal ore deposits. For shallow, subvolcanic intrusions, the crystallising magma typically reaches fluid saturation at conditions falling into the 2-phase field of the H₂O-NaCl system. In this case, two separate fluid phases, low-density vapour and higher density, saline brine are exsolved.

We present brine-melt, vapour-melt, and vapour-brine partition coefficients for over 30 elements, based on LA-ICP-MS individual fluid and melt inclusion measurements from coexisting assemblages in miarolitic quartz from the Torres del Paine intrusive complex in Chilean Patagonia. Calculated $K_D(\text{brine-melt})$ span almost 6 orders of magnitude between 0.001 and ≤ 600 ; and are highest for Cl-complexing fluid mobile elements such as Pb, Zn, and Ag. In comparison, $K_D(\text{vapour-melt})$ are more moderate with values between 1 – 100 for all fluid-mobile elements.

Combining these partitioning data with estimated amounts of vapour and brine exsolving at the magmatic-hydrothermal transition, we can project the relative amounts of a given element that are transferred into low-density vapour and higher density brine. For typical magmatic-hydrothermal systems in the upper crust, amounts of exsolved brine are significantly lower than for vapour. This counterbalances the commonly stronger partitioning of fluid-mobile elements into brine, and confirms that both fluid phases are relevant for mobilising and transporting elements in subvolcanic magmatic-hydrothermal systems.

Lecture

Topic: 4.5 Tectonic Systems (TSK Open Session)

Tectonic history of Eoalpine high-pressure rocks – new results and open questions

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The Eoalpine high pressure (HP) belt is part of the Austroalpine basement and reached eclogite facies conditions at 100 to 90 Ma during the Cretaceous Alpine orogenic cycle. It extends over 350 km from the Texel Complex in the west over the Saualpe and Koralpe units to the Pohorje Mountains in the east. While HP to ultra HP conditions are well established, there is still debate on the tectonic history of these rocks. Early studies suggest a continuous subduction along the suture of the Meliata ocean. Other studies suggest a younger intra-continental subduction zone, which formed along a pre-existing weakness caused by Permian rifting. Also, the exhumation mechanisms of these rocks remain unclear. Exhumation through an extrusion wedge has been suggested for the rocks of the Saualpe. The contact toward the hanging wall is interpreted as a low-angle normal fault active during extrusion of the HP rocks. Based on crystallographic preferred orientation (CPO) data, exhumation in an extensional regime along a low angle detachment fault was proposed for the Koralpe. Slab extraction has been proposed for both the Koralpe and the Pohorje units, based on pseudosection modeling, which suggests a common exhumation path for the HP units with their hanging wall starting at 1.0 GPa. We will present new CPO data of both metabasalts and the surrounding gneiss matrix from the Koralpe as well as the Pohorje mountains, which will shed some light on the deformation mechanisms active during exhumation and on the overall tectonic history of these rocks.

Lecture

Topic: 11.3 Young Scientist Session

Organic geochemical data of higher plant coals from Svalbard and Northeast Greenland reveal implications for a connected Paleogene setting

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The organic geochemistry of Paleogene coals from central Spitsbergen (Longyearbyen and Grumantbyen) and northeast Greenland (Thyra Ø Island and Kronprins Christian Land), which were sampled during a BGR expedition in 2018, was studied using Rock-Eval and gas chromatography-mass spectrometry.

Rock-Eval data and biomarker distributions of the coals (e.g. hopanoids and hopanoic acids) demonstrate a low coal rank for both, but a lower thermal maturity of coals from Greenland compared to those from Svalbard. The generally high abundance of hopanoids implies a strong bacterial reworking of the organic matter, whereas sulphur occurrences indicate a marine influence after organic matter deposition. A great variety of higher plant biomarkers was detected in all coals. Distinctive compounds recorded in the coals are aliphatic and aromatic diterpenoids as well as partly aromatised picones, indicating strong input of conifers and angiosperms. The oxicity of the paleo-swamps was determined with pristane and phytane based ratios: Tentatively organic matter was deposited in a fluvio-deltaic setting at both sites.

This study provides a detailed geochemical investigation of so far understudied coals from northeast Greenland. Moreover, it aims to enhance our understanding of formerly connected Paleogene settings from Spitsbergen and Greenland in terms of their paleoecology, primary input into coal swamps and individual thermal history. Our data also give insights into an Arctic environment that existed at comparably high latitudes as today, but at times close to the Paleocene-Eocene Thermal Maximum (PETM), where it supported the development of extensive swamps and forests.

Poster

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

Phosphate inhibition of schwertmannite nucleation

Helen Elizabeth King, Sergej Seepma, Mariette Wolthers

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The iron(III) phosphate mineral schwertmannite has shown potential for the removal of oxyanions such as phosphate and arsenate through their adsorption [1,2] and incorporation into the schwertmannite structure [3]. Here we have used dynamic light scattering (DLS) to explore the inhibitory effect of mM concentrations of phosphate on the nucleation dynamics of schwertmannite at different temperatures. Our experiments show that potential prenucleation clusters are present in the solutions prior to nucleation of schwertmannite. In the presence of phosphate these become increasingly stabilized and in long-term experiments are observed to grow slowly. Nucleation of schwertmannite was determined as a change in the system behavior, where a sudden increase in the size of the scattering particles was observed. After nucleation, particle growth was characterized by a much faster rate until the particles began to settle from the solution. Both the growth rate after nucleation and the induction time increased with increasing phosphate concentration, but, were even more retarded by decreasing temperature. Phosphate likely alters the system dynamics through direct interactions with the iron(III) as evident even at the ion pair level in UV-Vis spectroscopy measurements and the incorporation of phosphate into the schwertmannite structure based on X-ray diffraction analysis.

References

1. Eskandarpour et al. 2007 ISIJ International 47, pp. 563.
2. Burton et al. Environmental Science and Technology, 43, 9202.
3. Regenspurg & Peiffer 2005 Applied Geochemistry, 20, pp. 1226.

Lecture

Topic: 8.1 Geosciences and Waste Management

High resolution LA-ICP-MS mapping for the determination of partition coefficients using the example of natural barite

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In deep geological repository systems, containers for highly radioactive waste may encounter groundwater, which ultimately leads to the release of radionuclides. For the exploration of new atomic waste repositories, the retention of these radionuclides in hydrothermally grown barite and calcite has drawn much attention recently. Here, partition coefficients are important parameters as they are helpful to evaluate the immobilization potential. To derive meaningful partition coefficients, only parts of the crystals in equilibrium with their host fluid should be considered. Differences in partition coefficients between synthetic and natural calcite have been observed and might at least partially stem from such analytical complications. This study presents a method which combines both, the advantages of visualizing growth structures at the μm scale and element sensitivity down to the ppm level via LA-ICP-MS. Objects of investigation are natural barites from a borehole in the Äspö Hard Rock Laboratory, Sweden, that have been sampled together with their host fluid. High-resolution mappings with a spot size of $2\ \mu\text{m}$ allow us to define discrete growth zones and calculate equilibrium partition coefficients based on pixel clusters that represent the latest crystallization events. Additional LA-ICP-MS spot analyses substantiate the lower error values of our method and provide partition coefficients for twelve elements. La and Sr are assumed to behave like radionuclides, due to similar chemical properties. Preliminary barite partition coefficients for La and Sr are 3-4 orders of magnitude below calcite values of the same sampling location, indicating a much lower immobilization potential of barite compared to calcite.

Lecture*Topic:* 1.5 Fundamentals and applied aspects of nucleation and crystal growth**Additive-controlled synthesis of single crystalline gold nanoparticles****Felizitas Kirner, Elena V. Sturm**

Ludwig-Maximilians-Universität München, Germany

Nowadays, applications of nanomaterials increasingly demand for monodisperse nanoparticles (NPs), since their defined properties form the basis for a wide range of applications. Gold NPs are of special interest due to their fascinating optical properties related to localized surface plasmons. This plasmonic behavior is highly responsive to extrinsic factors (physical-chemical environment, temperature, interactions of particles, stabilizing agent, etc.) and their morphology (size, shape, quality of surface). We present a three-step seed mediated synthesis for highly monodisperse single crystalline Au NPs stabilized by hexadecylpyridinium chloride (CPC) in variable sizes (24-90 nm) with an adjustable ratio of the cubic and octahedral facets.^[1] This synthesis thus circumvents the common reproducibility drawbacks of CTAB-dependent syntheses.^[2] The effect of the additive KBr and reducing agent ascorbic acid on shape and growth kinetics was systematically investigated and an explanation for the switching of the Au NPs morphology from cubic to octahedral is provided. The plasmonic response of individual particles and their assemblies is demonstrated using spatially resolved EELS to show the optical behavior of the particles, which is far superior to that of lithographically fabricated Au nanostructures.^[3] These particles may then be used to assemble mesocrystals. Such superstructures of crystallographically aligned NPs may lead to strong directional and additional novel collective properties that cannot occur in any other structure of the same size range.^[4]

[1] F. Kirner et al., DOI: 10.1039/d0tc01748e.

[2] R. G. Rayavarapu et al., DOI: 10.1021/la100166f.

[3] M. Mayer et al., DOI: 10.1002/anie.201708398.

[4] E. V. Sturm et al., DOI: 10.1039/c6cs00208k.

Lecture

Topic: 1.7 Experimental Petrology and Geochemistry

Experimental constraints on reactive flow in the lunar mantle and high-Ti magma petrogenesis

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Basaltic lunar mare volcanism has erupted a variety of melt compositions that far exceeds that of terrestrial basalts. Most notably, TiO₂ contents of lunar basalts vary by almost two orders of magnitude and can reach up to 18 wt.% in red/black primitive pyroclastic glasses [1]. Such high Ti contents point to a role for ilmenite-bearing cumulates (IBC), which are predicted to form near the end of solidification of the lunar magma ocean [2]. No experimental study investigating the melting of pure IBC or mixtures of IBC and peridotite [e.g., 3] has, however, succeeded in reproducing the composition of high-Ti lunar basalts.

We propose that lunar high-Ti basalts originate as IBC partial melts, but have their composition modified through reactive flow in the lunar mantle. We simulate this process by experimentally reacting an IBC partial melt composition [3] with high-Mg# olivine and orthopyroxene crystals at 1400-1500 °C and 1.5 GPa in a piston cylinder press. This leads to a peritectic reaction where orthopyroxene undergoes dissolution-precipitation to form a more Ca- and Ti-rich rim, in addition to Fe-Mg exchange between IBC melt and minerals. The composition of the reacted melt shifts to lower Mg# and overlaps with that of high-Ti basalts. No growth of ilmenite or clinopyroxene is observed, thus satisfying the condition that high-Ti melts lack these phases at high-pressure multiple saturation.

[1] Delano (1986) *JGR* **87** A171–A181; [2] Ringwood & Kesson (1976) *LPSC Proc.* 1697–1722; [3] van Orman & Grove (2000) *MAPS* **35** 783–794.

Lecture

Topic: 10.3 Geoscientific museums and collections in the area of responsibility between science and public relations

Mineralogical museums are attractive and special places of learning

Dorothee Kleinschrot

Universität Würzburg, Germany

Minerals in beautiful colors and shapes still attract visitors to museums. Whereas in the past it was hobby collectors, today it is also interested people who want to find out more. Dusty showcases filled with systematically arranged minerals are no longer in demand. Current topics from science do, especially if they are related to everyday life. The exhibition about minerals in Smartphones in the Würzburg University Mineralogical Museum attracted a large number of visitors from different age and professional groups. Exhibitions with artists reach a different group of visitors. Accompanying the exhibitions, a museum educational program is offered with original illustrative material and models as well as presentations on current scientific results, prepared in an understandable way. As part of the museum's public relations work, school classes are among the most important visitors. Enthusiastic pupils are multipliers and our future students. The aim is to arouse children's curiosity about science. A visit to the museum serves as an ideal supplement to the curriculum-related lessons at all types of schools. Symmetry operations in the primary school mathematics curriculum can be supplemented very well by symmetry exercises on original crystals and by making crystal models in the museum. At Bavarian secondary schools, the subject of geology is offered as an alternative curriculum in the upper grades. The Mineralogical Museum has been a training partner of these schools for many years. In the teaching-learning laboratory, the students get to know the various geoscientific working methods and identify minerals and rocks accompanied by students.

Lecture

Topic: 6.1 Earth surface processes in extremely water-limited environments

Tracing life in the Atacama Desert by multi-isotope analyses of sulfates

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Calcium sulfates are the dominating salts in soils of the Atacama Desert (Chile) but respective sulfate sources are debated. Various sulfate sources comprise distinct isotopic compositions. To map the spatial distribution of sulfate sources and to identify biological sulfate recycling, we determined $\Delta^{17}\text{O}_{\text{SO}_4}$, $\delta^{18}\text{O}_{\text{SO}_4}$, $\delta^{34}\text{S}_{\text{SO}_4}$, and $^{87}\text{Sr}/^{86}\text{Sr}$ of surface samples from Atacama Desert soils taken along four W-E transects from the Pacific coast to the Pre-Andean Cordillera.

Distinct mass-independent ^{17}O anomalies in sulfates originate from atmospheric oxidation of reduced sulfur species derived from volcanic emissions or dimethyl sulfide (DMS) a biogenic sulfur gas that emits from the ocean. Marine aerosols represent a mixture of marine sulfate and atmospherically oxidized DMS and thus comprise elevated $\Delta^{17}\text{O}_{\text{SO}_4}$. Biological sulfate recycling leads to oxygen isotope exchange with ambient water, resulting in $\Delta^{17}\text{O}_{\text{SO}_4}$ values that converge towards 0‰ and generally increasing $\delta^{18}\text{O}_{\text{SO}_4}$ values because water in the Atacama Desert is highly evaporated. Volcanic and marine sulfate aerosols are effectively distinguished by $\delta^{34}\text{S}_{\text{SO}_4}$. The combination of $\delta^{34}\text{S}_{\text{SO}_4}$ and $^{87}\text{Sr}/^{86}\text{Sr}$ allows to identify dissolution and re-precipitation of sulfate.

Our dataset reveals the distribution of sulfate sources for Atacama Desert soils. Post-depositional bio-alteration processes lead to changes in the isotopic composition allowing to draw conclusions on bio activity and water availability in such hyper-arid environments like the Atacama Desert.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

Improving the Interoperability of Established Geochemical Databases

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Global geochemical datasets are increasingly used to solve ever more complex research questions exploiting sophisticated computational methods. However, standards to guide geochemical data publication and facilitate uniform access to such large datasets are largely lacking. In their absence, the GEOROC database provides access to a curated compilation of igneous and metamorphic rock and mineral compositions from >20,000 publications. GEOROC is also a major contributor to the EarthChem Portal, a single point of access to six independently curated databases with a common data schema.

Whilst providing findable, accessible and reusable data has been GEOROC's mission for 23 years, interoperability between geochemical data systems, let alone with other disciplines, remains difficult. To improve the FAIRness of global geochemical data and ensure it can be harvested by other disciplines (e.g. through the NFDI4Earth programme), the field of digital geochemistry first needs to be further developed and strengthened. In collaboration with EarthChem, our DIGIS project is revising the IT infrastructure of the GEOROC database (data model, vocabularies, etc) to enable greater interoperability between the two data systems. For the long-term success of this effort, international stakeholder engagement as well as support by publishers, funders and the international geochemical societies is crucial. Together with EarthChem and other participants of the OneGeochemistry initiative, we are therefore actively engaging with the global geochemistry community to improve data services and to develop community-endorsed best practices for geochemical data publication.

Lecture

Topic: 8.1 Geosciences and Waste Management

Contaminant mobilization from an abandoned polymetallic sulfide mine, Mt. Bobija, Serbia

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On top of Mt. Bobija, located in Western Serbia and mainly composed of silt- and limestone, outcrops of a massive triassic sulfide ore body with pyrite, sphalerite, galena, tetrahedrite, and barite mineralizations were mined until the late 20th century. Since then, waste-rock dumps located at 1100 m a.s.l. close to the mine were subject to weathering, potentially releasing harmful elements in dissolved or particulate form to downhill freshwater systems (Orovička reka) via erosion channels. In order to screen the distribution of pollutants and their speciation and evaluate the impact of the mine-waste dumps on downhill freshwater systems, sediment samples were taken along erosion channels up to 3800 m from the waste-rock dumps. The samples were air-dried, sieved <2 mm, and analyzed for their bulk chemistry and mineralogy using XRF spectrometry and XRD, respectively. Speciation of potential pollutants was investigated using the BCR sequential extraction method. Bulk chemistry data of waste-rock dumps showed high contents of Cu (247-7360 mg/kg), Pb (873-87360 mg/kg), and Zn (441-37520 mg/kg) as well as elevated concentrations of As (994-2344 mg/kg), Sb (844-2810 mg/kg), and Hg (350-1108 mg/kg). In this talk, we will specify (1) pollutant concentration trends along erosion channels, (2) the speciation of pollutants with increasing distance of the contamination source, and (3) the potential impact of Mt. Bobija mine wastes on downhill freshwater systems.

Lecture

Topic: 5.3 Warm climates in Earth History as a future analogue

Assessing Eocene hydrological pattern by reconstructing seasonally enhanced fluvial discharge into marginal seas

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Shifts in the hydrological cycle, such as the location and magnitude of seasonal precipitation, are changing as a result of current climate change. The Eocene, as the warmest epoch during the Cenozoic, is increasingly used as a test of our understanding of how broad-scale features of the climate system respond to greenhouse gas forcing. Here we demonstrate an attempt to reconstruct hydrology of northwest Europe by assessing the riverine input into the Anglo-Paris Basin (an adjacent basin to the Paleo North Sea) during the Lutetian. Marginal seas, like the Anglo-Paris Basin, are well-placed to track seasonal atmospheric variations as well as changes in fluvial discharge.

For our reconstruction we measured stable oxygen ($\delta^{18}\text{O}$) and clumped isotopes (Δ_{47}) in combination with spatially-resolved Ba/Ca ratios in pristinely preserved bivalve shells (*Venericor planicosta*). The combined isotope systems were used for the calculation of temperature as well as to identify salinity changes. Barium was simultaneously employed as proxy for terrigenous input. To further evaluate the terrigenous origin of the elevated barium that is frequently observed within these samples, we also measured spatially-resolved strontium isotopic ratios ($^{87}\text{Sr}/^{86}\text{Sr}$) by LA-MC-ICP-MS.

The Ba/Ca record displays an invariant background with large, reoccurring peaks, indicating episodic enhanced riverine input into the basin. The periodic freshwater discharge is also visible within the isotope record that shows a variable $\delta^{18}\text{O}_{\text{SW}}$ (+2 to -4‰), pointing to major changes in salinity. These periods are preferentially linked to warmer temperature, therefore representing a primary wet season during summer times.

Lecture

Topic: 4.5 Tectonic Systems (TSK Open Session)

Physics of microfabric generation: insights from a new deformation theory

Falk H Koenemann

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The mechanics of solids theory from the 18th C is obsolete since energetic physical thinking, thermodynamics, and bonds in solids were discovered in 1840-1870. Elastic deformation is by nature a change of state in the sense of the First Law of thermodynamics; this cannot be concluded from the common theory. A proper approach to elastic deformation – stress – must begin with the equation of state, and be based on the First Law. – The thermodynamic theory (in scalars P, V, T) is isotropic by nature. It has been transformed into vector field form (f, r, T) to consider anisotropic boundary conditions. The displacement field has a contracting eigendirection [ED] at 111° , an extending ED at 11° to the foliation plane. EDs can neither rotate nor shear. The maximum shear directions, the bisectors between the EDs, are also the directions of maximum angular velocity. Therefore, the common idea of crystallographic glide planes aligning with the bulk shear direction, thereby permitting unlimited dislocation glide, is unrealistic. Not the glide planes control the fabric orientation, but the maximum material anisotropy aligns with the extending ED. The crystals populating a maximum are in a locked position, they cannot glide. It follows that extended plastic flow by dislocation glide alone is physically impossible. Secondary processes must be active simultaneously, such as grain boundary glide, recovery, heterogeneous shear zones. The new approach correctly predicts all observed features of plastic simple shear, such as S-C, sigma-delta clast systematics, and microfabric obliquity.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Gabbro glacier or sheeted sills? How the lower crust of fast-spreading oceanic ridges is accreted

Jürgen Koepke¹, Dieter Garbe-Schönberg², Dominik Mock¹, Samuel Müller²

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Based on a newly established profile through the fast-spreading oceanic crust of the Oman ophiolite and on cores drilled within the ICDP Oman Drilling Project (OmanDP), we present here the results of 10 years research, focusing on the nature of the magmatic accretion of the deep crust beneath fast-spreading mid-ocean ridges. We established a 5 km long profile through the whole crust of the Oman ophiolite by systematic outcrop sampling in the Wadi Gideah (Wadi Tayin Block near Ibra), providing the reference frame for the two 400 m long crustal OmanDP drill cores GT1 and GT2, drilled into the same Wadi.

The results allow implication on the mechanism of accretion of fast-spreading lower oceanic crust. Depth profiles on bulk rock and mineral compositions, crystallization temperature and microstructures combined with petrological modeling reveal insights into the mode of magmatic formation of fast-spreading lower oceanic crust, implying a hybrid accretion mechanism. The lower 2/3 of the crust (mainly layered gabbros) formed via the injection of melt sills and in situ crystallization. Here, upward moving fractionated melts mixed with more primitive melts through melt replenishments, resulting in an upward differentiation trend. Since the fraction of crystallization is only small, upmoving melts could easily transport the latent heat produced by deep crystallization upward. The upper third of the gabbroic crust is significantly more differentiated, in accord with a model of downward differentiation of a parental melt originated from the axial melt lens located at the top of the gabbroic crust.

Lecture

Topic: 10.3 Geoscientific museums and collections in the area of responsibility between science and public relations

Education through fascination: looking for ways to promote geoscience

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The course of recent debates on global warming, biodiversity crises, pandemics and anti-pandemic measures, racism, or military conflicts demonstrates how quickly societies become emotionally driven and unsusceptible to evidence. Changes in the use of media indicate impatience of the users, limiting the attention span that would be needed to comprehend complex causalities. Are we witnessing the decline of classic natural sciences, whose approach is genuinely explorative and requires collecting facts prior to arranging them in models?

Earth sciences gather knowledge on the development of geo- and biosphere through time, exemplified in collection objects such as minerals, rock samples and fossils. Visitors are attracted by the beauty, age, authenticity of the specimens or the complexity of processes that led to their formation. Most frequently, however, museum exhibitions present original specimens alongside their interpretation, while the process of research remains underrepresented. This hampers a general broad understanding of science among non-specialists.

Museums and collections can help promoting geosciences for a broader audience by combining methodological insight with the fascination of the object. Apart from the traditional ways of communicating science via popular talks and publications, new formats like science slams, cross-over exhibitions and especially digital tools that can be integrated in exhibitions are designed to facilitate access to research methods and principles.

Reliable visitor analytics is needed to evaluate the success of science communication in limited model projects. Determining best practices and sharing them within the geoscientific community should contribute to arousing awareness and understanding for Earth sciences in the society.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

GARNET GROWTH IN A KYANITE-BEARING PERALUMINOUS PEGMATOID FROM THE MOLDANUBIAN ZONE (BOHEMIAN MASSIF, AT)

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An 8 mm sized almandine-spessartine garnet from the Moldanubian Gföhl Unit (Bohemian Massif, AT) displays asymmetric morphology and several zoning types, reflected by varying inclusion microstructures and garnet colour. Different characteristics of oscillatory, sector, concentric and non-concentric zoning serve to decipher several phases of garnet crystallization from pegmatoid melt.

Directed garnet growth is corroborated by (i) asymmetric crystal morphology with irregular shape on one side and idiomorphic facets on the other, (ii) asymmetric compositional zoning, (iii) absence of two rim zones on the irregular side which are clearly discernible on the idiomorphic side and (iv) presence of a garnet reaction rim on the irregular side exclusively.

The garnet composition and microstructural zoning are not necessarily spatially correlated. Major element composition can show continuous trends, despite striking microstructural changes. Contrastingly, domains with the same microstructural characteristics can display differences in compositional details. Therefore, compositional and microstructural zoning seem to be governed by different parameters that change during garnet crystallization.

Sector and oscillatory zoning are reflected by inclusion microstructure and colouring of the garnet host. Grt{110} and Grt{112} growth sectors contain various inclusion types in different ratios, where dodecahedral sectors show prevalence of phosphates over rutile, vice versa for trapezohedral sectors. In addition to non-concentric zoning, these observations indicate a local and crystallographically assisted inclusion origin. Instead of external forcings (Jamtveit 1991, Am Min 76), oscillatory zoning is interpreted to reflect a self-organized process at the garnet-melt interface (Allègre et al. 1981, Nature 294).

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Lecture

Topic: 1.7 Experimental Petrology and Geochemistry

The role of S_3^- in molybdenum transport by hydrothermal fluids revealed by in situ X-ray absorption spectroscopy

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The knowledge of molybdenum speciation under hydrothermal conditions is a key for understanding the formation of porphyry deposits which are the primary source of Mo. Previous studies have revealed a complex speciation of Mo including (hydrogen)molybdate ions, their ion pairs with alkalis, oxy-chloride species, and thiomolybdate complexes. However, these available data are unable to account for the observed massive transport of Mo in porphyry-related fluids revealed by fluid inclusion analyses demonstrating 100s ppm of Mo (e.g., Kouzmanov and Pokrovski, 2012). A potential missing ligand for Mo may be the trisulfur radical ion, which is predicted to be abundant in sulfate-sulfide rich acidic-to-neutral porphyry-like fluids.

We performed X-ray absorption spectroscopy (XAS) measurements at the Mo K-edge (20.0 keV) in a hydrothermal autoclave available at BM30 of ESRF synchrotron (Testemale et al., 2005) to study the molybdenite solubility in model S_3^- rich aqueous solutions at 300°C and 500 bar. We found that Mo can be efficiently transported by S_3^- -bearing fluids at concentrations of several ppm, whereas the available data on OH-Cl-S complexes predict negligibly small (<100 ppb) Mo concentrations at our conditions. Work is in progress to extend the experiments to wider T-P-composition range of porphyry fluids and to quantitatively assess the role of S_3^- in Mo transport by geological fluids.

K. Kouzmanov and G.S. Pokrovski, Soc. Econ. Geol. Spec. Pub. 16 (573–618), 2012; D. Testemale et al., Rev. Sci. Instr. 76 (043905), 2005.

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Lecture

Topic: 3.2 Composition and evolution of deep planetary interiors

Strength and anisotropy of textured ϵ -FeSi at extreme conditions

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The cores of terrestrial planets are comprised of Fe-Ni alloys, with around 5-10 weight % of the light elements. They account for the observed core density deficit compared to the Fe-Ni alloy at high-pressure high-temperature conditions. Silicon has long been considered as a major light element of the cores due to its high cosmic abundance and ability to incorporate into the Fe-Ni alloy during core formation. Thus, Fe-Si alloys and compounds are likely to be present in the cores of terrestrial planets such as Mercury.

The seismological observations indicate that compressional waves travel slower through the equatorial plane of the Earth's core compared to the waves traveling along the polar axis. This anisotropy is likely related to the plastic deformation of the inner core material. Yet, the effect of light elements on the plasticity of iron is poorly known.

Here we investigate lattice strains and textures of ϵ -FeSi up to 50 GPa at 300 K and 1100 K. We employed the radial x-ray diffraction technique using diamond anvil cells as deformation apparatus. We used our data to determine yield strength of ϵ -FeSi and to assess the sound-velocity anisotropy of the polycrystalline ϵ -FeSi as a function of pressure and temperature. Upon compression, FeSi aggregate does not develop strong textures and, as a result, shows weak sound-velocity anisotropy. The strength of the material is nearly temperature-independent. Thus, we infer the constraints on the silicon budget in planetary deepest interior by demonstrating that strong sound-velocity anisotropy is incompatible with the high silicon content.

Lecture*Topic:* 4.1 Magmas and Fluids in the Crust**Revisiting the B isotope fractionation and partitioning systematics in synthetic MORB****Sebastian Kommesch¹, Felix Marxer², Florian Pohl², Francois Holtz², Renat Almeev², Ingo Horn², Raúl O. C. Fonseca¹**¹Ruhr Universität Bochum, Germany; ²Leibniz Universität Hannover, Germany

Boron isotope systematics allow tracing of *e.g.* fluid-mediated mobilisation of subducted material in subduction zones. The associated B isotope fractionation factors are constrained by *e.g.* analysis of synthetic samples.

Here we investigate the effect of temperature, and water content as a function of pressure, on the B isotope composition of a basaltic melt and coexisting fluid. The MORB-like starting material was doped with a ~ 450 µg/g aliquot of the NIST951a B isotope reference material. Synthetic MORB are produced using internally heated pressure vessels (IHPV). Experiments were performed between 1250 and 1000 °C and 1 and 2.5 kbar, ($fO_2 \sim \Delta QFM + 3.3$).

Boron isotope compositions were determined using *fs*-LA MC-ICP MS, intermediate precision of NIST610 is $\delta(^{11}\text{B}/^{10}\text{B})_{\text{NIST951a}}$, hence $\delta^{11}\text{B} = -1.43 \pm 0.82 \text{ ‰}$ (2 s.d., average of 5 sessions, total average ($n = 134$) is $-1.46 \pm 0.16 \text{ ‰}$, 95% c.i.). Our MORB glass yields an intermediate precision of $\delta^{11}\text{B} = +0.05 \pm 0.11 \text{ ‰}$ (2 s.d. of 5 sessions, total average ($n = 153$) = $+0.01 \pm 0.02 \text{ ‰}$ (95% c.i.).

Boron melt-fluid partition coefficients are below unity ($D^{\text{melt}/\text{fluid}} < 1$), $\delta^{11}\text{B}$ decreases from ± 0 to -1.5 ‰ with increasing total water content. Our results show that B will be concentrated in the fluid at magmatic temperatures. Moreover, it is shown that the degassing of fluid from a basaltic melt likely leads to measurable B isotope fractionation (tentative $\Delta^{11}\text{B}_{\text{melt-fluid}} = -2.2 \pm 0.6 \text{ ‰}$), with potential implications to our interpretation of the $\delta^{11}\text{B}$ of degassed, water-rich basaltic magmas.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

Evidence for a non-classical dissolution-reprecipitation reaction path in natural high pressure-low temperature rocks

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Dissolution and precipitation of minerals in the presence of a hydrous fluid is commonly assumed to occur predominantly by hydrolysis of the outermost monolayers of the reacting crystal and subsequent incorporation of atoms from aqueous solutions into favorable sites at the product surface. However, experiments have shown that different parts of this classical reaction pathway are facilitated and enhanced by the presence of nanoparticles and/or amorphous phases.

We show in natural high-pressure/low temperature rocks, which experienced metamorphic conditions in the order of 500°C at 1 GPa, that an alkali-Al-Si-rich amorphous material can be found in nm-sized metamorphic porosity [1]. The gel-like water-rich material contains about 15wt% total dissolved solids (TDS), which is more than ten times higher than expected for aqueous solutions at these metamorphic conditions. High-resolution TEM observations show that the amorphous material forms directly by depolymerization of the crystal lattice of amphiboles and clinopyroxenes. Depolymerization of the minerals starts along grain or phase boundaries, dislocation cores within the crystal lattice or lattice defects in general that serve as effective element exchange pathways and are sites of porosity formation. High hydrogen concentrations in such dislocation cores within nominally anhydrous clinopyroxene has been confirmed by Nano-SIMS measurements and indicates hydrolysis and recrystallization within mineral grains.

The resulting amorphous material occupies large volumes in an interconnected porosity network which has been documented in 3D imaging. Precipitation of product minerals occurs directly by repolymerization of the amorphous material at the product surface.

Reference:

[1] Konrad-Schmolke et al. 2018, Nature Communications 9: 1637.

Poster

Topic: 7.1 Geo-Biosphere interactions through space and time: new analytical and experimental approaches to the fossil record

Fungal bioerosion in fossil dinosaur bones from the Kenton quarries (Late Jurassic, Morrison Formation, Oklahoma): Implications for bone fossilization processes

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After death, bone is exposed to various abiotic and biotic processes. Microbial bioerosion has been reported from recent, archaeological and palaeontological bones and is deemed to have been caused by fungi, cyanobacteria or bacteria. It is recognizable as microscopic tunnelling, caused by microbial enzymes. However, fossil (i.e., fully permineralized) bone exhibits strikingly few signs of bioerosion. Fossilization only happens if bone is preserved long enough to allow diagenesis by mineral uptake and loss of collagen.

Upper Jurassic sauropod dinosaur long and girdle bones from Kenton quarries 1, 5, and 6 (Oklahoma, Morrison Formation) present abundant and distinctive filamentous microstructures. This kind of preservation is absent in hundreds of other Morrison Formation dinosaur bone samples studied.

Methods used to evaluate the nature of microstructures include literature research (comprehensive review of palaeontological and archaeological literature) and thin section analysis. Polarized light microscopy was used to describe the general bone histology, ontogeny, and density and distribution of bioerosive microstructures. The aim of this work is to identify bioerosive microstructures and to elucidate possible causative agents, bioerosive mechanisms and invasion patterns. The conclusion is that the filamentous microstructure are most likely Wedl tunnels caused by fungal attack. Presence of tunnelling seems to be unrelated to the specific quarry, ontogenetic stage, taxon, and bone type.

Further research on the taphonomic and depositional environments of the Kenton quarries are needed to identify the cause of these unique microstructures. Heavily bioeroded bone and its rarity allows to constrain hypotheses regarding bone fossilization.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Re-distribution of platinum-group elements in supergene ores of the Merensky Reef, Eastern Bushveld Complex, South Africa

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The Merensky Reef of the Bushveld Complex, South Africa, is one of the largest resources of platinum-group elements (PGE) worldwide. Near-surface supergene ores of the Merensky Reef contain high grades of PGE and are economical ore bodies. Unfortunately, the recovery rates of these ores are low. This is the first study that investigates the variation of PGE in pristine and supergene samples of the Merensky Reef from the eastern Bushveld.

The whole-rock PGE distribution was investigated via ICP-MS and the platinum-group mineral (PGM) distribution with reflected light microscopy, SEM, and microprobe. Pristine samples reveal that the PGEs occur mainly as discrete PGMs and in solid solution in sulfides (especially Pd in pentlandite). The PGMs in the pristine ore are PGE-sulfides, e.g. cooperite-braggite or laurite; and subordinate PGE-bismuthotellurides and PGE-arsenides. During weathering, sulfur and, to a lower extent, Pd, were removed resulting in a PGE mineralogy that mainly consists of relict PGM, Pt-Fe alloys, and Pt-oxides/hydroxides. Additionally, PGEs (mainly Pd) are hosted by Fe-hydroxides and secondary hydrosilicates (e.g., chlorite or serpentine).

The highly variable distribution in the supergene ore results in very low and thus uneconomic recovery rates. The PGEs in the weathered samples occur only partly as discrete PGMs and therefore the processing is not as effective. The PGEs are also hosted by hydrosilicates and Fe-hydroxide and thus hydrometallurgical or pyrometallurgical processing of the bulk rock is necessary for the extraction of PGE, which is still uneconomic and thus new chemical bulk-leaching methods would need to be developed.

Lecture

Topic: 8.1 Geosciences and Waste Management

Anthropogenic Gadolinium and Other Emerging Contaminants in the Southern North Sea and the Elbe, Ems and Weser Estuaries

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In the last decades, many trace elements that were hitherto only used as geochemical proxies gained societal and economic importance due to their increasing use in high-technology applications including medicine and renewable energies. The increasing application of such metals results in a tremendously growing and unconstrained input from anthropogenic sources into the environment. Knowledge of the environmental behavior and the toxicity of these compounds are for many of these elements still in their infancy. The minute concentrations in the natural environment and complex matrices pose additional analytical challenges.

This contribution presents results on the anthropogenic and geogenic inputs of gadolinium, a major component in MRI contrast agents, and other emerging contaminants into the southern North Sea from the Elbe, Ems and Weser estuaries. The water samples were collected during research cruise M169 "TRAM" ("Tracing geogenic and anthropogenic critical high-technology metals in the southern North Sea") with R/V Meteor.

Using Seafast-QQQ-ICPMS, we provide evidence for the widespread anthropogenic input/distribution of the wastewater-derived contaminant Gd in the southern North Sea, including the Wadden Sea World Heritage. Complementary ultrafiltration and DGT passive sampling data show that the anthropogenic Gd exclusively occurs in the truly dissolved element pool (< 1KDa) of the discharged river waters and is bound in a highly stable, inert complex that is not bioavailable. Our results corroborate the notion that the Gd-based contrast agents used during MRI scans may pass wastewater treatment plants unhindered and show a very conservative behavior during estuarine mixing, enabling its transport to the open sea.

Lecture

Topic: 10.3 Geoscientific museums and collections in the area of responsibility between science and public relations

Discovering minerals and rocks

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We all like to go on a discovery tour – regardless of age. And we like to use all our senses. But the most important thing in everything we do is that we UNDERSTAND what we are doing. Geoscientific collections in particular offer the potential to learn by TAPPING.

In German usage, „Verstehen“ and „Begreifen“ are to be used synonymously and it means to grasp with the hands, goes better into the memory, is better understood.

And that is what we do in practice in the museum, especially elementary and middle school students are very receptive here. Away from the strict theory and the classic guided tour, encourage the students to participate, to actively create. Practical examples, such as feeling in cloth bags, arranging selected rocks to form a rock cycle, actively getting to know physical properties such as hardness, fissility, density, fluorescence, etc. are presented using examples. Depending on the age, from KITA-age to senior, different modules are offered in the Mineralogical Collection of the University of Jena to get to know and "grasp" geoscientific contexts. There is a conscious decision not to use a lot of technology on site, and the focus is on working with the object. Thereby the uniqueness of the products of our nature is brought closer to the visitors, because only a conscious contact with nature can protect it!

Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

The struggle of choosing the “best” data basis for remote geomorphological analyses – Quality assessment of open-source digital elevation models in Northwest Namibia

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Today, digital elevation models (DEM) form the data basis for most geomorphological analyses. With the wide range of freely available, global DEMs, the question arises which option is the best choice for the desired analysis. The quality of DEMs of equal spatial resolution can be characterized by their vertical accuracy and precision. While the vertical accuracy describes the one-dimensional difference between the DEM and the Earth's surface, the precision describes the spatial error distribution within the dataset.

To study the geomorphologic evolution at the dry limit, the sparsely vegetated Northwest of Namibia provides a promising landscape due many ephemeral rivers incised differently far into the geologically complex Kunene Highlands and draining towards the Skeleton Coast, which is covered to a large extent by dune fields. This versatility, however, provides challenging condition for the assessment of DEMs, strongly dependent on the respective underlying remote-sensing technology. For this reason, we conducted a quality assessment of the commonly used SRTM, ASTER, ALOS and GLO-30 DEMs – all featuring an equal spatial resolution of one arc-second (~30 m). The absolute vertical error has been assessed by validation using geodetic ICESat-2 data. To quantify the precision of the DEMs in relation to the morphometric complexity of the terrain, surface roughness measures were applied. In addition, it was investigated whether the lithology has an impact on the accuracy and precision. In conclusion, the GLO-30 turned out to be as yet the most accurate (RMSE = 1.1 m) and precise open-source DEM for Northwest Namibia.

Lecture

Topic: 11.3 Young Scientist Session

Towards a cost-efficient method to apply anthropogenic gadolinium as a pseudo-natural tracer in monitoring waste water-derived xenobiotics in tap water

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Anthropogenic Gd in the aquatic environment originates from very stable water-soluble Gd complexes used as contrast agents in magnetic resonance imaging (MRI). These contrast agents cannot be removed in waste water treatment plants and are released into surface waters with their clearwater discharge. Since the first discovery of anthropogenic Gd in tap water in Berlin in 1995, a strong increase was observed until 2012, mainly in the city's western districts. For a follow-up study in 2021, we sampled these sites again to monitor evolving anthropogenic Gd levels in tap water over the past decade.

We adapted a method for automated preconcentration of seawater samples with low REY concentrations using a seaFAST system to the analysis of tap water. Comparing the results of this new protocol to those derived via the established manual method, we demonstrate the excellent agreement between these two approaches.

The general trend of strongly increasing anthropogenic Gd anomalies observed between 2009 and 2012 continued until 2021, closely following the increase of the number of MRI scans performed in Berlin. While the general spatial distribution confirms earlier observations of much stronger anthropogenic positive Gd anomalies in western than eastern districts, several eastern districts where no anthropogenic Gd had been observed in the past, now also show pronounced positive Gd anomalies, revealing the presence of waste water-derived xenobiotics in the tap water.

Using automated preconcentration for REY analysis in tap water, the microcontaminant Gd may now be applied as a reliable and cost-efficient pseudo-natural tracer for waste water-derived substances.

Lecture

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Meteoric 10-Be as a tracer for water infiltration into deep weathering zones along a climate gradient

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In a semi-arid and a mediterranean study site in the granitoid Chilean Coastal Cordillera, we investigated drilled weathering profiles of 100 m depth and found significant differences in the depth of the weathering zone. Where rainfall is limited, fractures may be transport pathways for water to depth, inducing deep weathering. With more rainfall present, diffusive water transport through pore spaces allows surficial weathering in the profiles.

These distinct modes of water infiltration can be traced with the meteoric cosmogenic nuclide ¹⁰Be ($T_{1/2} = 1.4$ My) while stable ⁹Be is released during silicate weathering. By combining these isotopes, a ¹⁰Be/⁹Be ratio emerges in fluids that traces water infiltration and the element release by weathering. This isotope ratio is preserved in the “reactive” form as attached to amorphous Fe-oxides.

Concentrations of reactive Be ($[Be]_{\text{reac}}$) were determined in soil, saprolite, bedrock, and fracture surface samples. Both study sites show an increase in $[^9\text{Be}]_{\text{reac}}$ towards the surface. $[^9\text{Be}]_{\text{reac}}$ is higher on fracture surfaces compared to soil and saprolite, indicating that fractures and pore spaces are conduits for water flow. $[^{10}\text{Be}]_{\text{reac}}$ decrease from surface to depth in soil and saprolite, reaching detection limit at 2 m in the semi-arid, and at 25 m in the mediterranean study site. $[^{10}\text{Be}]_{\text{reac}}$ in deep fracture samples are close to detection limit although high $[^9\text{Be}]_{\text{reac}}$ indicate Be mobility by water flow. Decay and/or adsorption of ¹⁰Be during transport, or insufficiently low water infiltration, may explain why so little ¹⁰Be is found on fracture surface and at depth.

Poster*Topic:* 1.8 Minerals and Mineral Properties**On a new monoclinic SFC polytype****Biljana Krüger, Janina Grabowski, Volker Kahlenberg**

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Dark red crystals of a silico-ferrite of calcium (SFC) with composition $\text{Ca}_{5.34}\text{Fe}_{20.55}\text{Si}_{2.12}\text{O}_{40}$ have been obtained from synthesis experiments at 1250°C. The SFC phase crystallizes in space group C2/c with the following lattice parameters: $a = 9.981(4) \text{ \AA}$, $b = 15.283(6) \text{ \AA}$, $c = 5.303(2) \text{ \AA}$, $\beta = 99.88(4)^\circ$, $Z = 1$.

The structural formula of the new phase can be written as $^{\text{VII}}\text{A}_4^{\text{VI}}(\text{M1M2M3M4})_{\Sigma 12}\text{O}_4[{}^{\text{IV}}(\text{T1}_2\text{T2}_2)_{\Sigma 12}\text{O}_{36}]$, where A represents a seven coordinated Ca-site, $\text{M} = \text{Fe, Ca}$ are octahedral sites and $\text{T} = \text{Fe, Si}$ are tetrahedral positions. The structure is composed of spinel(S)- and pyroxene(P)-type modules.

The SFC structure is closely related to that of the minerals of the rhönite group (sapphirine supergroup) and synthetic so-called SFCA phases (Silico-ferrite of calcium and aluminum), where different polytypes composed of the same fundamental S- and P-modules have been observed.

The new monoclinic SFC phase exhibits disorder in the spinel module, representing a layer with edge-sharing zig-zag octahedral chains connected via tetrahedra. Two of three octahedral sites in these chains and the connecting tetrahedra are half occupied only. This enables two (left and right) orientations of the chains along $[-1\ 0\ -1]$. The same arrangement is observed in equivalent layers of a triclinic SFCA phase reported by Liles et al. (2016). However, in this compound two possible configurations of these layers allow for stacking faults.

Liles, D.C., de Villiers, J.P.R. & Kahlenberg, V. (2016): *Miner Petrol* 110:141–147.

Lecture*Topic:* 1.7 Experimental Petrology and Geochemistry**Water speciation in partially deuterated hydrous stishovite at 450 °C and 9 GPa****Nico Kueter^{1,2}, Kara Brugman², Francesca Miozzi², George D. Cody², Michael J. Walter², Jing Yang², Timothy A. Strobel²**¹Geological Institute, ETH Zürich, Switzerland; ²Carnegie Science - Earth and Planets Laboratory, Washington D.C., USA

The high-pressure SiO₂ polymorph stishovite is a major constituent of subducted oceanic crust and is stable over a wide range of pressures and temperatures ranging from the lower upper mantle to the lower mantle¹. Its capacity to store water (i.e., H, OH, H₂O) renders stishovite an important water conveyor to the transition zone and lower mantle². Previous studies demonstrated that Al-free Stishovite quenched from multi-anvil experiments can incorporate up to 3.2 wt% water (<550 °C, 10 GPa³⁻⁵). This was explained by a hydrogarnet substitution mechanism, where four H⁺ substitute for one Si⁴⁺ in the tetragonal stishovite lattice^{3,4}. In-situ X-ray diffraction experiments with diamond anvil cell (DAC) found stishovite containing up to 10 wt% water under pressure but showed that this water is lost upon decompression², suggesting that water also exists in a more mobile molecular form in the stishovite structure.

We investigated the water speciation in hydrous stishovite synthesized at 450 °C and 9 GPa from partially deuterated SiO₂ glass via ¹H-NMR. Water comprises 1.5–2.0 wt% of the stishovite and causes up to 0.4% unit-cell volume expansion as determined by X-ray diffraction. ¹H-NMR cannot rule out the presence of a hydrogarnet substitution mechanism, but spinning sideband intensities indicate that water is also stored as semi-rigid H₂O defects. Spectroscopic D/H analysis of the system components suggests a preferential partitioning of deuterons into the stishovite relative to the coexisting water. We further present a method to recover and preserve the quenched fluid from the experimental capsule.

¹Ono,S.(2001)*EPSL*,57-63; ²Lin,Y.(2020)*PNAS*,184-189; ³Spektor,K.(2011)*PNAS*,20918-20922; ⁴Spektor,K.(2016)*Am.Min.* 2514-2524; ⁵Nisr,C.(2017)*Am.Min.*,2180-2189.

Lecture

Topic: 6.4 Landslides – detecting, monitoring, modeling, assessing hazards, and coping with risks

Towards high efficacy Early Warning in Europe

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The Potsdam Conventus

Early Warning Systems for natural disasters are the most promising means of saving lives, property and societal integrity in cases of impending natural hazards. They are expected to be critically required, even more in the future, as either new and hitherto unknown phenomena are expected to become substantial threats, or climate change brings increasing intensity, impact and frequency of adverse weather related phenomena, or cascading hazardous processes appear more frequently. Since the 1994 Yokohama World Conference on Disaster Risk Reduction, Early Warning Systems are acknowledged as the most efficient elements of societal resilience, however the 'State of the Global Climate 2021' (World Meteorological Organization, WMO, 2022) concludes the very low implementation level and often extremely poor performance of existing systems. In order to foster the implementation and improvement of systems in all 193 Member States, the United Nations have declared the coming five years as 'Years of Early Warning'. Based on a broad range of practical and organizational experiences from 1980s events in Japan, the Yokohama World Conference, the 1998 Potsdam Early Warning Systems Conference, several successful scientific and technical development projects financed by the European Union, this contribution delivers an architectural design structure as well as a comprehensive roadmap for Early Warning implementation in Europe. It encompasses the necessary steps in national and international policies, in diverse fields of legislation, in various involved scientific and technical disciplines, and in the harmonization of ethical approaches. The creation of a European Centre for Early Warning Information is suggested.

Lecture

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

„Wer hat an der Uhr gedreht?“ Mechanisms of Rb-Sr age resetting revealed by high-resolution LA-ICP-MS/MS isotope mappings

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The Rb-Sr isotope system is sensitive to secondary processes that disturb or even completely reset the age signal in datable minerals like mica or feldspars. To interpret age signatures correctly, the factors governing isotope mobility in real-world minerals have to be identified. Three main processes are known to influence isotopic clocks: (1) diffusional re-equilibration of minerals with their surroundings, which is expected to be strongly temperature-sensitive provided that the matrix of a given mineral facilitates rapid isotope transport (2) fluid-mediated dissolution-precipitation and (3) deformation-induced dynamic recrystallization.

Distinction between these processes is notoriously difficult. However, different types of Sr isotope mobility should leave characteristic microscale isotope distribution patterns, with bell-shaped Sr diffusion patterns, preferential rejuvenation close to high-strain zones in the case of ductile deformation, and probably element zoning patterns resulting from fluid-driven precipitation. To recognize and to distinguish such patterns, two-dimensional images of the Rb/Sr elemental and Sr-isotope distribution would be required, in analogy to what has been done using Ar-Ar in K-feldspar [1],[2].

Visualization of such patterns has long been analytically impossible due to the absence of an in-situ method that provides sufficient Rb Sr-sensitivity, isotope selectivity and high spatial resolution. By combining state-of-the-art ICP-MS/MS spectrometry and a fast aerosol transfer lasing system, we developed a routine for rapid Rb-Sr age mappings of mica that offers resolution at the μm -scale. We present first age maps for muscovite crystals from metamorphosed granitic pegmatites.

[1] Wartho, J. A. et al. (1999) [https://doi.org/10.1016/S0012-821X\(99\)00088-6](https://doi.org/10.1016/S0012-821X(99)00088-6)

[2] Popov, D. V. et al. (2020) <https://doi.org/10.1016/j.chemgeo.2020.119841>

Lecture

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Millennial-timescale climate change over the last 800 kyrs evidenced by magnetic, colorimetric and ATR-FTIR data from the Suhia Kladenetz quarry loess-paleosol sequence (Pleven, Bulgaria)

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Eastern European loess-paleosol sequences (LPS) are excellent archives of past climate change. Millennial-timescale climate change is successfully evidenced in loess of the last and penultimate glacial periods. However, study designs with similar or lower sampling resolution strategies and/or single proxy investigations do not favor their identification for earlier glacials, which are generally scarcer, thinner and characterized by lower sedimentation rates. The high-sampling resolution multi-proxy study presented here demonstrates the first evidence of millennial-timescale climate change for periods older than MIS6 archived in an Eastern European LPS.

The Suhia Kladenetz 27 m long profile was sampled continuously at a 2 cm resolution for bulk sediment. Magnetic and colorimetric measurements are performed on all samples. ATR-FTIR data is acquired at the same resolution through loess units and at a 12 cm interval elsewhere, while grain size analyses are conducted continuously at a 12 cm interval. Rock magnetic data and microscopic observations, from our previous work, characterized a 20-cm-thick outcropping tephra in the MIS6 loess unit and identified several cryptotephra. Moreover, a correlative age model demonstrating that the LPS covers the last ~800 kyrs allowed to provide age estimates for the tephra and cryptotephra and thereafter to deduce their likely volcanic sources.

The integrated age model in combination with high-resolution colorimetry-based estimates of goethite and hematite concentrations, and clay mineralogy highlight a cyclicity undoubtedly driven by climate change within interstadials/stadials as shown by correlations with the NGRIP $\delta^{18}\text{O}$ ice core records for the last glacial/interglacial cycle.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

FAIR dissemination of laboratory data in the solid Earth sciences: an EPOS community portal for cross-disciplinary metadata

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The Thematic Core Service Multi-scale Laboratories (TCS MSL) is a community within the European Plate Observing System (EPOS) that includes a wide range of world-class laboratory infrastructures and that provides a cross-disciplinary platform for virtual access to data and physical access to solid Earth science labs.

Data coming from the MSL laboratories provide the backbone for scientific publications, but they are often available only as supplementary information to research articles. Moreover, the vast majority of the collected data remain unpublished, inaccessible, and often not sustainably preserved for the long term. To allow reuse of these valuable but often neglected data, the TCS MSL developed a full chain to support solid Earth science researchers from the long tail in the FAIR dissemination of their collected data.

This chain builds upon a community-driven metadata standard that allows for multiple discipline-specific detailed descriptions, a publication tool (metadata editor), and a community portal that gives access to DOI-referenced data publications at multiple research data repositories related to the TCS MSL context (<https://epos-msl.uu.nl/>). The portal is built on the CKAN repository toolkit and is driven by the richness of the TCS MSL metadata standard. Besides its importance for the TCS MSL community, it also provides a showcase of how to set up a CKAN-based environment as a cross-disciplinary catalogue for FAIR metadata exchange in a highly heterogeneous setting.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

New insights on the role of reverse weathering in determining seawater geochemistry: a lithium isotope study

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The lithium isotope composition ($\delta^7\text{Li}$) of ancient seawater is a fundamental proxy for the reconstruction of past conditions on Earth. At any given time, seawater $\delta^7\text{Li}$ depends on the magnitude and isotope composition of the major input and output fluxes, which themselves result from interactions between climate, Earth surface processes and tectonics. Characterizing lithium fluxes during modern times and past eras can thus help determining Earth surface response to environmental changes.

Despite a general consensus on the characterization of the major fluxes of lithium to seawater, questions remain regarding the fate of lithium during early-diagenetic reactions taking place at the ocean floor. In particular, the amount of lithium incorporated into new secondary aluminosilicates formed at the seafloor (i.e., reverse weathering), and the Li isotope fractionation associated with this, are poorly constrained.

Here, we tackle these questions with new lithium isotope data and lithium concentrations measured on the clay-sized fraction of terrestrial and marine sediments from the Chilean active margin. The dataset is composed of riverbed sediments from major rivers along the Chilean climatic gradient (26°S to 41°S), hemipelagic sediments from marine core-tops, and three gravity cores located at 36°S, 33°S and 30°S offshore. It allows us to a) detect a systematic overprint of terrestrial signals in the marine realm, explainable only by the formation of authigenic aluminosilicate phases at the ocean floor, b) determine the Li isotopic signature of reverse weathering products, and c) discuss the global modern fluxes of lithium into and out of seawater.

Poster

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

The TRR170-DB Data Repository: Improving Metadata for FAIR Planetary Replication Datasets

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TRR170-DB (<https://planetary-data-portal.org/>) is a re3data (r3data.org) referenced data repository that stores machine-readable replication datasets of the collaborative research center 'Late Accretion onto Terrestrial Planets' (TRR 170) and from other institutions in the planetary science community. The TRR170-DB framework aligns their data storage with the FAIR (Wilkinson et al., 2016) data life cycle as promoted by the German National Research Data Infrastructure Initiative (www.nfdi.de) and various national and international funding agencies and initiatives. The TRR170-DB repository will be permanently hosted by Freie Universität Berlin, which ensures long-term preservation of, and access to TRR170-DB's published data.

TRR170-DB has a flexible data-driven metadata system that uses tailored metadata blocks for specific data communities. Metadata and files of a published replication dataset can be exported in various open international metadata standards and file formats. This ensures that all published data are generally accessible for other external databases and repositories ("interoperability").

A major requirement for the reuse of data is metadata information that reflects up-to-date analytical developments. Currently, we are expanding metadata templates to incorporate additional standardized information on samples and materials, analytical methods and additional experimental data in the area of geochemistry. This ongoing process will involve international scientific communities and initiatives (OneGeochemistry, Astromaterials Data System, NFDI, etc.) by discussing and testing joint standards and practice. Our efforts on advancing metadata for geochemical analysis data parallel with establishing an interest group on 'metadata standards for instrumental analysis data in geochemistry' in the context of the German NFDI4Earth, a consortium of the NFDI Initiative.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

IEDA2: NEXT GENERATION DATA INFRASTRUCTURE FOR FAIR GEOSCIENCE SAMPLE DATA

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IEDA2 represents a unique collaborative data infrastructure of 3 complementary data systems: EarthChem, LEPR/ traceDs (Library of Experimental Phase Relations), and the System for Earth Sample Registration (SESAR) that jointly support researchers in the Geosciences. IEDA2 helps researchers share and access sample data following the FAIR data principles, and ensures open, reproducible, and transparent science practices. IEDA2 provides a framework for data publication; data synthesis; human- and machine-readable data access that facilitates data mining and computational analysis; and a digital environment that links and integrates physical samples with the modern digital research data ecosystem. The vision for IEDA2 is to advance data-driven and computational methodologies in geochemistry, petrology, and volcanology, and to optimize (re)use and analysis of data, inform peer review, and guide future research directions.

IEDA2 provides services for FAIR geochemical, geochronological, mineralogical, and petrological data with the EarthChem Library (ECL) and FAIR samples with the System for Earth Sample Registration SESAR. ECL and SESAR follow the TRUST principles for repositories, with services for online data submission, data templates, validation of data and metadata completeness, accuracy, and compliance; persistent identification (DOI, IGSN), moratorium periods, human- and machine-readable search and access interfaces, and long-term archiving. With renewed funding from the US NSF, IEDA2 will over the next 5 years focus on enabling user contributions to data synthesis; networking sample data resources; and enhancing usability while educating and engaging the 'Next Generation' of users and fostering a culture of collaboration and partnerships in the national and international Geoscience data space.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

The provenance of the sandstone used for the construction of temples in the World Heritage Site of Angkor, Cambodia

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Many of the Angkor temples with their magnificent decoration are built of sandstone. A greyish-green variety of arkose with an argillitic-chloritic binding was used typically, including the famous temple Angkor Wat.

The provenance of the “temple sandstone” can be located at the Eastern slope of the Kulen mountain as part of the Upper Triassic and Lower Jurassic Terrain Rouge formation. The properties of the building stones vary widely and this results in various forms of damage and decay. Therefore, knowledge of the deposits and the quarries is essential.

Using digital terrane models with data acquired in 2015 by the Cambodian Archaeological Lidar Initiative (CALI) the fieldwork was executed. Wide areas with flat pit-quarries were found in the densely forested area, some were known since the 1960s. Sedimentary structures and the tectonic fracture pattern could be detected in the digital terrane model.

Sandstone was quarried in many sites obviously at the same time in different stratigraphic levels due to the high demand during the construction of big temples within a relatively short time. Thus, different sandstone varieties occur in a single temple.

The quarries are often flat pits and tool marks are frequently observed. Preformatted blocks are still found in and near the quarries.

A schematic cross-section of the sedimentary sequence of the eastern slope of the Kulen Mountains could be documented particularly along a newly built road. The so far proposed stratigraphy needs a major revision.

Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

TephATA: A Tephrostratigraphic Framework for the Atacama Desert and its Application on Regional Sedimentary Archives

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A fundamental aspect to study past Earth surface process variations over time and to set local observations in a regional and global context is their temporal understanding. However, accurate dating of sedimentary archives documenting these variations can be hampered in extremely water-limited environments by applicable dating methods (type of archive/temporal range). Tephrostratigraphy and -chronology can be applied independent of the type of sedimentary archive and thus represent powerful tools for dating and synchronization of archives. In the Atacama Desert, tephra layers occur in various types of archives and on various time-scales. A tephrostratigraphic framework, which sets the tephra layers in a stratigraphic and chronological order and shows the regional dispersal of individual tephra layers is currently lacking. Within the CRC1211 "Earth-Evolution at the dry limit", the project TephATA aims at setting up a regional tephra database to develop the first comprehensive tephrostratigraphic framework for the Atacama. The database TephATA is currently integrated as a web-based part of the CRC1211 database and uses an extended IGSN metadata schema. TephATA combines existing and new chronological as well as stratigraphical information of tephra layers with their glass geochemical compositions, which is the backbone for reliable correlations of tephra layers and identification of widespread marker horizons. If the geochemistry-based approach allows a correlation of tephra layers, age information can be transferred to tephra layers that does not contain sufficient minerals for absolute dating. Particularly widespread tephra layers will function as independent tie-points for the synchronization of the various sedimentary records investigated within the CRC1211.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Geosciences Support Monument Conservation – 25 Years of German Apsara Conservation Project

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The Angkor region was the center of the historic Khmer kingdom, now Cambodia, from the 9th-15th centuries. The Angkor Park, with over 200 temples, has been a UNESCO World Heritage Site since 1992. The largest and most famous temple is the mountain temple of Angkor Wat, dating from the first half of the 12th century. It is built of sandstone over an artificial mountain with a substructure of laterite.

Angkor Wat is completely decorated with stone reliefs and houses the famous bas-reliefs depicting mythological scenes from Hinduism and the military feats of its builder God-King Suryavarman II on about 1.800 m².

The building stone of the temple is a clay-bound arkose. After more than 870 years of unprotected exposure in tropical climates, the stone shows some alarming weathering damage. Especially the weathering form of "scaling" threatens reliefs and building stones.

The German Apsara Conservation Project active for 25 years aims at the scientific conservation of sculptured surfaces at the temples in Angkor and other historical sites in Cambodia. Based on geoscientific investigations, the requirements for a conservation concept including materials and application could be formulated and adapted materials developed. A multidisciplinary project approach is followed together with other experts from engineering, microbiology, chemistry, and conservation sciences. Students from German and international universities are also involved.

A successful conservation concept needs highly trained practitioners for its implementation. About 20 Cambodian conservators work in the GACP, all trained in the project and meanwhile transferred to the Cambodian conservation authority APSARA.

Lecture*Topic:* 2.2 From dust to planets**The search for trace elements in stardust silicate grains****Jan Leitner^{1,2}, Peter Hoppe², Mario Trieloff¹**¹Ruprecht-Karls-Universität Heidelberg, Germany; ²Max-Planck-Institut für Chemie, Mainz, Germany

Isotopically anomalous dust grains that formed in the outflows of evolved stars and in the ejecta of stellar explosions are a minor, but important component of primitive Solar System materials. These grains carry records of stellar nucleosynthesis and evolution, circumstellar grain formation, and stars contributing material to the nascent Solar System. Silicates are the most abundant type of presolar dust available for single grain analyses [1]. Presolar SiC and graphite contain various amounts of trace elements [e.g., 2], while for O-rich grains, only one study reported Sr in an O-rich grain [3]. Here, we report on a search for trace elements in a large presolar silicate by NanoSIMS. Measurements were performed with the Hyperion RF plasma O-source using three different mass sequences. Strontium, Zirconium, and Cerium were identified, with Sr/Si in compliance with astrophysical models. Zr/Si and Ce/Si ratios exceed model predictions, indicating additional effects governing their incorporation. The ⁹⁰Zr- and ¹⁴⁰Ce-distributions are correlated with ⁴⁸Ti. For a gas of solar composition, Sr and Ce would condense into titanate, while Zr forms ZrO₂ at higher temperatures. Due to chemical similarities between Zr and Ti, ZrO₂ might have been incorporated into Sr- and Ce-bearing Ti-oxides, serving as condensation nuclei for the silicate [4].

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Lecture

Topic: 8.1 Geosciences and Waste Management

Determining Dilute Condition Dissolution Rates with Stirred Reactor Coupon Analysis

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With many countries deciding on deep geological disposal of high-level nuclear waste, the corrosion behaviour of the glassy waste matrix is of utmost importance. Multiple studies determined glass dissolution rates under various conditions, resulting in a general rate behaviour scheme of a high initial rate, followed by a low residual rate (plus a potential late-stage increase).

To simulate the impact of groundwater contact with the waste matrix, robust dissolution rate parameters are crucial, but thus far a protocol for interlaboratory comparability was missing.

As part of a waste form development program at Pacific Northwest National Laboratory, the Stirred Reactor Coupon Analysis (SRCA) test method was developed over the last years and used to determine the three dilute rate model parameters [rate constant, activation energy, and pH power law coefficient] for many glass compositions.

The SRCA reactor design is composed of a stirred solution contained in a large volume baffled reactor in which glass coupons are suspended. Dissolution rates are determined by height differences between masked and unmasked areas of each coupon measured post mortem with, e.g., profilometer analysis.

To evaluate the robustness of the method, a round-robin study was initiated with 12 international groups testing four glass composition under various pH/temperature conditions.

With the method proving useful for this application and showing strong potential for use as a bulk measure of glass corrosion, we are attempting to establish a consensus standard procedure recognized by ASTM International. Naturally, applications of the method to other fields of mineralogy and geochemistry are encouraged.

Poster

Topic: 1.8 Minerals and Mineral Properties

Quantification of radiation damage in zircon and other accessory minerals using rare-earth element μ -photoluminescence spectroscopy

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Many accessory minerals, i.e., zircon, incorporate variable amounts of actinides, whose radioactive decay creates structural defects in their crystal structures. The increased susceptibility of radiation-damaged zircon to chemical alteration or aqueous leaching is of enormous importance as these processes may bias results of chemical and isotopic age determinations. Here, we present a new concept based on the luminescence emission of REE³⁺ that provides an estimate of the amorphous fraction from laser-induced PL measurements using state-of-the-art confocal spectrometers with spatial resolution in the μm -range. A careful investigation of PL spectra from self-irradiated zircon samples from Sri Lanka and Mt. Malosa (Malawi) reveal that the Dy³⁺-luminescence emission in zircon is basically a superposition of emissions from Dy ions in various, structurally different sites. The relative integrated area of a fitted model spectra from an amorphous reference sample in relation to the full integrated area of the obtained emission gives a good estimate of the amorphous fraction present in the probed sample volume. This opens up the possibility to investigate the accumulation of radiation damage in single crystals of zircon in great detail and give rise to direct comparison with damage accumulation in heavy ion irradiation experiments.

Acknowledgments

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Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Dissecting the Sadisdorf Sn-W-Li vein and greisen system

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The Sadisdorf Sn-W-Li-Cu prospect, Germany, comprises magmatic-hydrothermal greisen and vein-style mineralization associated to a small alkali-feldspar granite porphyry. Petrographic and fluid inclusion data across the full extent of the deposit is used to understand the temporal and spatial evolution of the mineral system and the key factors controlling ore formation.

Four mineral associations have been recognized from proximal to distal to the intrusive stock. These are hosted within quartz-mica veins or greisen bodies: 1) oxide-dominant cassiterite-wolframite-molybdenite association, 2) cassiterite-(stannite) associated with Cu-Zn-Pb-As sulfides mixed association, 3) sulfide-dominant chalcopyrite-sphalerite-galena-arsenopyrite-tennantite-pyrite association, and 4) late-stage fluorite veins and cavity infill.

Fluid inclusions (FI) in quartz, topaz, cassiterite and sphalerite consist of H₂O-NaCl or H₂O-NaCl-CO₂±CH₄ fluids. Irrespective of association most FI show the same range in homogenization temperatures (Th; 202-420°C) and salinities (0-13 wt.% NaCl eq.). FI hosted by late-fluorite, however, are marked by lower Th (<269°C) and salinities (0-5 wt.% NaCl eq.).

Results imply that the ore fluid was a low-salinity and high-temperature vapor-rich fluid. Despite the distinct mineralogical zoning within the system, significant spatial variations of temperature or salinity could not be identified. Hence, we propose that zoning is a result of systematic variations in oxygen fugacity and/or availability of reduced sulfur along the fluid flow path, either attributed to consumption of oxygen by early oxides, fluid-rock interaction and/or potential volatile loss. Conversely, the lower salinity and temperatures of the late fluorite association reflects the dilution and cooling of fluids with time and likely the ingress of meteoric water into the system.

Poster

Topic: 7.3 Assessment of the Earth System through Micropaleontology

Temperature calibration for high Mg-calcite planktic Foraminifera shells from the Gulf of Aqaba

Noy Levy^{1,2}, Adi Torfstein^{2,3}, Ralf Schiebel¹, Natalie Chernihovsky^{2,3}, Klaus Peter Jochum¹, Ulrike Weis¹, Brigitte Stoll¹, Gerald H. Haug^{1,4}

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Hypersaline, oligotrophic seas have been shown to accommodate planktic Foraminifera (PF) with enriched Mg/Ca in their calcareous shells, compared to other marine environments. Although Mg/Ca is a widely used proxy applied as a paleothermometer, its systematics in extreme hypersaline systems is not well understood.

We measured element ratios using LASER ablation ICP-MS on the tests of the two abundant PF species, *Globigerinoides ruber albus* and *Turborotalita clarkei*, obtained from monthly resolved time series sediment traps at various water column depths in the northern part of the GOA.

Globigerinoides ruber albus shows a positive relationship between Mg/Ca and surface water temperatures of the surface mixed layer down to 60 m water depth. Although *T. clarkei* does not show the same positive relationship, it exhibits high Mg/Ca during water column mixing (March–April) possibly reflecting the movement of two water masses in the water column.

Using common calibration equations (Anand et al., 2003; Kisakürek et al., 2008; Gray et al., 2018), the high-Mg (5–25 mmol/mol) provided higher than measured in-situ (IS) ambient seawater temperatures ($T_{Mg/Ca}$ and T_{IS} , respectively). The high salinity at the GOA (>40) is assumed to be the main reason of the high shell-bound Mg.

Comparing surface dwelling *G. ruber albus* versus subsurface dwelling *T. clarkei* may facilitate reconstruction of the absolute and relative seasonal development temperature and surface water stratification. We suggest that species specific Mg/Ca-T calibrations for the GOA provide more accurate regional palaeoceanography and paleoclimate reconstruction of hypersaline environments.

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

In-situ sulfur and lead isotope evidence for Eoarchean crustal recycling in southern West Greenland peridotites

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Previous bulk sulfur isotope measurements of Eoarchean peridotites from south of the Isua Supracrustal Belt in southern West Greenland have revealed evidence for the presence of recycled surface material in the form of nonzero $\Delta^{33}\text{S}$ values [1]. In order to confirm these results, identify potential heterogeneity related to multiple sulfur sources, and confirm the Eoarchean origins of the sulfides in these rocks, we combined petrography and mineral chemistry with *in-situ* multiple sulfur and lead isotope analyses of sulfide minerals via SIMS. Sulfides measured by SIMS were found to be composed primarily of pentlandite and pyrrhotite, with some pentlandite-like compositions consistent with horomanite, which is crystallographically distinct from pentlandite. Our *in-situ* isotope results confirm the existence of predominantly sediment-derived (positive $\Delta^{33}\text{S}$) material recycled from Earth's surface in these rocks. Average SIMS $\Delta^{33}\text{S}$ results for measured samples were generally in good agreement with previously measured bulk rock data. The lead isotope compositions confirm an Eoarchean age of the sulfides and show the typical high- μ signature that is observed in other Eoarchean rocks from the area [2]. We observe that highly unradiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ isotope ratios in some sulfides plot close to the least radiogenic Pb isotope compositions measured in galenas from Isua.

[1] Lewis et al. (2022) EGU 22-5226

[2] Kamber et al. (2003) CMP 145, 25-46.

Poster

Topic: 8.1 Geosciences and Waste Management

Thermodynamic investigation of the Li₂O-MnO system in a certain composition region relevant for slag tailoring in the field of lithium-ion battery (LIB) recycling

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New developments of energy-efficient recycling processes and systems for LIB recycling are required from the perspective of resource circulation, raw material supply and sustainability. One promising approach is based on a combined pyro- and hydrometallurgical treatment. However, tailoring respective slag compositions and processing conditions is a challenging task in terms of increasing recycling efficiency. It requires a fundamental understanding of the phase development in the slag. For this, thermodynamic data and models are needed to predict phase formation and fractions under certain compositions and solidification conditions. The influence of manganese in LIB slag systems is not fully understood. An important base system is the Li₂O-MnO system, for which no thermodynamic model-compared data are available in the literature that are in a composition range relevant for LIB slags. In this work, the Li₂O-MnO system is studied thermodynamically. Different compositions of Li₂O-MnO in a LIB relevant slag composition field are synthesized and investigated with respect to their caloric and thermal properties with STA measurements under respective solidification conditions, such that solid-liquid transitions, as well as specific heat capacities of the mixtures, are obtained. Based on the experimental data gained in this study, model parameters of the modified quasichemical model (MQM) are optimized in the CALPHAD framework, such that the liquid phase of this system can be modelled thermodynamically for several compositions. This first survey contributes to a deeper understanding of the influence of manganese on the phase formation during solidification in lithium-containing systems.

Poster

Topic: 7.1 Geo-Biosphere interactions through space and time: new analytical and experimental approaches to the fossil record

Fossilization of Triassic marine reptile bones from southwest China – bone diagenesis at elevated temperature

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The preservation of fossils over long periods of geological history usually has special characteristics, and the specific conditions for successful fossilization have not been established yet. Triassic bones from SW China are characterized by an exceptionally broad variation in the style of preservation. This region presents a perfect natural lab for the study of conditions advantageous for bone preservation. Twenty-five specimens of marine reptiles from the Middle to Late Triassic black shales were sampled and examined in petrographic thin sections, by Raman spectroscopy and wavelength-dispersive X-ray spectroscopy. Our results revealed evidence that the bones were heated, possibly by hydrothermal fluids or by regional geological events, and we observed fluorite in fossil bone for the first time. We discriminate five stages of bone alteration: 1) no alteration beyond diagenetic mineral precipitation in the bone porosity; 2) weak alteration of apatite and migration of kerogen from the shale into the fossil bone; 3) formation of authigenic fluorite needles; 4) Recrystallization of bone apatite to idiomorphic apatite while bone structure is still present; 5) complete loss of bone structure and replacement by idiomorphic apatite. Systematic carbon Raman thermometry returns temperatures up to 150-180°C, indicating that loss of histological information might be linked to temperatures near to low-grade metamorphism. This study provides reference data for different stages of bone alteration, which is important for the study of bone diagenetic processes in dependence of higher than near-surface temperatures.

Poster*Topic:* 3.2 Composition and evolution of deep planetary interiors**Complex electronic, magnetic, and structural transformations in FeO****Xiang Li¹, Elena Bykova^{2,4}, Georgios Aprilis^{2,3}, Denis Vasiukov^{2,3}, Stella Chariton², Valerio Cerantola⁵, Maxim Bykov², Anna Pakhomova⁵, Fariya Akbar², Elena Mukhina⁶, Davide Comboni⁵, Catherine Mccammon², Aleksandr Chumakov⁵, Carmen Sanchez-Valle¹, Leonid Dubrovinsky², Ilya Kupenko¹**¹University of Muenster, Germany; ²Bayerisches Geoinstitut (BGI), Germany; ³Laboratory of Crystallography, Material Physics and Technology at Extreme Conditions, Universität Bayreuth, Germany; ⁴Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany; ⁵ESRF – The European Synchrotron (ESRF) France; ⁶KTH Royal Institute of Technology, Sweden

Iron oxides are important materials for Geoscience but also for basic science and applied technologies (Kupenko et al., 2019). Iron monoxide is likely to be the final constituent of the evolution of subducted banded iron formations and might be a source of the low-velocity zones at the Earth's core-mantle boundary (Dobson and Brodholt, 2005). The stability and high-pressure properties of Fe_xO could, thus, determine the fate of banded iron formations and their potential role in processes in Earth and planetary interiors, including controls on redox cycles.

Fe_xO has the NaCl (B1) structure at ambient pressure and temperature and transforms into rhombohedral distorted-B1 phase (rB1) at about 16 GPa. A further transition from a rhombohedral rB1 phase to a hexagonal B8 phase has been proposed at 74 GPa and 900 K (Fei and Mao, 1994). Although numerous studies were focused on the investigation of the electronic and magnetic properties and phase diagram of Fe_xO, information on the Fe²⁺/Fe³⁺ interplay, magnetic and structural coupling of Fe_xO at high pressures and high temperature are very limited.

We will present our investigation on the pressure dependence of the electronic, magnetic and structural properties of Fe_xO by means of Synchrotron Mössbauer Source spectroscopy and Single-Crystal X-ray diffraction with diamond anvil cells up to 94 GPa and 1200 K. We will discuss the interplay between Fe²⁺ and Fe³⁺ and its effects on the electronic and magnetic properties of Fe_xO and their potential role in the mineralogy, chemistry, and physics of the Earth's deep interior.

Ramdohr-Poster

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Microstructural investigations of the interaction between embedded fuel particles and Portland cement clinker

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In view of current climate and energy policies, the cement industry is striving to save emissions and is increasingly using alternative fuels (AF) for the clinker burning process. AF are generally more coarse-grained and have a higher probability to fall incompletely burned onto the clinker bed, where they become embedded and can lead to changes in the material by locally causing reducing conditions. However, the qualitative and quantitative understanding of relationships between fuel particle sizes and the resulting material properties of the clinker is still limited. Here, we show experimentally that local reducing conditions can indeed lead to the reduction of iron and thus to local changes of the phase assemblage. The altered oxygen partial pressure within the pore volume of the sample also causes a brown coloration of the clinker. The extent of the changes was found to depend on the fuel particle size and the residence time of the embedded fuel particles in the clinker bed in the kiln. The new qualitative and quantitative data enable the optimization of the clinker burning process, which in turn can lead to an increasing use of AF in the future.

Poster

Topic: 3.1 Novel isotopic insights into high-temperature geochemical processes

Potassium isotope systematics in ocean island basalts from Madeira (East Atlantic) imply recycling of distinct portions of subducted oceanic crust

Haiyang Liu^{2,3}, Ying-Yu Xue^{2,3}, Jörg Geldmacher¹, Uwe Wiechert⁴, Tinggen Yang^{2,3,5}, Fanfan Tian^{2,3,5}, Hai-Ou Gu⁶, He Sun⁶, Kun Wang⁷, Wei-Dong Sun^{2,3,5}

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Subduction of oceanic lithosphere is widely considered as the primary cause of mantle heterogeneity as reflected by the chemical variation of ocean island basalts. However, the fate of deeply subducted oceanic lithosphere (i.e., remaining intact, getting segmented or completely destroyed and intermixed with ambient mantle) is still largely unknown. Based on trace element and radiogenic isotope systematics, it has been suggested that the geochemical difference of shield and post-erosional stage lavas of the volcanic Madeira archipelago reflects recycling of different portions of subducted lithosphere (e.g., Geldmacher and Hoernle, 2000, *EPSL* 183; Gurenko et al. 2013, *Lithos* 170-171). Accordingly, the geochemical composition of the shield stage magmas reflects altered upper oceanic crust, while the isotopically less enriched post-erosional magmas preferentially stem from less-modified, lower crustal/lithospheric mantle portions of the recycled slab. New, high precision potassium ($\delta^{41}\text{K}$ of -0.75‰ to -0.50‰) and oxygen ($\delta^{18}\text{O}$ of 4.90‰ to 5.21‰ in olivine phenocrysts) isotope data from Madeira lavas support this model. Subduction dehydration can cause large K isotope fractionation in the upper, seawater-altered parts of oceanic crust resulting in lighter K isotopes (lower $\delta^{41}\text{K}$) in ocean island basalts containing such material. The measured $\delta^{41}\text{K}$ represents the lowest range among oceanic basalts published so far and overlaps with obducted eclogite, indicating the involvement of dehydrated oceanic crust. The correlation of light K with light O and enriched radiogenic isotope ratios supports the model that Madeira's magma source contains different portions of subducted oceanic crust, which were preserved over millions of years without significant intermixing.

Poster

Topic: 6.3 Fractionation of metal(loid) stable isotopes during low-temperature Earth surface processes

High-precision Cd isotope analysis of soil and rock by double spike MC-ICP-MS

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Cadmium (Cd) is a trace element on Earth and causes health problems to humans. A monitoring of the Cd level of, for example, arable soil is therefore of utmost importance. Even though Cd isotopes are a valuable proxy for such a monitoring, the low concentration of Cd in soil and rock challenged its determination hitherto. Thus, here we developed a novel high-precision Cd isotope measurement method for soil and rock samples. First, we developed a one-step anion chromatography method using micro-columns. Second, we developed a MC-ICP-MS method using double spike approach to correct for instrumental mass-dependent isotope fractionation. Parameters affecting the precision and accuracy of the Cd isotope composition ($\delta^{114/110}\text{Cd}$) were systematically tested. These tests included molarity and concentration mismatches between purified samples and the bracketing standard NIST SRM 3108, and the variation in double spike and sample ratio. We also evaluated potential mass biases caused by molecular and isobaric interferences. The long-term external precision for $\delta^{114/110}\text{Cd}$ is better than $\pm 0.05\text{‰}$ (2 SD). Cd isotope compositions of fifteen international reference materials were determined, including soils and igneous rocks of different Cd concentrations and a manganese nodule. The $\delta^{114/110}\text{Cd}$ values of the reference materials ranged from $-0.25 \sim 0.63\text{‰}$ for soil samples, and from -0.20 to 0.10‰ for rock samples. The large variations in $\delta^{114/110}\text{Cd}$ in soils and igneous rocks suggest the application of Cd isotopes to gain more detailed insights into magmatic processes and the biogeochemical cycle of Cd in terrestrial ecosystems.

Lecture

Topic: 8.1 Geosciences and Waste Management

The Effect of Mineral Dissolution-Precipitation Reactions on the Diffusivity of Porous Media: Innovative Experiments & Reactive Transport Modelling

Mara Iris Lönartz, Jenna Poonosamy, Yuankai Yang, Guido Deissmann, Dirk Bosbach

Institute of Energy and Climate Research (IEK-6) Nuclear Waste Management and Reactor Safety, Forschungszentrum Jülich GmbH, Germany

A reliable assessment of the evolution of geological repositories for radioactive wastes requires a profound understanding of coupled hydrogeochemical processes across various temporal and spatial scales. At barrier interfaces, chemical and thermal gradients promote mineral precipitation reactions, reducing the porosity and potentially leading to clogging of diffusion-controlled porous media [1]. Recent experiments and pore-scale modelling investigations conducted to benchmark continuum-scale reactive transport models revealed the deficiency of conventional and revised porosity-diffusivity relationships based on Archie's law to account for changes in effective diffusivity of evolving porous media [1-2]. To identify key parameters at the pore-scale that might explain the discrepancies between experimental and modelling studies, we designed a "lab-on-a-chip" approach for counter-diffusion precipitation experiments, combining time-lapse optical microscopy and *operando* Raman spectroscopy. As the 2D microfluidic pore network became clogged, the transport of deuterium through the evolving microporosity of the precipitated celestine was visualized by Raman imaging, demonstrating the dynamic nature of porosity clogging. Pore scale simulations were conducted on the 2D images of the evolving pore network to determine its effective diffusivity. The application of a revised porosity-diffusivity relationship improved the agreement between modelling results and experimental observations, but also strongly emphasised the need for further pore-scale investigations. Our innovative combination of microfluidic experiments and pore-scale modelling opens new possibilities to validate and identify relevant pore-scale processes and provides data for upscaling approaches to derive key relationships for continuum-scale reactive transport simulations.

[1] Chagneau et al. (2015), *Geochem. Trans.* 16, 13.

[2] Deng et al. (2021), *Water Resour. Res.* 57(5), 1-16.

Lecture

Topic: 1.7 Experimental Petrology and Geochemistry

From natural observations to an experimental investigation of a potential miscibility gap between Fluorapatite and Fluorbritholite-(Ce)

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Evidence for a miscibility gap between fluorapatite (FAP) and fluorbritholite-(Ce) (FBri) has been observed in various natural occurrences, inferred by significant compositional gaps between Ca + P (FAP) and REE + Si (FBri) chemical components.

This presentation delves into the observation of coupled exsolution microtextures of FAP in FBri and vice versa at the Rodeo de los Molles REE Prospect, in Argentina. The existence of a miscibility gap as a function of temperature between FAP and FBri was explored via a series of simple experiments performed at 500°, 600°, 700°, and 1100 °C and 200 MPa. A series of combinations involving synthetic CePO₄ or FAP and CeF₃ plus H₂O and SiO₂ and a series of reactants, i.e. Na₂Si₂O₅, NaOH, NaF, CaF, KOH, and Ca(OH)₂ was utilized. Experiments involving CePO₄ and Na₂Si₂O₅ and NaOH were the most reactive, while experiments involving KOH and Ca(OH)₂ produced neither FBri nor FAP. This suggests that Na might play a major role in the formation of FBri.

On a T vs FAP-FBri composition plot, the miscibility gap of natural samples is situated between FAP₉₂FBri₈ and FAP₃₀FBri₇₀ at T below 350 °C. At T above 350 °C the gap narrows down to FAP₈₀FBri₂₀ and FAP₆₈FBri₃₂. In the experiments, FBri-(Ce) shows a continuous compositional range from FAP₇₈FBri₂₂ to FAP₂₈FBri₇₂ for T = 500 °C, FAP₇₆FBri₂₄ to FAP₅₂FBri₄₈ for T = 600 °C and FAP₈₀FBri₂₀ to FAP₆₀FBri₄₀ for T = 700 °C. This indicates that there is no miscibility gap ≥ 500 °C between fluorapatite and fluorbritholite-(Ce).

Lecture

Topic: 9.4 Chemical sediments and mineral deposits in basins: archives of paleoclimatic, hydrogenetic, biogenic, hydrothermal, and diagenetic, processes throughout Earth's history

Superimposed diagenetic and hydrothermal processes – the key to high grade Zn mineralization in sedimentary basins

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Clastic-dominant (CD-type) deposits typically comprise huge base metal and sulfur anomalies ($> 10^6$ tons) that are concentrated in a small number of Proterozoic and Phanerozoic basins. Some Phanerozoic deposits also contain barite in the succession hosting mineralization. Traditional models invoke sedimentary exhalative (SEDEX) processes to explain the formation of CD-type deposits, whereby metalliferous hydrothermal fluids were vented into a euxinic (H_2S -bearing) water column, resulting in syn-sedimentary sulfide precipitation. Arguments for SEDEX activity are primarily associated with stratiform ore textures and highly positive $\delta^{34}S$ values in pyrite. Recently, however, two Late Devonian CD-type deposits at Macmillan Pass (Selwyn Basin, Canada) have been the focus of 3 new approaches aimed at understanding how seawater paleoredox, diagenesis, and hydrothermal processes were interconnected: 1) Fe and Mo based paleoredox proxies provide evidence that anoxic non sulfidic (ferruginous) conditions were dominant during host rock deposition. 2) In situ $\delta^{34}S$ values from pyrite and barite can be explained by diagenetic processes associated with the sulfate methane transition zone. 3) Detailed petrographic and fluid inclusion studies have described a comprehensive mineralogical paragenesis, whereby the introduction of hot ($300^\circ C$) hydrothermal fluids into the shallow subsurface (<1 -km depth) resulted in the thermal degradation of organic matter, barite dissolution, and sulfide mineralisation. Importantly, the Macmillan Pass deposits represent subseafloor replacement systems in which there was potential for positive feedbacks between diagenetic and hydrothermal processes, resulting in highly efficient ore-forming systems. These results are also relevant to other Phanerozoic basins in which stratiform barite deposits are spatially associated with sulfide mineralization.

Poster*Topic:* 1.3 Bridging length and time scales in the modelling of geomaterials**A normal to incommensurate phase transition in malayaite, CaSnOSiO₄****Thomas Malcherek¹, Michael Fischer², Boriana Mihailova¹, Carsten Paulmann¹**¹Universität Hamburg, Germany; ²Universität Bremen, Germany

Malayaite, the tin analogue of titanite, has been shown to develop an incommensurately modulated phase with a modulation vector of $q=0.26b^*$ at a temperature of 20K [1]. The occurrence of the modulated phase confirms density functional perturbation calculations of the phonon dispersion, indicating phonon softening in this particular range of k-space. Single crystal X-ray diffraction experiments at beamline P24 of PETRAIII/Desy at variable temperatures between 20 and 100K indicate a transition temperature of $48\pm 3K$ for the corresponding normal to incommensurate phase transition. On approaching the phase transition temperature from below, the modulation vector remains almost constant, while the intensity of the satellite diffraction maxima decreases. The crystal structure transforms from the $C2/c(0b0)s_0$ superspace group to $C2/c$. The phase transition is discussed in relation to further anomalies observed between 90K and 400K by single crystal X-ray diffraction and Raman spectroscopy and in particular in relation to mode softening of a low frequency Bg-mode involving Ca-motion parallel to [001]. This mode softening is observable over the entire temperature range between 400K and 90K and culminates in the modulated low temperature structure of malayaite, as evidenced by the corresponding instability observed in the calculated phonon dispersion.

[1] Malcherek T., Paulenz B., Fischer M., Paulmann C. (2020) Acta Cryst. B76, 316-321

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

 $^{146,147}\text{Sm}$ - $^{142,143}\text{Nd}$ systematics of the Acasta Gneisses: New insights on the formation of Earth's oldest rocks

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Reconstructing the earliest evolution of the silicate Earth remains a major geological challenge because of the scarcity and incomplete preservation of rocks older than 3.8 Ga. Isotope variations produced by short-lived radionuclides, such as ^{146}Sm , have the potential to trace the early formation of distinct chemical reservoirs within the silicate Earth, and at the same time can also help decipher the petrogenesis of the oldest-preserved cratonic units.

Here, we present coupled $^{146,147}\text{Sm}$ - $^{142,143}\text{Nd}$ systematics of layered gneisses from the Acasta Gneiss Complex (AGC) in northwest Canada. In addition, U-Pb dates of zircon extracted from individual layers and whole-rock major and trace element data are used to constrain the emplacement ages of the gneiss protoliths and their petrogenetic history. Mafic and felsic layers yield average $\mu^{142}\text{Nd}$ values of +2.7 and -7.5 ppm (± 2.5 ppm, 2 S.D.), respectively, documenting the existence of both Hadean mantle and crustal components within the sources of the AGC. Within individual layers, zircon U-Pb data form bands along concordia suggesting ancient Pb loss, with major clusters at 3.5–3.6 Ga for the felsic layers and 3.65–3.75 Ga for one mafic layer. Using these ages, the felsic layers yield consistently negative $\varepsilon^{143}\text{Nd}$ values of about -5, while the mafic layers have near-chondritic $\varepsilon^{143}\text{Nd}$. Variations in $\varepsilon^{143}\text{Nd}$ and $\mu^{142}\text{Nd}$ are tightly correlated, suggesting correct age assignment and intactness of the long-lived ^{147}Sm - ^{143}Nd system since zircon crystallization. Thus, the studied samples likely record primary $^{142,143}\text{Nd}$ variations, implying that multiple sources were involved in the formation of the AGC protoliths.

Lecture

Topic: 11.2 Latest Achievements in Scientific Ocean and Continental Drilling

Sedimentology and sequence stratigraphy of the Aalenian from southern Germany

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Aalenian sedimentary deposits in southern Germany have accumulated in a shallow-marine shelf environment and are typically dominated by thick claystones and argillaceous siltstones, with increasing percentages of sand towards the top. The sedimentary evolution and paleoclimatic significance of these often poorly exposed deposits remain largely unexplored. Here we present a suite of high-resolution x-ray fluorescence (XRF) core scanning data from southern Germany to identify Transgressive-Regressive cycles during the Aalenian stage. Results are based on three scientific drill cores that have been analyzed with an Avaatech XRF Core Scanner at a 10 mm sampling interval, an energy of 10 keV and a current of 500 μ A to measure element intensities ranging from aluminum through iron. Resulting trends in elemental ratios that are indicative for subtle grain-size variations have been used to reconstruct shoreline trajectories and establish a sequence stratigraphic framework for the thick and largely homogenous, lower Aalenian Opalinuston Formation.

Lecture*Topic:* 4.3 The role of fluids in metamorphic and metasomatic reactions**The mysteries of jadeite jade, a monitor of subduction-zone fluids****Walter Viktor Maresch¹, Andreas Hertwig², Hans-Peter Schertl¹**¹Ruhr-University Bochum, Germany; ²Ruprecht-Karls-University Heidelberg, Germany

Jadeite jade is the rare variety of jade at present known only from 20 localities of high-pressure, subduction-zone serpentinite mélangé. Jadeite jade is tough, hard and brilliant when polished. It has been of special mystic meaning in Mayan and Chinese cultures for up to 8000 years. Much discussion surrounds jadeite-jade genesis: origin by direct precipitation from a high-pressure aqueous fluid? Or metasomatism of a precursor rock like trondhjemite/plagiogranite? Present evidence suggests both processes are actually closely related; densification and decrease in volume during reaction of plagiogranite to jadeite jade is a key factor. Until recently, the plagiogranite protoliths were considered to be of mid-ocean-rift origin and brought into subduction zones by cold descending oceanic crust. Jadeite jade was assumed to be mainly formed at $T < 500^{\circ}\text{C}$. Recent work (e.g., Angiboust *et al.*, *J. Metam. Geol.*, **39**, 473-500, 2021) indicates a surprising second source: Adakitic melting of basaltic crust at depth can produce trondhjemite intrusions that initiate the formation of jadeite jade at high temperatures as well. Since the 1950's, jadeite is known to be a high-pressure mineral, but only in silica-saturated environments. Thus it is enigmatic why quartz is rarely found in jadeite jade (Harlow *et al.*, *Short Course Handbook, Min. Ass. Canada*, **44**, 305-374, 2014). Recent studies (e.g., Hertwig *et al.*, *Russ. Geol. Geoph.*, **62**, 496–524, 2021) indicate the answer. Remnants of quartz are found as tiny, inconspicuous relict inclusions in jadeite crystals, but quartz has been removed from the rock matrix by later desilication.

Poster

Topic: 1.6 Probing (bio)geochemical reactions at mineral interfaces using micro- to nanoscale techniques

Latest analytical developments of the SwissSIMS Lausanne

Johanna Marin Carbonne¹, Anne-Sophie Bouvier¹, Elias Bloch¹, Daniela Rubatto²

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The SwissSIMS is a national facility equipped with a Cameca 1280 HR2 installed at the University of Lausanne, which is open to all scientists. Here we present the latest analytical developments that allow the measurement of smaller mineral grains and of high resolution depth profiles. Depth profiles of Ti concentration in experimental zircon have revealed that diffusion parallel to the crystallographic c-axis is 4-5 order of magnitude faster than perpendicular to the c-axis. This study has important implications for Ti in zircon thermometer. We will also present latest results on Cl isotope in melt inclusions that provide new insights on element recycling in subduction zones. Fe isotope compositions of micropyrates from ancient and modern microbialites can be thus used as a biosignatures of Fe microbial reduction but also emphasize that pyrite formation record very local conditions. Perspectives on future analytical developments at the SwissSIMS will be also provided.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Micropyrrite in stromatolite : a time capsule of ancient metabolisms

Johanna Marin Carbonne¹, Marie Noelle Decraene¹, Juliette Dupeyron¹, Julien Alleon¹, Virgil Pasquier¹, Nicolas Olivier², Christophe Thomazo³

¹University of Lausanne, Switzerland; ²Magma and Volcanoes, University of Clermont Ferrand, France; ³Biogeosciences, University of Burgundy, France

The identification of ancient microbial signatures preserved in the geological record is crucial for understanding life evolution during the Early Earth. Stromatolites and microbialites are considered among undisputable oldest trace of life but their biogenicity is sometimes disputed. Archean stromatolite contain small sulfides hereafter designed as micropyrrite, often enclosed with organic material, that can be formed either by abiotic processes (reaction between H₂S and Fe(II)) or by metabolic activity like microbial sulfate reduction (MSR) or dissimilatory iron reduction (DIR). Iron and sulfur isotope compositions offer the most direct means to track the biogeochemical cycling of these elements through time, but their joint use as biosignatures of specific metabolic activity has been relatively limited to date. We have developed a microscale approach using correlative microscopy and SIMS and NanoSIMS analyses that allow to document Fe and S isotope composition at the mineralogical scale of the pyrite grains. Here we will present results obtained on the Tumbiana Formation (2.7 Ga, Western Australia), on the Buck Reef chert (3.41 Ga, basal member of the Kromberg Formation, South Africa), and on the Moodies Group (3.2 Ga, South Africa). Our approach allows to decipher the post-depositional metasomatic influence from the primary microbial signatures inherited during diagenesis. Our results also highlight that pyrite formation record very local conditions at the sediment-interface or at the microbial mats. Our results demonstrate the existence of microbial iron respiration as early as 3.26 Gyr ago, providing new time calibration of the tree of life for this type of metabolism.

Lecture

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

Unraveling orogenic processes through U–Pb garnet petrochronology

Horst Marshall¹, Gerdes Axel¹, Millonig Leo¹, Albert Richard¹, Beranoaguirre Aratz^{1,2}, Hezel Dominik¹

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Orogenic processes typically proceed through a number of tectonic stages in which rocks are subjected to burial, heating, exhumation and cooling. The rates and durations of the prograde stages are commonly poorly constrained, because the minerals typically used for age dating mostly form late in the process during decompression and the onset of cooling, or they possess closure temperatures that are lower than the metamorphic peak temperatures of metamorphism.

In-situ garnet U–Pb geochronology is an emerging technique that has the potential of unraveling the prograde- and peak-metamorphic history and may thus be the ideal petrochronometer that is needed to investigate mountain-*building* processes, where most other chronometers only record the collapse and exhumation of orogens.

At FIERCE, we perform garnet laser-ablation MC-ICPMS U–Pb geochronological analyses of metamorphic garnet with typically <0.1 µg/g U. Distinct growth zones of garnet from polymetamorphic granulites that experienced ultra-high temperature (UHT) metamorphic conditions above 900 °C were analyzed.

We find that ages of older garnet growth zones are not reset during subsequent UHT-metamorphism, and conclude that the U–Pb system in garnet has a closure temperature at UHT conditions that may only be rivaled by zircon. Consequently, garnet U–Pb ages from crustal metamorphic rocks have to be interpreted as crystallization ages. LA-ICPMS garnet U–Pb dating thus complements the information obtained from other geochronometers, as it provides accurate and precise insight into the prograde to peak metamorphic *P–T–t* history of (poly)metamorphic terrains and the formation of orogens.

Lecture

Topic: 5.6 Natural archives as recorders of past climate and environmental conditions – processes, methods and applications

Millennial hydrological variability during the MIS3-2 in a lowland freshwater ecosystem of the northern Neotropics

Luis Rodrigo Martínez Abarca¹, Michelle Abstein¹, Frederik Schenk², Liseth Perez¹, Thorsten Bauersachs³, Antje Schwalb¹

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We inferred environmental changes in the northern Neotropics using geochemical and mineralogical data from the sediment record of Lake Petén Itzá (Guatemala), covering the Marine Isotope Stages (MIS) 3 (57-29 cal ka BP) and 2 (29-15 cal ka BP). Our study focused on past changes in runoff, lake evaporation, organic matter sources and changes in redox conditions associated with water-level variations. Wet conditions, higher primary productivity and anoxic bottom waters were inferred for MIS3. The transition from MIS3 to MIS2 (39.0-23.0 cal ka BP) was characterized by increasing lake evaporation and oxic bottom waters, possibly associated with lower water-levels. These conditions reversed during the Last Glacial Maximum (23.0-18.0 cal ka BP) when our data suggest higher runoff and lake productivity and a return to anoxic bottom waters as a result of rising water-levels. Our high-resolution geochemical record reveals the presence of short-term climate stages globally known as Heinrich Stadials (HS), Greenland Interstadials (GI) and Greenland Stadials (GS). The Lake Petén Itzá record indicates that HS and GS were generally dry, while the GI were characterized by higher runoff and wet conditions. This variability in runoff correlates with shifts in the average position of the Intertropical Convergence Zone during the Late Pleistocene. The northern Neotropics are strongly affected by current global warming; our data provides important information regarding the potential future behaviour of the northern Neotropics both in long-term and short-term climate change scenarios.

Poster

Topic: 10.1 Geoscience Communication and Education

Three years communicating geosciences in social networks: Divulgacion Terrologa

Luis Rodrigo Martínez Abarca¹, Sandra García León²

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Social networks have become important communication bridges between the scientific community and society. For this reason, on June 11, 2019, “Divulgacion Terrologa” was created. This is a Facebook and Instagram site in Spanish whose objective is to accurately and clearly disclose the different processes that intervene in the dynamics of our planet. In this initiative, periodic publications are made about the different terrestrial spheres. In addition, we promote the research work of undergraduate and postgraduate geoscientists in the “Young Researchers Wednesday” section. Likewise, in the “Geoscientists in Action” section, we disseminate the work activities of geoscientists from outside the academy. On Facebook as of May 31, 2022, about 360 posts have been made. Total followers are 5200, however, the average number of people reached per post is 2200. The most viewed post reached nearly 60 thousand views. 49% of the followers are women while 51% are men. The followers of the page reside in Latin America, the United States and Europe. Our publications have been translated into English, French and German. The results obtained during this time suggest the importance of science communication in the imparting of Earth Sciences.

Poster

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Towards a more robust assessment of internal K-content for single-grain feldspar luminescence dating.

Linda Maßon, Svenja Riedesel, Anja Zander, Tony Reimann

University of Cologne, Germany

Accurate dose rate determination is essential in luminescence dating studies and when using feldspars, the internal K-content has to be considered. Until recently it was common practice to base the estimates for the internal content of ^{40}K and ^{87}Rb of feldspar extracts used for infra-red stimulated luminescence dating on literature values. However, in some regions of the world (e.g. Atacama, Java), feldspar extracts prepared for single-grain luminescence analyses exhibit a complex mineralogy affecting the reliable determination of the internal dose rate (e.g. Sontag-González et al., 2021). A proof of concept study on luminescence dating in the central Atacama Desert for example demonstrated that values suggested by literature overestimate the K-content of the luminescent feldspars (Zinelabedin et al., 2022).

Here we test and evaluate different methods to determine the K-content of feldspar grain separates and its impact on single grain luminescence dating. For a set of chemically and structurally different samples from various geological origins, we compare the labour-efficient determination of the K-concentration on 100 μg subsamples utilising a β -counter with two more time-consuming techniques (EDX, micro-XRF) measuring the K-content of the individual grains.

We test the validity of the time- and cost-efficient β -counter dose rate estimation procedure in comparison to more cost- and labour-intensive alternatives. We aim at establishing a methodological foundation for spatially-resolved and single-grain luminescence-based analysis of feldspar samples with the ultimate goal to investigate geomorphological processes on the μm -scale in the Atacama Desert.

References:

Sontag-González et al. 2021, QG 65, 101181.

Zinelabedin et al. 2022, QG 101341.

Lecture

Topic: 11.3 Young Scientist Session

Impact of Glaciation and Glacial Erosion on the Stress Field in Forearcs

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In the late Cenozoic, many mountain belts were glaciated and experienced enhanced glacial erosion. Glacial erosion modulates the topography of mountain belts, which alters the state of stress and can trigger a tectonic response. In the past decades, the interaction between glacial erosion and tectonics has received much attention, but the effects of glacial erosion on the stress field in forearcs of subduction zones remain poorly understood. Here, we use two-dimensional finite-element models to constrain the stress changes caused by glacial erosion. The models are generic but use a geometry that is adjusted to the subduction setting of the southern Andes, which were covered by the Patagonian ice shield throughout the late Cenozoic. We construct different models to evaluate how a reduction in mountain height, a shallowing of the trench depth due to trench sedimentation, the development of a broad central valley, and changes in surface slope in the high mountains influence the stress field. The preliminary results show that the different effects of erosion can have contrasting effects on the stress field. For instance, a lowering in mountain height and trench sedimentation tend to increase the compression, while a steepening of the surface slopes in the high mountains and the load of an ice shield reduce the compression. Our findings suggest that the effects of glacial erosion can cause complex modifications of the stress field that may support or suppress a tectonic response.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

Distribution and isotope fractionation of traces during carbonate mineral formation from amorphous precursors

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The formation of calcium carbonate from an amorphous precursor phase is a crystallization route selected by a large number of marine calcifiers. To date, however, only little is known about the fate of traces and their isotopes during the transformation process of the initial amorphous phase to the final crystalline product, although they are routinely used for environmental reconstruction. Here we report on our recent findings on the chemical and isotopic compositions of Mg and B in calcite and aragonite that formed via the crystallization of an amorphous phase precursor and we compare them with the results obtained during classical overgrowth experiments. During the formation of the amorphous precursor a weak Mg isotope fractionation occurs between the solid and aqueous phases, whereas the transformation of the precursor to the final crystalline product yields Mg isotope compositions that resemble near equilibrium values. This behaviour contradicts the strong kinetic effects that were reported earlier during calcite classical growth at low degrees of solution supersaturation with respect to this mineral. In the case of boron, which is commonly used as a pH proxy, the obtained results suggest that calcite formed at pH = 8.9 is in good agreement with the boron pH proxy and the presence of only borate ions in the solid. In contrast formation of calcite at pH=8.3 and aragonite deviate from the values measured earlier in overgrowth experiments but are in good agreement with the ab-initio calculations by Balan et al. (2018).

Balan et al. (2018) GCA 222,117-129.

Lecture

Topic: 6.1 Earth surface processes in extremely water-limited environments

New data on the formation of the enigmatic zebra stripes in the Atacama Desert – towards unravelling key mechanisms and time scales of geomorphic processes under extreme hyperaridity

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The most enigmatic hillslope forms in the hyperarid core of the Atacama Desert are the so-called zebra stripes, covering slopes between the coastal range and the pre-Andean cordilleras. They are defined as contour-parallel, lateral bands of loose angular gravels resting on hillslopes between 4° and 30°. While a previous study argued that they represent fossil evidence of overland flow, recent investigations documented a remarkable form-concordance with deposits from experiments on segregation-induced granular fingering, suggesting that dry granular flow may play a role in their formation. Here, we add new data on key mechanisms and time scales of geomorphic processes related to zebra stripe formation based on UAV-derived aerial photos, geomorphological and sedimentological investigations, different monitoring techniques, as well as terrestrial cosmogenic nuclide concentration measurements and OSL rock surface dating. OSL results show long exposure, no overturning, and inactivity at the northern, and Pleistocene/Holocene activity and clast overturning at the southern study site. ¹⁰Be and ²¹Ne measurements at this southern active site suggest downslope increasing TCN concentrations and clast transport on Pleistocene time scales and faster transport rates on steep slopes. While no stripe activity was detected during a Mw 5.4 earthquake, the monitoring results document clast overturning by freeze-thaw processes during a period of snow and frost in July 2019. This suggests a significant role of freeze-thaw processes in zebra stripe formation due to selective, long-term and subtle clast overturning and the evolution of the typical sorting pattern, potentially allowing for using zebra stripes as an indicator of paleo-climatic conditions.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

FID GEO: promoting cultural change towards Open Access and FAIR data in the German geoscientific community

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The rise of Open Science practices is impacting the entire scientific publishing culture. The transition to Open Access for text publications goes hand in hand with the growing demand to make scientific data and software available to the general public. The FAIR data principles play a key role in this, designed to make research and the underlying data easily findable, accessible, interoperable, and reusable for humans and machines. Geosciences data are as diverse as their content. They range from large real-time data streams of international observing networks to small data sets produced by individual researchers at their laboratories. Consequently, there need to be different strategies for data management and publication in which research data repositories can be important partners for the researchers.

The Specialised Information Service for Geoscience (FID GEO) is a DFG-funded project that is promoting a holistic approach of Open Science that includes scholarly literature, data, samples, and scientific software equally and pushes for their interlinkage. FID GEO has become an important player for connecting researchers, data repositories, information infrastructures, German geoscientific societies, and publishers. FID GEO actively provides data and text publishing services through its affiliated repositories GFZ Data Services and GEO-LEOe-docs, as well as on-demand digitization of printed geoscience literature and maps. In addition, FID GEO aims to inform the German-based geoscience community about all aspects of Open Science and FAIR data by bringing the discussions to the individual disciplines through various communication channels.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

New insights into the crust-mantle transition zone beneath fast-spreading mid-ocean ridges: the role of Cr-spinel composition.

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The formation of oceanic crust at mid-ocean ridges is one of the dominant processes in the chemical differentiation of our planet. Oceanic crust formed at fast-spreading ridges exhibits a relatively uniform seismic stratigraphy and is regarded as layered and relatively homogeneous in mineralogy. Because of the lack of natural in-situ exposures at the base of the crust of recent oceans, existing models on the geodynamics of the deep processes during crustal accretion have never been tested directly using natural samples. Using the CM1 and CM2 drill cores penetrating the Oman ophiolite sequence, the best analogue for fast-spreading crust on land, recovered by the ICDP Oman Drilling Project, we started a study combining experimental work and investigations on samples of the drill cores in order to shed light on the nature of this the poorly understood crust-mantle transition. The drill cores CM1 and CM2 cover the upper mantle harzburgites at the bottom, followed by a 90 m thick massive dunite layer with layered gabbros at the top. Ni and Mg# in olivine as well as Cr#, Mg# and trace elements in chrome spinel were analyzed by EPMA and fs-LA-ICP-MS. The data reveals a homogeneous harzburgite composition, followed by homogeneous dunite in the lower part and an upper dunite section showing decreasing Mg#, and therefore more differentiated compositions towards the top. We conclude that only the upper half of the 90 m thick dunite has a cumulative origin. The lower dunite section may be formed as a result of reactions with harzburgite.

Lecture

Topic: 10.1 Geoscience Communication and Education

Geoscientific teaching material for teachers and students

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In Germany, the geosciences are not part of the school curriculum as an independent teaching unit. At present, basic knowledge in the geosciences is only taught in mostly isolated geography lessons and occasionally also in the form of examples in physics or biology lessons. However, to deal with the upcoming global problems such as climate change, scarcity of resources or geohazards, which all are major geoscientific topics, it is becoming more and more important that geoscientific knowledge is taught on a broad level in school. In order to achieve this goal, in particular geography teachers must be given more qualified geoscientific training during their studies.

The first videos and accompanying texts and figures for a series of educational videos on the System Earth have recently become available on the DGGV website. Basic geoscientific knowledge shall be presented here in short videos in an easily understandable form. The videos are intended specifically for teachers in schools, but also for students and interested laypersons. Videos, texts and figures can be downloaded and used by teachers free of charge for teaching purposes.

The new video series has just started with its first 9 instructional videos that are already available for download. In the near future, many more videos and texts will follow, which should give a comprehensive overview of the System Earth.

Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

The behaviour of tin in skarns of the Variscan Erzgebirge – the Geyer skarn system as a case study

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This study focuses on the mineralogy and petrography of pro- and retrograde skarn stages at the Geyer Sn system in the Erzgebirge, Germany. These data are used to constrain how tin is distributed amongst silicate minerals and cassiterite, and how given tin-bearing minerals are related to the temporal fluid evolution. Skarns at Geyer are associated to comparatively thin (> 2 m) but laterally extensive marble layers and immediately adjacent mica schists that occur within meta-sedimentary successions of the Saxothuringian basement.

Prograde skarn stage I is characterized by diopside-rich skarnoids with locally reddish garnet. Prograde stage II comprises garnet-pyroxene skarns with massive greenish garnet. The early retrograde stage III is characterized by epidote and amphibole, whereas the late retrograde stage IV is associated with pervasive chloritization. Calc-silicates of stage I have low tin contents and discrete tin minerals are absent. In contrast, garnet of prograde skarn stage II contains up to 0.25 apfu and malayaite occurs locally. Early retrograde epidote and amphibole have elevated tin contents with up to 0.25 apfu and 0.4 apfu, respectively, whereas most of the cassiterite is associated with late retrograde chlorite of stage IV. The retrograde overprint is hence associated with a redistribution and possibly renewed introduction of tin and eventually results in the formation of cassiterite during the late retrograde stage. The observations imply that inheritance of Sn from meta-sedimentary host rocks is negligible. Sn mineralization also post-dates the contact metamorphism (skarnoid) and hence suggest that Sn is mainly introduced by the hydrothermal fluid.

Lecture

Topic: 2.2 From dust to planets

Accretion of Rocky Planetary Bodies: Chemical Constraints

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All rocky materials originating from small and undifferentiated bodies of the Solar System have similar and close to solar abundances of refractory elements and are depleted to various degrees in moderately volatile elements. This depletion correlates with the respective condensation temperatures of the elements. In contrast, the element abundance pattern in bulk silicate Earth (BSE) is different. Its depletion in the moderately volatile lithophile elements does not show a correlation with their respective condensation temperature, rather these elements show chondritic relative abundances.

The element pattern of BSE can be modeled as a mixture of three distinct components with different volatile element depletions and oxidation states. Component A is volatile-element depleted and strongly reduced; Component B has chondritic abundances of the refractory and moderately volatile elements and is highly oxidized; Component C has element abundances similar to carbonaceous chondrites. These components make up ~85%, ~15% and ~0.4% of BSE, respectively, and require a specific sequence of events by which they were added. The major part of the Earth accreted early under strongly reducing conditions during which it underwent metal-silicate differentiation. Addition of the oxidized and volatile-richer second component was followed by a second core formation under more oxidizing conditions by segregation of a sulfide melt. The last component was added as a “late veneer”. Combining this evolution of element abundances in BSE with constraints from U-Pb and Rb-Sr systematics suggest the combination of Component A with B occurred at 4.50 Ga and corresponds to the Moon-forming event.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

The behaviour of Sn and W at the magmatic-hydrothermal transition: Insights from natural and synthetic fluid inclusions

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Tin (Sn) and tungsten (W) have been established as strategic metals, whose resources are mainly related to highly evolved, volatile-rich granitic systems and related hydrothermal fluids. Their transport and enrichment results from a combination of melt- and fluid-driven processes. To evaluate the relative importance of these processes, we propose to combine the study of natural and synthetic fluid inclusions (FIs). Natural FIs occurring in early (associated with cassiterite) to late hydrothermal (associated with wolframite) quartz of the Argemela magmatic-hydrothermal system (Central Portugal) are mainly of aqueous (average $X_{H_2O} = 0.94 \pm 0.04$) L+V±S type. Raman spectrometry revealed an evolution from V-rich CO_2 - CH_4 - N_2 to L-rich CO_2 ± N_2 - CH_4 inclusions through the transition and graphite is present in several early inclusions, suggesting relatively reduced conditions and a potential inheritance from the source. In addition, and because further work is needed to understand the fluid/melt partitioning of Sn and W, several experiments were conducted at 700 and 800°C, 200MPa and variable fO_2 and salinities to synthesize FIs. A synthetic glass was produced to mimic the major element composition of the Argemela highly peraluminous intrusion and concentrations of W, Sn, P and Li were varied. Inclusion-free quartz were used to trap the fluids. First results prove the feasibility of the study. Microthermometry and LA-ICP-MS analyses are in progress for both natural and synthetic FIs.

Lecture*Topic:* 1.3 Bridging length and time scales in the modelling of geomaterials**Polarons in amphiboles: evidence from resonance Raman scattering and DFT calculations****Boriana Mihailova¹, Simone Bernardini^{1,2}, Naemi Waeselmann¹, Giancarlo Della Ventura^{2,3}, Wei Xu⁴, Augusto Marcelli^{3,5}, Jochen Schlüter⁶**¹Universität Hamburg, Germany; ²Università di Roma Tre; ³INFN Laboratori Nazionali di Frascati; ⁴Institute of High Energy Physics, Chinese Academy of Sciences; ⁵RICMASS; ⁶Mineralogisches Museum, Leibniz-Institut zur Analyse des Biodiversitätswandels

The properties of rocks are determined from the physical properties of minerals composing the rock, which in turn ultimately depend on the crystal phonon modes and electron density of states. Amphiboles ($AB_2C_5T_8O_{22}W_2$, $C_5 = M1_2M2_2M3$) are among the major hydrous-silicate mineral constituents of the lithosphere, whose structure consists of strips of 6-membered TO_4 -rings attached to MO_6 octahedra. To elucidate the atomistic origin of the rock conductivity observed in peculiar geological settings, we have studied single crystals of MFe -containing amphiboles from different subgroups by in situ high-temperature polarized Raman spectroscopy and density-functional-theory calculations of the electron band structure of grunerite ($^{A-}Fe^{2+}_2Fe^{2+}_5Si_8O_{22}(OH)_2$) as a model pure- $^MFe^{2+}$ amphibole [1]. Above a certain temperature resonance Raman scattering occurs, due to the formation of small polarons arising from the coupling between polar optical phonons and electron transitions within $Fe^{2+}O_6$ octahedra, the mobility of which through the mineral bulk is strongly anisotropic. The FeO_6 -related polarons coexist with delocalized H^+ , that is, at elevated temperatures typical of lithosphere Fe-bearing amphiboles are conductive and exhibiting two types of charge carriers: electronic polarons and H^+ cations, regardless of the oxygen fugacity. However, the presence of external oxygen favours the ejection of H^+ and electrons from the crystal. Therefore, at lithospheric temperatures Fe^{2+} -bearing amphiboles can be in a unique metastable state with an anisotropic surface-to-bulk gradient in the chemical potential. Same phenomena are expected for other rock-forming minerals sharing a similar structural feature with amphiboles: linked TO_4 -rings and MO_6 -octahedra.

[1] Mihailova et al. *Commun. Mater.* **2**, 57/1-10 (2021)

Poster

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

The controls on sedimentary pyrite formation in Southern Ocean deep-sea sediments

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The formation of pyrite in deep-marine sediments is typically limited by organic carbon or/and reactive iron availability. The Southern Ocean generally exhibits an iron deficiency, limiting bioproductivity and thus the sequestration of CO₂ from the atmosphere. Based on iron deficiency in the photic zone, it could be assumed that the formation of pyrite is iron-limited, too.

To evaluate the controls on sedimentary pyrite formation, sediments from ca. 4 Ma to recent, recovered during IODP Expedition 382 (Iceberg Alley) in the Scotia Sea, were examined for their carbon, nitrogen, sulfur, major and minor element contents.

The organic carbon and sulfur contents in the sediments have a mean value of c. 0.4 and 0.3 wt.%, respectively, whilst iron has a mean value of c. 4 wt.%. Organic carbon and sulfur demonstrate a good correlation and a significant increase from c. 1.25 Ma toward the stratigraphically younger. Further, the relationship between iron, sulfur, and organic carbon suggests that sulfur is fixed in pyrite.

The good correlation between sulfur and organic carbon points to a organic carbon limitation for pyrite formation. Also, the excess of iron speaks against an iron limitation for pyrite formation. Therefore, the increase in sulfur and organic carbon contents from the onset of the mid-Pleistocene transition might demonstrate higher export of organic carbon from the photic zone to the ocean floor, and an enhanced formation of pyrite in the sediments.

Poster

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

Mantle metasomatism constraint: LA-ICPMS U-Pb dating of single garnet xenocrysts from the V. Grib kimberlite, Russia

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Mantle metasomatism largely controls the physical and chemical properties of the lithospheric mantle and exerts control over the genesis of kimberlitic magmas and diamond formation. In this context, garnet xenocrysts from kimberlites are fundamental for decoding metasomatic events in the lithospheric mantle and to decipher the variation in rock types with depth. However, dating mantle lithologies and processes is complicated by high ambient temperatures that allow the equilibration of most isotopic systems up to the time of kimberlite eruption.

In this study we investigate garnet xenocrysts from the ~376 Ma V. Grib kimberlite, Russia to evaluate the potential of garnet for dating metasomatic events in the subcontinental lithospheric mantle. Based on major and trace element compositions and REE patterns, harzburgitic, wehrlitic, lherzolitic (4x) and megacrystic garnet xenocrysts are distinguished.

Our preliminary data indicates that garnet can record the ages of different metasomatic events. Garnet from harzburgitic and lherzolitic lithotypes indicate at least 30 myr of mantle metasomatism prior to kimberlite eruption. This age spread reflects distinct metasomatic events, but partial resetting of the U-Pb isotope system also has to be considered.

Lecture*Topic:* 1.2 Methods in Geochemistry and Mineralogy**Diffraction intensities of ordered omphacite, measured from precession electron diffraction****Nobuyoshi Miyajima, Lucas M. Calvo, Tiziana Boffa Ballaran, Greta Rustioni**

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Cation ordering in minerals at high temperatures is important for understanding the metamorphic processes in the interior of the Earth. Omphacite, $(\text{Na}_{0.5}\text{Ca}_{0.5})(\text{Al}_{0.5}\text{Mg}_{0.5})\text{Si}_2\text{O}_6$ undergoes an order transition from $C2/c$ to $P2/n$ at about 865 °C. In the transition, the degree of Mg, Al order on two alternate M1 sites is coupled with the Ca, Na ordering on two alternate M2 sites to maintain local charge balance. The determination of diffraction intensities related with cation ordering in omphacite is, therefore, important to understand the kinetics of the cation ordering in omphacite and its thermal history in metamorphic rocks. Here we report the determination of diffraction intensities of an ordered omphacite by using precession electron diffraction (PsED) in a transmission electron microscope (TEM). An ordered omphacite ($\text{Jd}_{39}\text{Hd}_4\text{Acm}_1\text{Di}_{52}$) from a kyanite-free eclogite in the Münchberg Massif, Bavaria, Germany was investigated. The selected area electron diffraction (SAED) pattern of the omphacite is recorded on a CCD camera using a precession mode in TEM. To evaluate the degree of the cation ordering in omphacite, the intensities of the reflections with $h + k = \text{odd}$, e.g., (050) and $h + k = \text{even}$, (060) were integrated with a gaussian function. The obtained intensity ratio of 0.06(1) in the (050)/(060) reflections from the PsED was comparable with 0.067(5) of the single crystal X-ray diffraction data of the omphacite from the same rock. Using PsED in TEM, we measured pseudo-kinematical diffraction intensities of omphacite, resulted in evaluating the cation ordering state in omphacite at the submicrometer scale.

Poster

Topic: 4.1 Magmas and Fluids in the Crust

In-situ fractionation at the decameter scale in lower oceanic crust

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As the best-preserved fragment of paleo oceanic crust on land, the Samail ophiolite (Sultanate of Oman) allows extensive field studies on fast-spread lower oceanic crust. Drill core GT1 of the Oman Drilling Project in the frame of ICDP (International Continental Scientific Drilling Program) spans about 400 m from the layered gabbros between ~1200 and 800 m above the crust-mantle boundary (maM). The drilled samples are mostly gabbros or olivine gabbros and we applied petrological, geochemical, and microstructural methods to identify those magmatic processes relevant for the lower crust accretion. Mg# (Mg/Mg+Fe x 100; molar basis) in olivine and clinopyroxene and the Ca# (Ca/Ca+Na x 100; molar basis) in plagioclase show parallel fractionation trends from 800 to 1070 maM which can be subdivided into four 25 to 80 m-thick smaller trends. Above 1070 maM, phase compositions change towards more primitive compositions over a 15 m-thin horizon, revealing decameter-scale fractionation over the uppermost 80 m of the core. These trends are confirmed by bulk rock Mg# and Cr/Zr ratios and thermodynamic modeling suggests that they can result from in-situ fractionation by a crystallization degree of less than 30 mol% followed by primitive melt replenishment. Thus, the necessity of removing latent heat which is regarded as critical in terms of in-situ crystallization is only limited, because most melt migrates upwards, without crystallizing. Our results suggest that magma replenishment and fractional crystallization are the key processes responsible for the accretion of the layered gabbro section of the Oman paleocrust.

Lecture

Topic: 10.1 Geoscience Communication and Education

Virtual field trips – a powerful tool to complement teaching in earth sciences

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The corona pandemic faced earth science lecturers and students around the world with an essential conflict: field trips as practical parts of their studies were strictly reduced to a minimum and the theories learned in the lecture hall could not be applied to observations made in the field. As a consequence, digital tools are required to make visual features of outcrops experiential and to provide students the opportunity of home-based field experiences.

We set up a concept of virtual field trips (VFT), based on a combination of 360° panorama photographs, detailed pictures, 3D models and thin section photomicrographs, allowing the integration of heterogeneous types of data (e.g. audio, videos, texts) in order to enhance the learning experience. By going without virtual or augmented reality headsets or environment for now, the VFT can be experienced by everyone with a computer and internet connection, regardless of physical or financial abilities which is a clear advantage compared to real field trips. With the goal of a semi-automatic and low-level access VFT platform for geologists, we tested our concept for the Wingertsbergwand outcrop in the Eifel consisting mainly of ash and pumice tephra from the Laacher See eruption 13 ky ago. Although getting the real touch with nature cannot be replaced by a screen-based virtual experience, we are confident that people can benefit from VFTs not only by accessing the deposited data but also due to the great chance of complementing lectures by visual accents which make scientific contents much easier to understand.

Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Mineralogy and Processing experiments of an unusual parasite bearing REE ore from northern Vietnam

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The carbonatite-hosted Namxe rare earth element (REE) deposit in northern Vietnam has a total rare earth oxide (TREO) content of up to 2 wt% which is mainly hosted by parasite in the southern part of the deposit. Detailed mineralogical investigation of the rather complex mineralization revealed that parasite occurs in two geochemical varieties with slightly differing REE₂O₃/CaO ratios (5.8 ±0.2 vs. 6.8 ±0.35). Parasite occurs in dykes together with carbonates (ankerite, calcite) and barite and is often intergrown with fine-grained (sub 100µm size fraction) barite-celestine group minerals. The recognition of remnants of corroded bastnaesite suggest that REE enrichment is a result of a multi-stage process involving Sr- and CO₃-rich fluids with mantle signature (δ¹³C values of -6.8 ‰ to -2.89 ‰) with no or little additional REE input.

We applied state-of-the-art techniques to propose a possible processing route of the ore, including experiments using sensor-sorting, selective comminution, magnetic separation (HIMS and WHIMS) and froth flotation. Sensor sorting turned out to be quite efficient as the basaltic host rock can be separated from the dyke material, resulting in a mass reduction of about 30% and a REE loss of less than 2%. Selective comminution experiments revealed similar results with the rejection of 27% of barren material and a slightly higher loss of REE (3.5%). Two step froth flotation of a model blend led to a concentrate with >40% TREO content.

Randohr-Poster

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Pressure anomaly of the ATP hydrolysis rate facilitates life of extremophiles

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Life is prevalent on Earth even in extreme environments, e.g., near black smokers. This biological community has to face temperatures of up to 120 °C and pressures of 40 MPa. To maintain vital reactions, extremophiles have developed various mechanisms to survive. The stability of the energy-storing molecules adenosine triphosphate (ATP) and adenosine diphosphate (ADP) are of essential importance because reactions involving these phosphates constrain the range of life. ATP is limited by the non-enzymatic hydrolysis, which is kinetically enhanced at high temperatures. If this abiotic process is too rapid, metabolism as we know won't be possible anymore. The effect of elevated temperatures on the hydrolysis rate constants of ATP is widely known and is best described by an Arrhenius relationship. In contrast to previous studies, our first findings showed a decelerating effect from 0 – 60 MPa with a minimum in the reaction rate at 20 – 40 MPa at 100 °C. The rate constants of the non-enzymatic hydrolysis of ATP are decreasing from $5.8 \times 10^{-4} \text{ s}^{-1}$ at 0.1 MPa to $4.2 \times 10^{-4} \text{ s}^{-1}$ at 20 MPa at 100 °C. The corresponding half-lives are 1195 s and 20 MPa. This observation is extremely fascinating as Takai et al. (2008) have seen a similar pressure anomaly at extreme temperatures for *Methanopyrus Kandleri*.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Effects of water level rise on the dynamic behavior of land uplift in abandoned mines, Germany

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The terrain elevation changes resulting from the rising water level caused by stopping dewatering or flooding in abandoned mines area can damage surface construction or make the surface area useless. Estimation up to 2051 depicts a rise in uplift velocity between 0.5–3.0 mm/year and noticeably a total uplift of up to 300 mm.

This study used the system dynamics approach to identify the variable interaction, analyze the managerial decisions, establish a comprehensive model to consider land uplift's dynamic deformation and provide a mathematical relationship based on the causality relationship loop diagrams. Six sub-model of Casual-Loop Diagrams (CLD) are considered, including the effect of dynamic interaction of *groundwater extraction, vertical & horizontal stress, land usage, pumping costs*, and the impact of *water pollution* and *effective stress* on the land uplift rate for the next 100 years. As a result, increasing the groundwater pollution in abandoned mine areas caused to increase in the land uplift rate. Furthermore, a 2°C rise in the average temperature in the area of study (Wasserprovinz Haus Aden area, Germany) reduces the groundwater level in abandoned mines by about 19%, which causes to decline in the total land uplift by around 4.3%—furthermore, increasing of 10% in rainfall results in about 12% increase in the land uplift rate.

Such CLDs define dynamic interaction between the numerous variables and simulate the uplift trend throughout nonlinear feedback loops, illustrating the result of any managerial decision and regulating the new decisions in case of need.

Poster*Topic:* 6.2 Rates and Dates of Earth Surface processes: Methods & Applications**Applications of fallout plutonium at the University of Cologne to resolve Anthropocene Earth (sub-) surface processes****Joel Mohren¹, Steven A. Binnie¹, Erik Strub², Stefan Heinze³, Tibor J. Dunai¹**¹Institute of Geology and Mineralogy, University of Cologne, Germany; ²Division of Nuclear Chemistry, University of Cologne, Germany; ³CologneAMS, Institute of Nuclear Physics, University of Cologne, Germany

Anthropogenic fallout radionuclides (FRNs), in particular ¹³⁷Cs, are frequently measured to investigate Anthropocene sediment or soil particle redistribution patterns and rates. However, applications of ¹³⁷Cs can be complicated due to contaminations from nuclear power plant accidents. In addition, decreasing global ¹³⁷Cs activities mean that it will become increasingly difficult to measure in coming decades. Fallout ²³⁹⁺²⁴⁰Pu measured by Accelerator Mass Spectrometry (AMS) remains largely unaffected by these issues and allows more precise measurements on smaller sample sizes. There is thus much potential for ²³⁹⁺²⁴⁰Pu in modern Earth (sub-)surface processes investigations. The Institute of Geology and Mineralogy, together with the Division of Nuclear Chemistry, and the Centre for Accelerator Mass Spectrometry (CologneAMS), University of Cologne, have developed ²³⁹⁺²⁴⁰Pu capabilities, calibrated against published and externally referenced in-house standards. Measurement uncertainties regularly achieved are < 5%. Based on these preconditions, we now aim to comprehensively exploit the wealth of possible ²³⁹⁺²⁴⁰Pu applications to decipher modern Earth (sub-)surface processes. We present a selection of ongoing projects, in which we assess deflation processes (South Africa, northern Chile), aspect-induced differential soil erosion (central Chile), seismic-induced boulder slip rates (northern Chile), and sediment transport through natural pipes associated with sapping processes (Germany). Furthermore, we test the application of ²³⁹⁺²⁴⁰Pu as proxy for rainfall in the Atacama Desert (northern Chile). Our approaches contribute to a better understanding of Earth (sub-)surface processes in the Anthropocene, and, where applicable, we seek to compare these data to longer-term background rates of topography formation.

Lecture*Topic:* 6.2 Rates and Dates of Earth Surface processes: Methods & Applications**Measuring fallout plutonium activities in soils to trace the fate of soil organic matter in arable land, Republic of South Africa****Joel Mohren¹, Hendrik Wiesel^{2,3}, Wulf Amelung⁴, Alexandra Sandhage-Hofmann⁴, Erik Strub², Steven A. Binnie¹, Stefan Heinze⁵, Tibor J. Dunai¹**¹Institute of Geology and Mineralogy, University of Cologne, Germany; ²Division of Nuclear Chemistry, University of Cologne, Germany; ³Advanced Nuclear Fuels GmbH, Lingen, Germany; ⁴Institute of Crop Science and Resource Conservation, University of Bonn, Germany; ⁵CologneAMS, Institute of Nuclear Physics, University of Cologne, Germany

The Free State Province comprises one of the major agricultural regions in the Republic of South Africa. Here, the loss of soil organic matter (SOM) from arable land bears the risk to pose a serious threat to regional crop production yields. For agricultural land located within the Free State Province, previous studies have found a strong relationship between (decreasing) SOM contents and the total time period soils were subject to cropping practices. While wind erosion and mineralisation processes have been identified to be the dominant factors causing this pattern, their individual contribution to SOM loss remained difficult to quantify. Datasets obtained from monitoring stations measuring soil redistribution by wind rarely cover timespans exceeding a few years of observation. To overcome this problem, we measure fallout ²³⁹⁺²⁴⁰Pu inventories in topsoils sampled from agricultural plots with different cropping histories. Plutonium inventories are frequently quantified to infer fluvial soil redistribution patterns and rates during the Anthropocene, but their application to investigate wind erosion is still at an early stage of development. The approach we follow allows us to identify strong correlations between SOM loss and decreasing radionuclide inventories during the second half of the 20th century. Furthermore, cropped soils lost about 50% of their initial ²³⁹⁺²⁴⁰Pu, indicating that the decrease of SOM contents over time is predominantly caused by wind erosion. Our results, which are in good agreement with ¹³⁷Cs data, underscore the necessity to tackle unsustainable cropping practices in the Republic of South Africa and in comparable settings on Earth.

Poster

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

A multi-methodological approach to investigate the erosion of arable land caused by the July 2021 flood event in Erftstadt-Blessem, Germany

Joel Mohren, Steven A. Binnie, Matthias Ritter, Tabea Kautz, Sabine Tiegelkamp, Tibor J. Dunai

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Severe flooding in July 2021 has caused massive erosion of arable land located close to the village of Erftstadt-Blessem, Germany. Backward incision formed local drainage networks, evacuating Quaternary sediments towards a gravel pit located to the north of the village. The fluviially shaped topography was largely preserved after the flooding, providing the opportunity to characterise the mode of erosion and to identify factors that governed the manifestation of processes involved. The presence of somewhat exotic erosive features (e.g. amphitheatre-shaped channel heads, natural pipes) leads us to the hypothesis that groundwater sapping could have played a major role in eroding the arable land and underlying sediments. To test this hypothesis, we use Structure-from-Motion Multi-View Stereo photogrammetry to reconstruct drainage geometries (drone imagery provided by the Kreisverbindungskommando Köln, M. Wiese; supported by T. Gersthofer, ESRI Deutschland GmbH) and for in-situ density measurements of subsurface layers. Subsurface characteristics are further assessed by grain size analyses and X-ray diffractometry. The data are used to compare the post-flood topography of Erftstadt-Blessem to sapping-shaped topography on Earth and Mars. Furthermore, $^{239+240}\text{Pu}$ activities are measured in pipe infills to investigate hypothetical spatial connections to the uppermost soil horizons. Burial dating techniques (cosmogenic $^{26}\text{Al}/^{10}\text{Be}$ and optically stimulated luminescence) are used to constrain the age of the eroded sediments. Our overarching goal is to use our data as input for landscape evolution modelling to assess the importance of individual factors (e.g. substrate properties, vegetation cover) on the severity of erosion in Erftstadt-Blessem and comparable settings.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Melt mixing and transport across the Whale Head Rock contact aureole of the Albany-Fraser Orogen, Western Australia

Jo Moore¹, Jack Gillespie², Katy Evans², Lukas P. Baumgartner¹

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The processes that facilitate the production of granitoids are elucidated by the study of exposed lower crustal sections. The focus of this study is an exposure of the lower crustal portion of Albany-Fraser-Orogen (AFO) of Western Australia. This outcrop, located at Whale Head Rock in the western AFO, preserves the interface between an intrusive body and migmatized sedimentary rocks. Detailed mapping, petrography and thermodynamic modelling are combined to characterize the sources and distribution of melt generations in the aureole. U-Pb dating of zircon indicates that the tonalite crystallisation and migmatization of the metapelitic units were coeval at ca. 1.3 Ga. While thermodynamic modelling yields conditions of ca. 820°C and 0.5 GPa, in metapelites throughout the area. The contact zone evolves from igneous dominated textures to migmatitic sediments, dominated by concordant, internally derived leucosomes. The distribution of mineral assemblages and mineral chemistry across this section indicates that the mixing between intrusive and internally generated melt is structurally constrained. The back reaction with late stage, more evolved, melts within this mixing zone indicates that it acts as a pathway for continued melt removal and transport. This study represents an outcrop scale model for the complex processes that are involved in the production of granitoids at high temperature, medium pressure conditions. Giving further insight into the generation and extrapolation of melt from thinned crustal settings.

Lecture

Topic: 6.1 Earth surface processes in extremely water-limited environments

Atacama Desert soils as potential habitat for life at the extreme dry limit

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In the soils of the Atacama Desert its evolutionary history is buried and thus memorized. This is because of the extreme and prolonged dryness, which enabled the preservation of organic residues of life. Until now it is not known if and how life has survived under such conditions. Therefore, we aimed at quantifying and identifying different sources and hotspots of organic matter (OM) along four west-east directed transects, spanning the Atacama Desert from north to south and selected soil profiles which were dug to 0.6-3.4 m depth. Soil organic carbon (SOC) concentrations were determined by temperature-dependent differentiation; *n*-alkane and PAH signatures, as markers for plant residues and atmospheric, external inputs of OM, respectively, were detected using gas-chromatographic separation and mass-sensitive detection; potential hotspots of OM accumulation were identified by soil moisture content, electric conductivity and microbial community structure. We found that with increasing aridity SOC stocks decreased from 53±53 to 4±1 t ha⁻¹ in the topsoil. In the subsoil, SOC concentrations peaked between 40 and 150 cm depth, also in hyper-arid regions, adding 74.0-94.3% of subsoil SOC to the topsoil SOC stock. Biomarker analyses revealed that OM was partly derived by plant growth, some came by atmospheric transport and that there exist habitats of life at greater soil depth. Now further studies are needed to investigate how much of this OM is derived from the atmosphere or was built in-situ and what keeps the deep biosphere alive and who is colonizing it.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

NanoExtreme: Nano-focus end-station with double-sided CO₂ laser heating for experiments at ID27@ESRF

Wolfgang Morgenroth^{1,2}, Mohamed Mezouar², Gastón Garbarino², Anna Pakhomova², Björn Wehinger², Markus Herrmann³, Sandro Jahn³, Lélia Libon¹, Max Wilke¹

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The ESRF has built a new high pressure beamline for nano-focused X-ray diffraction, fluorescence and imaging at the extremely brilliant source EBS. The upgraded beamline is in operation since end of 2021.

In the framework of the joint BMBF-funded project 'NanoExtrem', research groups from the Universities of Potsdam and Cologne have been contributing to the construction of this end-station by providing personnel and instrumentation:

- 15 – 60 keV in monochromatic mode, additional 'pink' beam mode
- beam focus of down to ~250 nm at 17.00 keV to achieve pressures >500 GPa
- XRD detection using EIGER2 X CdTe 9M detector
- sample goniometers for nano-focusing, YAG and CO₂ laser heating or heavy duty experiments like Paris-Edinburgh cell or a 4 K cryostat
- in preparation: new experiments exploiting coherence of the beam and providing X-ray imaging capabilities.

This 'high-flux nano-XRD' beamline is optimized for the needs of the geo- and materials-science community for *in-situ* XRD and XRF studies at extreme conditions. It will be possible to study materials relevant to processes of the deep Earth or other planetary bodies in an unprecedented manner. We will present the overall design and provide first insights to performance parameters commissioned and used in first user experiments.

We acknowledge many divisions within the ESRF for construction and the German BMBF for financial support. BMBF project 'NanoExtrem' 05K2019: 05K19IP2 (Potsdam) and 05K19PK2 (Köln).

Poster*Topic:* 1.6 Probing (bio)geochemical reactions at mineral interfaces using micro- to nanoscale techniques**Feedbacks in silicate glass alteration studied by *in operando* fluid-cell Raman spectroscopy****Gerrit Müller^{1,2}, Moritz Bernd Karl Fritzsche², Lars Dohmen³, Thorsten Geisler²**¹Utrecht University, The Netherlands; ²University of Bonn, Germany; ³SCHOTT AG, Germany

The alteration of silicate glasses (and minerals) is involved in most biogeochemical cycles and poses challenges in several technical applications. The mechanism(s), kinetics and rate-determining factors have been extensively studied in an attempt to eventually arrive at a quantitative, predictive process description. However, this has proven challenging, because of the non-linear progression of the alteration process, which is affected by several reaction-inherent feedbacks. We investigated the interplay of such feedbacks through Raman spectroscopic fluid-cell experiments, enabling *in operando* visualization and rate measurements of reactions at the altering glass surface. One experiment with a low surface area-to-solution volume (SA/SV) ratio exhibited a transient acceleration of initial dissolution rates, followed by continuously rapid glass dissolution along with slow growth of a smectite-based surface alteration layer (SAL), apparently limited by glass-derived Mg. Contrastingly, in a high SA/SV experiment, glass dissolution monotonically decreased after the onset of rapid SAL growth, which was followed by the formation of carbonate coating and pore-space fillings, as well as by zeolite precipitation. Growth conditions and resulting properties of the SAL seem to exert dominant, non-linearly decelerating effects on glass dissolution, but are opposed by (re-)accelerating effects of glass cracking, pitting, and SAL delamination. In turn, SAL formation depends on precipitation kinetics and the accumulation of glass-derived solutes at the reaction front. However, dissolution and precipitation may also feedback with solution chemistry and transport processes. Such mechanistic insights from *in operando* experiments help understanding silicate alteration processes and can assist the improvement of predictive models.

Lecture

Topic: 9.4 Chemical sediments and mineral deposits in basins: archives of paleoclimatic, hydrogenetic, biogenic, hydrothermal, and diagenetic, processes throughout Earth's history

Systematics of submarine 'forward' and 'reverse' weathering

Gerrit Müller, Appy Sluijs, Jack J. Middelburg

Utrecht University, The Netherlands

Submarine weathering reactions associated with cation-rich ('forward') and cation-poor ('reverse') materials are significant, yet poorly understood parts of marine biogeochemical cycles, especially in coastal zones, where abundant lithogenic material is delivered by rivers and mixes with marine biogenic particles. Because of their different reaction stoichiometry, forward and reverse weathering processes have opposing effects on inorganic carbon, alkalinity and major element cycling in the ocean. The dominance of either forward or reverse weathering processes has been demonstrated to vary at different coastal marine sites, fueling speculation about controls of rates and stoichiometry of these diagenetic weathering reactions. We constructed a simple kinetic box model of coupled organic and inorganic particle diagenesis in river-influenced coastal systems to disentangle effects of (1) pH-Eh regimes, driven by prevalent microbial pathways of organic matter decay, and of (2) mineralogical variability of sediment substrates, i.e., the mixture of different terrestrial and marine inputs. In theory, highly pre-weathered and biogenic silica-rich substrates altering in suboxic settings dominated by microbial iron reduction favor solute and alkalinity consumption by reverse weathering. In contrast, alteration of cation-rich, volcanogenic and basaltic material in CO₂-enriched oxic or methanogenic zones may rather drive a forward weathering process and alkalinity generation. Because the spatial distribution of both factors, sediment input and local redox processes, likely has changed during Earth's history, substantial variability of differential element fluxes in submarine weathering processes would be expected, confounding our current understanding of weathering feedbacks in the Earth system.

Lecture*Topic:* 3.2 Composition and evolution of deep planetary interiors**Silicon and Carbon content in the Earth's inner core constrained from sound velocities at extreme conditions****Susanne C. Müller¹, Efim Kolesnikov¹, Georgios Aprilis², Alexandr Chumakov², Davide Comboni², Michael Hanfland², Ilya Sergeev³, Lélia Libon⁴, Wolfgang Morgenroth⁴, Max Wilke⁴, Xiang Li¹, Hannah Koppetz-Mitra¹, Arno Rohrbach¹, Jasper Berndt¹, Carmen Sanchez-Valle¹, Ilya Kupenko¹**¹Westfälische Wilhelms-Universität Münster, Germany; ²ESRF European Synchrotron Radiation Facility, France; ³Deutsches Elektronen Synchrotron, Germany; ⁴Universität Potsdam, Germany

The inner core is comprised of iron and nickel as the main components. However, the composition of the Earth's core remains enigmatic to date. The comparison of densities and seismic velocities between pure Fe-Ni alloys and seismological models reveals a density deficit and reduced velocities in the core. These observations can be explained by the addition of 3-7 wt% light elements to Fe-Ni alloys. Possible candidates are H, C, O, Si, and S. To understand the formation, evolution, and dynamics of the core of the Earth and other terrestrial planets, constraining the light element budget is crucial. Silicon could be the dominant light element because of its partitioning behaviour, isotope fractionation, and chemical properties. The low shear velocity (V_s) and high Poisson ratio in the inner core could be explained by the addition of carbon. Indeed, recent *ab initio* calculations proposed that simultaneous incorporation of Si and C can provide a good match both for density and sound velocities.

In search of the light elements and their amounts, we carried out nuclear inelastic scattering (NIS) and x-ray diffraction experiments in diamond anvil cells at pressures up to 160 GPa. We determined the sound velocities of the Fe-2wt%Si-0.4wt%C-alloy at high pressures and used thermoelastic parameters extracted from the NIS data to extrapolate them to core conditions. Here, we will present the results and discuss the availability of silicon and carbon in the inner core, as well as the possible amount of each element to match seismic observations.

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

Taking the pressure out of the Archean Metamorphism: The role of CO₂ in assessing metamorphic conditions of the Isua supracrustal belt, W-Greenland

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The Eoarchean Isua Supracrustal Belt (ISB), West Greenland exposes one of the oldest rock records on Earth. Its tectonic setting is still subject of debate with interpretations ranging from plate tectonics to vertical tectonics. Information on the origin (mantle rocks vs. cumulates) and metamorphic P-T-X evolution of ultramafic lenses exposed in the Western part of the ISB may hold the key to shed substantial light on the geodynamic evolution. While the geochemical signatures are non-conclusive in view of the origin, there is a general agreement of high to ultrahigh pressure conditions for the metamorphic overprint based on the presence of titanian clinohumite and titanian chondrodite, phases typically reported as indicative for high pressure metamorphism in ultramafics.

In this contribution we present results assessing the role of CO₂ using a combination of textural analysis and thermodynamic calculations. It is shown that the stability fields of the observed mineral assemblage is strongly controlled by the fluid composition (XCO₂). While high pressure conditions (> 2 GPa) are limited to a narrow range of fluid composition, thermodynamic modelling reveals that the formation of the observed reaction textures including the formation of the Ti-phases can be readily achieved via cooling at amphibolite facies conditions (580 to 500 °C at 1 GPa) in the presence of a CO₂-bearing fluid in agreement with the PT conditions determined for the rest of the ISB. Hence, the general wisdom of Ti-clinohumite and Ti-chondrodite being unequivocal indicative of high to ultrahigh pressure conditions in ultramafic rocks has to be abandoned.

Lecture

Topic: 1.8 Minerals and Mineral Properties

Thermoelastic properties of partially metamict zircon: Indication of multi-stage recrystallization processes

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Radioactive decay of unstable isotopes causes damage to zircon, which significantly reduces its elastic stiffnesses (e.g., Özkan, 1976). These damages can be partially healed by temperature treatment of the zircon crystal. In order to study in situ the recrystallization of metamict zircon, thermoelastic properties, and thermal expansion data were collected between 100 K and 1600 K utilizing resonant ultrasound spectroscopy and dilatometry, respectively. The investigated samples of natural gem-quality zircon belong to the damage stage I introduced by Holland & Gottfried, 1955, i.e. the damage in the crystal structure is mainly dominated by the accumulation of isolated point defects.

While non-metamict zircon samples display a linear decrease in elastic stiffnesses, the partially metamict zircon samples undergo strong irreversible effects detected in both utilized methods. The elastic stiffnesses increase starting at about 600 K, while the thermal expansion decreases. The severity of this effect becomes more pronounced with an increasing initial state of damage and thus can be related to the healing of defects induced by metamictization. A second effect sets in at about 1200 K, likely related to a transition from static to dynamic behavior. This supports the idea that reducing radiation damage is a multi-stage process, including point defect healing and recrystallization of an amorphous fraction.

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Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

Geomorphological significance of the Atacama Pediplain as a marker for the climatic and tectonic evolution of the Andean forearc

Sebastián Muñoz-Farías¹, Benedikt Ritter², Tibor J. Dunai², Jorge Morales-Leal¹, Eduardo Campos¹, Richard Spikings³, Rodrigo Riquelme¹

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The Atacama Pediplain (AP) is a major element in the Atacama Desert landscape, commonly used as an indicator of climatic and tectonic stability. We choose the El Salado Canyon area (26°S) that longitudinally exposes the AP to study its relationship with the Andean forearc evolution, combining geomorphologic and stratigraphic observation with new geochronological data (⁴⁰Ar/³⁹Ar biotite ages on ignimbrites, and ²¹Ne exposure ages on quartz-clasts). The AP alluvial deposition occurred in two episodes of alluvial backfilling spatially and temporally separated from each other (Early Miocene - Mid Miocene in the Precordillera, and Mid Miocene – Early Pliocene in the Central Depression), and both triggered by semiarid to arid conditions restricted to the higher Precordillera. Both episodes occurred despite the regionally recorded Mid Miocene onset of hyperarid conditions, revealing the local control of the upstream humidity in the downstream sedimentation. Clustered exposure ages from the Pliocene reveal the abandonment of the alluvial plains due to the incision of the El Salado Canyon, whereas younger and individual exposure ages from the Early Pleistocene, explained by minor surficial activity, reveal a climatic control on the surfaces after the incision that ended with the increase of the Pleistocene hyperaridity. Therefore, the development of alluvial deposition despite the regional Mid Miocene hyperaridity, and the development of a deep canyon incision after the last recorded Andean uplift, reveals that the AP has been strongly influenced by local conditions that do not allow its use as a general marker of a single climatic or tectonic event.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Estimating the upper limit of the Proterozoic petrographic carbon (PC) flux

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Atmospheric oxygen levels in the Proterozoic are highly debated with estimates reaching from >0.1 – 24 % PAL. A new approach to model Proterozoic atmospheric oxygen levels, based on concentrations of recycled PC in Proterozoic strata, indicates that atmospheric oxygen was potentially between 2 and 24 % PAL. However, this model lacks some precision because oxygenation rates and the Proterozoic riverine flux of petrographic carbon are poorly constrained.

This study focuses on deep marine shales of the 658 - 653 Ma-old Tapley Hill Formation (Adelaide Basin, south Australia) that were deposited during an eustatic transgression following the Sturtian glaciation. These shales contain 0.04 - 0.73 wt.% TOC and experienced burial diagenesis with temperatures of 195 – 220 °C based on Raman spectroscopic characterization. However, 14.4 - 58.7 % of the OM within these rocks is recycled graphitic PC indicating metamorphic temperatures as high as 650°C. The amount of PC increases with decreasing TOC values, resulting in total PC concentrations of 0.02 – 0.1 wt.% (average 0.05 wt.%).

Because of the likely exceptionally high post-glacial erosion rates we presume that the average of 0.05 wt.% marks an upper limit for recycling of graphitic PC in the Proterozoic. However, the diagenetic overprint in combination with petrographic similarities between graphitic and disordered OM both indicate that the actual concentration of total recycled PC is higher. Therefore, we conclude that the upper limit of the Proterozoic PC flux was similar to the upper limits found in modern marine sediments 0.1 – 0.2 wt.%.

Lecture

Topic: 4.5 Tectonic Systems (TSK Open Session)

Structural and geochemical data of the Mourne nappe near Kerames (Crete): Constraints on the tectonometamorphic evolution of the Uppermost Unit

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The Uppermost Unit of Crete is attributed to the Internal Hellenides and consists of different nappes derived from an Upper Cretaceous arc (Asterrousia), and a late Jurassic to Cretaceous subduction-accretion complex (Vatos, Arvi, Miamoux).

Blueschists of the subduction-accretion complex of central Crete (Preveli nappe, T = ca. 350°C, P = ca. 1.2 GPa) are resting on top of Pindos rocks and are overlain by Cretaceous Vatos flysch, Jurassic ophiolites and a second sequence of blueschist-facies rocks referred to as Mourne nappe.

The Mourne blueschists show a large variety of amphiboles, such as glaucophane, riebeckite, richterite, ferri-winchite, barroisite, magnesio-hornblende, edenite and actinolite. K-Ar dating of barroisite and phengite yielded late Jurassic ages (Seidel et al., 1977).

Top-to-the SW shearing under epidote blueschist-facies conditions led to the dominant foliation of the Mourne metabasites, which is characterized by the shape-preferred orientation of blue amphibole, omphacite (as relics), epidote, rutile and titanite.

Growth of barroisite, magnesio-hornblende and epidote indicate isothermal decompression under epidote-amphibolite facies conditions.

Cooling and further decompression is indicated by several generations of younger veins mineralized with albite, quartz, epidote, actinolite (greenschist facies) and actinolite, epidote, prehnite, calcite (prehnite-actinolite facies).

The youngest deformation led to discrete foliation-parallel shear zones under brittle conditions, related to the emplacement of the Mourne nappe on top of the ophiolites.

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Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Provenance of prehistoric lithic materials in the Arsanjan area (south central Iran); a geoarchaeological study

Nima Nezafati¹, Akira Tsuneki², Fereidoun Biglari³

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The Arsanjan area is located in the middle of the Zagros thrust zone, south central Iran, and consists of a series of ranges and plains. The study area is situated in the east and southeast of the Arsanjan city, where several Paleolithic and late prehistoric cave sites have so far been recorded. One of the largest cave sites is Tang-e Eshkan that opens to the southwest and faces a large plain at the junction of two valleys. The cave has been archaeologically excavated in 3 seasons from which numerous Middle Paleolithic and Upper Paleolithic lithic materials have been unearthed.

One of the questions raised from the study of the archaeological lithic artifacts was the source of the huge amount of lithic materials recovered from the cave. In this regard, the major aim of this study was to search for the possible sources used by the Paleolithic people for manufacturing their lithic tools. For this purpose, the surrounding area of the cave was surveyed and sampled. The samples were then compared with the lithic artifacts exhumed from the cave from the viewpoint of their color and appearance as well as their petrographic and geochemical characteristics.

Based on the field and hand specimen observations and the petrographic and geochemical investigations, both high-silica materials from the riverbed and the surrounding rock outcrops could have been used by Paleolithic hunter-gatherers in the Arsanjan area.

Ramdohr-Poster

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Deriving basin-wide erosion/denudation rates of basaltic rocks using cosmogenic Kr isotopes, volcanic complex Vogelsberg, Germany

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The Vogelsberg area located in Hessen, Germany, comprises the largest contiguous volcanic complex in Central Europe, covering an area of about 2300 km². After volcanic activity ceased during the Mid Miocene, the complex was subject to extensive erosion and weathering. Fluvial erosion has shaped the area, which is now characterised by Pleistocene valleys and a radial river system exposing primitive alkali basalts and basanites. The inference of time-integrated erosion rates from regularly measured cosmogenic nuclides (e.g. ¹⁰Be, ²⁶Al) remains challenging in such an environment due to the apparent mafic and thus quartz-poor composition of the local bedrock. However, the application of cosmogenic Kr isotopes on the weathering-resistant mineral zircon provides a novel tool to infer basin-wide denudation rates from quartz-poor lithologies. In our project, we aim to exploit the advantage of the applications of Kr and sample zircons from sediments of six streams radially draining the Vogelsberg. After zircon purification, these samples will be measured at the Cologne Noble Gas Mass Spectrometer to quantify Kr concentrations in these samples and to assess the time-integrated erosion patterns shaping the volcanic complex.

Lecture*Topic:* 1.7 Experimental Petrology and Geochemistry**Quantifying diffusion-driven metal stable isotope fractionation in olivine through powder source experiments****Martin Oeser¹, Ralf Dohmen², Julius Eschenauer², Stefan Weyer¹**¹Leibniz Universität Hannover, Institut für Mineralogie, Germany; ²Ruhr-Universität Bochum, Institut für Geologie, Mineralogie & Geophysik, Germany

Chemical and isotopic zoning in olivine has frequently been used to determine timescales of magmatic processes by diffusion modeling. Furthermore, combining the information from chemical- and Fe-Mg- or Li isotopic zoning has been shown to be a powerful tool to elucidate complex crystal growth and diffusion histories [1,2]. However, the extent of diffusion-driven Fe-Mg-Li isotope fractionation in olivine (typically termed as β_{Fe} , β_{Mg} , and β_{Li}) and the parameters that control them, are not yet well constrained. The latter may bear a potential to better determine the boundary conditions of diffusion in order to (1) better unravel complex diffusion histories and (2) receive more precise diffusion timescales. Here, we have performed a series of diffusion experiments in which a powder source was used to produce Fe-Mg- and Li chemical and isotopic diffusion profiles in crystallographically oriented San Carlos olivine crystal cubes. Chemical and isotopic diffusion profiles were analyzed by electron microprobe (Fe-Mg concentrations), by femtosecond-laser ablation-ICP-MS (minor and trace elements), and by fs-LA-MC-ICP-MS (Fe-Mg and Li isotopic variations). We have been investigating the dependence of β_{Fe} and β_{Mg} on temperature, crystallographic orientation, and composition, and additionally the dependence of β_{Li} on $f\text{O}_2$. Our preliminary results indicate that the Fe-Mg isotope fractionation during diffusion parallel to the crystallographic a- and b-axes is larger than that for diffusion along the c-axis. Furthermore, Li diffusion and the associated Li isotope fractionation appear to be strongly influenced by $f\text{O}_2$.

References:

[1] Sio & Dauphas, *Geology* 2017.[2] Oeser et al., *American Mineralogist* 2018.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

Depth profile sampling by femtosecond-LA-(MC-)ICP-MS for high spatial resolution analyses of chemical and isotopic diffusion profiles

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Femtosecond laser ablation coupled to MC-ICP-MS has been proven to be a powerful means to analyze isotope ratios of “non-traditional” stable isotope systems with high spatial resolution, precision and accuracy. The technique has been successfully applied e.g. to investigate diffusion-generated Li- and Fe-Mg isotopic zoning in magmatic crystals. Here, we present a novel sampling technique employing a fs-LA system that is equipped with a CNC-controlled laser stage. This set up allows to perform depth profile analyses of major and trace elements as well as metal stable isotope variations (Li-Mg-Fe) and is particularly suitable for experimental samples with a well-defined crystal interface. Samples are ablated in circular patterns with diameters of 100-200 μm and the integrated signal of one layer represents one data point of the depth profile. Depth resolution is between 300 nm and 2.5 μm and depends on the scan speed and the repetition rate of the laser. We have tested this technique by analyzing chemical diffusion profiles in olivine crystal cubes which are compared to “horizontal” profile data acquired by electron microprobe analyses. Furthermore, Fe-Mg isotopic depth profiles were analyzed in a diffusion couple consisting of a ²⁵Mg- and ⁵⁷Fe-doped olivine thin film in contact with a natural olivine crystal cube. Our results indicate (i) that concentration data acquired by LA depth profiling match well with electron microprobe data, and (ii) that precise and accurate $\delta^{25}\text{Mg}$, $\delta^{26}\text{Mg}$, $\delta^{56}\text{Fe}$ and $\delta^{57}\text{Fe}$ data can be obtained.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Geochemical Reconstruction of the Provenance, Tectonic Setting and Paleoweathering of Lower Paleozoic Black Shales from Northern Europe

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Lower Paleozoic black shales from Estonia, Sweden, and Russia were analyzed for major and trace elements to reconstruct the provenance, tectonic setting, and paleoweathering conditions of these shales. The black shale is highly enriched in U, V, Mo, and Pb (except in samples from Sweden where Pb is slightly enriched), slightly enriched in SiO₂, Fe₂O₃, K₂O, and TiO₂ and highly depleted in CaO, Na₂O, and MnO, with respect to average shales. The provenance signatures (Th/Sc versus Zr/Sc, Al₂O₃ versus TiO₂, Zr versus TiO₂ plots, and Zr/Sc ratio) of the Baltoscandian black shales suggest that they were derived from rocks of intermediate to felsic composition and from recycled sediments. The likely provenance region was the Paleoproterozoic igneous and metamorphic basement of southern central and southern Finland, which consists predominantly of felsic to intermediate metamorphic (acidic to intermediate gneisses, felsic volcanics, microcline granites and migmatites) and igneous rocks (small granitic intrusions and large rapakivi granite intrusions), and reworked older Ediacaran and Lower Cambrian sediments; however, the proportion of clastic input from these sources is not uniform in the three regions studied. The discrimination of the tectonic settings of source materials of the black shale using the SiO₂ versus K₂O/Na₂O plot and a new discriminant method (APMdisc) favors a passive margin setting. The Chemical Index of Weathering (CIW) indicates that the clastic material in the black shale of the studied regions has experienced an intense degree of chemical weathering. Weathering indices show that the black shale has experienced significant secondary potassium enrichment.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Imperial Porphyry, a famous dimension stone from Egypt

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Imperial Porphyry is a porphyritic rock of trachyandesite to dacite composition, providing U-Th-Pb zircon ages of 609-600 Ma (Abu El-Enen et al. 2007). It shows a spectacular purple color that is due to fine grained flakes of hematite, formed by pervasive hydrothermal alteration under oxidising conditions. The famous dimension stone was quarried in the Mons Porphyritis area in the Eastern Desert of Egypt from the first to the fifth century. During this period, the valuable material was processed as decorative stone for objects of art, reserved exclusively for the Imperial court of the Roman Empire. Careful polishing of the rock achieved a highly reflective finish, the characteristic purple color being regarded as an imperial status symbol. The different steps of extraction and the transport from the mountainous outcrops down to the river Nile involved masterly technical performances, all the more as a wide-spaced joint pattern allowed the production of large, cleavage- and fracture-free blocks, suitable for manufacturing of monolithic or sectioned columns, sarcophagi, magnificent giant bowls and sculptures. For instance, individual segments of Constantine's Column in Constantinople attain weights of up to 45 tons. Obviously, the Roman engineers had a fundamental knowledge on geological survey to detect occurrences suitable for quarrying. After the Roman period, antique spoils of Imperial Porphyry, now known as Porfido rosso antico, were extensively re-used for sculpturing.

Abu El-Enen MM, Lorenz J, Ali KA, von Seckendorff V, Okrusch M, Schüssler U, Brätz H, Schmitt R-T (2007) Int J Earth Sci 108:2393-2408

Poster

Topic: 1.7 Experimental Petrology and Geochemistry

Solid bitumen in shales from the Middle to Upper Jurassic Banik section of northernmost Iraq: Implication for reservoir characterization

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Iraq is the sixth largest oil reserve in the world, with current proven reserves of 115 billion barrels of oil (BBO) and 110 trillion cubic feet (TCF) of gas. The study area is situated within the Kurdistan Region of Iraq which is estimated to contain about 39% of Iraq's total barrels of oil reserves. Petrographic, organic, and inorganic geochemical analysis of the solid bitumen and host shales from the Middle and Late Jurassic-age Sargelu and Naokelekan Formations of the Banik section, northernmost Iraq, were undertaken with the aim of understanding their derivation and preservation, as well as examining the carbon and oxygen isotopes, and paleoredox proxies under which the solid bitumen and host sediments were deposited. Petrographic analysis of both formations revealed the presence of solid bitumen high reflectance (first phase) and solid bitumen low reflectance (second phase). The equivalent vitrinite reflectance indicates that the solid bitumen of the Sargelu and Naokelekan Formations probably accumulated within the shale reservoirs following oil migration from source rocks located within the same formations. Mineralogical study (XRD and SEM - EDX) revealed that the shales hosting the solid bitumen also contain clay minerals (illite, rectorite, chlorite, montmorillonite, and kaolinite) as well as carbonate minerals, quartz, alkali feldspar, and pyrite. Carbon and oxygen isotope data along with paleoredox indicators suggest that both the solid bitumen sources and host shales in the Sargelu and Naokelekan Formations formed within a shallow-marine setting, most probably under anoxic conditions where water circulation was restricted.

Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

From lithium mineral to chemical: challenges and opportunities

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About half of the global supply of lithium for the battery market is extracted from lithium minerals, such as spodumene. Conventional extraction of lithium from spodumene concentrate proceeds via calcination, acid roasting, leaching, purification and crystallisation of lithium hydroxide. The process achieves high lithium recoveries and lithium hydroxide purities but suffers from large energy, chemical and by-product footprints, as well as inflexibility to accommodate low grade sources or variations in concentrate mineralogy. The strict specifications for spodumene concentrate suitable for calcination result in large proportions of spodumene ore reporting to waste streams. Furthermore, common late-stage alteration of spodumene to muscovite and cookeite leads to partial melting and clinker formation during calcination, degrading lithium recovery from altered ore. With the recent focus on more sustainable production of energy and technology critical raw materials, the above challenges need to be addressed to keep lithium extraction from mineral sources viable in the future. The presentation will illustrate the challenges but also focus on opportunities to make lithium extraction more sustainable.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

GFZ Data Services – A domain repository for geosciences data

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GFZ Data Services is a domain repository for geosciences data comprising the Earth, Space and Environmental Sciences. It assigns digital object identifier (DOI) to data and scientific software since 2004. Hosted at the GFZ German Research Centre for Geosciences (GFZ), the repository has a focus on the curation of long-tail data by domain scientists on one hand, but also provides DOI minting services for several global monitoring networks/observatories in geodesy and geophysics and collaborative projects. Furthermore, as Allocating Agent for the International Generic Sample Number (IGSN), the globally unique persistent identifier for physical samples, GFZ is providing IGSN minting services for physical samples.

GFZ Data Services increases the interoperability of long-tail data through (1) the provision of comprehensive domain-specific data description via standardised and machine-readable metadata with controlled domain vocabularies. Metadata is (2) complemented with comprehensive and standardised technical data descriptions or reports; and (3) by embedding the research data in wider context by providing cross-references through Persistent Identifiers (DOI, IGSN, ORCID, Fundref) to related research products (text, data, software) and people or institutions involved.

In addition to the task as a research data publisher, GFZ Data Services is the central node for research data management at the GFZ with information on metadata, data formats, the data publication workflow, FAQ, links to different versions of our metadata editor and downloadable data description templates. Specific data publication guidance is complemented by more general information on data management, like a data management roadmap for PhD students.

Poster

Topic: 4.5 Tectonic Systems (TSK Open Session)

U-Pb dating of fluid interactions: Hidden tectonic events in the Telemark domain (southern Norway)

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Regional tectonic events are difficult to detect in a stable continental crust, especially in the absence of major tectonic structures. Tectonic events may, however, trigger crustal fluid migration, leading locally to the formation of alteration zones in uraninite and uranium-bearing minerals. Accordingly, these events may be assessed, for example, by U-Th-Pb dating.

The Evje-Iveland pegmatites intruded at the end of the Sveconorwegian orogeny into the metamorphic basement of the Telemark tectonic domain of southern Norway. After magmatic crystallization, several fluid interactions lead to the alteration of igneous minerals and to the formation of discrete secondary mineral assemblages. We investigated uraninite and secondary uranium-phases from a range of Evje-Iveland pegmatite localities.

Pegmatites in the Landsverk area have been subjected to a prominent hydrothermal brecciation event, leading to the crystallization of hydrothermal minerals, including quartz, albite, epidote and titanite assemblages. A broad age group around 500 Ma is also obtained from hydrothermally altered domains of the Einkerken uraninite. In addition, secondary uranium phases uranophane- β and uranophane yield chemical ages corresponding to the Early Cretaceous and Paleogene. The post-Sveconorwegian mineralisation can tentatively be related to the Caledonian orogeny, opening of the North Sea rift system, and Scandinavian uplift, respectively.

Distinct age populations from hydrothermally overprinted uranium ores can be correlated with regional tectonic events, not otherwise detected in a stable continental crust.

Lecture*Topic:* 1.2 Methods in Geochemistry and Mineralogy**A new approach for high-precision triple oxygen isotope analyses of CO₂****Andreas Pack, Malte Seefeld, Oliver Jäger, Greta Viktoria Simon, David Bajnai**

Universität Göttingen, Germany

Detection of small variations in triple oxygen isotope ratios ($\Delta^{17}\text{O}$) of rocks, minerals, and water has opened new applications in the field of isotope geochemistry (1,2). A long-standing problem is extending the approach to CO₂ and carbonates because of analytical difficulties getting precise $\Delta^{17}\text{O}$ of CO₂. Direct measurement of $\Delta^{17}\text{O}$ of CO₂ by means of high-resolution gas source mass spectrometry has been successfully demonstrated but requires measurement times of days for reaching a precision <10 ppm (3). Here, we present data of high-precision analyses of carbonate-derived CO₂ and CO₂ from the conversion of air O₂ using a tunable infrared diode laser absorption spectroscopy (TILDAS) attached to a custom-built inlet system controlled by free software (PHP, Python, JavaScript, CSS, HTML) and low-cost electronic hardware, i.e., Raspberry Pi. With this device, we now achieve an external reproducibility as small as ± 5 ppm. This opens new application fields, of which some will be presented.

1. A. Pack and D. Herwartz, The triple oxygen isotope composition of the Earth mantle and understanding $\Delta^{17}\text{O}$ variations in terrestrial rocks and minerals. *Earth Planet. Sci. Lett.* **390**, 138-145 (2014).
2. E. Barkan and B. Luz, High precision measurements of $^{17}\text{O}/^{16}\text{O}$ and $^{18}\text{O}/^{16}\text{O}$ ratios in H₂O. *Rapid Commun. Mass Spectrom.* **19**, 3737-3742 (2005).
3. G. A. Adnew, *et al.*, Determination of the triple oxygen and carbon isotopic composition of CO₂ from atomic ion fragments formed in the ion source of the 253 Ultra High-Resolution Isotope Ratio Mass Spectrometer. *Rapid Commun. Mass Spectrom.* **33**, 1363-1380 (2019).

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Two different parental melt trends for the Deccan Trap main sequence

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The lava flows of the Deccan Large Igneous Province (DLIP) cover at least one million years of continuous magmatic activity across the Cretaceous-Paleogene boundary (Schoene et al. 2021) likely representing the initial stage of the Réunion plume. Earlier studies suggested that the geochemical signatures of basaltic rocks from the DLIP main sequence originated from melts of the depleted upper mantle and Réunion plume that mixed within magma chamber systems (e.g. Peng et al. 1994). In this scenario, the compositional range of the DLIP is best explained by subsequent assimilation of varying proportions of crustal and lithospheric components during ascent.

The major and trace element as well as Sr-Nd-Hf-Pb isotope data of this study covers the entire stratigraphy of the DLIP main sequence and casts doubt on the generally accepted interpretation. Most notably, Pb isotopes as well as high field strength element systematics suggest two separate magma differentiation trends in the petrogenetic pathway of DLIP melts. The observed trends are best explained by two mafic endmembers that tap different mantle source reservoirs. Our isotope and trace element data suggests that melts from these reservoirs, namely the depleted upper mantle and lower mantle (Réunion plume) assimilated crustal and lithospheric components to a variable degree. Consequently, lava flows within single volcano-stratigraphic formations of the DLIP likely originated from different parental melts that did not interact during ascent. Previously, such fast-changing contributions from different mantle reservoirs have been underestimated for the Deccan volcanic rocks.

Peng et al. 1994. GCA

Schoene et al. 2021, GChron

Lecture

Topic: 2.2 From dust to planets

Depletion of Titanium in the mantle of the Earth

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Many authors have used the chemical composition of peridotitic rocks from a variety of geological settings to estimate the composition of the upper mantle of the Earth, (PUM-primitive upper mantle). This composition should represent the bulk Earth mantle after core formation and before the onset of mantle melting. The basis for this estimate are linear negative correlations of refractory element such as Al and Ca with MgO and positive correlations with Ni and Co in peridotitic rocks (see [1] and references therein). One implication is that refractory lithophile elements occur in chondritic ratios in PUM. A close inspection of recent data on mantle rocks (e.g., [2]) showed, however, that Al/Ti ratios in these rocks are generally above 20, compared to the chondritic ratio of about 18. This signature is present in many suites of mantle rocks, even considering the often poor quality of Ti analyses in chondrites and mantle rocks. It appears that Ti is depleted in PUM by 10 to 15%.

The depletion of Ti in the mantle of the Earth may either reflect very reducing conditions during early Earth accretion or strong metal-silicate partitioning of Ti under extreme conditions of temperature and/or pressure. Recently metal-silicate partition coefficients at high pressures and temperatures were experimentally determined. Preliminary results indicate that some Ti may indeed partition into metal during core formation.

Lit.: [1] Palme H. and O'Neill H.St.C. in *Treatise on Geochemistry* (2nd ed., vol.3, 1-39. [2] Carlson R.W. and Ionov D.A. (2019) *GCA* 257, 206-223.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

Multi-Step Crystallization Pathway of Vivianite

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Vivianite is a poorly soluble iron (II) phosphate phase found in modern and ancient anoxic soils and sediments. It plays an important role in the biogeochemical cycling of Fe (II) and P and is also a promising P recovery source from waste water. Despite this, the mechanisms and kinetics of vivianite formation are still unknown. Here we present results from a study where we followed the pathway of nucleation and growth of vivianite in solution, starting from aqueous iron (II) and phosphate ions. We aimed to shed light on whether vivianite – like many other sparingly soluble phases – forms via a classical or a non-classical nucleation and growth pathway. To address this, we employed a series of cross-correlated *in-situ* and *ex-situ* approaches to followed the time resolved formation reactions using UV-vis spectrophotometry, scanning and transmission electron microscopy, powder X-ray diffraction, infrared spectroscopy, simultaneous thermal gravimetric-differential thermal analyses and synchrotron-based X-ray absorption experiments. These complementary approaches helped us unravel the various stages of nucleation and crystallization of vivianite at high and low supersaturation. Our data indicates that vivianite nucleates via distinct stages in solution and not via a single step, thus following a non-classical nucleation and crystallization pathway. We also demonstrated how one can stabilize and characterize the structure, chemical composition of the intermediate phases and discuss the factors influencing their stability and transformation to the more thermodynamically stable crystalline vivianite.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

Au analysis by pressed-powder-pellets (PPP)-LA-ICP-MS

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Analysis of Au in geological materials has been proven useful for understanding geological processes related to the formation of various Au-rich ore deposits. However, the Au concentration in the source rocks is extremely low and the methodologies allowing analysis at sub-ng/g levels are time-consuming, costly and generally involve handling of dangerous chemicals. Here we present a new, faster, cheaper and safer method for low Au concentration analysis by Laser-Ablation Inductively-Coupled-Plasma Mass-Spectrometry (LA-ICP-MS) of pressed-powder-pellets (PPP), which has been developed in the Laboratory for Environmental and Raw Materials Analysis (LERA) at Karlsruher Institut für Technologie (KIT). Fine instrumental tuning for key parameters such as ICP-MS sample gas flow, torch position, RF power, laser frequency, ablation style and laser gas flow allows us to increase the Au sensitivity while keeping oxide production low. Indeed, the latter is critical when analysing low concentration Au samples as the ICP-MS analysis is generally impaired by Ta¹⁸¹O¹⁶ and the Hf¹⁸⁰O¹⁶H¹ interferences. Reducing the oxides allows the PPP-LA-ICP-MS method for better quantification and correction of these interferences. The new method improves the detection limit down to 0.05-0.1 ng/g Au. Routine analysis of reference materials shows that Au analysis by PPP-LA-ICP-MS is both accurate and precise. This contribution highlights that the method is suitable for investigating Au distribution and behaviour in Au depleted rocks.

Lecture

Topic: 2.2 From dust to planets

Experimentally Induced Thermal Fatigue on Lunar and Eucrite Meteorites – Influence of the Mineralogy on Rock Breakdown

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Understanding regolith formation and evolution on airless planetary surfaces at the spatial scale from meters to microns is crucial. Diurnal temperature variations on airless planetary surfaces is a common feature of planetary bodies that play a role in regolith evolution [e.g., Molaro and Byrne, 2012; Delbo et al., 2014]. In a new laboratory experiment we investigated the effects of thermal fatigue in vacuum between 200K and 375K on the lunar anorthosite breccia Northwest Africa (NWA) 11273 and the eucrite Northwest Africa (NWA) 11050. A liquid nitrogen-cooled cryostat is evacuated and predefined temperature cycles are carried out automatically while monitoring the temperature. The samples are investigated via scanning electron microscopy (SEM) and micro-computed tomography after 0, 10, 20, 50, 100, and 400 cycles.

NWA 11050 responds to thermal cycling with the formation and extension of cracks, but the crack formation rate is only ~50% of that for samples studied previously. Lunar anorthosite breccia NWA 11273 shows extensive micro-flaking – a phenomenon reported here for the first time due to thermal stresses. We propose that surfaces exposing solid primary rocks (e.g., eucritic basalts) are less likely producing fine-grained soil by thermal fatigue but larger fragmented (blocky) regolith. Mature regolith rocks with high abundance of (impact) glasses such as the lunar anorthosite breccias are contributing to a fine-grained, tenth-of- μm -sized, soil.

References:

Molaro J. L. and Byrne S., (2012) *Journal of Geophysical Research* 117:E10.

Delbo M. et al. (2014) *Nature* 508:233-236.

Warren, P. H., and Korotev, R. L. (2022) *Meteoritics & Planetary Science* 57:527-557.

Lecture

Topic: 1.7 Experimental Petrology and Geochemistry

The stability of Tuite [γ -Ca₃(PO₄)₂] in peridotitic bulk systems and its significance for volatile and trace element transport into the deep Earth

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Apatite is an important host for halogens and incompatible trace elements, in particular for LILE and REE. The *P-T* stability of its high-*P* breakdown product tuite and its potential role as deep-Earth volatile and trace element carrier, however, is still largely unconstrained in both subduction zone and convecting mantle *P-T* regimes.

To investigate the upper *P-T* stability limit of tuite and its compositional evolution, multi-anvil experiments were conducted at 15 to 25 GPa and 1600 to 2000 °C, using a spinel lherzolite doped with β -Ca₃(PO₄)₂, halogens, and a trace element mix containing selected LIL, HFS and REE as starting material. The phases stable in this *P-T* range include tuite, majoritic garnet, ringwoodite, forsterite, clinoenstatite, bridgmanite, Ca-perovskite, ferropericlase, and melt.

Preliminary SIMS data indicate that Ca-perovskite and tuite are the major REE reservoirs. At 20 GPa/1600°C, REE_{tuite}/REE_{Ca-Pv} concentration ratios are 0.17 for Ce, 0.28 for Gd and 0.09 for Lu. At 25 GPa/1600°C these ratios are 0.09, 0.09, and 0.04, respectively. Both tuite and Ca-Pv strongly fractionate LREE, resulting in steep chondrite-normalized [1] REE-patterns. At 20 GPa/1600°C, for example, Ce_N/Lu_N ratios are 21.8 and 11.2 for tuite and Ca-Pv, respectively. This partitioning behaviour indicates that Ca-Pv is likely to be the major host for REE in primitive mantle, whereas tuite is an additional important REE-carrier and the most important P-carrier in metasomatically altered mantle.

[1] Barrat, J.A. et al., (2012) *Geochimica et Cosmochimica Acta* 83: 79–92.

Poster

Topic: 8.4 Post-mining: Opportunities and challenges

Mobile GIS as an innovative method for Geomonitoring of post-mining processes

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The use of geographic information systems in the field is often referred to as mobile GIS. This method makes it possible to collect, edit data with a smartphone application using GNSS locations. Especially important in scientific research is the verification of the obtained results. Mobile GIS allows the integration and implementation of data from various in-situ measurements such as soil sensors or thermometer. In this paper we will present results of mobile GIS application in projects: C₂M₂ - Climate Change | Management and Monitoring, Digital Twin- Integrated Geomonitoring and KaMonSyS - System for monitoring the installation and safety to cavernous storage facilities using satellite and drone-derived data, carried out by Research Center of Post-Mining at Technische Hochschule Georg Agricola.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Analysis of changes of the vegetation condition on the area of the closed Prosper Haniel mine using multispectral satellite and drone images.

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Mining and post-mining processes have a significant impact on the environment. An important current task and challenge is therefore the continuous monitoring of mining areas. The project "Digital Twin - Integrated Geomonitoring" financed by RAG Stiftung (no. 20-0013) and carried out in cooperation with the Geological Survey of North-Rhine Westphalia develops an integrated geoscientific workflow to monitor the former mine Prosper-Haniel, (Bottrop). This paper describes a method of environmental geo-monitoring using vegetation indices, which allow long-term, temporal-spatial observation of changes and trends at the land surface. The freely available EU-Copernicus Data with its multispectral Sentinel-2 as well as the NASA Landsat-8 data provide a giant data repository for this investigation. To validate the results a subsurface model of the overburden and tectonic elements of the mine is integrated. The results show the full valorisation of integrated geoscientific workflows to understand changes at the surface above a former mine.

Lecture

Topic: 11.3 Young Scientist Session

Relative importance of poroelastic effects and viscoelastic relaxation for postseismic velocity fields after normal and thrust earthquakes: insights from 2D finite-element modelling

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Earthquakes on faults in the brittle upper crust cause sudden changes in pore fluid pressure as well as viscoelastic flow in the lower crust and lithospheric mantle, which affect the postseismic stress and velocity fields in the crust. However, the relative importance of these processes during the postseismic phase has not been systematically studied. In this study, we use 2D finite-element models for intracontinental dip-slip faults to investigate the interaction of pore fluid pressure changes and postseismic viscoelastic relaxation during the earthquake cycle. In different experiments, we vary the permeability of the crust and the viscosity of the lower crust or lithospheric mantle, while keeping the other parameters constant. The results show that the earthquake induced pore pressure changes dissipate within a few days to decades, depending on the permeability of the crust. Therefore, poroelastic effects dominate the velocity field in the first few months, but still affect the velocity field years after the earthquake if the permeability of the upper crust is sufficiently low. Viscoelastic relaxation may also occur in the early postseismic phase for sufficiently low viscosities and then dominates the velocity field from about the second postseismic year onward. Depending on the viscosity, the viscoelastic flow may persist for several decades. Our findings imply that both poroelastic effects and viscoelastic relaxation may overlap earlier and over longer time periods than previously thought, which should be considered when interpreting aftershock distributions, postseismic Coulomb stress changes and surface displacements.

Lecture

Topic: 1.6 Probing (bio)geochemical reactions at mineral interfaces using micro- to nanoscale techniques

Structural incorporation of arsenate into vivianite

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Vivianite is a stable ferrous iron phosphate [Fe^{II}₃(PO₄)₂·8H₂O] that forms in oxygen-poor, Fe²⁺- and organic-rich environments. Isomorphic substitution of divalent cations (e.g. Mg and Mn) for Fe(II) in the structure are typical in natural vivianites. However, anion substitution is rare; and in particular, arsenate [As^VO₄³⁻] substitution has never been reported for natural vivianites and only partial substitution has been reported for synthetic analogues although parasymphesite [Fe^{II}₃(AsO₄)₂·8H₂O] exist in natural environments. In this study, we synthesized As(V)-substituted vivianites (Fe^{II}₃[(PO₄)_{1-x}(AsO₄)_x]₂·8H₂O) with systematically increased degrees of substitution (0.22 ≤ x ≤ 0.95), forming a complete solid solution between end-members vivianite and parasymphesite. The As(V)-substituted vivianites crystallized in a monoclinic C2/m like both end-members, and kept the platelet crystal habit of As-free vivianite even at high degrees of As(V) substitution. The local bonding environment data derived from Fe and As K-edge X-ray absorption spectroscopy and crystal chemical information from infrared spectroscopy analysis confirmed that As(V) was successfully incorporated into the vivianite crystal structure. Furthermore, the scanning transmission electron microscopy coupled with energy dispersive X-ray elemental maps revealed a homogenous distribution of As in the vivianite samples. Our data shows that As(V) can be incorporated into the vivianite structure (up to 95 mol% or 25 wt.%). In natural environments, this could provide a stable sink for arsenic immobilization in both modern and ancient ferruginous settings.

Lecture

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Alteration of basalt mineral surfaces at hydrothermal conditions: Insights into reaction mechanics during solid-fluid interactions.

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The analysis of solid-fluid interactions in nature is crucial for our understanding of material fluxes and sub-surface stability. However, there is still a significant quantitative and qualitative difference between dissolution data obtained in nature and laboratories. With modern surface-analysis techniques like AFM, VSI, SEM and Raman Spectroscopy, we can observe alteration on mineral surfaces on a high nanometer to low micrometer scale. This enables us to figure out microscopic reactions that can lead to macroscopic changes at rock surfaces.

To gain insights into a natural basaltic system, a subsurface observatory has been installed in a borehole at Surtsey volcano off the southwest coast of Iceland ^a. In the observatory, mineral surfaces of olivine (Fo90) and basaltic tephra were exposed to hydrothermal conditions at 41°C and 96°C respectively.

Laboratory experiments were performed with the same material under conditions similar to those in the Surtsey borehole. With the help of data from both experimental studies, we examined different gradients of palagonization reactions at glass surfaces as well as a beginning serpentinization of olivine at high temperature conditions. At low temperatures, especially olivine surfaces examined etch pits as a result of dissolution reactions. These differences in surface alteration demonstrate the complexity and the influence of various mechanics that play a role at solid fluid reactions and surface alteration. Furthermore, ongoing experiments address the role of microbe-mineral interactions in controlling the rates and mechanisms of mineral dissolution and precipitation.

^aTürke et. al.: Design of the subsurface observatory at Surtsey volcano, Iceland, 2017.

Lecture

Topic: 9.4 Chemical sediments and mineral deposits in basins: archives of paleoclimatic, hydrogenetic, biogenic, hydrothermal, and diagenetic, processes throughout Earth's history

Triple oxygen isotope compositions of iron oxide-apatite deposits – a window into ore formation processes and the ancient atmosphere

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Iron oxide - apatite (IOA) deposits are magnetite- and apatite-rich rock assemblages that are hosted by intermediate to felsic magmatic rocks, and are frequently mined for iron. The geological formation mechanisms of IOA deposits were suggested to involve either high-temperature silicate, iron oxide and/or sulfate melts or, alternatively, hydrothermal processes at more moderate temperatures. Here, we show that magnetite and apatite samples from the type locality of the deposits in the Kiruna district, northern Sweden, contain up to tens of atom percent oxygen from evaporitic sulfate, as is demonstrated by their anomalously low $\Delta^{17}\text{O}$ values. In order to explain this observation in conjunction with field evidence for an igneous origin of the deposits from Kiruna, we propose that the IOA assemblage of Kiruna crystallised from iron-rich sulfate melts and/or from sulfate-rich iron oxide melts. The iron-rich sulfate melts would have formed when evaporite-rich sediments melted by anatexis and scavenged iron from magmatic sources, whereas sulfate-rich iron oxide melts could have formed, e.g., when iron oxide liquids exsolved from silicate magmas and then assimilated evaporites. An inventory study shows that several other Proterozoic and Cambrian IOA deposits have anomalously low $\Delta^{17}\text{O}$ values similar to Kiruna, whereas post-Cambrian IOA deposits, in contrast, have more moderate $\Delta^{17}\text{O}$ values. IOA deposits may therefore ubiquitously contain evaporite-derived oxygen, with variations in the lowermost $\Delta^{17}\text{O}$ values of the deposits reflecting the changing isotope composition of atmospheric O_2 through time; and therefore providing an unexpected window into global bioproductivity and atmospheric $p\text{CO}_2$ levels of the ancient Earth.

Poster

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

The export of barium into the marine benthic realm assessed through Ba/Ca of benthic foraminifera – approaching a novel calibration

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Global warming and changes in precipitation patterns are of increasing concern for populations in the Mediterranean region. Exploiting regional paleoenvironmental archives helps to understand how climatic parameters changed regionally in past periods which serve as future climate analogues. Prominently, benthic foraminifera serve as proxy carriers to unravel variability of paleo-temperature, -salinity, -pH, -productivity and -oxygenation. Besides the faunal composition of a defined sediment sample, the geochemical signature recorded in the shells is a constantly investigated proxy signal. Recently, the Ba/Ca has been proposed to track changes in barium content of marine bottom waters. In fact, barium concentrations in the benthic (shallow) marine environment either reflect directly riverine input or export productivity via barite as part of the organic matter sinking to the seafloor. We use core-top material of dead and live (Rose Bengal stained) specimens from a water depth range of 600-1500 m throughout the Northern Aegean Sea, to quantify variability of Ba/Ca across two different species with hyaline shells (*Melonis baarleanus* and *Uvigerina mediterranea*) and different sediment sampling depths. Using Laser Ablation ICP-MS we can further assess the intratest variability of Ba/Ca_{foram}. Moreover, we compare the Ba/Ca_{foram} to measured bottom water [Ba/Ca] from the same locality and consider a multitude of factors for approaching this novel core-top calibration. First results show that the species-specific partition coefficients are matching those of published laboratory experiments and core-top calibrations for hyaline benthic foraminifera. We show the application of high-resolution sampling techniques in the benthic environment to assess the complex present-day situation.

Poster

Topic: 8.1 Geosciences and Waste Management

Measurement of the dusting behaviour by means of continuous fall and determination of the asbestos content by scanning electron microscopy of technical building materials

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Asbestos fibres are still an important topic today due to their strong carcinogenic effect, especially in demolition, renovation, and maintenance work. Due to the various matrices and asbestos fibre bonding in different materials, it is assumed that the fibre release potential will vary accordingly. This fibre release potential is investigated in this study. Additionally, the analytical method described in the TRGS 517 is applied regarding the determination of the mass content of asbestos in fine-grained products.

Mortared building materials with different asbestos mass contents are processed using the DusTower. The occupied filter is then processed and analysed using a scanning electron microscope (SEM) according to IFA/BIA 7487. By measuring the asbestos fibres regarding their length and diameter, the mass content on the filter and in the product can subsequently be calculated.

The analysis shows that it is not possible to determine the mass content of asbestos in the product with this method. However, the fibre release potential behaves differently with the materials and some materials release more fibres than others. This depends on both the grain size and the fibre bond. We can draw important conclusions regarding methodology and more importantly, with respect to the fibre release potential of different materials which are being handled on building sites every day.

Lecture

Topic: 1.7 Experimental Petrology and Geochemistry

Alkali depletion as a trigger for degassing of hydrous melts in magma injection processes

Patricia Louisa Petri, Anja Allabar, Marcus Nowak

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The injection of mafic magma into a hydrous felsic magma chamber is a potential trigger mechanism for bimodal explosive volcanism. Contact of hot mafic magma with cooler, H₂O-rich rhyolitic magma causes a decrease in H₂O solubility <300 MPa to trigger vesicle formation. Mixing processes at the interface may reinforce vesicle formation (Caricchi et al. 2021).

Bimodal decompression and reference experiments were performed with basaltic and rhyolitic melts. Pre-hydrated rhyolite- and basalt-cylinders were perfectly contacted, heated, and equilibrated to experimental conditions. The initial sample properties were determined by a bimodal reference experiment, quenched immediately after equilibration. To simulate the magma ascent, three bimodal samples, and a rhyolite-rhyolite decompression experiment for testing the experimental setup were decompressed to the final pressure and then quenched.

The rhyolite reference experiment showed homogeneously distributed H₂O vesicles throughout the sample, verifying the two-cylinder design. In all bimodal samples, a hybrid zone formed between the end-members, due to diffusion-induced mixing processes. An enhanced vesiculated zone developed in the rhyolite-dominated hybrid zone compared to the unmixed endmembers. This results from the rapid diffusive loss of alkalis from the mildly peralkaline rhyolitic melt into the basaltic melt. The decreased Na₂O concentration reduces the H₂O solubility (Allabar et al. 2022) and promotes H₂O supersaturation in the depleted rhyolitic melt during decompression.

This suggests that injection of a basaltic melt into a hydrated peralkaline rhyolitic melt reservoir can lead to significantly enhanced H₂O vesicle formation in the hybrid zone. Increased degassing and the associated triggering of explosive eruptions can be expected.

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

New avenues in isotope analyses: The Thermo Scientific™ Neoma™ MC-ICP-MS/MS

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Multicollector inductively coupled mass spectrometry (MC-ICP-MS) is irreplaceable in modern isotope ratio mass spectrometry of metals. The advent of this technique paved the way to analyze large parts of the periodic table to investigate scientific questions with up to single ppm precision. However, the application is limited by the presence of Ar-based interferences inherent to the Ar plasma source and by the need to elaborately purify samples by chemical treatment to overcome isobaric interferences.

The introduction of single-collector ICP-MS/MS instruments opened a new way of on-line chemical separation during the measurement by using a mass filter prior to a collision/reaction cell. A confined mass range can be introduced into the reaction cell where different chemical behavior of the elements allows selective mass shift reactions into another mass range that has been cleared by the mass filter for interference-free analyses. Great potential of this application has been identified in the field of *in situ* geochronology of beta-decay systems such as Rb-Sr.

The Neoma MS/MS combines for the first time the unprecedented precision of MC-ICP-MS with a proprietary pre-cell mass filter and the chemical selectivity of a collision/reaction cell in a commercially available instrument. Earlier analytical concepts were improved by a novel pre-cell mass filter and hexapole collision/reaction cell to guarantee the full performance of the standard Neoma MC-ICP-MS while adding the new abilities of MS/MS. Here, we report on the benefits for a variety of new applications within geosciences.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Dating of weathering and oxygenation events in the Keonjhar Paleosol, Singhbhum Craton, East India

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The chemical inventory of Archean paleosols provides crucial constraints on early paleoclimate and paleoredox conditions. However, it often remains ambiguous whether recent weathering has also affected such early signals. This is especially crucial for understanding when free oxygen was present in Earth's atmosphere. Although there is multi-proxy geochemical evidence for episodes of early oxygenation prior to the GOE, some claims for early oxygenation signals in near-surface rocks may have resulted from modern terrestrial weathering. Among the rare occurrence of Archean paleosols, the ca. 3.0 Ga Keonjhar Paleosol in the Singhbhum Craton of East India has received particular attention in this regard, as the occurrence of Ce anomalies has been interpreted to originate from the presence of free oxygen in Earth's Mesoarchean atmosphere [1]. To test this hypothesis, we applied ¹³⁸La-¹³⁸Ce geochronology [2] to various sections of this paleosol that reveal a ¹³⁸La-¹³⁸Ce age of 115±54 Ma, which precludes Archean oxygenation and rather reflects late Mesozoic weathering. In addition, we have also determined ¹⁴⁷Sm-¹⁴³Nd and ¹⁷⁶Lu-¹⁷⁶Hf ages for this paleosol, of 1058±56 Ma and <84 Ma, respectively. This result is surprising, as the ¹⁷⁶Lu-¹⁷⁶Hf system seems to be fully overprinted by young weathering compared to the ¹⁴⁷Sm-¹⁴³Nd system. The Sm-Nd age may reflect partial REE remobilization during Proterozoic orogenic overprint [3].

[1] Mukhopadhyay et. al., GEOLOGY, 2014, 42, 10, 923–926.

[2] Tanaka and Masuda, Nature, 1982, 300, 515-518.

[3] Ghosh and Bose, JMPS, 2020, 115, 70-87.

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

Access for free: How to get free-of-charge access to Earth scientific research labs through EPOS-NL and EXCITE

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Access to top research equipment facilitates top research. However, the research equipment needed may not always be available within individual institutes, while access to external facilities may not in all cases be affordable. This restricts the research that any individual can do and hampers scientific breakthroughs, particularly across disciplines. To overcome this limitation, two collaborative infrastructure networks were recently initiated: EPOS-NL (European Plate Observing System- Netherlands) and the EXCITE network. Both these networks pool facilities present at multiple institutes and provide free-of charge access to these, for Earth Scientists worldwide. Specifically, EPOS-NL (www.EPOS-NL.nl) provides access to geophysical labs in the Netherlands, for research within rock physics, microscopy, tomography and analogue modelling of tectonic processes. These labs can provide the means and expertise for research into the mechanical behavior and transport properties of the Earth's crust and upper mantle. The EXCITE network (www.EXCITE-network.eu) provides trans-national access to 24 state-of-the-art microscopy and tomography facilities in Europe. As such it can help you gain insight into the processes governing the behavior of the Earth crust through microchemical analyses and 2D- to 4D imaging, and down to nanometer resolution. Access to EPOS-NL and EXCITE can be requested by applying to a bi-annual call, posted on their respective websites. This involves submitting a short (1-2 page) research proposal. Research proposals are peer-reviewed on the basis of excellence but generally have a high chance of success (~80% in previous rounds). Interested? Have a look on the EPOS-NL and EXCITE websites – and apply!

Poster

Topic: 7.3 Assessment of the Earth System through Micropaleontology

Neoflabellina reticulata (Reuss 1851) – The Fossil of the Year 2022

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The Paläontologische Gesellschaft (Palaeontological Association) has been awarding the title Fossil of the Year since 2008. Every year an important fossil is chosen to promote palaeontology in the public. This year, after presenting several vertebrate, invertebrate and plant fossils, a microfossil was selected for the first time. Arguments for the selection of the foraminifer *Neoflabellina reticulata* are:

- *Neoflabellina reticulata* is a beautiful fossil.
- *Neoflabellina reticulata* is an index fossil of the Maastrichtian, thus underlines the utility of microfossils in biostratigraphy. The Maastrichtian is the last stage of the Cretaceous and ends with the best known mass extinction event.
- *Neoflabellina reticulata* lived in marine shelf environments below the storm wave base, i.e., it can be used as palaeoecological indicator.
- *Neoflabellina reticulata* can be found in practically all chalk environments of the Maastrichtian and is documented from such well known sites as the chalk cliffs of Rügen island.
- The first description of *Neoflabellina reticulata* was published by August Emil Reuss in 1851, in the period of the establishment of micropalaeontology as a science.
- The locus typicus of *Neoflabellina reticulata* are the chalk marls of Lemberg, today's Lviv in Ukraine. This underlines the connectivity of science.

The Fossil of the Year was presented in a public lecture in the Pommersches Landesmuseum in Greifswald 22 May 2022. Here, we provide more information on our poster.

Lecture

Topic: 6.3 Fractionation of metal(loid) stable isotopes during low-temperature Earth surface processes

Tracing silicate weathering using lithium isotopes: from the lab, to the field and the past

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Silicate weathering is the primary mechanism by which atmospheric CO₂ is removed and stored for long periods of time. It is therefore a key biogeochemical mechanism in controlling the present and past climate, and may also have a significant role in future carbon dioxide removal. However, tracing silicate weathering is difficult in the modern environment, and have proven particularly challenging during geological history.

Lithium isotopes appear to be a tracer with significant potential in this field, because they only trace silicate weathering, and are apparently unaffected by biological processes.

Here we will present the behaviour of Li isotopes during weathering experiments and in the field. We will then demonstrate how this relates to Li isotope excursions through climatic events in Earth history, and what Li isotope data tell us about the operation of the "weathering thermostat" – the purported temperature-dependent stabilisation mechanism of the climate.

Lecture

Topic: 4.3 The role of fluids in metamorphic and metasomatic reactions

Fluid flow characteristics recorded in continental eclogites of the Münchberg Massif

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Eclogite-facies metamorphic veins provide records of fluid flow dynamics during high-pressure metamorphism. Here, we evaluate the inventory of quartz-rich metamorphic veins and segregations in Variscan eclogites from the Münchberg Massif (NE Bavaria) to investigate the fluid origin and the scale of fluid flow. These eclogites experienced peak P-T conditions around 3 GPa and 700°C, and a continental rather than oceanic mafic igneous protolith setting is proposed.

Isolated, mm-sized quartz pockets with euhedral high-pressure minerals are common in the Münchberg eclogites, but continuous veins that may have allowed focused fluid flow to beyond specimen scale are rare. Nevertheless, where such veins occur, they can contain eclogite assemblages including minerals such as omphacite, garnet, rutile, kyanite, and phengite. Oxygen isotope thermometry of quartz-garnet, quartz-phengite, and quartz-kyanite pairs yield temperatures around 700°C. $\delta^{18}\text{O}$ values of quartz (+6.1 to +10.5‰) from almost all the veins are identical to predicted (from mass balance modelling at 700°C based on host rock $\delta^{18}\text{O}$ values from +4.0 to +7.9‰) equilibrium $\delta^{18}\text{O}$ values of host rock quartz.

The veins and pockets are mostly in equilibrium with their host eclogites regarding texture, mineralogy, mineral chemistry, and oxygen isotopes. They seem to represent former cavities filled by internally-derived fluids, whereas indications for fluid transport beyond specimen scale are rare. The abundance of isolated quartz pockets and scarcity of more extended veins suggest that rather low quantities of fluid were produced. This may be typical for continental eclogites, which are supposed to have experienced little pre-subduction hydration compared to oceanic eclogites.

Lecture

Topic: 8.1 Geosciences and Waste Management

A lab on a chip concept for rationalizing hydro-geochemical processes at the pore scale and their integration into larger scale analyses

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Deep geological repositories with a multi-barrier concept are foreseen by various countries for the disposal of high-level radioactive waste. Advanced simulation tools based on a detailed process understanding need to be developed for a close-to-reality description of repository evolution scenarios over time scales of some hundred thousand years. The construction of underground galleries and geotechnical barriers in the host rock formation and the emplacement of nuclear waste packages will create perturbations induced by chemical, thermal and pressure gradients at the interfaces of the different barriers, leading to mineral dissolution and precipitation to achieve re-equilibration. These processes can lead to an alteration of permeability, diffusivity and other physical characteristics of the rock matrix that can have significant effects on subsurface solute and gas transport. The understanding of these phenomena at the pore scale is a prerequisite for the development of predictive conceptual approaches to describe the evolution of the subsurface. Our lab on a chip concept, which combines microfluidic experiments and reactive transport modelling has proven to be a powerful tool to (i) evaluate the impact of hydraulic heterogeneity on nucleation mechanism, (ii) decode oscillatory zoning exhibited by solid solutions crystallizing in porous media, (iv) assess the effects of confinement of crystallization, and finally (v) parameterize porosity-diffusivity relationships with respect to coupled mineral dissolution-precipitation reactions. In this work, we discuss how this pore-scale knowledge can be integrated into reactive transport models to achieve a realistic description of coupled processes at perturbed interfaces.

Poster

Topic: 1.8 Minerals and Mineral Properties

The elastic tensor of natural topaz: the effect of OH/F ratio

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Topaz $\text{Al}_2\text{SiO}_4(\text{OH}_x\text{F}_{1-x})_2$ is a crustal mineral, typical of magmatic and hydrothermal environments, but also present in metamorphic orogenic settings. It is characterized by high density and mechanical properties that make it a popular precious stone. Although apparently simple, the chemical composition of topaz shows a wide variability in the ratio OH/F, which has attracted researchers interested in connecting it to their geological settings, and for provenance analysis to identify the sources of commercial stones. We present a study of the full elastic tensor of a set of four, well characterized, natural Topaz crystals from different geological settings and with different OH/F ratios. The substitution of F with OH produces a general softening of the elastic coefficients of topaz. We present and interpret the compositional dependence of the individual tensor coefficients and the aggregate moduli in connection with the consequences of OH/F substitution in the crystal structure of topaz.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

OneGeochemistry; Paving the way to true Interoperability in Geochemistry Data

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Geochemical data have been collected since the 19th century and are essential for geoscientific research as well as contributing to solving societal issues. Typically local or regional questions are solved with single datasets that can be measured in megabytes. However, solving more complex research questions requires many datasets to be compiled into single large ones to find answers through multidimensional analyses, statistics, AI and ML. Compiling such collections to allow computations is often a painstakingly lengthy and manual process.

Coming to an age in which we are dealing with global challenges, only large scale geochemical data collections can contribute to solving these. Projects such as EarthChem and GEOROC have come a long way and continue to set the bar. Whilst these projects have made geochemical data easily findable and accessible, interoperability to other global data systems is still lacking. To make these data truly FAIR, a minimum set of standards and best-practices for data publication need to be agreed on by the global geochemical community. And rather than re-inventing the wheel, we should follow the example of the highly standardized sample and data management strategies of, e.g., IODP cruises, NASA missions, or the seismology and OneGeology communities.

The recently formed OneGeochemistry initiative aims to bring together and ensure that all decisions are made in conference with the international geochemical community. The large international societies will have to play a key role here, their message supported and amplified by funders and national initiatives across the globe.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

Observing high pressure melting and crystallization of silicates utilizing MHz diffraction at the European X-ray free electron laser

Clemens Prescher¹, Guillaume Morard², Marzena Baron³, Ryan Stewart McWilliams⁴, EuXFEL community proposal #2292⁵, EuXFEL community proposal #2605⁶

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The opening of the European X-ray Free Electron Laser near Hamburg (EuXFEL) offers promising new experimental opportunities for studying materials. It can deliver X-rays with energies up to 25 keV and its brightness is so large, that a single pulse exhibits enough intensity to generate a diffraction image. In combination with the 4.5 MHz (220 ns separation) rate of pulse delivery, and new detector technologies (AGIPD), the EuXFEL enables unique capabilities for time resolved diffraction experiments.

Coupling these new capabilities with laser heated diamond anvil cells, enables the study of materials under planetary conditions with unprecedented time resolution, possibly overcoming previous issues with chemical reactions between the sample and its environment as well as the study of transient phenomena such as phase transformations.

We will present first results and challenges of experiments investigating silicates under extreme conditions at the "High Energy Density" (HED) instrument of the European XFEL during two community proposals which brought together around fifty international participants (proposal numbers #2292 and #2605).

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

Optical clumped isotope thermometry of carbon dioxide and methane

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Clumped isotope thermometry exploits the relative abundance of doubly substituted isotopologues to decipher the formation temperature of minerals. Here we present a promising approach based on mid-IR laser absorption spectroscopy for high-precision measurements of $^{13}\text{C}^{18}\text{O}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}_2$, $^{13}\text{CH}_3\text{D}$, and $^{12}\text{CH}_2\text{D}_2$ isotopologues in CO_2 and CH_4 . This optical approach offers rapid analysis on a 10-20 minutes scale, compared to hours or days needed for mass spectrometry. The currently reached sub-‰ precision is sufficient for the realization of an optical isotope thermometer for many geochemical applications.

Poster

Topic: 4.1 Magmas and Fluids in the Crust

Age differences between separate magma pulses in two laccoliths (Halle Volcanic Complex): insight into processes of silicic magma formation

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The Halle Volcanic Complex includes several laccoliths emplaced during Carboniferous-Permian flare-up (Breitzkreuz & Kennedy, 1999). Previous dating of the laccoliths yielded a range of ages from 301 ± 3 Ma (Landsberg) to 292 ± 3 Ma (Petersberg). Textural and whole rock chemical composition of samples from several depths from both laccoliths suggest formation of the laccoliths in several pulses and in this study we have checked if a complementary record is preserved in chemical composition of accessory phases. Altogether seven depths have been analyzed from two laccoliths including electron microprobe analyses of zircon and apatite and U-Pb SHRIMP dating. Additionally four depths were analysed for U-Pb zircon age by CA-ID-TIMS. Zircon is chemically homogenous within and between laccoliths and has similar sets of inclusions. On the other hand, apatite shows variable Nd contents decreasing with depth for both laccoliths and apatite from Petersberg has more Cl, when apatite from Landsberg has more Na. The implication is that apatite chemistry is better at recording magma evolution than zircon. SHRIMP ages are scattered over 30 Ma for a single sample, which suggests the presence of antecrysts and lead-loss, or alternatively indicates formation of the laccoliths over a prolonged period of time.

Acknowledgements: The research was funded by the National Science Centre (Poland) the OPUS project UMO-2017/25/B/ST10/00180 to APietranik.

Breitzkreuz, C., Kennedy, A. (1999) Magmatic flare-up at the Carboniferous/Permian boundary in the NE German Basin revealed by SHRIMP zircon ages. *Tectonophysics*. 302, 307-326.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Petrographical and petrophysical properties of tight siliciclastic rocks from the Ibbenbueren coal mine with regard to mine flooding

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With regard to high production costs and the energy transition, German hard coal mining was phased out in 2018. As mine water drainage becomes economically and technically redundant, the mine water rebound may change the local stress state inducing ground movements, microseismicity, and gas anomalies. Geomechanical approaches that attempt to couple subsurface stress changes and surface ground movements require geological and petrophysical information of the subsurface. This study provides petrographic and petrophysical data of Upper Carboniferous (Westphalian B–C), fluvial, tight (most porosities <10 %, most permeabilities <1 mD) siliciclastic rocks from the former Ibbenbueren coal mine in NW Germany where the ground water currently rebounds. Measured compressional (3809–6656 m/s) and shear wave velocities (2126–3723 m/s), and calculated Young's moduli (31.3–80.9 GPa) vary significantly and are related to Cretaceous maximum burial. Thus, predominantly mechanical compaction and subordinately quartz cementation altered the textural framework of the rocks. Grain size (0.008–1.1 mm) determined by the depositional environment represents the major control on wave velocities and Young's moduli. Calculated Poisson's ratios (0.09–0.31) in contrast are a function of the stress history, initial mineralogy, and diagenetic alterations. Therefore, the variations observed in texture, mineralogy, wave velocities, and derived Young's moduli and Poisson's ratios are crucial for the poroelastic behavior of the subsurface and need to be considered in case studies, which model post-mining ground movements as a result of mine flooding.

Lecture

Topic: 5.6 Natural archives as recorders of past climate and environmental conditions – processes, methods and applications

Radiocarbon depleted intermediate water masses during the LGM in the equatorial Indian Ocean

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Ocean circulation and changes in ventilation represent one of the crucial regulation screws in the Earth's climate system. For the Last Glacial Maximum (LGM, 21 kyr BP), characterized by a 100 ppm lower atmospheric CO₂ concentration, growing evidence exists for enhanced storage of CO₂ in the deep-sea. However, inasmuch the intermediate depth of the oceans opposed or amplified this sequestration is poorly constrained.

Here we present coupled ²³⁰Th/U and ¹⁴C measurements on scleractinian cold-water corals retrieved from ~450m water depth off the Maldives in the Indian Ocean. Based on these measurements we calculate $\Delta^{14}\text{C}$, $\Delta\Delta^{14}\text{C}$ and Benthic-Atmosphere (B_{atm}) ages in order to understand ventilation dynamics of Indian Ocean intermediate water masses.

Our results exhibit radiocarbon depleted intermediate water masses as low as -340 ‰ ($\Delta\Delta^{14}\text{C}$), corresponding to ~2100 years (B_{atm}) at the LGM. Such extremely radiocarbon depleted intermediate water masses suggest abyssal upwelling of southern-sourced deep-water masses, being strongly enriched in respired carbon and thus highlighting the oceanic carbon storage capacity even at upper thermocline depth. Nevertheless, B_{atm} ages reveal a pronounced short-term centennial variability, that demonstrates the dynamic nature of this oceanographic phenomena.

Thus, reduced intermediate ocean ventilation off the Maldives and resulting carbon storage may help to improve our understanding of the role of the thermocline Ocean with respect to the Earth's carbon cycle.

Ramdohr-Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

CaSO₄ crust as potential habitat for microbial life in the extreme hyperarid Atacama Desert and their reciprocal effects

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The Atacama Desert is one of the most extreme landscapes and environments on Earth. Due to its predominant hyperarid climate and high UV radiation, life is mostly absent. Prolonged aridity causes the formation of CaSO₄-rich soils and crusts from mostly atmospheric deposition and aeolian input, creating a blanket covering vast landscapes. Water as the defining pre-requisite for life is scarce, however, infrequent precipitation events, fog and dew are potential moisture sources. CaSO₄-rich soils in the Atacama Desert are cemented due to secondary modification (dissolution, transport and re-precipitation) of CaSO₄ minerals (Gypsum-Basanite-Anhydrite) and other soluble salts, which form an indurated surface cover with several dm to meters thickness. Within these CaSO₄-rich soils, cavities and cracks are partly covered with recrystallized evaporitic minerals indicating the temporal presence of water activity (of unknown state and volume). Harsh environmental conditions on the surface contrast life in the subsurface. Microbial communities from different groups of bacteria, archaea and eukaryotes inhabit such endolithic environments, living from captured moisture within the soil, or potential from hydrated CaSO₄. Their presence and interaction, however, can also influence pedogenic processes, contributing to CaSO₄ dynamics as landscape forming agent and as preconditions for higher developed life. We present some initial results from a CaSO₄-rich soil crust study from the Atacama Desert, using XRD, ICP-OES, and SEM imaging along with the lipid-biomarker analysis to explore and characterize the CaSO₄-rich soil as habitat for microbial life, and to unravel the potential impact of microbial life on landscape forming processes, i.e. CaSO₄ soil dynamics.

Lecture

Topic: 10.2 Geoethics – fostering ethical perspectives in Geosciences

Skeletons in the closet: ethics, law, and politics in palaeontology

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Palaeontology is unique among scientific disciplines in that it thrives on the exchange of information across diverse communities, both academic and non-academic. However, palaeontological research does not always best serve these communities. A practice that is prevalent in palaeontology is "parachute science", referring to the practice whereby researchers drop into, collect data and leave without the involvement or interaction with the local community. Put simply, these parachuting palaeontologists are benefitting from the resources of a country and often, the efforts of local people, without giving anything back. Lack of paleontological and scientific involvement with communities in the Global South may be a remnant of colonial-era palaeontology. The history of natural science is inseparable from the history of European colonialism when local specimens were brought to the homeland of the colonisers to be repositied and studied in museums for the sake of the "greater scientific good". The culture of theft and plunder, a legacy of colonialism perpetuates in palaeontology, even now. The drive for discovering the next new extraordinary fossil can be linked to several ethical and legal issues, where fossils are excavated without record and smuggled across borders to finally end up in collections across the world.

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

Identifying Li-bearing phases by μ EDXRF based automated mineralogy

Dieter Rammlmair

Germany

The automated identification and quantification of Li-bearing phases in core samples and hand specimen has gained interest due to increasing industrial demand for lithium. Despite the fact, that Li cannot be directly detected by μ EDXRF, the spectral signatures of a number of Li-bearing phases such as spodumene, lepidolite, amblygonite and others are characteristic enough to differentiate them from non-Li phases. By applying hyperspectral ENVI software and its spectral angle mapper (SAM) algorithm a supervised classification based on an endmember data bases can be used to image the phase distribution. SAM considers all ratios of available band based on total signal intensity per pixel per selected spectral region to offer a measure to compare an unknown pixel with all available endmembers of a database. A good knowledge of the paragenesis of each investigated system is key to limit ambiguities between Li phases, and non-Li phases carrying elements, such as H, Be, B, which cannot be detected either. This will be achieved by tailoring the endmember database according to these premises. Quantitative μ EDXRF-based mineralogy is based on interpretation of chemical signatures, but shows some limitations regarding isochemical phases, isochemical mixtures at grain boundaries and sporadically strong diffraction signals of one or the other grain. Results which can be obtained are modal mineralogy, grain area size distribution, grain aspect ratio and sample and grain area chemistry.

Poster

Topic: 8.1 Geosciences and Waste Management

Chemical and mineralogical characterization of Li- and Mn-bearing slags to increase the recycling efficiency of lithium from lithium-ion-batteries (LIB)

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Within the framework of the BMBF-funded project „PyroLith“ (FKZ: 03XP0336C), which deals with the recovery of lithium from NMC-type LIB via a combined pyro- and hydrometallurgical process route, two slag sample series of a simplified five-component system $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO-Li}_2\text{O-MnO}$ were characterized using XRD, SEM-MLA, EPMA, XRF, ICP-MS and UVC radiation. The focus of the investigations was on crystalline and amorphous Li-bearing phases, their crystal growth and degree of intergrowth.

The results show that the slags generally solidified in a vesicular to compact, fine-grained, holo- to hypocrySTALLINE, heterogeneous microstructure with a silicate matrix. Euhedral, anhedral and/or dendritic crystals up to 900 μm in size are embedded in the groundmass. In addition to variable contents of amorphous components, a total of six crystalline Li-containing phases ($\gamma\text{-LiAlO}_2$, $\beta\text{-eucryptite}$, Li-Mn-Al spinel, LiAl_5O_8 , $\text{Li}_5\text{AlSi}_2\text{O}_8$, $\text{Li}_2\text{MnSiO}_4$) and two crystalline Li-free phases (melilite, glaucocroite) could be identified and quantified. Based on their chemical composition, two amorphous phases are distinguished. $\gamma\text{-LiAlO}_2$, which is considered most important for an effective recovery of lithium in the selected process route, shows a characteristic green luminescence colour with distinct phosphorescence under short-wave ultraviolet radiation (254 nm). An influence of manganese on the crystallization of $\gamma\text{-LiAlO}_2$, as described in [1] and [2], could not be observed.

[1] LIBRI (2011): Entwicklung eines realisierbaren Recyclingkonzeptes für die Hochleistungsbatterien zukünftiger Elektrofahrzeuge. Abschlussbericht, 132 S., Hanau

[2] Wittkowsi A., Schirmer T., Qiu H., Goldmann D. & Fittschen U.E.A. (2021): Speciation of Manganese in a Synthetic Recycling Slag Relevant for Lithium Recycling from Lithium-Ion-Batteries. *Metals* 2021, 11, 188

Poster

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Investigating Te and other volatile trace elements in sediments as proxies for flood basalt volcanism

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Linking the timing and eruption rate of flood basalt volcanism with the sedimentary record is critical to understanding how large volcanic events cause environmental change during periods of mass extinction. We investigated the trace elements Te, Re, Cd, As, Sb, Tl which are highly enriched in volcanic gas relative to crustal rocks, as potential proxies for past volcanism. We analysed sediments from the Permian-Triassic, Pliensbachian-Toarcian and Cretaceous-Paleogene boundaries where mass extinction events have been linked to Siberian, Karoo-Ferrar and Deccan flood basalt volcanism respectively.

At the P/Tr boundary at Spitsbergen, Te concentrations and Te/Th ratios increase by a factor of 10 together with Hg at the Late Permian Extinction level, and decrease gradually over 300-400 kyr into the Griesbachian. Two Lower Jurassic sections (Portugal, France) show similar enrichments in Te during and after the Toarcian Oceanic Anoxic Event, and at the Pl/To boundary. Late Maastrichtian and early Danian sediments at Elles (Tunisia) record several peaks in Te/Th below and above the K/Pg boundary, possibly corresponding to 100 kyr pulses of Deccan volcanism, and a 'spike' due to extra-terrestrial Te in the K/Pg boundary clay.

Te/Th does not appear to vary systematically with sediment lithology, or with changes in environmental conditions. We suggest that the Te enrichments are volcanic in origin, and together with Hg and Hg/TOC ratios, may be used as a proxy for the intensity of volcanic activity. In contrast, Cd, Tl and Re concentrations in sediments from these sections are at least partly influenced by environmental factors.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Archaeometry - tracing the past human footprint with geosciences

Thilo Rehren

The Cyprus Institute, Cyprus

Recent debates around the recognition (or otherwise) of an Anthropocene, and the impact of climate change on the human experience emphasize the fact that 'we humans' are an integral part of System Earth. Thus, research methods and approaches developed within the Earth Sciences are eminently suitable to study our interaction with it. At the same time, the inherent understanding of time, and the change that comes with it, further predestines methods of the Earth Sciences for the study of the human past – i.e. doing archaeology.

In this lecture, I will explore the two sides of the human – environment interaction, and discuss the role of Archaeometry / Archaeological Sciences bridging the two domains of earth sciences and anthropology, respectively. Traditionally, mining & metallurgy, and more recently also oil & gas extraction are commonly associated with a particularly heavy 'footprint' of humans on the environment. However, most of my examples will be drawn from the study of ancient glass and its production as one proxy to study human mobility, complementing a much wider array of tools and approaches to the many facets of this topic.

Poster

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

Sweet death – lead glazed Renaissance ceramics and their interaction with acidic foodstuffs

Thilo Rehren¹, Thomas Delbey², Brunella Santarelli¹, Giulia Fogarizzu¹, Kaare Rasmussen³

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We present analyses of lead glazes from dishes and storage bowl from six Renaissance (1536 to 1660 CE) sites in southern Denmark and northern Germany. All are high-lead silicates, ranging from 55 wt% to 75 wt% PbO, with only silica and alumina routinely exceeding c 1 wt%. The underlying bodies are ferruginous clays with 15 to 20 wt% Al₂O₃ and <10 wt% Fe₂O₃.

Here, we discuss the relationship between the PbO content in the glaze with the amount of lead entering acidic foodstuffs stored or served in these vessels. The experiments used 4 wt% acetic acid, similar to common foodstuffs preserved with vinegar such as pickles. This concentration is high enough to be effective in preserving food, while low enough to taste good. It also approximates official test methods for the release of Pb for glass hollowware in contact with food according to ISO 7086-1.

We found a strong exponential correlation between lead leaching and lead oxide content in the glaze, reaching toxic levels in the leachate solution after short periods of exposure (less than 1 day) for PbO contents above c 70 wt% PbO. Our research shows that widely distributed lead-glazed ceramics had the potential of being a main source of Pb in human bodies. How the pottery was actually used, in combination with kitchen wares fashioned from other materials, might explain why lead-glazed ceramics might not have had quite the poisonous consequences the etching experiments suggest.

Lecture

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

Dissecting a granulite-facies migmatite: Leucosome – melanosome – bulk rock relationships and the role of garnet (Namaqua Metamorphic Province, South Africa)

Jürgen Reinhardt, Aidan Leetz, Russell Bailie

University of the Western Cape, South Africa

A geochemical-mineralogical study carried out on a migmatite from the granulite zone of the Bushmanland Domain in the Grenville-cycle Namaqua-Natal Belt in southern Africa reveals an anatexis process largely controlled by biotite dehydration melting that resulted in leucosome compositions which are less siliceous and which have a higher maficity compared to the melanosomes. The rocks show an unusual internal S-L structure with a dominantly linear, parallel arrangement of isolated leucosome patches within a melanosome matrix. Although the leucosome proportion is high (between 40 and 60 vol%), there is very little local interconnectivity between adjacent leucosome patches, with no clear evidence for either larger-scale melt accumulation, or for melt escape channels along or across the rocks' structural anisotropy. Geochemical evidence indeed points to anatexis without significant melt loss, whereby the resultant leucosome and melanosome segregations combine in the bulk rock to a composition that corresponds to a pre-anatexis metapelitic protolith. The leucosomes show no evidence for the involvement of externally-derived melts.

Garnet plays a critical role for the major and trace element distribution between leucosome and melanosome, as it is concentrated in the former, lowering the Si content relative to the bulk rock and increasing FeO, MnO, Sc and HREE. The high concentration of peritectic garnet within the newly formed melt would also have increased its density markedly. In conjunction with the particular (constrictional deformation-related) distribution of unconnected leucosomes in these migmatites, this may well have impeded effective melt loss from the source rock, despite the high melt proportion.

Lecture

Topic: 10.1 Geoscience Communication and Education

Non-formal and Informal Geoscience Education in a South African Science Centre

Tanja Reinhardt

University of KwaZulu-Natal, South Africa

Informal educational settings such as science centres play an important role in science education around the world. Science centres are known to have a positive influence on promoting visitors' curiosity, interests, and knowledge of science because visitors can interact with real objects and engage with exhibits in a relaxed informal environment, watch science shows, or consult websites. In addition to informal education, learning in science centres can also be non-formal through organized, systematic, educational activities such as workshops.

The aim of science centres in South Africa is to develop programs, workshops and undertake outreach programs, which focusses on creating awareness, promoting and teaching science and technology particularly in disadvantaged communities, e.g. rural areas and townships.

The Science and Technology Education Centre at the University of KwaZulu-Natal (STEC@UKZN) in Durban which includes the Geology Education Museum, is one of these science centres. It is a place of hands-on science learning with an emphasis on Geoscience education. Over the years, STEC@UKZN was involved in the development of numerous low-cost geoscience-related activities, exhibits and educational material using an informal and non-formal education approach. While we usually operate face to face, the Covid-19 crisis had us adopt alternatives ways and we had to move some of our activities online.

In our presentation we will highlight our various geoscience initiatives, be it non-formal or informal, face to face or online that take place in the science centre.

Poster

Topic: 2.2 From dust to planets

Stable iron isotope fractionation in metal sulfidation at 600–1200 °C

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Iron metal and troilite co-exist in ordinary chondrites and iron meteorites [1,2]. Here, we present results from Fe metal equilibrium sulfidation experiments in evacuated silica glass tubes at 600–1200 °C. The two distinct phases, Fe and FeS, were analyzed for their $\delta^{56}\text{Fe}$ and $\delta^{57}\text{Fe}$ compositions with MC-ICP-MS (Thermo Scientific Neptune Plus). The materials were ablated using a Spectra-Physics Solstice femtosecond laser ablation system at the Institute of Mineralogy, University Hannover, see [3] for analytical details.

At 600–1000 °C the sulfidation reaction occurred in the solid state and Fe metal is coated by FeS, whereas above 1000 °C we observe Fe and FeS melts. We insured isotopic equilibration by running experiments with different durations. At 600 °C and 71h we observed kinetic fractionation effects, whereas after 260h the sulfide coating was isotopically homogeneous. Overall, FeS is systematically heavier compared to the Fe metal, and the isotopic fractionation decreases with increasing temperature from 600–1200 °C. However, a comparison of the experimental results with $\delta^{56}\text{Fe}$ data from ordinary [1] and iron [2] meteorites shows the opposite fractionation trend. In the meteorites the FeS is always isotopically lighter compared to the Fe metal. We suggest that this is due to kinetic fractionation effects that occur during cooling of Fe-FeS melts in the meteorites, whereas our quenched experiments retained the equilibrium $\delta^{56}\text{Fe}$ fractionation.

[1] Needham A. W. et al. (2009) *GCA* 73:7399–7413. [2] Williams H. M. et al. (2006) *EPSL* 250:486–500. [3] Horn I. (2007) *Spectrochim. Acta B* 62:410–422.

Poster

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

First Lu-Hf ages of garnet-bearing lithologies from the Saxonian Granulite Massif

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The Saxonian Granulite Massif is an antiformal gneiss dome with granulite facies rocks in the core, enwrapped by uppermost amphibolite to lower greenschist facies metasediments. Their subduction and exhumation histories during the Variscan orogeny are still poorly understood. Samples of two garnet-bearing serpentinites and one eclogite from the dome-core, as well as one garnet-cordierite gneiss from the lowermost schist-cover were dated using Lu-Hf chronometry.

The granulitic core mostly consists of leucocratic granulites with scarce and laterally discontinuous slivers of mafic and ultramafic rocks. All samples were taken at the largest occurrence of ultramafics at the Rubinberg, where granofelsic eclogites (CPx, Grt, Pl, Rt) are found as two 1 m-thick, foliation parallel layers within foliated garnet-bearing serpentinites (Grt, relics of CPx, Amp, Ol, Spl). Garnet is better preserved within eclogites than in serpentinites. Within eclogites, EPMA major element zoning profiles of garnet blasts show a prograde metamorphic path, partially modified by diffusional relaxation leading to flattening of chemical zoning profiles. Complete homogenization of major elements is characteristic for all pyrope-rich, strongly kelyphitic garnets in the serpentinites. Garnet blasts within the garnet-cordierite gneiss (Pl, Grt, Sil, Bt, Crd, Qtz, Ilm, Spl) reveal complex compositional zoning profiles with a prograde metamorphic zonation pattern in the core and a secondary increase of Ca and Mn in the rims.

The eclogite yielded a Lu-Hf age of 347.5 ± 6.7 Ma, which is interpreted to indicate the timing of peak metamorphism within the granulitic core, predating the retrograde exhumation-related fabrics. Ages of serpentinites and gneisses are still pending.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Microseismicity in relation to the rise of the mine water level and the regional stress field in the eastern Ruhr area

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Using data from permanent seismological stations of the Ruhr University and the temporal short-period FloodRisk network in the eastern Ruhr area, microseismicity in the area of the former coal mine “Bergwerk Ost” is observed. The database is supplemented by the levels of the mine water table, which are regularly measured and made available by Ruhrkohle AG (RAG) at various measuring points distributed over the study area. A special focus is on the relation of the microseismicity to the rising mine water level after the end of mining.

Since the beginning of the flooding, more than 2000 induced events in a magnitude range from -0.7 up to 2.6 M_{LV} have been localised. The spatial distribution of hypocentres is divided into two areas, with few events in the central study area and over 95% of earthquakes in its eastern part. Many of these events are spatially clustered and some show quite high waveform similarity. This allows relative localisation to increase the accuracy of the location.

Comparing the old galleries, which today serve as the main underground waterways, with the localisations from the relative seismicity localisation, strong correlations can be seen. The measured temporal trend of the mine water level, after pumps were shut down in mid-2019, shows a strong correlation with the temporal evolution of the observed microseismicity.

In addition to investigating the spatial and temporal distribution of seismicity, fault plane solutions could be determined for larger seismic events. These are compared with the regional stress field derived from independent investigations.

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Poster

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

The new Cologne Noble Gas Laboratory – Extraction and Analysis of cosmogenic Ne Isotopes

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We established a new laboratory for noble gas mass spectrometry that is dedicated to the development and application to cosmogenic nuclides at the University of Cologne. At the core of the laboratory are a state-of-the-art high-mass-resolution multicollector Helix MC Plus (Thermo Fisher Scientific) noble gas mass spectrometer and a novel custom-designed automated extraction line. The mass spectrometer is equipped with five combined Faraday multiplier collectors, with 10^{12} and 10^{13} Ω preamplifiers for faraday collectors. We installed and build up a new extraction line to conduct Ne isotope analysis, including laser extraction and cryogenic automated separation. Except for the laser, the extraction process is completely automated and allows a high standard of reproducibility, which prevents variations due to manual operation. Performance tests were conducted using gas of atmospheric isotopic composition (our primary standard gas), as well as CREU-1 intercomparison material, containing a mixture of neon of atmospheric and cosmogenic composition. The precision in determining the abundance of cosmogenic ^{21}Ne is equal to or better than those reported for other laboratories. The absolute value we obtain for the concentration of cosmogenic ^{21}Ne in CREU is indistinguishable from the published value. We now regularly perform analysis of samples for cosmogenic neon for running projects and are open to new collaborations. For further information we refer to our publication *Ritter et al. 2021 - Technical Note: Noble gas extraction procedure and performance of the Cologne Helix MC Plus multi-collector noble gas mass spectrometer for cosmogenic neon isotope analysis – Geochronology - <https://doi.org/10.5194/gchron-3-421-2021>*

Poster

Topic: 6.3 Fractionation of metal(loid) stable isotopes during low-temperature Earth surface processes

Mobilization of non-crystalline uranium (U) and related U isotope fractionation in biotic environments

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Environmental uranium (U) contaminations may be remediated by using microbes to reduce mobile hexavalent [U(VI)] to more immobile tetravalent U [U(IV)]¹. However, the subsurface stability of U(IV), usually present as solid-phase non-crystalline U, can be affected by reactions with ligands, oxidants or bacteria. Uranium isotopes have the potential to monitor and assess these mobilization/immobilization processes, however, currently detailed knowledge of their fractionation in all involved individual processes is lacking.

Here, we present laboratory experiments, investigating the efficacy of *Acidithiobacillus (At.) ferrooxidans* to mobilize non-crystalline U(IV) and associated U isotope fractionation. As starting material an U(VI) isotope standard was reduced by *Shewanella oneidensis* MR-1 in a phosphate-containing medium (WLP) in order to produce non-crystalline U(IV). *At. ferrooxidans* mobilized between 74% and 91% U after one week, and interestingly, U mobilization was observed for both, living and inactive cells. This finding raises doubts on the long-term sustainability of in-situ bioremediation measures at U-contaminated sites.

In contrast to mobilization with ligands, which results in ²³⁸U enrichment in the mobilized phase², mobilization by *At. ferrooxidans* did not cause U isotope fractionation, potentially because of a layer effect³. Thus, isotopic signatures found in nature are more likely associated with other processes such as U reduction, abiotic oxidation, or mobilization with ligands.

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Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

NFDI4Earth – First steps towards a national ESS research data infrastructure

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As part of a major German effort towards a national research data infrastructure, the NFDI4Earth (www.nfdi4earth.de) brings together researchers in the Earth System Sciences, their data, tools, and services to address their digital needs. NFDI4Earth is a community-driven process providing researchers with access to FAIR, coherent, and open ESS data, innovative research data management (RDM) and data science methods. It will do so by developing a central infrastructure that provides access to all ESS data sources, and tools via the OneStop4All to access, connect, visualise and generally research these.

The NFDI4Earth aims from early on for an open communication to and active involvement of the ESS community and the interested public, particularly its participants and interest groups. The structure of the NFDI4Earth was already presented on previous editions of this conference series and will therefore only be briefly summarised. The focus of this talk will be on the developments within the NFDI4Earth, its services and products. A lot has happened since its official start in January 2022, e.g., decisions on the software stacks, consideration of the various use cases, development of the knowledge hub and living handbook, starting of various interest groups, start of 14 pilot projects. Most importantly, we will point out where you can (and hopefully will) engage in the further development of the NFDI4Earth services and products because it is your feedback and participation that will allow us to develop the NFDI4Earth as close to the needs and expectations of the community as possible.

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

Nine-tailed data monsters? Lessons learnt in the compilation of GlobalID

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Lead isotope data are an important tool for the reconstruction of raw material provenances of non-ferrous archaeological materials. The quality of the provenance reconstruction depends, among other factors, on the comprehensiveness of the reference data the archaeological samples can be compared to. When compiling such databases, three major challenges typically emerge: (a) Access to the respective publications, many of them scattered in conference proceedings and local journals; (b) a huge variety and often incompatibility and incompleteness of meta-information; and (c) language barriers. To overcome these obstacles, a group of colleagues started to tame this data monster in 2018 through the compilation of the global lead isotope database GlobalID. Its aim is to create in a community-driven process a FAIR database and an associated web application which provides easy access to the database and visualisation tools for people with different backgrounds and knowledge levels. Prototypes were published in late 2021 and work is still ongoing.

Many obstacles had to be overcome; many more are already looming on the horizon. After a short summary of the project, some of them will be presented, which we perceive as general challenges in taming such data monsters, and the solutions we came up with. Subsequently we will discuss where we are in urgent need from the scientific communities and related research data infrastructures for tools that allow us to fully tame the data monster into a truly FAIR database.

Ramdohr-Poster

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

The impact of fluid and mineral composition on experimental carbonate silicification

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The pseudomorphic replacement of carbonate minerals by silica is an omnipresent diagenetic process. However, the parameters that influence the silicification process are incompletely understood and experimental studies are sparse. Here, we present the results of batch experiments at normal conditions designed to replace various carbonates (calcite, aragonite, dolomite, magnesite, and marble) by amorphous silica. The experiments were conducted at variable pH (2–7), dissolved silica concentration (100–400 ppm), and duration ranging from 7 to 21 days. We used a multi-method analytical approach with XRPD, EPMA, Raman spectroscopy, and SEM to characterize the parent and product phases and the rich array of replacement features. After 21 days at pH 2–3, calcite and aragonite dissolve, disordered amorphous silica particles (<1 µm) precipitate, and an up to 150 µm thick replacement rim forms. During the initial calcite replacement phase, porous honeycomb-like structures form and relict rhombs remain. In a second phase, residual dissolved silica precipitates inside pore space at the replacement interface and forms dense networks of amorphous silica nanoparticles. Dense silica aggregates also form during the pseudomorphic replacement of fibrous aragonite. At the same experimental run conditions, neither dolomite nor magnesite show dissolution or precipitation features. Our results show that at low pH rim thickness increases with time and reaches its maximum at initial pH 2.5. At dissolved silica concentrations <200 ppm, no precipitation of amorphous silica was observed. The pseudomorphic carbonate-silica replacement proceeds via an interface-coupled dissolution-precipitation mechanism, in which carbonate dissolution induces silica precipitation.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Das „Puzzle Bodenbewegung“ im Kavernenfeld Epe

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Die Überwachung der Bereitstellung von Georessourcen stellt eine komplexe Herausforderung dar. Bildlich gesprochen handelt es sich um ein Puzzle, bei dem nicht alle Teile vorhanden sind und nicht vollständig klar ist, welches Motiv entsteht. Gleichzeitig ist es notwendig, das Motiv zu erklären. Dieser Prozess ist bereits für Geowissenschaftler:innen herausfordernd, stellt aber eine Vielzahl an Beteiligten und Betroffenen vor große Probleme, hier ein vollständiges Prozessverständnis aufzubauen. Die Forschungskooperation Epe hat das Ziel, die Bodenbewegung am Kavernenspeicher Epe erklärbar zu machen und hier Transparenz in die Einflussfaktoren der Bodenbewegungen aufzubauen. Hierzu besteht die Forschungskooperation aus der Stadt Gronau, der Bürgerinitiative Kavernenfeld Epe e.V., der Firma EFTAS, Münster und dem Forschungszentrum Nachbergbau der Technischen Hochschule Georg Agricola, Bochum. Zusätzlich wird dieses Vorhaben durch die Betreiber im Kavernenfeld unterstützt. In der Forschungskooperation werden die Ergebnisse der flächigen Radarinterferometrie mit den vor-Ort verfügbaren öffentlichen Geodaten fusioniert, umso ein Gesamtbild zu erzielen. Gleichzeitig werden diese technischen Arbeiten mit einem öffentlichen Beteiligungsprozess begleitet. Die Forschungskooperation stellt somit erstmalig eine direkte Zusammenführung unterschiedlichster Beteiligter in einem bergbaulichen Projekt dar, um mit transparenten Werkzeugen ein gemeinsames Prozessverständnis aufzubauen.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

The taphonomic fate of biominerals in hydrothermal sulfide systems – implications for the reconstruction of microbial life in deep time

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Hydrothermal sulfide systems are among the most ancient habitats on Earth and are widely considered potential sites for the emergence of life. Deposits from such settings are thus of great evolutionary significance, but the geobiology of our planet's most ancient hydrothermal sulfide systems remains largely unexplored. This is mainly due to a limited understanding of the formation and preservation of microbial biosignatures in such settings, particularly over geological timescales. Here we present our strategy to explore the geobiology of ancient hydrothermal sulfides by integrating analytical and experimental methods from geology, geochemistry, and microbiology. Specifically, we expose synthetic and biogenic Fe-minerals to physical and chemical conditions relevant to microbial niches in hydrothermal environments on early Earth (<121°C, anoxic, sulfidic). We characterize the resulting precipitates with analytical imaging techniques, mineralogical methods, and geochemical approaches (e.g., SEM-EDS, μ XRD, Raman spectroscopy, sequential Fe extraction). By comparing the observed characteristics with those of minerals in modern and ancient hydrothermal sulfide deposits, we are able to identify primary biogenic mineral precipitates and their transformation products. This integrative approach will allow us to develop an in-depth understanding of the formation and preservation of biosignatures in hydrothermal environments. This, in turn, is critical for the reconstruction of microbial life in deep time.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Extraction of Cr during mantle melting: Experimental constraints on the role of peridotite composition and the effect of water

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Chromium (Cr) is considered to be one of the most economically important critical raw materials. The most economically significant mineral for Cr exploitation is Chromite which can be found in podiform Chromite deposits that are associated with ophiolite complexes from Supra-Subduction Zone (SSZ) settings. In Europe, such deposits are located in northwestern Greece and the Balkans in general. The precise nature of podiform chromitite generation is not fully understood and still under debates and could be the result of a complex sequence of enrichment processes.

To improve our understanding of Cr extraction during mantle melting a series of experiments were performed on natural peridotite samples from the Pindos Ophiolite, Greece. Our experiments were conducted under pressure (1.0-1.5 GPa) and temperature (1350-1400°C) conditions that are relevant for the genesis of intra-oceanic arc magmas. To study the effect of hydrous conditions, the amount of water in the system was varied from 1 to 10 wt%. The samples had various modal proportions of olivine, ortho- and clinopyroxene and a different degree of alteration.

All experiments produced Cr-enriched melts (up to 7000 µg/g Cr) with a positive dependence of Cr content on the degree of melting and on the concentration of water added to the system. Based on the obtained results we have developed forward numerical models to constrain the Cr-enrichment process in magmas during mantle melting. Our study demonstrates that previous estimates on the extraction efficiency of Cr during mantle melting in SSZ should be reconsidered.

Poster

Topic: 9.4 Chemical sediments and mineral deposits in basins: archives of paleoclimatic, hydrogenetic, biogenic, hydrothermal, and diagenetic, processes throughout Earth's history

Revised lithostratigraphy of the Paleoproterozoic Porkonen banded iron formation and associated sulphidic shales, Northern Finland

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Aristotle University of Thessaloniki, Greece

The Palaeoproterozoic (~2.0 Ga) Porkonen Formation in the Kittilä greenstone belt (or terrane) in northern Finland is an exceptionally well-preserved succession of banded iron formation, shale-dominated units and submarine lava. The Formation comprises six distinct lithological units that from the base upwards include: a. massive chert b. banded magnetite±siderite-chert (iron ore) c. (Mn)siderite±chlorite-chert d. iron sulphide-rich black shale and breccia (3) tuffaceous shale and tuff and, (4) andesite/rhyolite.

The iron ore has a thickness of approx. 8 meters, laterally discontinuous (<12 km) and an average Fe content of 30.5%. The overlying manganese-rich siderite horizon (3-5m) has an average of 2% Mn, whereas the following 7m thick, sulphide-rich black shale averages at 27% Fe showing a maximum content of 47.9% Fe in one-meter interval. The latter shows elevated contents in Zn, Cu, Ni, Ag, Cd and Au.

All lithological units consist of low-grade metamorphic mineral assemblages, exhibiting primary sedimentary and early diagenetic features, and have contacts typically conformable and gradating.

Single-grain layering of micron-sized magnetite alternating with micritic carbonate, apatite and chert characterize the iron-oxide bands whereas primary colloidal textures, abundant contractional fractures, graphite-stylolites and crackle microbreccia characterize the chert bands. In the shale-dominated units the rhythmic, planar-parallel lamination of authigenic carbonates, diagenetic pyrite, and chert and pyrite nodules, have been contorted by penecontemporaneous soft-sediment deformation manifested by slump structures, load casts, and intraformational breccia with angular graphite fragments in a massive iron-sulphide matrix.

The lithostratigraphy may predict a layered -in oxygen ocean with hydrothermally-dominated Fe-Mn-rich deep water mass.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Mantle response to ridge re-organization

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The local preservation of depleted Nd-Hf and Os isotopic compositions in abyssal peridotites contrasts with the lack of such extreme isotopic signatures in erupted MORB [1]. This is likely a consequence of different preservation potentials of melts from enriched and depleted portions of mantle [2]. Indeed, fertile and geochemically enriched components produce melts hosting the majority of incompatible elements, concealing the chemical fingerprint of the depleted counterparts [3]. However, Mid Ocean Ridges are dynamic environments, where geodynamic responses to far field forces may cause change in ridge-geometry and/or re-organization of the ridge axis. This contribution discusses how this process affects melting regimes, reducing the effect of mixing [5,6]. I will consider study cases from large-offset oceanic transforms from the Mid Atlantic Ridge (Doldrums and Charlie Gibbs Fracture Zones), and from the highly asymmetric Knipovich Ridge, in the Arctic Ocean. Variations in chemistry of basalt and associated peridotites are used to show the coupled effect of cooling at the ridge-transform intersections and/or re-melting the sub-oceanic mantle. Changes in melting regime may cause preferential melting or enriched or depleted mantle domains, uncovering an intrinsic heterogeneity otherwise difficult to assess.

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Poster

Topic: 4.1 Magmas and Fluids in the Crust

Basalts from the intratransform domain at the Doldrums Megatransform (7-8° N MAR) reveal mantle re-melting

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In the Equatorial Mid Atlantic Ridge at 7-8°N the Doldrums Fracture Zone (FZ) is located: a complex transform system characterized by four 'intratransform' ridge segments (ITRs) bounded by five active transforms (Skolotnev et al., 2020). We determined major element, trace element and Sr, Nd, Hf and Pb isotope compositions for on-axis lavas erupted along the entire fracture domain. Basalts from the central ITRs are selectively enriched in alkalis ($\text{Na}_2\text{O}+\text{K}_2\text{O}=4.3$ wt%; Na_8 up to 3.7) and LREE ($\text{La}/\text{Sm}_N=0.86-0.97$), in agreement with low melting degrees in a cold intra-transform regime. Despite this, they have the most depleted Sr and Pb isotope compositions in the entire Equatorial MAR (i.e. $^{87}\text{Sr}/^{86}\text{Sr}=0.70237$ and $^{206}\text{Pb}/^{204}\text{Pb}=18$), coupled with comparatively less depleted Nd and Hf isotope compositions, which instead plot in the field of regional MORB ($^{143}\text{Nd}/^{144}\text{Nd}=0.5131-0.5232$; $^{177}\text{Hf}/^{176}\text{Hf}=0.2831-0.2832$). Hence, the magmatism at the ITRs was predominately sourced by a depleted mantle source, melted at very low melting degrees. On this basis we suggest that the upper mantle currently melting beneath the central portion of the Doldrums FZ has previously undergone partial melting at the MAR axis, consuming the most fertile, isotopically enriched heterogeneities.

Skolotnev, S.G., Sanfilippo, A., Peyve, A., Muccini F., Sokolov, S. Y., Sani, C., Dobroliubova, K.O., Ferrando, C...& Ligi, M., 2020. Large-scale structure of the Doldrums multi-fault transform system (7-8°N Equatorial Atlantic): preliminary results from the 45th expedition of the R/V AN Strakhov. *Ofioliti*, 45(1), 25-41.

Lecture

Topic: 11.2 Latest Achievements in Scientific Ocean and Continental Drilling

Paleoclimate Controls on Borehole Geophysics Signals in Lacustrine Deposits of Lake Chalco, Central Mexico

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Understanding the moisture history of low latitudes from the most recent glacial period of the latest Pleistocene to post-glacial warmth in continental tropical regions is hampered by the lack of continuous time series. We conducted downhole spectral gamma ray and magnetic susceptibility logs over 300 m of lacustrine deposits of Lake Chalco (Mexico City) to reconstruct an age-depth model using an astronomical and correlative approach, and to reconstruct long-term moisture availability. Our results suggest that the Lake Chalco sediments contain several rhythmic alterations with a quasi-cyclic pattern comparable to the Pleistocene benthic stack. This allows us to calculate a time span of about 500,000 years for this sediment deposition. We have developed three proxies for moisture, detrital input, and salinity, all based on the physical aspects of gamma ray spectroscopy and magnetic susceptibility. Our results indicate that Lake Chalco formed during Marine Isotope Stage 13 (MIS13) and the lake level gradually increased over time until the interglacial of MIS9. Moisture content is generally higher during interglacials than during glacials. However, two periods, namely MIS6 and MIS4, have higher moisture contents. We developed a model by comparing the obtained moisture proxy with climatic drivers, to understand how different climate systems drove effective moisture availability in the Chalco sub-basin over the past 500,000 years. Carbon dioxide, eccentricity, and precession are all key drivers of the moisture content of Lake Chalco over the past 500,000 years.

Poster

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Magnetic properties of Iron-Phosphate mineral in Early Quaternary lacustrine deposits of Niederschönhagen, NW Germany — a paleoclimate implication

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The Early Quaternary lacustrine deposits in the Niederschönhagen area (Detmold, NW Germany) represent an important archive for the paleoclimate record in continental northwestern Europe during the transition from the warm Pliocene to the cold Pleistocene. Niederschönhagen belongs to a subsidence series in the Weser Uplands in northwestern Germany. These subsidence structures were formed by the leaching of subsurface evaporitic rocks during the early Cenozoic. A large collapsed structure at Niederschönhagen resulted in the deposition of 170 m thick lacustrine deposits that span the latest Pliocene/earliest Pleistocene to present. Magnetostratigraphic analysis suggest a time span of ~2.7 – 1.9 Ma for the deposition of the lacustrine deposits at Niederschönhagen.

Our sedimentologic observation combined with X-ray diffraction (XRD) analyses indicate the presence of vivianite minerals in the context of greyish mudstone, which occurs between 140 m and 148 m. Vivianite is an authigenic ferrous iron phosphate mineral ($\text{Fe}_3(\text{PO}_4)_2 \cdot 8\text{H}_2\text{O}$), associated with the development of redox conditions at the bottom of lakes. Dependence of magnetic susceptibility (MS) on the temperature of natural iron phosphate mineral are studied. The thermal MS curves for vivianite on heating curves shows an increase at 420 – 480 °C, and unstable magnetite (maghemite) is produced.

Our results suggest that northwestern Germany experienced a wet period during the latest Pliocene and earliest Pleistocene. This abstract is part of ongoing research, the main goal of which is to establish a rigid stratigraphic framework for the 170 m long lacustrine deposit of Niederschönhagen.

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Investigation of chalcophile element fractionation processes in the oceanic crust by trace element analysis of magmatic sulphides

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The fractionation of chalcophile trace elements during magmatic processes is strongly controlled by the segregation of immiscible sulphide liquids, which is a common feature in convergent and divergent plate margins [1-2]. To constrain the partitioning behaviour of these elements during magmatic processes, in-situ LA-ICP-MS analyses were performed on magmatic sulphide droplets and related fresh volcanic glass from mid-ocean ridges, back-arc basins, island arcs and the Troodos ophiolite on Cyprus. Minerals associated with the sulphide droplets are mainly olivine in mid-ocean ridge basalts and Fe-Ti oxides in more evolved island arc rocks, suggesting a different timing of sulphide saturation. Reduced mid-ocean ridge magmas seem to segregate a sulphide liquid in an early stage, whereas more oxidised magmas in subduction zones form a sulphide liquid in a later stage triggered by redox changes [3]. Surprisingly, systematic differences in trace element contents and partition coefficients between sulphide liquid and silicate melt were not observed, despite the different redox conditions and differences in the timing of sulphide segregation between these settings. However, within each sample, a great variance in the trace element contents of sulphide droplets is observed. Whether this is related to variations in the chalcophile element contents of the primary magmas between plate tectonic settings remains unknown [4].

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Poster

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Orbital forcing of past climates

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The annually laminated oil shale from the Eocene maar lake at Messel (Germany) provides an exceptional sedimentary archive to study the early to middle Eocene climate in central Europe. In a new approach we combine borehole logging and highly resolved X-ray fluorescence (XRF) core scanning data to get insights into the short-term climate variability stored in the Messel sediments. To obtain lithological information from the sediments we applied multivariate statistics that resulted in three distinct lithological units. To allow for the comparison of regional and global paleoenvironmental and paleoclimatological data to other archives, we propose a newly reconstructed age model based on astronomical tuning of the borehole logging data, which show climate variability in the Milankovitch range (e.g. precession). Based on our results we derived an age range for the lower to middle Messel formation of 48.2 to 47.2 Ma. The here presented high resolution data provides local insights into the middle Eocene greenhouse climate dynamics.

Lecture*Topic:* 2.1 Changes of solid Earth's processes through deep time**Thallium isotope ratios record amphibole-dominated fractionation of Earth's earliest continental crust****Mathias Schannor^{1,2}, Heye Freymuth², Jesse Reimink³, Mark Rehkämper⁴, Helen Williams²**¹Freie Universität Berlin, Germany; ²University of Cambridge, UK; ³Pennsylvania State University, USA; ⁴Imperial College London, UK

Earth's oldest continental crust is found in cratonic nuclei comprised of tonalite-trondhjemite-granodiorites (TTGs). However, the nature of the source materials that formed TTGs, as well as the timing and mechanisms of its formation remain controversial. Current models for the formation of Archean TTGs are (i) vertical subduction and partial melting of the subducting hydrated oceanic crust, (ii) partial melting at the base of plume-generated oceanic plateaux within the garnet stability field, and (iii) fractional crystallization of mafic-intermediate magmas and accumulation of plagioclase ± amphibole [1, 2, 3]. The thallium stable isotope composition of magmatic rocks identify distinct components in modern subduction zone settings [4] and thus can be exploited to address early continental crust formation. Here we report Tl isotope compositions for rocks from the Acasta Gneiss Complex (AGC) in Canada, which contains the oldest known evolved crust, with igneous crystallization ages ranging from 4.03 to 2.95 Gyr [5]. Tonalitic gneisses of the ~4 Gyr old Idiwahaa unit have $\epsilon^{205}\text{Tl}$ values in the range of -4.0 ± 0.3 to -1.1 ± 0.4 that correlate with decreasing Dy/Yb and Dy/Dy*. The correlation follows indices of magmatic differentiation, which is consistent with extensive amphibole fractionation at shallower depths than the garnet stability field.

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Poster

Topic: 8.1 Geosciences and Waste Management

Asbestos in construction waste – presence and recognition of asbestos containing materials

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Construction waste (CW) from demolished buildings delivers a vast amount of resources for recycling material (RCM). RCM can be used as gravel, recycling-concrete or potentially for more precious applications. Hazardous pollutants in CW, like asbestos, threaten this applications, regarding health and environmental risks. Risks for human health induced by asbestos fibres, like asbestosis and mesothelioma are well known. The industrially used mineral asbestos has contaminated many parts within buildings (e.g. floor, ceiling, roof, seals, etc.) and technical constructions and products. Once, the asbestos-containing materials (ACM) reach the construction waste, the recognition of ACM becomes quite difficulty and time consuming. In the first instance we are developing a manual including attributes of different ACM to identify them on site, within the possibly very heterogenic CW. Additionally we are conducting experiments using modelled piles of CW in order to better understand the presence and visibility of ACM in piles. Here the appearance of ACM-substitutes is counted on the surface of modelled piles. The grain size distribution of demolished ACM will be quantified and analysed accordingly, to understand which amounts and distributions of particles of ACM may contaminate the CW. This may potentially be utilised to support the development of methods for the removal of ACM from CW.

The obtained results will lead to a better understanding of ACM in CW, which will increase and ensure the quality of RCM.

Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

Palaeomagnetic analyses in the Atacama Desert - challenges and chances

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Magnetic polarity stratigraphy and magnetic palaeointensity stratigraphy is often used on sedimentary rocks to correlate outcrops and establish chronologies. The concept is based on the assumption that dipolar geomagnetic variations are globally synchronous and independent of climate and depositional conditions. The strengths of the method include the wide dating range and the applicability to a large variety of sediments and rocks. Best results are gained if long continuous sequences with high and uniform sedimentation rates are available. In the Atacama Desert, however, these perfect conditions are rare, as the landscape is strongly influenced by tectonic processes and extreme climatic conditions. Within the CRC1211 "Earth Evolution at the Dry Limit" magnetic stratigraphy is used to improve the age control of long drill cores from the claypans PAG, Huara, and Paranal, and of discrete samples from the marine Bahia Inglesia Formation. In addition, a first methodological attempt is being made to validate the potential of gypsum wedges as possible palaeomagnetic archive. The analyses are particularly carried out in order to specify the time covered by these geoarchives. Challenges for the palaeomagnetic analysis of the different archives arise from the often quite brittle nature of the unconsolidated sediments, the weak magnetizations and the complex magnetic mineralogy, potentially biased by diagenesis. Here we present challenges of the ongoing studies, as well as first results and perspectives.

Poster*Topic:* 1.5 Fundamentals and applied aspects of nucleation and crystal growth**Crystal Growth and Characterization of the 12L-Perovskite Ba₄CeIr₃O₁₂****Henrik Schilling, Petra Becker**

University of Cologne, Germany

Highly frustrated magnetic systems are of great interest due to their exceptional properties and are topic of active research in solid state sciences. Within these systems, there are promising structures to investigate, such as perovskites with a 12L stacking sequence. The 12L-perovskites are characterized by isolated M₃O₁₂ triples of face-sharing [MO₆] octahedra ("trimers") [1]. For Ba₄CeIr₃O₁₂ it is expected that for each [Ir₃^{IV}O₁₂] trimer a total magnetic moment $S \neq 0$ will result which can lead to competing intra- and inter-trimer magnetic interactions at low temperatures.

For investigation of their magnetic properties, large single crystals of Ba₄CeIr₃O₁₂ are necessary. However, so far in literature only powder samples are reported [1] and no information about the phase diagram is available for this compound. With the aim of growing large single crystals of Ba₄CeIr₃O₁₂ we examined the ternary system of BaO – CeO₂ – IrO₂ with focus on the stability of the 12L-perovskite phase. Through our investigations it was possible to grow single crystals of Ba₄CeIr₃O₁₂ of up to 100 μm in size. The crystals were grown from melt solution using a BaCl₂ flux and a cooling rate of 3 K/h between 1300 K and 800 K. The crystal structure was determined by X-ray diffraction and the temperature-dependent phase stability was investigated by simultaneous thermal analysis (STA).

[1] Y. Shimoda, Y. Doi, M. Wakeshima, Y. Hinatsu, *Inorg. Chem.* **48** (2009) 9952-9957

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Vital effects on lithium isotope fractionation – Insights from Recent and Albian molluscs

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Molluscs have great potential as geochemical archive due to their wide spatial and temporal abundance. For lithium isotope compositions ($\delta^7\text{Li}$), a proxy for reconstructing weathering intensity, they would offer a valuable possibility of obtaining data unobscured by clay contamination which is known to be an obstacle when working with sediment samples.

However, recent studies have shown the potential challenge of accounting for vital effects when interpreting $\delta^7\text{Li}$ data from mollusc shells. Here, we assessed the potential of mostly aragonitic molluscs, mainly cephalopods, as an archive for $\delta^7\text{Li}$.

We analysed Recent cephalopods such as *Argonauta hians*, *Nautilus pompilius*, *Spirula spirula* and *Sepia officinalis*. This selection includes species that build both exo- and endoskeletons, and provides us the opportunity to assess whether this feature imposes different vital effects on lithium isotope fractionation. Furthermore, we sampled Albian molluscs including nautiloids (two specimens of *Cymatoceras* sp.) and ammonites (*Cleoniceras* sp. and *Desmoceras* sp.) as well as the bivalves *Arca cucullaea* and *Cardium* sp. from the Mahajanga Basin in Madagascar which show exceptional aragonite preservation.

Preliminary data for the modern specimens *A. hians* (a species that precipitates high-Mg calcite), *S. spirula* and *N. pompilius* show a narrow range of offsets from seawater $\delta^7\text{Li}$ that resembles the fractionation between water and inorganically precipitated aragonite for biologically relevant growth rates.

For the Albian cephalopods and bivalves, we observe a narrow range of $\delta^7\text{Li}$ values which hints towards possibly similar biomineralisation strategies among molluscs and thus, offsets caused by vital effects compared to their modern aragonitic relatives.

Poster*Topic:* 1.2 Methods in Geochemistry and Mineralogy**New matrix-matched reference material for SIMS analysis of oxygen isotopes in gem corundum****Sebastian Schmidt¹, Axel K. Schmitt¹, Andreas Hertwig¹, Ilya Bindeman², Andreas Pack³, Kevin McKeegan⁴**¹Institute of Earth Sciences, Heidelberg University, Germany; ²Department of Earth Sciences, University of Oregon, USA;³Geoscience Center, University of Göttingen, Germany; ⁴Department of Earth, Planetary, and Space Sciences, University of California – Los Angeles, USA

The aluminum oxide (Al₂O₃) corundum is of high economic interest, not least because of its rare gemstone varieties sapphire and ruby. Geochemical analyses are helpful to gain a better understanding of the geographical origin and distribution of corundum. In addition to trace elements, O-isotopes ($\delta^{18}\text{O}$) are a powerful tool to identify provenance of gem-quality corundum. High spatial resolution analysis by secondary ionization mass spectrometry (SIMS) plays an essential role for this because it can identify intracrystalline heterogeneity and thus more reliably identify genetic processes. However, accurate SIMS analysis requires suitable matrix-matched reference materials. Some in-house reference materials for corundum are currently in use by different SIMS labs, but these materials generally lack comprehensive chemical and isotopic characterization. Moreover, crystal-orientation effects can create bias in SIMS analysis. Therefore, it is timely to develop appropriate matrix-matched reference materials for SIMS analysis of corundum.

We have investigated O-isotopic homogeneity and composition of a synthetic laser ruby single-crystal. A rod of it was cut symmetrically from the interior to the rim and analyzed in bulk by laser-fluorination technique in two different laboratories. A preliminary average value of $\delta^{18}\text{O} = +18.3\text{‰}$ is reported, with no systematic variability across the rod. An adjacent slice of the rod was sectioned in four prominent crystallographic orientations confirmed by EBSD. SIMS results show homogeneous O-isotopic values independent of crystallographic orientation (2SD = 0.18‰ in $\delta^{18}\text{O}$, n = 4, six measurements on each orientation). Besides O-isotopes, abundances and homogeneity of key trace elements will be characterized by electron microprobe and SIMS.

Lecture*Topic:* 4.3 The role of fluids in metamorphic and metasomatic reactions**Externally- vs. internally-derived H₂O as control on reaction progress during high-pressure metamorphism****Simon Schorn**

University of Graz, Austria

The progress of metamorphic reactions at high-pressure is commonly limited by kinetics. Relatively low temperatures, absence of deformation, short timescales and particularly the paucity of fluid may hamper transformation, thereby promoting the preservation of lower-pressure assemblages at eclogite facies conditions. However, minute amounts of H₂O can trigger the prograde breakdown of plagioclase to denser high-pressure assemblages. In the case of dry protoliths such as gabbro/granulite, H₂O must be added to the system to cause metamorphism, for example via fluid infiltration. The 'eclogitization' of granulites however can occur in a closed system due to the partial breakdown of igneous biotite. Both the addition of external H₂O as well its liberation from biotite leads a localized increase in chemical potential ($\mu_{\text{H}_2\text{O}}$), causing H₂O to be transported into nearby anhydrous minerals. If external H₂O is added to metagranitoids at high pressure, it is mainly accommodated in phengite growing at the expense of K-feldspar. Upon decompression, such hydrated rocks would dehydrate, thereby causing fluid-assisted retrogression and loss of diagnostic eclogite-facies assemblages at lower pressure. By contrast, mafic eclogites have a limited capacity to store H₂O in minor hydrous minerals such as amphibole. Even when fully saturated at high pressure, the crystallographically-bound H₂O is insufficient for dehydration to occur during exhumation, thus favoring the preservation of garnet–omphacite-bearing assemblages. These mechanisms explain the discrepancy between peak pressures recorded in cogenetic mafic eclogites and orthogneisses observed in classic (U)HP terranes such as the Western Gneiss Region (Norway) and Dabie Sulu (China).

Lecture

Topic: 8.1 Geosciences and Waste Management

Formation and hydraulic reactivity of an alite-rich material from post-treated basic oxygen furnace slag

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Basic oxygen furnace slag (BOFS) is a by-product of steelmaking of which about 10.4 Mt are produced annually in the EU. BOFS is mostly used in road construction, earthwork and hydraulic engineering. However, in this use, the iron bound in BOFS is lost and the opportunity to produce higher value products from BOFS is forgone.

In recent decades, many researchers have investigated a thermochemical process to reduce iron oxides to metallic iron in molten BOFS. The metallic iron formed separates from the reduced slag due to its higher density and can be recovered. An advantage of this process is that simultaneously the chemical composition of the reduced slag is adapted to that of the Portland cement clinker and the hydraulic reactive mineral alite is formed.

In this study, BOFS was reduced in a small-scale electric arc furnace using petrol coke as reducing agent, and the hydraulic properties of the reduced, low-iron BOFS were investigated. Despite a chemical and mineralogical composition similar to that of Portland cement clinker, the reduced BOFS produced less heat of hydration, and its reaction was delayed compared to Portland cement. However, the addition of gypsum, as is also done in cement production from Portland cement clinker, has been found to accelerate the hydration rate of reduced BOFS.

Further research to improve the hydraulic properties of the reduced slag is essential. If successful, the production of a hydraulic binder and crude iron from BOFS could have economic and ecological benefits for both the cement and steel industry.

Poster

Topic: 1.8 Minerals and Mineral Properties

Thermoelastic properties of highly porous mullite ceramics

Jürgen Schreuer¹, Jan-Frederick Hörster¹, Mariano Talou², Andrea Camerucci², Hartmut Schneider³

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Mullite is one of the most important constituents of oxide ceramics because of its outstanding thermo-mechanical properties in oxidizing environments at high temperatures. In order to study the influence of porosity on elastic stability, mullite ceramics with porosity up to about 57% were prepared with a novel technique based on starch consolidation casting and sintering of commercial mullite powders with approximate 3/2-composition at temperatures up to 1923 K [1]. Their coefficients of thermal expansion and elastic stiffnesses were determined between 100 K and 1600 K employing dilatometry and resonance ultrasound spectroscopy, respectively. Additionally, the microstructures were investigated employing scanning electron microscopy and X-ray tomography.

Although size (ca. 5 – 20 μm), shape and distribution of pores appear chaotic in high magnification scanning electron microscopic images, their distribution is quite homogeneous at a larger scale. The thermal expansion of the porous ceramics is very similar to the ones of dense mullite ceramics [2]. However, the bulk and Young's moduli decrease strongly with the porosity as expected for materials having spherical pores. A critical porosity of about 71% is derived where the mullite ceramics probably lose integrity. The deviations from Cauchy-relations of the porous mullite ceramics are significantly smaller compared to the ones of dense mullite materials, reflecting the limitation of elastic interactions to the thin pore walls of the porous ceramics.

[1] Talou M.H., Camerucci M.A.: J. Eur. Ceram. Soc. 2015; 35: 1021-30.

[2] Krenzel T.F., Schreuer J., Laubner D., Cichocki M., Schneider H.: J. Am. Ceram. Soc. 2019; 102: 416-26.

Lecture*Topic:* 1.8 Minerals and Mineral Properties**Thermoelastic properties of olivine-type sinhalite and chrysoberyl****Jürgen Schreuer, Heimes Hednrik**

Ruhr-Universität Bochum, Germany

Similar to the mullite-types, the structures of olivine-type materials are dominated by parallel chains of edge-sharing MO_6 octahedra. The large number of crystal species belonging to these groups makes it possible to systematically study the influence of different cations and of different types of linkage of the octahedral chains on their properties. Therefore, we determined full sets of the coefficients of thermal expansion and elastic stiffnesses of orthorhombic sinhalite, $MgAlBO_4$, and chrysoberyl, Al_2BeO_4 , in the temperature range from 100 K to 1273 K and, respectively, from 100 K to 1473 K, employing a combination of dilatometry and resonant ultrasound spectroscopy. At ambient conditions the elastic behavior of sinhalite is more anisotropic than the one of chrysoberyl [1]. Both crystal species follow the general trend of increasing bulk modulus with increasing oxygen packing density as observed in many oxides with hcp-like packing of oxygen atoms. With bulk moduli of 178 GPa and 233 GPa sinhalite and chrysoberyl belong to the stiffest olivine-type materials known so far. While in chrysoberyl the softening of the elastic stiffnesses at high temperatures can be well explained by lattice vibrations, certain stiffness coefficients of sinhalite soften at an increasing rate above about 600 K. The anomalous behavior is probably related to the increasing instability of the tetrahedral BO_4 groups that eventually leads to decomposition of sinhalite at about 1400 K.

[1] Wang H., Gupta M.C., Simmons G.: J. Geophys. Res. 80 (1975) 3761-3764.

Lecture*Topic:* 2.2 From dust to planets**Heterogeneity of Bulk Oxygen Isotopic Compositions in Anhydrous Interplanetary Dust Particles****Birgit Schulz¹, Christian Vollmer¹, Lindsay P. Keller², Peter Hoppe³**¹Institut für Mineralogie, Westfälische Wilhelms-Universität Münster, Germany; ²XI3, ARES Division, NASA Johnson Space Center, Houston, USA; ³Max-Planck-Institut für Chemie, Mainz, Germany

Anhydrous interplanetary dust particles are among the least altered ancient solar system materials. While hydrous IDPs are ¹⁶O-poor, likely due to the interaction with isotopically heavy H₂O [1], oxygen isotopes of anhydrous IDPs seem to be highly variable, although data is scarce [2]. Bulk oxygen isotopic compositions of 70 nm thin ultramicrotomed sections of three anhydrous IDPs were measured by NanoSIMS. $\delta^{17}\text{O}_{\text{SMOW}}$ ranges from $-24.2 \pm 5.4 \text{ ‰}$ (1σ) to $7.8 \pm 3.4 \text{ ‰}$ and $\delta^{18}\text{O}_{\text{SMOW}}$ from $-25.3 \pm 3.6 \text{ ‰}$ to $9.5 \pm 3.1 \text{ ‰}$, with the heavier isotopic compositions attributed to the particles that show signs of mild thermal alteration. Isotopic heterogeneity is best explained by contribution of grains sampling different O isotope reservoirs in the protoplanetary disk, created by self-shielding and photodissociation of CO [3]. This process resulted in ¹⁶O-rich CO gas and ¹⁶O-poor H₂O in the outer disk. H₂O froze as ice-mantles onto dust grains and evaporated from grains transported to the inner disk, enriching it in ¹⁷O and ¹⁸O [4]. Therefore, anhydrous IDPs contain a mixture of materials from different times and spaces in the protoplanetary disk, as has been described for material from comet 81P/Wild2 revealed by the STARDUST mission [5].

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[2] Starkey N.A. and Franchi I.A. (2013) *Geochimica et Cosmochimica Acta* 105:73-91.

[3] Yurimoto H. and Kuramoto K. (2004) *Science* 305:1736-1766.

[4] Krot A. et al. (2020) *Science Advances* 6:eaay2724.

[5] Brownlee D. (2014) *Annual Review of Earth and Planetary Sciences* 42:179-205.

Lecture

Topic: 1.3 Bridging length and time scales in the modelling of geomaterials

Solute-solvent interactions in supercritical water: density-, and temperature-dependent effects on the Krichevskii parameter of different monovalent salts

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Reliable models describing chemical equilibria of aqueous fluids at high temperatures (T) and pressures (P) are crucial to several areas of the geoscience, ranging from problems in ore deposit geology to the use of geothermal energy systems.

Despite this importance, to date there is no model that can accurately predict the thermodynamic properties of supercritical aqueous fluids at and near the critical point (CP) of water.

This is due to the strongly divergent nature of certain thermodynamic properties of solutes, such as partial molar volumes (PMV), whose derivatives approach infinity at the critical point and are therefore difficult to constrain experimentally. Therefore, it is important to find ways to avoid direct treatment of anomalously behaving solution properties under CP conditions.

In this context, the Krichevskii parameter A_{Kr} is considered a promising key variable, which is closely related to the PMV of a solute and is known to describe a smooth function even in the vicinity of the CP of water. In an effort to better understand the behavior of A_{Kr} of different monovalent salts, we perform classical molecular dynamics (MD) simulations of supercritical aqueous solutions in a wide range of temperatures and densities. We describe the effect of solute type, T and water density on the behavior of A_{Kr} and draw connections to the molecular structure of water under the respective conditions. Our observations contribute to a deeper understanding of solute-solvent interactions under supercritical conditions and serve as part of a molecular-level guide for the development of future thermodynamic models.

Lecture

Topic: 6.4 Landslides – detecting, monitoring, modeling, assessing hazards, and coping with risks

Comparing data-driven landslide susceptibility mapping methods and the impact of modifying the study area and sampling method in the Hunza Valley (Pakistan)

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Federal Institute for Geosciences and Natural Resources, Germany

We compared artificial neural networks (ANN), frequency ratio (FR), logistic regression (LR), and weights of evidence (WoE) for landslide susceptibility mapping in the Hunza Valley, Pakistan. We applied different data manipulation techniques (e.g. feature masking and sampling) to analyze their effects on the model. The landslide inventory was collected using Google Earth satellite images. The corresponding potential causative factors were derived from a geological map, a digital elevation model, and satellite imagery data. We evaluated the models with receiver operating characteristics curves using cross validation. Using the validation data, ANN showed the best performance, followed by LR, WoE, and FR. All applied procedures achieved good and comprehensible results. However, the susceptibility patterns show substantial differences. Modifying the study area (e.g. excluding trivial areas, such as glaciers) and using different sampling strategies significantly impacts the susceptibility patterns in all models. We recommend the use of WoE and FR in large areas with few causative factors, despite their lower performance, as their models are more robust in areas with few observations compared to LR and ANN. ANNs unfold their potential for landslide susceptibility mapping only completely in areas with many non-linear correlated continuous data sets, where they are superior to other methods. Modifying the study area and sampling technique can have a bigger impact on the final susceptibility model than using another data-driven landslide susceptibility mapping method.

Poster

Topic: 1.7 Experimental Petrology and Geochemistry

Melting and subsolidus reaction in the system $\text{Mg}(\text{OH})_2\text{-MgCO}_3$ between 2 and 12 GPa

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CO_2 and H_2O are the most abundant volatile components in the Earth's crust and mantle. The presence of CO_2 , H_2O and mixtures of $\text{H}_2\text{O-CO}_2$ effect the phase relations of mantle lithologies. The $\text{H}_2\text{O-CO}_2\text{-MgO}$ system, providing the basis for more complex systems, is poorly constrained from some quenched experiments. Here we investigated by in - situ X-ray diffraction measurements using the large volume press at P61B at PETRA III (DESY) the subsolidus and melting reaction of magnesite mixed with 16 wt% brucite.

We report the melting reaction of magnesite + periclase + vapour à liquid between 6 and 12 GPa and the subsolidus reaction magnesite à periclase + vapour between 2 and 4.8 GPa. These reactions meet at an invariant point at about 5 GPa and 1500 °C. This invariant point was reported at lower pressure of 3.2 GPa by Ellis [1] who investigated the topology of subsolidus and melting reactions in the $\text{H}_2\text{O-CO}_2\text{-MgO}$ system theoretically. Between 5 and 12 GPa and in the presence of a $\text{CO}_2\text{-H}_2\text{O}$ vapour phase, magnesite melts at a temperature about 90 °C lower than under anhydrous conditions. This improves previous results from quenched multi-anvil experiments locating the melting point of hydrous magnesite at 6 GPa 50 °C lower than the melting point of anhydrous magnesite [2].

1 Ellis and Wyllie, *Carbonation, hydration, and melting relations in the system $\text{MgO-H}_2\text{O-CO}_2$ at pressures up to 100 kbar*. American Mineralogist, 1979. **64**(1-2): p. 32-40.

2 Müller, Koch-Müller, Rhede, Wilke, and Wirth, *Melting relations in the system $\text{CaCO}_3\text{-MgCO}_3$ at 6 GPa*. American Mineralogist, 2017. **102**(12): p. 2440-2449.

Lecture

Topic: 3.2 Composition and evolution of deep planetary interiors

Core formation experiments at conditions of a deep magma ocean

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Models of core formation involve equilibration of metal and silicate in a deep magma corresponding to pressure and temperature conditions above 50 GPa and 3500 K (e.g. 1, 2). Over the last four decades, core formation experiments have been performed under limited P-T ranges, accessible with large volume presses such as piston cylinder or multi-anvil presses. Therefore, modeling the behaviors of elemental distribution between core and mantle during Earth's differentiation required thermodynamic extrapolations leading potentially to large errors. However, the last decade has proven the possibility of producing metal-silicate experiments using the Laser Heated Diamond Anvil Cell (LHDAC), the only static pressure device capable of producing the direct P-T conditions of core-mantle equilibration, despite technical hurdles linked to sample recovery, analyses at small spatial scales, and chemical equilibrium. This talk will review recent findings which revealed new processes that were unexpected on the basis of prior experiments or confirmed and precise some existing models. Using the partitioning results of a large number of siderophile elements, the conditions of core formation during accretion, the budget of light elements in the core, and the origin of volatile elements will be discussed.

(1) J. Siebert, J. Badro, D. Antonangeli, F.J. Ryerson (2013). Terrestrial accretion under oxidizing conditions. *Science*, 339, 1194-1197.

(2) D. Huang, J. Badro, J. Siebert. The niobium and tantalum concentration in Earth's mantle constrains the initial composition of its primordial magma ocean (2020). *Proceedings of the National Academy of Sciences*, doi: <https://doi.org/10.1073/pnas.2007982117>.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Experimental Simulation of Liquid Immiscibility in a Primitive Silicate-Carbonatite System

Antonia Simon^{1,2}, Roman Botcharnikov¹, François Holtz², Daria Voropaeva³, Marion Tichomirowa³, Stephan Buhre¹

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Despite being the most important source of rare earth elements (REE), the formation of carbonatites as well as the enrichment processes of rare metals in these rocks remain elusive. While direct partial melting from a carbonated mantle source may account for some carbonatite occurrences, most carbonatites are spatially associated with Si-undersaturated, peralkaline magmatic silicates. The latter form either by crystal fractionation from a silicate parental melt, by separation of immiscible carbonatite from a carbonated silicate magma or a combination thereof. Currently, most experimental studies on carbonatite formation focus on evolved or simplified systems. In existing experiments, rare metals partially favour silicate over carbonatite melts, contradicting proposed enrichment processes.

In this study, we report on experiments simulating a primitive silicate-carbonatite system. As a starting material we used a synthetic trace element doped silicate glass, modelled after perovskite-hosted melt inclusions from the Kola Alkaline Province. To generate liquid immiscibility, carbonatite powder was added in varying proportions and run with/without water. The glass-powder mixtures were heated to 1250 °C at 500 MPa in an internally heated pressure vessel. While high proportions of silicate over carbonatite led to the generation of a homogeneous, carbonated silicate glass, liquid immiscibility was reached at proportions of 1:2 (silicate:carbonatite) alongside crystallisation of calcite. Mixing silicate and carbonatite 1:1 with addition of water resulted in the separation of a silicate glass from quench carbonatite, the latter containing idiomorphic perovskite. The high compatibility of REE in perovskite can strongly affect the rare metal partitioning and mobility in the immiscible liquids.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Subsolidus fluid driven post-magmatic mineral formation in peridotite and ijolite rocks from the Kovdor and Ivaara complexes (Kola Alkaline Province)

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Rocks exposed in alkaline magmatic complexes and associated rare metal deposits are a product of multistage formation. Petrographic, mineralogical and geochemical characteristics suggest that post-magmatic metasomatic mineral reactions triggered by high flux of magmatic volatiles are very common. Release of magmatic fluids and rock permeability are pressure dependent, which may exert a depth control on metasomatic reactions altering intrusion related vertical magmatic zonation along the intrusive conduit. Fenites attest to fluid release to the wall rocks. High permeability in the contact to the wall rock causes intensive fluid-rock interaction and metasomatic products observed across the contact at a given exposure level are the integrated product of fluid flux with a significant density driven vertical advective component. Alkaline rocks may thus reflect input from various mantle and crustal sources situated at lower levels of the intrusive system.

Here, we present results of a mineralogical and isotope geochemical investigation of samples from the complexes of Kovdor and Ivaara (Kola Alkaline Province), which are considered to represent different levels in both intrusive alkaline systems. Peridotitic and ijolitic rocks show substantial subsolidus mineral reactions. In both cases mineralogical as well as Sr and Nd isotopic signatures suggest a complex and multistage post-magmatic metasomatic evolution mainly driven by magmatic fluids, in which, however, input from the wall rocks across the contact into the complex cannot be ruled out.

Poster

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Transport and reaction of light elements in pegmatitic systems at thermal disequilibrium – first insights from an experimental approach

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The transition from fossil towards green energy sources is one of the major challenges for our society. In order to accomplish this, large amounts of lithium are necessary as a component in Li-ion batteries. Such resources can be obtained from pegmatites. These magmatic rocks are often associated with highly fractionated granites and are therefore abundant all over the globe. Rare-element pegmatites, a sub-group of pegmatites, are often strongly enriched in Li and B and a variety of strategic elements (e.g. Ta, Nb, Be, Sb, W). There are many models for the formation of such pegmatites, however, the mechanisms leading to strong metal enrichment are yet poorly constrained.

With our experimental study we want to address, whether Li and B isotopes can be used as tracers for magmatic and hydrothermal processes in pegmatites. For this purpose, we investigate the isotope fractionation of Li and B during the interaction between a pegmatitic melt and a fluid phase in a closed system. We have developed an experimental setup, where melt and fluid coexist. Diffusive transport is directed from the pegmatitic melt through an aqueous fluid into a sink (e.g. aluminosilicate melt or muscovite). To mimic natural conditions, temperature gradients ≤ 10 K/cm along the sample can be adjusted. First results of associated diffusion couple experiments show that Li diffusion is 1) several orders of magnitude faster than B and 2) insensitive to melt composition. B diffusion, on the other hand, strongly depends on melt composition and is mainly controlled by melt viscosity.

Lecture

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

Deciphering the exhumation path of granulite facies rocks based on mineral reaction textures and monazite geochronology

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The formation of mineral reaction textures such as coronae or symplectites is commonly attributed to post metamorphic peak processes. Thus, they can be used to make implications about the retrograde exhumation history of high-grade metamorphic rocks. Here we present an example of aluminous paragneisses from the Loosdorf complex (southern Bohemian Massif, Austria) showing metamorphic peak conditions of ~1.0 GPa and ~800 °C with the peak assemblage garnet–biotite–sillimanite–plagioclase–K-feldspar–quartz–granitic melt ± ilmenite ± rutile. In their melanocratic layers, these rocks developed cordierite moats around garnet and cordierite + spinel ± corundum ± anorthite reaction textures at former garnet–sillimanite interfaces. Chemical potential relationships and phase diagram calculations using the local symplectite bulk composition are used to explain the process of texture formation and to estimate the corresponding *P–T* conditions. Our results indicate that the reaction textures formed in the course of a near-isothermal decompression path subsequent to metamorphic peak at conditions of ~0.3 GPa and ~750 °C. This relatively "hot" exhumation could be explained by the contemporaneous exhumation of large HP–UHT granulite bodies now underlying the Loosdorf complex. The timing of regional metamorphism affecting the granulites and the southern Bohemian Massif in general is well constrained and has its peak at ~340 Ma. However, monazite from Loosdorf paragneisses yielded a slightly younger age of ~335 Ma. Although the ages overlap within errors, they are interpreted to represent the age of the isothermal decompression and exhumation resulting in the formation of the observed reaction textures.

Lecture*Topic:* 1.7 Experimental Petrology and Geochemistry**Solubility of water in peridotite liquids and the prevalence of steam atmospheres on rocky planets****Paolo A Sossi¹, Peter M E Tollan¹, James Badro², Dan J Bower³**¹Institute of Geochemistry and Petrology, ETH Zürich, Switzerland; ²Institut de Physique du Globe de Paris, Université de Paris, France; ³Center for Space and Habitability, Universität Bern, 3012 Bern, Switzerland

Atmospheres are products of time-integrated mass exchange between the surface of a planet and its interior. On Earth and other planetary bodies, magma oceans likely marked significant atmosphere-forming events, during which both steam- and carbon-rich atmospheres may have been generated. However, the nature of atmospheres around rocky planets remains unclear for lack of constraints on their solubilities in liquids of appropriate composition. Here we determine the solubility of water in 14 peridotite liquids, representative of Earth's mantle, synthesised in a laser-heated aerodynamic levitation furnace. We explore oxygen fugacities (f_{O_2}) between -1.9 and +6.0 log units relative to the iron-wüstite buffer at constant temperature (1900 ± 50 °C) and pressure (1 bar). The resulting f_{H_2O} ranged from 0 to 0.027 bar and f_{H_2} from 0 to 0.064 bar. Total H₂O contents were determined by transmission FTIR spectroscopy of doubly-polished thick sections from the intensity of the absorption band at 3550 cm^{-1} and applying the Beer-Lambert law. The mole fraction of water in the liquid is found to be proportional to $(f_{H_2O})^{0.5}$, attesting to its dissolution as OH. The data are fitted by a solubility coefficient of $\sim 525\text{ ppm/bar}^{0.5}$, roughly 25 % lower than for basaltic liquids at 1350 °C and 1 bar. Higher temperatures (rather than more magnesian compositions) result in a decrease of water solubility in silicate melts. Because the solubility of water remains high relative to that of CO₂, steam atmospheres are rare, although they may form under moderately oxidising conditions on telluric bodies, given sufficiently high H/C ratios.

Lecture

Topic: 9.2 Energy and technology critical raw materials: from genesis to processing

Mineralogy determines Co and Ni extraction from laterites via bioleaching and chemical leaching

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Laterite deposits may contain economic grades of cobalt and nickel. Laterite ore processing is challenging, especially for iron-rich, limonitic laterites. The BMBF-funded CLIENT II project BioProLat aims to develop a biohydrometallurgical process for laterites from Brazil. Bioleaching experiments with different ore samples, addition of elemental sulfur and different cultures of acidophilic bacteria were conducted in 2L stirred tank bioreactors under aerobic or anaerobic conditions at different temperatures at low pH. Additionally, column experiments were performed to simulate heap bioleaching. Mobilisation of cobalt via bioleaching was in the range of 68-88 %, while dissolved nickel was between 17 % and 56 %. Mineralogical and geochemical analysis (XRD, SEM- MLA, DSC, LA-ICP-TOFMS, XRF) of the original ore samples as well as leaching residues was conducted to (i) identify mineral phases, which are attacked by bioleaching and (ii) estimate the portions of Co and Ni, which are released by bioleaching of different mineral phases. Cobalt was mostly hosted by Mn-rich mineral phases (e.g. asbolane), which were dissolved via bioleaching. Nickel was present in Mn-rich minerals (e.g. asbolane) and magnesium silicates (e.g. serpentine) also being dissolved via bioleaching. However, most of the nickel occurred in goethite which was almost not dissolved via bioleaching. Chemical leaching tests supported bioleaching results. For a high cobalt and nickel recovery a combined chemical leaching with bioleaching offers an option for laterite processing.

Poster

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Internal fluid-mineral oxygen exchange: equilibrium clumped isotope behaviour in the most extreme rock-buffered systems?

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Chemical exchange between carbonate and internal water populations represents the lowest possible water/rock fraction in natural materials: with molar ratios possibly lower than one percent. Despite their low abundance, internal water masses in fossils and mineral specimens can play an important role mediating exchange reactions: lowering the energetic barriers for resetting clumped isotopes, as well as supplying oxygen to reset carbonate $\delta^{18}\text{O}$ values. In heating experiments below 375°C, these reactions do not reach full clumped isotope equilibrium at the experimental temperature. Applying the dual-clumped isotope system to heated and unheated bivalve and coral carbonate reveals that this partial equilibration is due to a mixture of fully equilibrated and unaltered endmembers, as opposed to the carbonate uniformly reaching equilibrium at a cooler temperature. This interpretation appears to contradict the behavior of fluid inclusion $\delta^{18}\text{O}$ values, which appear to have equilibrated at a cooler temperature. We attribute this discrepancy to the existence of multiple populations of internal water, such as organic-bound water and “true” fluid inclusions of liquid water, which could have different exchange kinetics with the carbonate. Dual-clumped analyses reveal the possibility for calculating peak heating temperature of thermally altered minerals, and future work will focus on finding unambiguous indicators for thermal alteration. An unambiguous indicator for heating will enable the use of new climate archives that otherwise would be disregarded due to the possibility of heating by ancient humans (shell middens), or fossils geothermally heated during burial.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

Particle-mediated origins of mesocrystallinity in calcium sulfate single crystals

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Calcium sulfate minerals are abundant in natural and engineered environments in the form of three phases: gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), bassanite ($\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$), and anhydrite (CaSO_4). Due to their relevance in natural and industrial processes, the formation pathways of these phases from aqueous solution have been the subject of intensive research. A number of studies have already revealed that nucleation in the CaSO_4 - H_2O system is non-classical, where the formation of the different crystalline phases involves several steps including a common amorphous precursor.

In this contribution we show that the formation of the amorphous phase involves the aggregation of small primary particles into larger disordered aggregates exhibiting a "brick-in-the-wall" structure. The actual crystallization occurs by the restructuring and coalescence of the particles ("bricks") into a given calcium sulfate phase depending on the physicochemical conditions of the solution. Such a process yields a final imperfect mesocrystal, composed of smaller domains rather than a continuous single crystal structure.

These observations reveal that organic-free calcium sulfate mesocrystals grown by a particle mediated-pathway might preserve in the final crystal structure an "imprint" of their growth pathways. Indeed, by considering large anhydrite crystals from the famous Naica Mine we observed a suite of correlated self-similar void defects spanning multiple length-scales. These flaws, in the macroscopic crystal, stem from "seeds of imperfection" originating from an original particle-mediated growth. Hence, building a crystal could be viewed as Nature stacking blocks in a game of Tetris, whilst slowly forgetting the game's core concept and failing to fill rows completely.

Poster

Topic: 2.2 From dust to planets

Experimental quantification of the degassing of chalcophile and siderophile elements from metal and sulfide melts

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The chemical composition of magmatic iron meteorites provides fundamental insights into planetary accretion processes. They are distinguished based on their trace element compositions and could represent the cores of more than 50 parent bodies¹. The primary difference between the different groups is the degree of volatile element depletions, which increases from class I to IV iron meteorites². The volatile element loss could have occurred prior to (i.e. nebular) or during parent body accretion/differentiation, for example during exposure of a liquid core following a catastrophic impact³. Investigating the mechanisms of volatile loss from requires experimental constraints on their volatility, for example during evaporation. We therefore experimentally quantified the evaporation of the nominally volatile, transitional and refractory chalcophile and siderophile from Fe-C and Fe-S melts, respectively. Their evaporation was studied as a function of pressure (high vacuum to 1 bar), temperature (1573-1823 K), composition (Fe, FeS) and time (min's to hours). The results show that the volatilities are significantly different than previously assumed, and that their volatility may be strongly and distinctly affected by the composition of the melt from which they evaporate. The new data is discussed in light of current models that describe volatile element depletions in magmatic iron meteorite parent bodies.

(1) Goldstein et al. (2009) *Chemie Der Erde - Geochemistry* (2) Scott & Wasson (1975) *Rev Geophys* (3) Kleine et al. (2018) *LPS* 2083.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Boron isotopic composition in cold-water corals determined by LA-ICP-MS

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In this study, we present B isotopic data for cold-water corals at high spatial resolution determined by UV femtosecond laser ablation system coupled to a Nu Plasma II MC-ICP-MS. Boron isotope records in biogenic carbonates provide constraints on the evolution of seawater pH and insights into biomineralization processes. We investigated B isotopic ratios in recent cold-water corals (*Desmophyllum dianthus*) from a field experiment in the Comau Fjord (Chile) to resolve seasonal variations. Corals from the head and the mouth of the fjord and from different water depths were stained with calcein, replaced at the same location or cross-transplanted and observed for a whole year to investigate time-resolved environmental signatures and potential adaptation effects under new environmental conditions. B isotopic ratios were measured at the upper part of the calyx in transverse sections between septa at the skeletal increment. $\delta^{11}\text{B}$ values range between 23.5 and 27.0‰ and varies with seasonality and location in the fjord. Isotope signature of cross-transplanted corals do not differ significantly from those of local corals showing that the recorded signature is directly influenced by environmental conditions. B isotopic signatures correspond to an internal pH up-regulation for calcification of 0.78 to 1.14 pH units, which is likely controlled by ambient seawater pH and nutrient availability. These results show the potential of in situ techniques to decipher marine archive to reconstruct environmental conditions.

Lecture

Topic: 11.3 Young Scientist Session

Composition and distribution of sedimentary organic matter in the distal Wealden facies (KB Rehburg-2) of the Lower Saxony Basin, Germany

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New insights into the Lower Cretaceous sediments can be gained from a recently drilled core (KB Rehburg-2, Lower Saxony, Germany) covering 180 m of Berriasian strata. Stratigraphic assignment is based on ostracods and indicates Wealden 1-4. Palynofacies analysis was carried out to reconstruct the depositional environment of the sequence studied. This data was complemented by geochemical measurements (TOC, S_{tot} , $\delta^{13}C_{org}$ and RockEval pyrolysis) and sedimentological observations to reconstruct the paleoenvironmental conditions during the earliest Cretaceous in the LSB. The particulate organic matter (OM) shows good to very good preservation and is composed of diverse spores, pollen grains, algae and woody debris; marine particles such as dinoflagellates, acritarchs and prasinophytes occur only sporadically.

Data evaluation and integration reveals a predominantly lacustrine, freshwater to brackish depositional system with high continental OM input. Abundance peaks of *Botryococcus* algae occur throughout the sequence and indicate freshwater to brackish conditions. The rare occurrence of dinoflagellates and acritarchs can be interpreted as indicators of short-term marine incursions into the LSB. Prasinophytes point to repeated salinity changes. The scarce abundance of dinoflagellate cysts differs significantly from existing studies in the LSB by Schneider et al. (2017), but correlation with two marine transgressive events is tentatively proposed (TE 1-2). This difference may result from a potentially more terrestrially dominated depositional system represented by the Rehburg-2 core.

References:

Schneider, A.C., Heimhofer, U., Heunisch, C., & Mutterlose, J. 2017. The Jurassic-Cretaceous boundary interval in non-marine strata of northwest Europe – New light on an old problem. *Cretaceous Research* 87, 42-54.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

The crystallization of ikaite ($\text{CaCO}_3 \times 6\text{H}_2\text{O}$) in presence of mineral surfaces: Effects on formation and implications for nucleation pathways

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Ikaite is an essential calcium carbonate mineral especially in cold regions of Earth. However, the conditions leading to the formation of ikaite are poorly constrained. In a previous study (Chaka 2018), it was reported that the nucleation mechanism of ikaite likely does not compare to widely recognized mechanisms of more stable anhydrous CaCO_3 -minerals. Nucleation was rather attributed to a low energy pathway, which leads to the highly hydrated ikaite structure by assembling aqueous ion pair complexes. Whether such a nucleation mechanism is affected by foreign surfaces, as it was already shown for the formation of anhydrous calcium carbonate minerals (Li et al. 2014), remained unclear so far. This lack of knowledge is particularly serious as a better understanding of the nucleation of ikaite in presence of mineral surfaces could lead to profound insights of ikaite formation under natural conditions. In our study, new data on ikaite formation in presence of mineral surfaces were gained from cryo-mixed-batch-reactor and cryo-AFM experiments using quartz and mica surfaces as proxies for natural settings. Our experiments revealed similar effects of the presence of quartz and mica on ikaite nucleation. Both minerals caused a significant expansion of the supersaturation range from which ikaite forms instead of calcite or vaterite. For ikaite formation, therefore, the presence of mineral surfaces is at least as important as calcite-inhibiting substances. The latter, so far, were the only ikaite promoters recognized in natural settings. Furthermore, our results revealed low interfacial energies which imply a nucleation mechanism including a minimal energy barrier.

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

How does deep granite weather? Fractures matter but fracture size counts

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How the weathering zone propagates into un-weathered rock at depth is subject of increasing research. Some models suggest that the depth of the ground water table controls weathering zone thickness. Others predict that regolith thickness is pre-conditioned by fracture density. Still others invoke weathering-induced fracturing by iron oxidation.

To explore the influence of climate versus tectonic processes on weathering intensity and regolith thickness we drilled 5 cores in granitic bedrock along a climatic gradient within the EarthShape project (from N to S dry desert, semi-arid, Mediterranean, humid) along the Chilean Coastal Cordillera. We combined borehole logging with geochemical and geophysical analyses of core and soil samples to evaluate the controls on weathering. Based on this geochemical data set we are able to show that the studied weathering profiles consist of three main weathering parts characterized by distinct geochemical gradients. The first part comprises the soil layer and is characterized by high weathering intensities, the second part comprises the saprolite down to the bedrock and includes the weathering front, the third part is found below the weathering front and is associated with fractures. Thus multiple weathering zones developed at major fractures. We found that the depth of the weathering front is mainly controlled by the characteristics of the fracture network: fracture aperture and dip, whereas weathering intensity is controlled by a combination of fracture network and the influence of vegetation through soil CO₂ and organic acids. Generally, our data show that for a given fracture density fracture apertures control regolith thickness.

Lecture

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

Timescales of magmatism in the Eifel (Germany), from crustal growth to Quaternary volcanism - A xenolith perspective

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Xenoliths transported to the surface by ascending magmas are crucial to decipher the structure and composition of the Earth's crust and provide valuable insights into melt formation and magma storage conditions. This cross-crustal sampling is of particular importance in regions where no basement outcrops exist, such as the Eifel, Germany. Crustal xenoliths containing zircon are suitable targets for U/Pb geochronology to quantify the timing of intra-crustal magmatic and metamorphic events.

The Quaternary Eifel volcanic field consist of >300 volcanoes including maars, scoria cones and tuff rings. Precise eruption ages for these are rare and often inconsistent between the different methods. A promising approach to determine accurate eruption ages is to apply (U-Th)/He geochronology to zircon extracted from partially re-melted crustal xenoliths embedded in pyroclastic material.

So far, we collected >200 xenoliths from >35 volcanoes in the West- and East Eifel. We observe significant differences in xenolith abundance between the volcanic centers and a variety of xenolith types, including magmatic and metamorphic rocks with varying degrees of pyrometamorphic overprinting. Zircon crystallization ages range from ca. 2000 to 280 Ma, clustering around Variscan and Caledonian ages. Remarkably, the youngest U/Pb ages indicate post-Variscan plutonic magmatism reaching to the Permian, which has not yet been reported for this area.

Preliminary (U-Th)/He zircon eruption ages acquired for the Meerfeld and Gemünden Maar confirm the feasibility of the method. Future work on xenolith samples from additional centers will generate a comprehensive dataset of eruption ages to unravel the spatiotemporal evolution of the Eifel volcanic field.

Poster

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

Low-grade Blueschist-facies Metamorphism in the Central Yarlung Suture Zone, Southern Tibet

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Blueschists are mostly metamorphosed basaltic rocks that form at high-pressure and low-temperature conditions and characterize sodic amphibole as the major constituent mineral. Blueschists in southern Tibet are distributed as discontinuous blocks in sedimentary-matrix mélangé within the Yarlung Suture Zone (YSZ). In this paper, petrographic and mineral chemical studies and pseudosection modelling were carried out to constrain the metamorphic conditions and evolution of blueschists in the central YSZ. Blueschists from Sangsang area are characterized by presence of sodic amphibole, epidote, chlorite, muscovite, omphacite and sphene in the peak metamorphic assemblage. Sodic amphiboles in Sangsang blueschist are identified as magnesioriebeckite in chemical compositions. Pseudosection calculations and intersection of isopleths indicate peak metamorphic conditions of 7.8kbar at 355°C. Blueschists from Kadui area contain metamorphic assemblages of sodic amphibole, epidote, chlorite, omphacite with accessory sphene. The amphibole in Kadui blueschist shows zoned from actinolite core to ferrowinchite/riebeckite rim and actinolite outmost rim. The metamorphic conditions of Kadui blueschists are estimated to be 360°C and 7.5kbar based on available phase equilibria and sodic amphibole compositions. These P–T conditions are consistent with metamorphism in the low-grade blueschist facies, burial depths of 25–27 km and a thermal gradient of 13–14°C/km. Our new findings indicate that the blueschist in the central part of YSZ experienced low-grade blueschist-facies metamorphism at shallow depths in subduction channel as a response to a northward subduction of the Neo-Tethyan oceanic lithosphere during the initial India–Asia collision stage.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Dual clumped isotope thermometry and fossil eggshells: a way to better understand the dinosaur-bird transition

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Birds evolved from dinosaurs during the Late Jurassic and they are now one of the most widespread group of vertebrates on the planet. However, some aspects of the dinosaur-bird transition, like the timing of switch to an endothermic thermophysiology and the loss of an ovary, are still obscure. Modern reptiles, as living representatives of the reptiles-dinosaurs-birds lineage, can be used to determine the ancestral conditions for both dinosaurs and birds.

For this study, we analyzed the dual clumped isotopic composition of eggshells of modern reptiles, modern birds and *Troodon*, one of the last bird-like dinosaur. Dual clumped isotope thermometry (combined analysis of Δ_{47} and Δ_{48}) not only allows the determination of the carbonate precipitation temperature, but consent the identification of the kinetic effects prevailing during precipitation, hence opening way to a more comprehensive understanding of the (bio)mineralization process.

Our results suggest that *Troodon*, despite presenting bird-like body temperature, still presented a reptile-like eggshell mineralization process that not required involvement of Amorphous Calcium Carbonate as transitional phase. These results might also imply that *Troodon* was still in posses of two fully functional ovaries.

Critically, this work proves that dual clumped isotope thermometry can extract biological information from mineralized fossil material, allowing investigation of physiological information of extinct animals even in absence of reliable soft tissue evidence.

Poster

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Microscale Si isotope variations in radiolarian cherts from the Rhenish Massif

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The Rhenohercynian back-arc basin hosts a Lower Carboniferous chert-shale succession that documents variable radiolarian productivity, subareal volcanism and pelagic background sedimentation. To assess the potential of radiolarian cherts to record paleo-productivity and/or oceanic Si concentrations, we investigate silicon isotope ratios ($\delta^{30}\text{Si}$) of radiolarian shells, their secondary fills and the matrix in which they are embedded by fs-Laser ablation-MC-ICP-MS. We discuss causes of variations in $\delta^{30}\text{Si}$ among the analyzed compartments that either point to isotope fractionation during early silicification of the sediments or the presence of two silica sources.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Chert oxygen isotope ratios are driven by Earth's thermal evolution

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The $^{18}\text{O}/^{16}\text{O}$ ratio of cherts ($\delta^{18}\text{O}_{\text{chert}}$) increases monotonically by ca. 15 ‰ from the Archean to present. As oxygen isotope fractionation in the silica-water system is temperature-dependent, this trend has often been interpreted as long-term climatic cooling, with a hot Archean ocean at $>70^\circ\text{C}$. Alternative interpretations invoke a low- $\delta^{18}\text{O}$ Archean ocean or pervasive alteration of the Precambrian chert $\delta^{18}\text{O}$ record.

There is now increasing recognition that $\delta^{18}\text{O}_{\text{chert}}$ reflects the temperature and fluid $\delta^{18}\text{O}$ at the endpoint of the silica diagenetic pathway, in which amorphous opal-A is transformed via dissolution-reprecipitation reactions to microcrystalline quartz via an intermediate opal-CT phase. Here, we investigate how silica diagenesis may have varied over geological time and how this would have impacted the $\delta^{18}\text{O}_{\text{chert}}$ record. We introduce a 1D silica diagenesis model that tracks the transformation of silica polymorphs in the sediment column during burial heating, revealing the importance of reaction kinetics in controlling the depth, temperature and oxygen isotope fractionations associated with chert formation. Our results show that $\delta^{18}\text{O}_{\text{chert}}$ is a poor archive of seawater temperatures. Instead, $\delta^{18}\text{O}_{\text{chert}}$ is sensitive to changes in heat flow through ocean sediments, such that a large fraction of the Archean-Cenozoic difference in $\delta^{18}\text{O}_{\text{chert}}$ can be explained by reasonable changes in heat flow over Earth history. This removes the need for extremes in either seawater temperature or $\delta^{18}\text{O}$, pointing to a temperate to warm Archean with only slightly ^{18}O -depleted oceans, and satisfying all geochemical, palaeoclimatological and biological constraints.

Lecture

Topic: 4.4 Deciphering orogenic processes: Combining metamorphism, anatexis, metasomatism and geochronology

Tracking high-grade metamorphism: from partial melting to the detrital record

Mahyra Tedeschi

Federal University of Minas Gerais, Brazil / University of Bern, Switzerland

High to ultra-high temperature (HT-UHT) metamorphism (>800°C) drives changes in rocks that range from the production of chemical heterogeneities to the disturbing of isotopic systems. To disentangle the complex history of these rocks, a multi-prong approach is needed, due to the different sets of mineral reactions that produce melts and fluids of varying compositions at different times. Nanorock inclusions preserved in zircon are critical for retrieving primary melt compositions through re-homogenization experiments, especially in garnet-free rocks, that can be further compared to melt compositions from different scales of observation. These observed melt compositions may then be contrasted with those predicted by thermodynamic models to evaluate the pressure-temperature evolution of partial melting. Nanorock inclusions can further assist in the deconvolution of HT-UHT rocks intricate geochronological record since these rocks often reveal a protracted zircon record with dates smeared along the concordia curve. This smearing may result from the partial resetting of existing grains or prolonged metamorphism and introduces ambiguity into U-Pb dating from igneous, sedimentary, and metamorphic rocks. The HT-UHT metamorphism has implications for maximum depositional ages and tectonic setting determinations, and its extent depends on whether metamorphism took place in the source that will be eroded and then deposited or when the rock was already deposited. A detailed investigation enables identifying protoliths and reconstructing metamorphic histories. Hf isotope analysis allows zircon sources to be distinguished, minimum crystallization ages to be retrieved, and provides additional constraints on the conditions of anatexis (e.g., open versus closed system melting; role of coexisting minerals).

Lecture

Topic: 11.1 Shaping the future of geoscientific data: The path to FAIR data

From Field Application to Publication: An end-to-end Solution for FAIR Geoscience Data

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Creation of data starts with sample collection in the field and the assigning of a unique global IGSN sample identifier to samples, these samples are stored along with any subsequent analytical data in our fine-grained and detailed geochemical data models allowing visualising and publishing acquired datasets. This unique solution has been developed by Lithodat Pty Ltd in conjunction with the AuScope Geochemical Network (AGN) consisting of most Australian geochemical laboratories and can be accessed by the public on the AusGeochem web platform.

Using our field application users can enter and store all sample details on-the-fly during field collection, the data will be stored in the user's private data collection. After running subsequent geochemical analyses those results, including all metadata, can be stored in the relational database and be attached to the sample. Once uploaded, data can be visualised within AusGeochem, using data analytics via technique-specific dashboards and graphs. All data can be shared with collaborators, downloaded in multiple formats and made public enabling FAIR data for the research community.

Having all data stored in a clean and curated relational database with very detailed and fine-grained data models gives researchers free access to large amounts of structured and normalised data, helping them develop new technologies using machine learning and automated data integration in numerical models. Having all data in one place including all metadata such as ORCID IDs from involved researchers, funding sources, grant numbers and laboratories enables the quantification and quality assessment of research projects over time.

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

On the Analyses and Interpretation of Lithium Isotopes

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Lithium (Li) is one of the fundamental metals used in modern and future technologies. Even with how critical it is in modern society, demand for Li will only increase in the coming years. Lithium is used primarily in batteries, and as such is a key component for, e.g., electric vehicles. Most lithium is extracted from salars and Li-pegmatites. However, the behavior of Li in terms of its mobilization, transportation, and deposition are still poorly understood. Even the analyses of Li is challenging. This presentation will break this into three aspects; how is Lithium analyzed, what are Earth's Li geochemical signatures, and how does one get this range of fractionation. In this presentation, we will discuss diverse tested methods and their pros and cons, as well as the analytical hurdles faced and overcome in the field of Li geoscience. We discuss the diverse ranges of Li isotopes measured throughout the Earth's crust, with a particular focus on the ranges relevant to Lithium deposits. Finally, we will discuss the fractionation factors leading to the observed isotopic ranges, with emphasis made on the environmental effects that affect a given sample from deposition to erosion. Overall, Li is a complex system, and our goal is to show the methods with which one can investigate Li, the questions we ask, and what some of the answers are.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

X-ray emission setup to study electronic structure of iron bearing compounds *in situ* at high pressure and high temperature

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The determination of iron-bearing compounds' electronic structure under high pressure and temperature (HPHT) conditions is pivotal to understand the chemistry, physics and dynamics of the Earth's interior [1,2].

We present a setup for investigating the electronic structure of such compounds *in situ* at HPHT using (resonant) X-ray emission spectroscopy ((R)XES) and exemplify its capabilities showing results for hematite (α -Fe₂O₃) and siderite (FeCO₃). Conditions up to 80 GPa and 3000 K were achieved using diamond anvils cells in combination with a portable double-sided laser heating setup exploiting an Yb:YAG laser [3,4] and the (R)XES spectra were acquired utilizing a wavelength-dispersive von Hámos spectrometer in combination with a Pilatus 100K area detector [5].

This setup allows measurements of a full emission spectrum in a single-shot fashion. In combination with high intense synchrotron radiation available at beamline P01 of Petra III and a dedicated diamond anvil cell loading scheme, the measuring time is shortened such that *in situ* iron K β XES makes spin state imaging viable and provides simultaneously access to the valence-to-core emission. Furthermore, the use of miniature diamonds [6] enables RXES measurements at the iron K edge yielding detailed information iron's electronic structure and local environment.

[1] B. Orcutt et al. Deep Carbon (2019)

[2] Y. Kono et al. Magmas under pressure (2018)

[3] C. Albers et al. PRB 105 085155 (2022)

[4] G. Spiekermann et al. JSR, 27, 414 (2020)

[5] C. Weis et al. JAAS 34, 384 (2019)

[6] S. Petitgirard et al. JSR 24 (2017)

Lecture

Topic: 4.5 Tectonic Systems (TSK Open Session)

Melt-assisted strain localization in the upper mantle shear zone of northwestern Ronda (Spain)

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On the northwestern boundary of the world's largest exposure of subcontinental mantle a major shear zone crops out. A microstructural transect from mylonites to tectonites (0-700 m distance to the shear zone front) reveals a metasomatic history of multiple melt pulses with major impact on deformation and shear localization. Fe/Ti rich melts coming from a structurally deeper melting front inside the peridotite body, re-fertilized the entire shear zone area up to its present-day front and precipitated interstitial pyroxenes and spinel. The resulting mixed matrix of recrystallized olivine and interstitial grains localized the deformation in the entire melt-affected region. Microstructural characteristics are elongated olivines with film/wedge-shaped pyroxenes along the olivine grain boundaries and interstitial spinel. Melt-rock reaction textures such as indentations, highly irregular grain shapes and lobate boundaries are commonly present. Strong CPOs (olivine A-type) for all phases and the absence of amphibole in the mixed matrix indicate deformation under relatively dry conditions predominantly accommodated by dislocation creep. However, P-T estimates (1-2 GPa, 800-900 °C), average grain sizes of ~100 µm and the localization of deformation in the mylonitic area also indicate the activity of an additional grain size sensitive mechanism. Within the matrix, reacting pyroxene porphyroclasts form tails of pyroxene, olivine, amphibole and spinel neoblasts. Their similar or coarser grain sizes compared to the matrix and an equiaxial grain shape indicate no further strain localization in these tails. Their predominant B- or AG- CPO-types of olivine and the presence of amphibole suggest the presence of fluids during the tail formation.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

The trend towards renewable energies & the role of rare earths: How sustainable is it? China as an example!

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The global turnaround in the energy industry shows clear tendencies towards the further integration of renewable energy alternatives. While China is especially known for being the worldwide biggest producer and consumer of hard coal, it is also going high speed for the renewables. The recently announced goal of climate neutrality seems to support this new path. This is because a closure of hard coal mines and their substitution by renewable energies is being touted as the future potential of a green economic transition. Yet the rare earths used in large quantities for this are anything but green or recyclable. An example of the potential and the impact on ecology and human health of the rapidly increasing development and integration of renewable alternatives can be shown with the help of an exemplary life cycle assessment at the Bayan Obo Mine in Baotou, Inner Mongolia. Here, it is clear that the negative effects are long term and have a strong influence not only over land, air and water, but also on human development through induced diseases and inhibition of development. The method of the life cycle assessment is still highly underrepresented in this research field and needs more reliable data and calculations for improved policy decisions and strategic action in the future.

Poster

Topic: 7.1 Geo-Biosphere interactions through space and time: new analytical and experimental approaches to the fossil record

U-Pb analyses of a fossil crab cuticle from the Chattian Doberg strata (NW Germany)

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A high abundance of arthropod cuticles in the fossil record are well preserved, even at the microstructural level. The age of these fossils is usually constrained chronostratigraphically, but incorporation of radioactive trace elements during fossilization makes cuticles also amenable to radiometric dating. Our study aimed to assess to what extent the current mineralogical, chemical, and isotopic composition of fossil cuticles can provide a record of the long-term diagenetic evolution.

We combined electron microprobe element mapping, Raman spectroscopy, and laser ablation ICP-MS analyses to study the exoskeleton of a fossil raninoid crab from Chattian (Late Oligocene) strata of the Doberg (near Bünde, NW Germany). The investigated exocuticle had been replaced by apatite, while the endocuticle mostly consists of uraniferous calcite (up to 500 ppm U), yielding a LA-ICPMS U-Pb age of 17.5 ± 1.4 Ma (Burdigalian, Late Early Miocene). This age is consistent with the view that the present mineralogy formed millions of years after the death of the individual. A Late Early Miocene age, however, was also obtained from another Oligocene raninoid crab cuticle from Bodenburg (100 km to the ESE), suggesting a possible regional geological significance of this age within the Lower Saxony Tectogene.

In conclusion, fossilized arthropod cuticle can remain a closed U-Pb system over geologic time scales. However, the fossil cuticles were altered by distinct geological events affecting the diagenetic conditions in depositional basins, such as, for instance, an increased fluid flow. The U-Pb system of arthropod fossil cuticles might allow for tracing these long-term diagenetic processes.

Poster

Topic: 4.5 Tectonic Systems (TSK Open Session)

U-Pb zircon geochronology of the Siebengebirge Volcanic Field - Implications for the dynamics of the Lower Rhine Basin (Germany)

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The Oligocene Siebengebirge Volcanic Field (SVF) is located at the south-eastern termination of the extensional Lower Rhine Basin (LRB). Tuffitic deposits, repeatedly embedded within the siliciclastic basin sediments, provide a largely untapped record on the evolution of intracontinental volcanism and basin dynamics. With the aim to provide radiometric age constraints, we applied laser-ablation U-Pb zircon geochronology on trachytic rocks from Siebengebirge surface outcrops, and tuffitic layers within drill cores of the Köln Formation.

While the lithostratigraphic sequence of the LRB is perfectly established [1], previous attempts using K-Ar on trachyte tuff sandine returned conflicting results, possibly due to diagenetic alteration [2]. Sampled tuffitic layers within the Oligocene of the Köln Formation (archived drill cores Haus Ölgarten and Niederpleis, GD NRW) returned U-Pb zircon populations from the Horizons 05/06 transition, as well as from Horizon 08 to Horizon 1, that are identical to those from the Siebengebirge trachytic outcrops.

In accord with previous results from Ar-Ar sanidine [3], U-Pb zircon geochronology confirms that differentiated volcanism in the SVF is restricted to a single, relatively short time period. First results for the Köln Formation suggest that the trachytic volcanism should indeed be placed at the base of Horizon 06 within the lithological standard profile, whereas similar material in younger horizons had probably been reworked. As a consequence, the voluminous trachytic SVF volcanism seems to coincide with accelerated subsidence of the rift basin.

[1] Schäfer et al. (2004) *Newsl Stratigr*; [2] Todt & Lippolt (1980) *J Geophys*; [3] Przybyla et al. (2018) *IJES*.

Poster

Topic: 1.8 Minerals and Mineral Properties

Richardsite – a member of the stannite group?

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A new chalcogenide mineral, Richardsite, was proposed in literature with a composition Zn_2CuGaS_4 and crystallizing in the tetragonal stannite-type structure [1].

This compound can be viewed as a mixed crystal in the solid solution $2(ZnS) - CuGaS_2$. The composition of $2(ZnS)_x(CuGaS_2)_{1-x}$ with $x=0.5$ results in the Richardsite chemical composition. We have studied this solid solution series concerning the crystal structure of mixed crystals using powder samples synthesized by solid state reaction of the elements. Additional single crystals, aiming for a composition of Richardsite, have been grown by chemical vapour transport (CVT). The chemical composition of the synthesized material has been determined by WDX spectroscopy as well as EDX-analysis in the STEM.

Both end members are non-isotype: $CuGaS_2$ crystallizes in the chalcopyrite and ZnS in the zinc-blende structure. Rietveld analysis of X-ray diffraction data and TEM investigations revealed that the $2(ZnS)_x(CuGaS_2)_{1-x}$ system forms a solid solution series but with a broad miscibility gap ($0.2 < x < 0.5$). Within this gap two phases, as tetragonal domains in a cubic matrix, coexist. Thus the mixed crystal with $x=0.5$, corresponding to Richardsite, adopts the cubic zinc-blende structure.

We could not prove the existence of Richardsite, Zn_2CuGaS_4 , as a new member of the stannite group. Our findings show that Zn_2CuGaS_4 crystallizes not in the tetragonal stannite structure but in the cubic zinc-blende structure.

[1] L. Bindi, J. A. Jaszczak, Minerals 10 (2020) 467

Topic: 4.5 Tectonic Systems (TSK Open Session)

Two stages of Coseismic Rupturing separated by a stage of Postseismic Creep indicated by deformed pseudotachylytes from the Silvretta basal thrust

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Decoupling and movement of large crystalline nappes during orogenesis are controlled by episodic deformation at changing strain-rate and stress conditions. Deformed pseudotachylytes from the Silvretta basal thrust in the Central Alps, Austria, record two stages of pseudotachylyte formation separated by a stage of creep with quartz dynamic recrystallization at decreasing stresses at greenschist facies conditions. Amphibole (-101) mechanical twins indicate high strain rates and transient high differential stresses of >400 MPa during the formation of pseudotachylytes in amphibole-rich gneisses. Undeformed pseudotachylytes contain isometric rounded amphibole-gneiss clasts and quartz-rich clasts. The pseudotachylytes can be gradually transformed into ultramytonites containing deformed quartz clasts that are elongated parallel to the foliation of the fine-grained ultramytonitic matrix. The deformed quartz clasts are characterized by aggregates with an oblique shape preferred orientation and crystallographic preferred orientation indicating dislocation creep during ultramytonite formation. In other samples, pseudotachylyte injection veins within quartz-rich layers that underwent dislocation creep were foliated and folded. These deformed pseudotachylytes can be cross-cut by undeformed pseudotachylytes. The two stages of pseudotachylyte formation are reflecting coseismic rupturing. The intermediate stage of creep with quartz dynamic recrystallization at decreasing stresses is interpreted to represent postseismic creep with relatively slow stress relaxation, as opposed to a separate deformation stage. However, also quartz-rich host rocks deformed related to pseudotachylytes occur that show growth of new grains at quasi-isostatic conditions along the damage zone of coseismically generated cleavage cracks, without any evidence of creep after pseudotachylyte formation and thus representing relatively fast stress relaxation.

Lecture*Topic:* 4.1 Magmas and Fluids in the Crust**The effect of water on trace element diffusivities in silicic melts: A case study on Li, Rb, and Cs****Juliana Troch¹, Chris Huber², Nico Kueter³, Marcel Guillong³, Peter Ulmer³, Michael R Ackerson¹, Olivier Bachmann³**¹National Museum of Natural History, USA; ²Brown University, USA; ³ETH Zurich, Switzerland

Trace element diffusion is a powerful tracer for the kinetics of magmatic processes such as recharge and fluid exsolution. However, the dependence of diffusivities on melt water contents is poorly understood, and most trace element diffusivities have been determined in water-free melts unrealistic for most natural magmatic systems. Here, we investigate diffusion of the alkali trace elements Li, Rb, and Cs as a function of water content in metaluminous rhyodacite, high-silica rhyolite, and peralkaline rhyolite.

Homogenous hydrous glass cylinders were produced from trace element-doped and undoped powdered glass with 1-8 wt% H₂O. For the diffusion experiments, glass cylinders with the same water content but different trace element concentrations are paired along polished contact surfaces. Diffusion experiments were conducted between 720-1100 °C for 5-25 min using gas pressure vessels and a piston cylinder. Diffusion profiles were analyzed by LA-ICPMS and evaluated by a Monte Carlo iterative fitting procedure for full error propagation.

Measured logD values correlate linearly with melt water content, with one order of magnitude increase for D_{Li}, two orders for D_{Rb} and three orders for D_{Cs} from driest (1 wt%) to wettest (8 wt%) experiment. Variations in major element composition only have a minor effect. Comparing the dependence of Arrhenius parameters D₀ and E_a on melt water content, activation energies correlate linearly, while pre-exponential factors suggest negligible correlation. Quantifying these effects facilitates using the diffusion of alkali trace elements for tracking magmatic processes, such as the exsolution of fluids from long-lived shallow mushy magma reservoirs in the Earth's crust.

Lecture

Topic: 7.3 Assessment of the Earth System through Micropaleontology

Coastal Foraminiferal Assemblages along the southern coast of Oman: A biogeographic stepping stone for benthic foraminifera?

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The shallow water ecosystems of Oman are subject to intense seasonal upwelling and unlike many other oligotrophic tropical areas, are impacted by strong, seasonal nutrient-rich eutrophic conditions. The environmental conditions provide a setting for presumably unique foraminiferal faunal assemblages, but despite intensive research on tropical foraminifera, detailed studies on coastal foraminifera have not yet been conducted. Situated at a key position between the high-diversity Coral Triangle and the tropical Red Sea/eastern African coast, the coastal waters of Oman act both as a biogeographic steppingstone but also as a nutrient-rich and cold-water barrier for benthic foraminifera migrating from the east to west. Upwelling zones have a deep impact on coastal areas, displace oligotrophic water masses and influence the settlement of highly diverse tropical coral reef and foraminiferal faunal communities. We have examined foraminiferal assemblages from extremely shallow but diverse habitats along the southern coast of Oman to document their composition, diversity and habitat preferences. To place the Oman assemblages in a biogeographic context and to assess the role of the Oman area as potential steppingstone, we compare the foraminiferal fauna to assemblages from the Maldives, the Chagos Islands, the Coral Triangle and the Red Sea/eastern African faunal province.

Lecture

Topic: 1.3 Bridging length and time scales in the modelling of geomaterials

Modeling of Fe-bearing mineral surfaces towards understanding the reactivity of chemically modified nanozerovalent iron particles

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Chlorinated hydrocarbons (CHCs) such as PCE (perchloroethylene), TCE (trichloroethylene), and DCE (dichloroethylene) represent a serious contamination problem for water resources. Therefore, there is an urgent need to develop new effective *in situ* remediation technologies for removing CHCs from soil and groundwater.

In the past, laboratory and field studies showed nanoscale zerovalent iron (nZVI) particles as suitable material for removing CHCs. However, the application of this technology is still limited due to rapid particle corrosion and short longevity. There is an intensive effort to suppress nZVI corrosion and increase its longevity without negative effects on particle reactivity. Chemical modification such as sulfidation and recently also nitriding has been recognized as promising treatments to increase the particle longevity. Studies showed that FeS_x and Fe_xN mineral phases are formed during the chemical modification.

To further optimize chemical modification of nZVI, it is important to understand processes at surfaces at molecular scale. We built models of typical crystal surfaces of FeS_x and Fe_xN minerals detected in modified nanoparticles. They were used in modeling of interactions of CHCs molecules with these surfaces by using density functional theory method. In calculations, solvent effect was also included by using polarizable continuum model. Further, reaction paths of TCE dechlorination was explored by performing transition state calculations and molecular dynamics. We showed that the cleavage of the first C–Cl bond was the rate-limiting step for the dechlorination of CHCs at the γ -Fe₄N(001) surface, with the reaction barriers of 27.0, 29.9, and 40.8 kJ mol⁻¹ for TCE, PCE, and *cis*-DCE, respectively.

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

Investigating the late accretion history and convective homogenization of the terrestrial mantle – new perspectives from coupled Ru isotope and HSE abundance data

Jonas Tusch¹, Mario Fischer-Gödde¹, J. Elis Hoffmann², Carina Gerritzen³, Wolfgang Maier⁴, Martin Van Kranendonk⁵, Hugh Smithies⁶, Harry Becker², Carsten Münker¹

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The relative and absolute abundances of highly siderophile elements (HSE) present in the modern terrestrial mantle has been set during late accretion of meteoritic materials that the Earth received after cessation of core formation. In particular, the study of HSE abundances in komatiite melts that erupted between 3.5 and 2.9 Ga revealed the slow mixing of HSE-rich late accreted material into the terrestrial mantle and the progressive homogenization of primordial domains by continuing mantle convection.

Here, we report new Ru isotope and HSE abundance data for komatiitic rocks from the 3.46 Ga Dwalile greenstone remnant in the Kaapvaal Craton, SW Swaziland and from 3.5-3.2 Ga old komatiitic rocks from the Pilbara Craton, NW Australia. In contrast to ¹⁰⁰Ru excesses identified in 3.5-3.2 Ga old komatiites from the Pilbara, contemporaneous komatiites melts from Swaziland were found to have ¹⁰⁰Ru values indistinguishable from the modern mantle. Although HSE abundances in Dwalile komatiites show up to 2 times enrichment compared to primitive mantle estimates, the modern mantle-like Ru isotope composition of these rocks constrains that the Dwalile mantle source already fully equilibrated with the late accreted components by 3.5 Ga. These findings ultimately demonstrate that apparent HSE enrichments compared to the modern mantle may not necessarily reflect mass excesses of late accreted components. Therefore, our new data reveal that calculated HSE contents of mantle domains should be carefully interpreted with regard to the late accretion history of Earth and ideally combined with other sensitive tracers such as ¹⁰⁰Ru isotope systematics.

Lecture

Topic: 7.1 Geo-Biosphere interactions through space and time: new analytical and experimental approaches to the fossil record

Assessing diagenetic stability of enamel bioapatite oxygen isotope compositions by alteration in isotopically enriched tracer solution

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Oxygen isotope compositions in enamel bioapatite are considered as robust proxy archives for ingested drinking water, body temperature and physiology of fossil vertebrates. However, only few alteration experiments have tested this assumption.

Here we present the results of alteration experiments of dental tissues. Three mm-sized dental cubes, comprising both enamel and dentine, were cut from a modern African elephant molar and placed into acidic aqueous solution highly enriched in ¹⁸O (3.43 mols/mol%) and were reacted in sealed Teflon vials at temperatures of 30 to 90 °C for up to two months. The $\delta^{18}\text{O}_{\text{SIMS}}$ distribution across the reacted dental cubes were measured in-situ to determine the degree of bioapatite alteration via profiles with step distance as short as 20 μm .

In the 30 °C experiments only a few permil enrichment in $\delta^{18}\text{O}_{\text{SIMS}}$ occurred at the outer and inner enamel rim. In contrast, for 90 °C experiments enamel was strongly enriched (≈ 100 to 600 ‰) throughout the complete enamel transect, increasing with experimental duration. The ¹⁸O-enriched tracer solution penetrated the enamel and exchanged significant amounts of oxygen with all three different oxygen-bearing moieties PO₄, CO₃ and OH. Thus, even mm-thick mammalian enamel is susceptible to pervasive oxygen isotope alteration, including the PO₄-group, which is generally considered to be robust against abiogenic low temperature oxygen isotope exchange. This has implications for the reliability of enamel $\delta^{18}\text{O}$ values as palaeoclimatic and palaeoecologic proxy.

Lecture

Topic: 6.3 Fractionation of metal(loid) stable isotopes during low-temperature Earth surface processes

Are magnesium stable isotopes a valuable geochemical tool in agronomy?

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A sustainable use of soil resources is urgently required to cope with the increasing demand for agricultural products. Advanced soil cultivation methods like subsoiling were suggested but analytical tools to measure changes in the nutrient use efficiency of crops are still missing. Here we tested the applicability of Mg stable isotopes as novel evaluation tool in agronomy and validated our results with the nutrient uptake depth proxy $^{87}\text{Sr}/^{86}\text{Sr}$.

First, we conceptually demonstrated under which conditions changes in the Mg isotope composition ($\delta^{26}\text{Mg}$) of crops and the bioavailable fraction of Mg could be resolved from analytical uncertainty, when simulating subsoiling on soils with distinct Mg supply. Shifts in $\delta^{26}\text{Mg}$ values are only detectable if i) the crop uptake-related Mg isotope fractionation factor is high, ii) a high Mg uptake flux of crops faces a low Mg supply in soil, and iii) subsoiling causes a considerable deepening of the nutrient uptake depth.

Second, we tested our concept on field trials, where deep loosening with and without compost incorporation was conducted. Although $^{87}\text{Sr}/^{86}\text{Sr}$ indicates a deepening of the nutrient uptake depth after subsoiling with compost, shifts in $\delta^{26}\text{Mg}$ values of crops and the exchangeable fraction were mostly unresolvable from the analytical uncertainty. Yet, systematic shifts in $\delta^{26}\text{Mg}$ values among crops cultivated on and beside a melioration strip were found and attributed to the uplift of isotopically distinct compost-derived Mg. Still, Mg stable isotopes represent a valuable tool towards nutrient use efficiency measures on soils with low Mg supply, unless agricultural lime is applied.

Lecture

Topic: 8.4 Post-mining: Opportunities and challenges

Soil gas surveys for post-mining flooding monitoring

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A consequence of shutting down coal mines as it was done in Germany until 2018 is a rising mine water level posing the risk of possible mining damage. In the frame of the German BMBF funded project FloodRisk an interdisciplinary approach is applied to monitor such risks, in particular mine flooding induced seismicity. In this study geomechanical and geochemical methods were applied to detect active faults as a preparatory step for permanent mine flooding monitoring at the former German coal mine "Haus Aden". A selected section of a major normal fault in the area shows potential for critical stress indicating it as a preferred gas migration pathway. Short-term soil gas measurements showed correspondingly high concentrations of CO₂ and ²²²Rn. Both analysis results are a good indicator for a structurally controlled gas migration and thus evidence of the modelled fault outcrop. CH₄ which is normally the primary mine gas could not be detected, probably related to its oxidative decomposition with formation of CO₂. In the next step, selected gas sampling points will be equipped with new, low-cost, permanent gas sensors for long-term monitoring of potential post-mining induced seismicity.

Lecture

Topic: 11.2 Latest Achievements in Scientific Ocean and Continental Drilling

Cyclostratigraphic investigations with special emphasis on half-precession signals using XRF-data from ODP Site 663 (Eastern Equatorial Atlantic)

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The characteristics of half-precession (HP) cycles (~9,000 - 12,000 years) are still poorly understood, despite their appearance in numerous records. Previous studies on European terrestrial and marine records indicate a connection of the HP-signal to low latitudes. Consequently, we investigate HP-cycles in equatorial regions, which is the assumed origin of this signal.

Spectral analysis, evolutive approaches and correlation techniques are used on records from ODP Site 663 to identify the HP-signal in elemental ratios reflecting e.g. terrigenous input and/or bioproductivity. Filters that remove the classical orbital cycles (eccentricity, obliquity, precession) allow to isolate the HP-signal and to determine its temporal evolution.

We present first results of a larger project which has the overall objective to characterize the HP-signal during and beyond the Mid-Pleistocene Transition (MPT) at Site 663. The connection of (half-)precession to eccentricity implies a weaker influence of HP during the MPT, as the major driver of climate forcing during this period is the 41-kyr obliquity cycle. Further objectives of the investigations will be to link the orbital patterns of Site 663 to terrestrial records, e.g. from the ICDP project on Lake Bosumtwi (Ghana). This will contribute to a better understanding of paleoenvironmental processes in Equatorial Africa.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Hydrothermal alteration of pyrochlore from carbonatite: An experimental study

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Niobium is a critical metal used in various superconducting materials and alloys. It is predominantly mined from ores rich in pyrochlore-group minerals with the general formula $A_2B_2O_6Y$ ($B \geq 50\%$ Nb). Fluorcalciopyrochlore, $(Ca,Na)_2Nb_2O_6F$, is considered as primary magmatic pyrochlore. However, metasomatism by hydrothermal fluids, amongst other processes, can lead to a wide range of chemical compositions (Mitchell 2015). Different stages of pyrochlore alteration were assigned to specific p-T-ranges using associated minerals in the host rock ores. Enrichment in Ba for example is documented in low-temperature hydrothermal environments (Lumpkin & Ewing 1995).

However, it is difficult to unravel the role of temperature, pressure, fluid composition or time in alteration processes of primary fluorcalciopyrochlore in natural carbonatite systems. Therefore, alteration experiments using an autoclave are necessary to identify and quantify alteration mechanisms. To our knowledge, such experiments have only been conducted for microlite and betafite (Geisler et al. 2005), but not for pyrochlore *sensu stricto*.

Hence, we studied the interaction of natural fluorcalciopyrochlore with Cl-rich, acidic hydrothermal fluids of varying composition in teflon-lined hydrothermal reactor vessels at 200 °C. Here we will present preliminary results of our experiments and discuss consequences of hydrothermal alteration of pyrochlores, with application to Nb-rich carbonatite ores.

R. H. Mitchell, *Ore Geology Reviews*, 64, 2015; G. R. Lumpkin & R. C. Ewing, *American Mineralogist*, 80, 1995; T. Geisler et al., *American Mineralogist*, 90, 2005

Lecture

Topic: 8.1 Geosciences and Waste Management

Mineralogy and Leaching of Steel Slag (BOF/LD/Converter steel slag)

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Integrated steelworks produce steel from iron-ore. Co-produced are vast amounts of slags in the Blast Furnace process (~200-250 kg slag/ton of metal) and Basic Oxygen Furnace (BOF) process (~100 kg slag/ton of steel). Whereas BF-slag is in high demand for cement use, BOF-slag addition to cement doesn't create synergy, despite mineralogical similarity.

BOF slag mineralogy can be predicted using thermochemical modelling for the multicomponent system CMAFfSP, using FactSage, and petrological observations of BOF slag confirm phenocrysts of Magnesio-Wuestite (Liquidus-phase) followed by alpha-C₂S, in a groundmass of co-crystalizing Wuestite, Srebrodolskite (C₄AF), C₂S and lime. Incorporation of minor constituents (Ti, V, Cr) occurs in Wuestite (Cr) and C₂S (V) and C₄AF (V, Ti), but cannot be predicted for lack of solid solution models. Cr and V can cause leaching concerns for slag applications.

Studying hydration reactions on finely ground BOF slag indicates that hydrogarnet, hydrotalcite, portlandite and CSH-gel tend to form as product and that all primary slag phases contribute in the reaction. The leaching of Vanadium is pH-controlled during C₂S dissolution.

Application of BOF slag as secondary raw material requires adequate characterization. Grinding BOF slag to cement-fineness can produce a high-strength binder, however, requiring the aid of specific additives.

C=CaO; M=MgO; A=Al₂O₃; F=Fe₂O₃; f=FeO; S=SiO₂; P=P₂O₅; C₂S=Ca₂SiO₄

Lecture

Topic: 5.1 The co-evolution of Earth's atmosphere, oceans, and life from the early Archean until today

Stromatolites trace metal availability in microbial habitats of the Miocene hypersaline lagoon in the Oberpullendorf Basin, Austria

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Stromatolitic carbonates formed in ancient microbial mats and provide unique geochemical archives to reconstruct palaeo-environments of microbial life. In this study, we report C-O isotopes and trace metal concentrations of Miocene stromatolites from the Oberpullendorf Basin (Austria) that were formed during the Badenian salinity crisis at the north-western coast of the Paratethys Sea. The combined approach of trace element data with C-O isotopes of individual stromatolite laminae is used to reconstruct short-term variations of palaeo-environmental conditions in microbial habitats.

Stromatolitic carbonates in the lower units show negative $\delta^{13}\text{C}_{\text{carb}}$ values and typical seawater-like shale-normalized rare earths and yttrium (REY_{SN}) patterns with positive La_{SN} , Gd_{SN} anomalies, super-chondritic Y/Ho ratios, and heavy REY_{SN} enrichments to light REY_{SN} , indicating an open marine depositional setting. Stratigraphic upwards, stromatolitic carbonates show suppressed seawater-like REY_{SN} signatures and increasing $\delta^{13}\text{C}_{\text{carb}}$ values that reflect the development of a restricted environment. Seawater-like REY_{SN} patterns and homogeneously distributed negative $\delta^{13}\text{C}_{\text{carb}}$ values in the stratigraphic uppermost part resemble the transition to fully marine environmental conditions again. Enrichment factors of bio-essential elements (Fe, Mn, Co, Zn, Mo, W) reflect sufficient element availability during marine conditions but continuous limitation during the development of the (semi)closed lagoon.

We show that this approach may provide the groundwork for a better understanding of the evolution and development of microbial metabolisms under severely different atmospheric-hydrospheric conditions on planet Earth and beyond.

Poster

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

What does the temperature dependent magnetic susceptibility tell us about the depositional history of Lake Bosumtwi (Ghana)?

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Lacustrine archives may provide valuable point-data for studying past climatic and environmental changes. Lake Bosumtwi (Ghana) is of special interest as it recorded such oscillations throughout the last 1.07 million years in a potential key region of human evolution during this period. The prominent climatic- and environmental sensitivity of this geo-archive can be explained by its location on the interface of competing climate agents such as the Hamattan (hot and dusty winds from the Sahara) and the North African Monsoon both being dependent on the Intertropical Convergence Zone. These impacts may translate into diverse and complex ways regarding geo-scientific proxy data. In this context, the temperature dependent magnetic susceptibility $k(T)$ is promising to reflect magnetic-mineralogical changes that may indicate oscillating climatic and diagenetic effects and dust input. To better constrain the effects of all potential affecting parameters, we test a multivariate approach on the last glacial part of Lake Bosumtwi that integrates $k(T)$, the room temperature magnetic susceptibility, its frequency dependency and gamma ray logs. This approach is promising to increase our understanding of all parameters and their interdependency. Thus, we aim to shed new light on the relationship between $k(T)$ and the depositional history of Lake Bosumtwi.

Lecture

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

High relative humidity in the hyper-arid late Miocene Atacama Desert quantified by triple oxygen and hydrogen isotopes in gypsum

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³Departamento de Ciencias Geológicas, Universidad Católica del Norte, Chile

In the Chilean Atacama Desert, alternation of lacustrine evaporites and diatomites suggest that hyper-aridity has prevailed since the early Miocene, but was interrupted by recurring pluvial phases. Changes in lacustrine deposition, however, can be either climate- or tectonically-driven, which challenges a unique interpretation. Here, we demonstrate that an isotope model-data approach combining triple oxygen and hydrogen isotope data of paleo-lake water derived from gypsum hydration water with the Craig-Gordon evaporation model can provide quantitative information on local hydroclimate conditions in the past Atacama Desert.

We analyzed the isotope composition ($\delta^{17}\text{O}$, $\delta^{18}\text{O}$, $\delta^2\text{H}$) of structurally bonded water extracted from lacustrine and marine gypsum deposits in the Atacama Desert of Late Miocene and Pleistocene age, respectively. We used a Monte Carlo simulation to obtain the best-fit solution of input variables of the Craig-Gordon equation – notably, relative humidity, the isotope composition of source water and atmospheric water vapor – through isotope data of multiple gypsum samples from a single unit of the paleo-lacustrine formations. Gypsum ages were obtained by U-Pb dating.

Our results demonstrate that a generally more humid climate persisted over northern Chile 8.9 Ma ago, caused by distal vapour advection with significant rainout along the vapour advection pathway. The regional atmospheric circulation likely changed as a result of an overall weaker sub-tropical subsidence over the Miocene SE Pacific Ocean. Marine lagoon gypsum with an age of 1.8 ± 0.2 Ma were deposited under near-similar hyper-arid conditions in comparison to the present-day coastal climate.

Ramdohr-Poster

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

Transformation Processes and Kinetics in the Magnesium Phosphate Mineral System

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Phosphorous is an important nutrient for all living beings. Together with nitrogen, it is a crucial element for the global agriculture, yet it is a limited natural resource. The mineral struvite ($\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$) occurs in guano deposits, wastewater pipelines, and pathogenic urinary stones. It's recovery and reutilization as a slow release fertilizer has become a common process in wastewater treatment. However, it's instability under atmospheric conditions leads to transformation to other phosphate phases, a process that is still poorly understood.

We investigated this transformation by reacting synthetic, μm - and mm -sized struvite crystals at different temperatures in open and closed systems. We monitored the transformation of struvite with time using ex-situ X-ray diffraction (XRD) and processing with Rietveld refinement. Complementary, transformations of mm -sized crystals were investigated by imaging with optical and scanning electron microscopy and by analysis with Raman spectroscopy.

XRD analysis shows that struvite transforms to newberyite ($\text{Mg}(\text{PO}_3\text{OH}) \cdot 3\text{H}_2\text{O}$) at room temperature over several weeks by losing water and ammonium. Optical microscopy reveals newberyite as opaque, white or dark brown patches, inside crystals and at crystal sides. At elevated temperatures (37 and 60 °C), struvite predominantly transforms to dittmarite ($\text{MgNH}_4\text{PO}_4 \cdot \text{H}_2\text{O}$) with newberyite as minor product, indicating a temperature-driven loss of water that is faster than ammonium loss. The presence of newberyite and dittmarite was confirmed by Raman spectroscopy. Transformation rates of both the open and closed system were evaluated. These findings are important to understand long-term processes that may influence the properties of wastewater-derived struvite as slow-release fertilizer.

Lecture*Topic:* 1.2 Methods in Geochemistry and Mineralogy**Isotopic compositions and functional chemistry of meteoritic organic matter revealed by high spatial resolution mass spectrometry – synchrotron spectroscopy – electron microscopy techniques****Christian Vollmer¹, Jan Leitner^{2,3}, Charlotte L. Bays⁴, Ashley J. King⁴, Paul F. Schofield⁴, Tohru Araki⁵, Aleksander B. Mosberg⁶, Demie Kepaptsoglou⁶, Quentin M. Ramasse⁶, Peter Hoppe²**¹Institut für Mineralogie, Universität Münster, Germany; ²Max-Planck-Institut für Chemie, Mainz, Germany; ³Institut für Geowissenschaften, Universität Heidelberg, Germany; ⁴Planetary Materials Group, Natural History Museum, London, UK;⁵Diamond Light Source, Didcot, UK; ⁶SuperSTEM Laboratory, Daresbury, UK

The isotopic and chemical properties of organic matter (OM) in extraterrestrial samples record a combination of presolar, nebular, parent-body, and terrestrial processes, which can be disentangled by high-spatial resolution studies [e.g., 1]. These studies have the advantage that they also allow for analysis of the petrographic relationship to the matrix and require only minimal chemical treatment. Here we have investigated OM properties within two recent observed falls, Tarda and Winchcombe, by combined “in-situ” techniques. Carbon and nitrogen isotopic compositions were studied by NanoSIMS. OM was sectioned by the focused ion beam (FIB) technique (Hitachi Ethos NX5000). Scanning Transmission X-Ray Microscopy (STXM) was performed at the I08 beamline of Diamond Light Source. Low-kV electron energy loss spectroscopy (EELS) in the vibrational and core loss regimes was performed with a monochromated, aberration-corrected Nion UltraSTEM 100MC. Nitrogen and carbon isotopic compositions of OM aggregates and nanoglobules in Tarda show a range of $\delta^{15}\text{N}$ values from close-to-terrestrial to $\sim 600\text{‰}$ with close-to-terrestrial or slightly heavy $\delta^{13}\text{C}$ values. Single hotspots reach $>1000\text{‰}$ in $\delta^{15}\text{N}$ and $\sim 80\text{‰}$ in $\delta^{13}\text{C}$, but no negative $\delta^{15}\text{N}$ values similar to Maribo OM have been detected [2]. STXM analyses at the C K-edge show that OM in Winchcombe is typical for OM in primitive meteorites, with strong absorption at the aromatic C=C (~ 285 eV) and the ketone/aldehyde (~ 286.6 eV) bands. The presence of reactive double and triple C-N bonding is a strong indicator that some OM is still pristine.

[1] Van Kooten et al. GCA 2018, [2] Vollmer et al. SciRep 2020.

Lecture

Topic: Frontiers in Mineralogy Talk

How rock weathering sets Earth's thermostat

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Since its formation 4.5 billion years ago our blue planet contains liquid water at its surface. If all water were frozen as on our cold neighbour Mars, or if all water had disappeared into space as on hot Venus there would be no life on Earth. We owe Earth's habitability to the weathering feedback, balancing volcanic CO₂ additions from Earth's interior by CO₂ drawdown through silicate weathering, stabilising the greenhouse effect.

The isotope ratios in seafloor sediment show that this balance has shifted in the last 15 million years. According to ¹⁸O/¹⁶O it got colder, eventually leading to the northern hemisphere glaciation. ¹¹B/¹⁰B discloses that atmospheric CO₂ decreased, resulting in cooling by a reduced greenhouse effect. The cause of decreasing CO₂ is subject of a lively debate. One view holds that the rise, erosion, and increased weathering of mountain belts increased CO₂ drawdown. The other suggests constant weathering fluxes, as indicated by the ratio of the cosmogenic isotope ¹⁰Be rained out from the atmosphere to the stable isotope ⁹Be released from rocks by weathering (¹⁰Be/⁹Be). With a land surface that got increasingly more "weathering reactive" by geologic reworking, atmospheric CO₂ concentration would decrease even if CO₂ input and drawdown flux remained constant and balanced. Stable ⁷Li/⁶Li indeed confirms such change in the properties of the land surface in the past 15 million years.

Today a dramatic shift is imminent, because humans are massively interfering with this delicate balance through industrial CO₂ emissions, an experiment that better be discontinued fast.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Is it possible to date baddeleyite (ZrO₂) with the same precision as zircon (ZrSiO₄) with CA-ID-TIMS?

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Zircon (ZrSiO₄) is the most used mineral in geochronology. Recent methods let to date zircon with precision of 1-2% error (Schaltegger et al., 2015) by SHRIMP/SIMS (high-resolution ion microprobe/secondary ion mass spectrometry) and LA-ICP-MS (laser ablation inductively coupled mass spectrometry) with a precision of 1-3.2% (Sundell et al., 2021). In comparison to other methods, CA-ID-TIMS (chemical abrasion isotope dilution thermal ionization mass spectrometry) enables to date zircons with very high precision of only 0.1% error (>10 times more precise than other methods). Zircon cannot be always used for dating, because not all rocks have zircon in their composition. For example, carbonatites do not always contain zircons, but they contain baddeleyite, which also can be applied as a geochronometer. SHRIMP/SIMS and LA-ICP-MS are fast and inexpensive methods used to date different minerals, including baddeleyite. However, the precision of these methods is not adequate to define a sequence of magmatic intrusions. CA-ID-TIMS dating uses a standard chemical abrasion procedure (CA), which was developed especially for zircon and cannot be applied for baddeleyite. Therefore, the CA method must be adjusted for baddeleyite before the dating is possible.

Rioux et al. (2010) designed numerous experiments to adjust chemical abrasion procedures for baddeleyite dating and achieved some positive results. However, the same effective method of treatment for baddeleyite as for zircon has not yet been developed. In this study, we present the first results of experiments with baddeleyite. We significantly reduced the effect of Pb-loss and increased measurement precision to the values of zircon (0.1%).

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Highly siderophile elements reveal ancient subarc mantle beneath the South West Indian Ridge at Marion Rise

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The ultra-slow spreading South West Indian Ridge (SWIR) near Marion Rise comprises segments of thin crust and abundant abyssal peridotites exposed near the ridge axis. Zhou and Dick (2013) proposed that buoyant depleted mantle beneath the SWIR may represent Proterozoic melting residues recycled from Gondwana lithosphere, resulting in excess buoyancy at Marion Rise. In order to test this hypothesis, serpentinized harzburgites, dunites and scarce lherzolites were dredged and sampled by remotely operated vehicle along SWIR (36°54.0' E to 39°13.5' E) during expedition SO 273 in 2020. The major and trace element compositions of the peridotites (Mg# = 0.90-0.92) are similar to other depleted abyssal peridotites and mostly lack visible clinopyroxene. Here, we present new highly siderophile element (HSE) mass fraction and Os isotopes, that constrain the time of melt extraction, style of mantle melting and melt transport. Low HSE abundances (Ru = 0.07-0.3x primitive mantle) coupled with strongly fractionated HSE patterns (high Ru/Os, Ir/Os, Ru/Re) in studied peridotites exposed at normal faults suggest higher melting degrees than in most abyssal peridotites elsewhere. The HSE patterns are similar to those in harzburgites and dunites from ophiolites, interpreted to reflect sub-arc mantle lithosphere that was depleted by flux melting above subduction zones. Measured ¹⁸⁷Os/¹⁸⁸Os range between 0.119 and 0.142, possibly reflecting melt depletion at 1.4 Ga and interaction with sulfide-undersaturated melts or fluids with suprachondritic ¹⁸⁷Os/¹⁸⁸Os. The data provide evidence for locally strong depletion of mantle rocks at Marion Rise and the occurrence of ancient subarc mantle underneath a modern oceanic ridge.

Lecture

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Processes and “rates” of pedogenesis across a Late Quaternary chronosequence dated by in situ cosmogenic ^{10}Be – a case study from the coastal Atacama Desert (N Chile)

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Studies on soil formation under hyperaridity have so far focussed on the hyperarid core of the desert. Although the coastal sector of the Atacama Desert receives much larger amounts of moisture due to the orographic blocking of fog by the Coastal Cordillera, neither the pedogenic processes nor the timescales on which the coastal soils formed have as yet been studied. We therefore assessed physical and chemical soil parameters across a chronosequence of a coastal alluvial fan at Paposo, which is composed of four morphostratigraphic units. From each surface generation, we sampled four shallow soil profiles and multiple boulders for exposure dating using in situ cosmogenic ^{10}Be . The combined establishment of a pedostratigraphy and morphochronology allows us to indirectly assess rates of soil formation and to make use of a soil catena as an unprecedented palaeoenvironmental archive for the Atacama Desert.

Physicochemical soil properties mostly exhibit monotonic relationships with increasing time since abandonment of the first fan surface in the early Late Pleistocene. Pedogenic processes and weathering result in a loamification reflected in the soil texture by continuous fining with age. In contrast to typical Aridisols, trends towards desalinization as well as complete decalcification become apparent. Moreover, spectrophotometric soil colour measurements as well as the content of pedogenic iron oxides indicate that rubification plays a major role in the pedogenesis under coastal hyperaridity. Significant effects of biotic activity become apparent in organic carbon and phosphorus contents. Eventually, the results provide strong indications for in situ formation of clay-sized particles and colloids.

Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

Deciphering the Gypsum - Anhydrite Phase Transition in the Atacama Desert

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Present as gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$), bassanite ($\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$) and anhydrite (CaSO_4), calcium sulphates comprise a significant fraction of the surface and soil in the Atacama Desert.

Field observation suggest a secondary formation process for the dehydrated sulphates

These thermodynamically predicted phase transitions were ruled out by previous studies to occur by heating under ambient conditions of the Atacama Desert or by suppressing the water activity with simplified brine-solutions^[1]. Furthermore, high induction times for nucleation hampers anhydrite growth.

Recent studies^[2,3] have shown that precipitation of anhydrite can be achieved in flow-through reactors at room temperature even with high water-activity ($a_w = 0.98$).

Results from our own flow-through experiments with gypsum seeded with anhydrite under a variety of temperatures and salinities contradict the notion that the production of anhydrite is a consequence of simple hydrological factors. It appears essential to gain a deeper understanding of catalytic processes that stabilize anhydrite nuclei.

Possible responsible catalysts could be of ionic, nano-particulate or organic nature. The effects of these catalysts have been studied in the literature extensively^[4] and especially nanoparticles and ions from soluble salts are abundant in Atacama Desert sediments.

We show results from experiments performed on natural and synthetic samples that systematically explore the domains of solution flow, ionic contamination and nanoparticles.

[1] Ossorio, M., et al., Chemical Geology 386 (2014): 16-21.

[2] Dixon, E., et al., Journal of Geophysical Research: Planets 120.4 (2015): 625-642.

[3] Miller, Kayla., (2017).

[4] Cody, R. D., and A. B. Hull., Geology 8.10 (1980): 505-509.

Lecture

Topic: Frontiers in Mineralogy Talk

Applied mineralogy for sustainable use of materials

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Adapting nature offers a wide variety of opportunities to create advanced materials in the laboratory that find their templates in natural minerals. Materials, which are nowadays gaining increasing importance, are mainly those related to economically, environmentally and socially sustainable processes. Minerals and their synthetic counterparts are used, for instance, for purification processes, energy conversion and storage materials, or as bio-inspired materials with structures and properties mimicking those of natural materials.

One example of a success story in which minerals provide the original for synthetic materials used on a large scale is zeolites. Natural zeolites, microporous aluminosilicates, are mostly formed in volcanic rocks by a hydrothermal transformation of e.g. volcanic ashes at low temperatures and almost without pressure. The formation conditions may sound relatively simple but the reconstruction of synthetic zeolite analogues is much more complex than might have been expected at first. The fascinating crystal structures with different channel and pore architectures have opened a wide field of technical applications. Both natural and synthetic representatives are used on a large scale in industry and agriculture. Zeolites are utilized as absorbers for water purification, gas-cleaning processes and catalysis. For the understanding of their physical and chemical properties, detailed information about formation conditions and crystal structures is essential.

The profound knowledge of minerals, their synthesis, crystal chemistry and characterization methods makes applied mineralogy and crystallography indispensable disciplines in the development of new and exciting materials for sustainable processes.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Geobiological significance of organic matter preserved in 3.5 Ga hydrothermal barites from the Dresser Formation (Pilbara Craton, Australia)

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3.5 billion-year-old bedded barite of the Dresser Formation (Pilbara Craton, Australia) contains abundant primary fluid and solid inclusions. The fluid inclusions contain volatiles like H₂S, COS, and CS₂, as well as simple organic compounds (e.g., acetic acid, organic polysulfanes, thiols) [1]. As the bedded barite may have been formed from hydrothermal fluid discharge into an evaporitic caldera [2], these compounds could have acted as fertile substrates for early life forms thriving in this environment [1]. The solid inclusions consist of minerals (metal sulfides, carbonates, silicates) and insoluble organic matter (kerogen) [1,3; this study]. The latter are analysed in greater detail here. High-resolution Raman mapping and microscopy revealed three populations of kerogen inclusions based on their location in the barite deposit: (i) inclusions at the edges of single growth zones of barite crystals, (ii) inclusions within barite crystals, and (iii) inclusions in secondary quartz veins. Peak metamorphic temperatures for these three kerogen populations were determined using Raman spectroscopy. Near edge X-ray absorption fine structure (NEXAFS) measurements revealed a highly aromatic nature of the kerogen. Taken together, the combination of various analytical techniques provides valuable insights into the nature and origin of organic matter in the 3.5 Ga old barites, which significantly advances our understanding of some of Earth's most ancient habitats.

[1] Mißbach, H. et al. (2021), Nat. Commun. 12, 1101

[2] Van Kranendonk, M.J. (2006), Earth Sci. Rev. 74, 197–240

[3] Philippot, P. et al. (2007), Science 317, 1534–1537

Lecture

Topic: 4.1 Magmas and Fluids in the Crust

Constraining the heat transfer from convecting upper-crustal magma reservoirs to hydrothermal fluid flow systems

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Heat transfer through the upper crust is primarily controlled by magma flow, heat conduction and hydrothermal fluid flow. The interplay between magma and fluid flow processes is essential for geothermal systems, ore formation and volcanic processes, but is not well constrained due to a lack of accessibility. We developed a coupled numerical model that can resolve both magma and hydrothermal flow to quantify the influence of magma convection and rock permeability on heat transfer. The results demonstrate how magma convection enhances the energy transfer towards the magma-hydrothermal interface, leading to an accelerating effect of up to 15% on the cooling of the reservoir. However, at high brittle-ductile transition temperatures and high host rock permeabilities, magma flow can also prevent efficient permeability creation and entrainment of hydrothermal fluids at the edges of the reservoir, leading to a secondary decelerating effect on the cooling rate. Using different initial melt compositions (basaltic to rhyolitic), our numerical simulations can further constrain the varying timescales of magma evolution from shorter-lived, lower-crystallinity convecting magma reservoirs to longer-lived, higher-crystallinity magma mushes where convection has seized.

Poster

Topic: 6.1 Earth surface processes in extremely water-limited environments

A 16 ka record of high-amplitude precipitation events from the southern part of the hyperarid Atacama Desert.

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The Atacama Desert in Chile is known to be one of the driest deserts on Earth, with dominating hyperaridity since the Miocene. During recent times, however, especially the southern part of the Atacama repeatedly experienced exceptional precipitation events, like in 2015 and 2017. Locally, these events with rainfall rates of >50 mm within 48 hours caused catastrophic floods with significant destruction and human fatalities. Although the meteorological drivers of these heavy rains are widely understood, only little is known about the frequency and amplitude of similar events on geological timescales.

Here we present the results of a study in an endorheic claypan from the southern edge of the hyperarid core of the Atacama, an area with mean annual precipitation of 5 mm/a. A modern ground-truthing approach applying remote-sensing and meteorological as well as climate-modelling data indicate that during the past 30 years, the claypan reacted very sensitive to local precipitation, with events >20 mm of rain causing sufficient surface run-off in the catchment to partially flood the basin. A short sediment core recovered from the center of the claypan covers approx. the past 16,000 years. First sedimentological, mineralogical, and geochemical findings imply strong variations in the amplitude of the recorded precipitation events over time, with a clear shift from more intense to lower-amplitude events from the late Pleistocene to the Holocene. The results of the study shed new light on the glacial-interglacial precipitation variability in the Atacama Desert and its driving mechanisms.

Lecture

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

GlobaLID – a community-driven global lead isotope database with interactive web application

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Lead isotopes are the most universally used method to reconstruct the raw material origin of archaeological objects made of lead, silver, copper, gold and their alloys, but also are routinely applied in e.g. ore deposit geology and environmental geochemistry. For all research utilising lead isotope signatures, a comprehensive compilation of existing reference data is essential. GlobaLID, a FAIR global ore lead isotope database coupled with an interactive web application, was set up as an open access repository and visualisation tool. The database was enriched by locally versed contributors with meta-information on geography, mineralogy, geology, metallogeny and analytical set-up of the original published data to allow their utilisation for a diverse range of research topics. The web application primarily serves the visualisation of the database. Different options for screening, filtering and plotting of the data are available, including the possibility to upload and plot user data and automatically match them to GlobaLID's database.

A first version of the database and prototype of the web application were launched in late 2021. Feedback from the scientific community identified major issues to tackle in the on-going work on GlobaLID, e.g. the complete standardisation of revised datasets, the possible integration of further data and material types, and the additional implementation of statistical tools. The core team will create and implement a common standard for these tasks together with other researchers. Our presentation will first highlight GlobaLID's most important features and subsequently present plans for its future development as a community-driven project.

Lecture

Topic: 2.1 Changes of solid Earth's processes through deep time

Mantle melting, mineralogy and (maybe) magma oceans: the metal stable isotope perspective

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Many studies of high- μ stable isotope systems (e.g., Mg, Si, Fe, Ni, Zn, Ti, Ca, Cr, V) in terrestrial magmatic rocks and silicate achondrite meteorites aim to link equilibrium mineral- and redox-specific stable isotope partitioning (equilibrium fractionation) effects with observed variations in isotopic composition, with the objectives of reconstructing the chemistry, mineralogy and redox state of their mantle source regions. In this presentation, I will discuss how these stable isotope systems can be used in conjunction with phase equilibria models to predict the coupled behaviour of different isotope systems during partial melting of different mantle lithologies under different conditions, and the implications for using these isotope systems to reconstruct the mineralogical and chemical evolution of planetary interiors.

Soderman, C. R., Matthews, S., Shorttle, O., Jackson, M. G., Ruttor, S., Nebel, O., ... & Williams, H. M. (2021). Heavy $\delta^{57}\text{Fe}$ in ocean island basalts: A non-unique signature of processes and source lithologies in the mantle. GCA

Soderman, C. R., Shorttle, O., Matthews, S., & Williams, H. M. (2022). Global trends in novel stable isotopes in basalts: Theory and observations. GCA

Poster

Topic: 6.3 Fractionation of metal(loid) stable isotopes during low-temperature Earth surface processes

Evolution of fluid flow and carbonate recrystallization rates in deep-sea sediments of the Equatorial Pacific

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Fluid flow and carbonate recrystallization rates were determined for deep-sea sediments from the Equatorial Eastern Pacific (IODP Exp. 320/321) using $\delta^{44/40}\text{Ca}$ values of pore water and corresponding sediments. The drill sites are located along a transect of decreasing crustal age, showing different characteristic geochemical pore water depth profiles. An overall isotopic equilibration with the sediment in the upper part of the sedimentary column can be identified, while in the lower part of these Sites, the $\delta^{44/40}\text{Ca}$ of the pore water increases back to seawater-like values at the sediment/basalt interface, forming a bulge-shaped pore water profile. The magnitude of this bulge decreases with increasing age of the oceanic crust and sediment cover, resulting in seawater-like $\delta^{44/40}\text{Ca}$ -porewater values throughout the whole sedimentary column of the oldest two Sites. These findings indicate that after sedimentation carbonate recrystallization processes start to enrich the pore water in ^{40}Ca with a subsequent input of a seawater-like fluid from the underlying crust into the sediment. After a time of carbonate recrystallization and cooling of oceanic crust, a flow of seawater-like fluid starts to move through the sedimentary column, shifting porewater back to seawater-like $\delta^{44/40}\text{Ca}$. We established a carbonate recrystallization and fluid flow model to quantify these processes. Our determined carbonate recrystallization rates indicate that the fluid flow within the investigated sites of IODP Exp. 320/321 depends on the sedimentary composition and location of the specific site, especially the proximity to a recharge or discharge site of a hydrothermal convection cell, which form the so-called 'hydrothermal siphon'.

Poster

Topic: 8.3 Archaeometry - tracing the past human footprint with geosciences

The Origin and Relationship of Bronze Blades from the “Sögel-Wohlde-Kreis” – a holistic (Isotope-) Geochemical Approach

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Determining the origin of archaeological bronzes and their metal sources is one of the great desiderata of archaeologists. Answering these questions is often difficult with archaeological and typological methods alone, which is why isotope and elemental compositions of metals have since become important components. While the methods for the analysis of copper are more or less straightforward, determining the origin of the tin sources is still limited. However, owing to the high inter-deposit variations of Sn isotope compositions, their analysis alone is not a reliable tool for determining the origin of tin in bronzes. Due to this fundamental limitations, recent works pursued a multi-isotope approach with Pb, Cu and Sn isotopes coupled with trace elements in two case studies searching for evidence of source mixing and/or recycling. This is beyond the mere proving for sources, which in turn may help to reconstruct relationships between artefacts of different origins and reveal cultural and trade networks. The approach is now investigated on a much larger scale in our recent project. For this, about 300 blades of the Sögel and Wohlde type from the Nordic Early Bronze Age are to be isotopically and chemically analysed and compared with counterparts in southern central Europe and south-eastern Europe. Ultimately, the origin of the artefact types, their metal sources and their socio-economical entanglements will be disclosed, but at the same time a critical evaluation of analytical data will be undertaken against the background of metal/ore mixing and recycling.

Lecture

Topic: 6.2 Rates and Dates of Earth Surface processes: Methods & Applications

Denudation and weathering rates of carbonate lithologies from meteoric $^{10}\text{Be}/^9\text{Be}$ ratios

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During the past decades, cosmogenic nuclides, such as in-situ produced ^{10}Be , evolved as state-of-the-art tool to quantify millennial-scale denudation in quartz-rich landscapes. However, applications of cosmogenic nuclides to carbonate-dominated lithologies are still rare, even though carbonate dissolution is a major weathering process that may compensate anthropogenically elevated CO_2 levels over centennial-millennial timescales.

Recent advances in quantifying carbonate erosion have been made using cosmogenic ^{36}Cl and of carbonate weathering using dissolved loads (e.g.^{[1],[2]}). As these integrate over two distinct time-scales we developed a method that records such rates simultaneously: the cosmogenic meteoric ^{10}Be over ^9Be ratio ($^{10}\text{Be}/^9\text{Be}$). We adapted a framework^[3] combining a known atmospheric flux tracer, meteoric ^{10}Be ($T_{1/2}=1.4$ My), with stable ^9Be , a trace released from rocks by weathering, to the limestone-dominated French Jura Mountains. We analyzed water, soil, sediment, and bedrock for $^{10}\text{Be}/^9\text{Be}$, major/trace elements, and Sr and C isotopes, to quantify i) Be contribution from carbonate vs. silicate minerals and ii) from primary vs. secondary carbonate phases, iii) solid-solute load partitioning, and iv) deep (sediment) vs. surficial (soils) weathering and erosion. Our results indicate average denudation rates of $300 \text{ t/km}^2/\text{yr}$, denudation being dominated by weathering flux (W/D ratios of 0.7-0.97), and a consistently higher contribution from deep weathering. These rates agree to decadal-scale denudation rates from combined suspended and dissolved fluxes within $< 2x$ which highlights the great potential of this method for future Earth's surface studies.

^[1]Ott et al., JGR-ES, 2019.

^[2]Ben-Asher et al., GSA-Bull., 2021.

^[3]von Blanckenburg, F, Bouchez, J. and Wittmann, H., EPSL, 2012.

Lecture

Topic: 2.2 From dust to planets

Constraining Volatile Element Loss Processes by Germanium Isotopic Investigations of Iron Meteorites

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The concentrations of Ge and other moderately volatile elements (MVE) in iron meteorites vary by orders of magnitude, however, the origin of these variations is poorly understood and nebular as well as planetary processes have been proposed. To better constrain the origin(s) and process(es) of MVE depletion among planetary bodies, we measured the Ge concentrations and mass-dependent Ge isotopic compositions of a set of iron meteorites, using a newly developed Ge double-spike technique.

In total, three IAB, four IC, eight IIAB, five IID, nine IIIAB, and one IIIE iron meteorites were investigated. The Ge concentrations are consistent with reported literature data and range from ~35 ppm for the IIIAB meteorites up to >300 ppm for the IAB irons. The Ge stable isotopic compositions of the analyzed samples, including the first Ge isotopic data for IC, IID, IIIAB, and IIIE irons, are relatively uniform ($\delta^{74/70}\text{Ge} \approx 1$). There is no resolved within-group variability for most of the investigated groups. Only the IID and IIIAB irons seem to show some internal variability which, however, is neither attributable to fractional crystallization nor to cosmic ray exposure effects. Despite large variations of Ge concentrations, the different iron meteorite groups lack significant Ge isotopic variations among each other, but such variations would be expected for simple evaporative loss of Ge during magma degassing. As such, the new data for magmatic irons do not seem to support the idea that the volatile-depleted nature of their parent bodies is the result of planetary processes.

Lecture

Topic: 8.1 Geosciences and Waste Management

Treatment of metallurgical by-products for metal winning and use as construction material

Christoph Wölfler

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Every year, millions of tons of by-products from the metal producing industry are dumped as waste and this amount is continuously rising. A competence network, involving Montanuniversität Leoben and seven international partners from industry, was formed to treat this topic. The project "COMMBY- Competence network for the assessment of metal bearing by-products" consists of three areas: characterisation and evaluation, process development and optimisation, as well as the development of an evaluation procedure for secondary resources.

Among other metallurgical by-products, special attention is paid to the slags generated during lead production. After metallurgical treatment for metal winning, the newly produced slag is evaluated for being used as construction material. Contrary to other approaches, in which these are used as cement substitutes, the focus lies on the substitution of sand. One advantage over the use as cement substitute is the larger particle size and the resulting improvement in eluate values. To achieve this, one possibility is to modify the basicity and investigate its effect on the enclosing behaviour of the slag with respect to environmentally critical compounds such as ZnO and PbO. After evaluating the best conditions for slag production, next steps will include the determination of the optimal amount of sand being replaced by slag without negative impact on the mechanical and chemical properties of the concrete.

Poster

Topic: 1.2 Methods in Geochemistry and Mineralogy

The chemical composition of basaltic and anorthositic lunar soil samples determined by ICP-MS

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Using quadrupole ICP-MS, we determined the chemical composition of five basaltic Apollo 12 and six anorthositic Apollo 16 soil samples, the cataclastic lunar anorthosite 60015 and the reference samples BHVO-2 and AN-G.

The aim was to evaluate the processes affecting soil compositions and to provide data that allows for accurate spike additions for isotope dilution analyses of volatile elements and double-spike Cd isotope analyses, while consuming only a few mg of precious sample powder. Of the 56 elements analyzed, Ta, W and Bi for BHVO-2 and Be, P, As, Zr, Cd, Sn, Sb, W, Tl, Bi and U for AN-G deviate by more than 20% from reference values (mostly GeoReM). Deviations are not due to secondary fluorite precipitation, but may reflect residual memory and blank issues and incorrect reference data. The latter is evident for Cd in AN-G, as ICP-MS and double-spike data agree within 6%, while the compiled value is 170% higher.

Apollo 16 soils are dominated by feldspathic highland terrane compositions and Apollo 12 soils are dominantly mixtures between mare basalt and Procellarum KREEP terrane compositions. Higher incompatible element abundances in 12032 and 12033 reveal a larger KREEP component. Of the most volatile elements, Tl displays the least variation in soil samples, Cd and especially In scatter more. Their abundances do not correlate with soil maturity, suggesting that micrometeorite bombardment has no major effect on volatile element abundances. In Apollo 12 soils, the Cd and In abundances may be controlled by the basaltic microbreccia or the basalt component, respectively.

Poster

Topic: 2.2 From dust to planets

Chemical composition and petrography of recent type 1 and 2 carbonaceous chondrite falls

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We analysed the recent (2019 - 2021) brecciated carbonaceous chondrite falls Flensburg (C1), Tarda (C2,) Kolang (CM1/2), Aguas Zarcas (CM2), and Winchcombe (CM2) together with Murchison and Paris for their chemical composition using ICP-MS and for Hg abundances using a direct mercury analyser. Chemical variations were evaluated considering new and published petrological and mineralogical data.

Aguas Zarcas #1 is enriched in Hg relative to a CI reference value of 258 ng/g, while Flensburg, Kolang, Winchcombe and the fusion crust-rich samples Aguas Zarcas #3a and 3b are depleted. The Hg contents in Aguas Zarcas #2 and 4 and both Tarda specimens are roughly similar to those extrapolated from plateau volatile element abundances, with a best fit if a CI Hg content of about 210 ng/g is assumed.

For Flensburg, Kolang, Aguas Zarcas #1 and 2, Murchison and Paris, elements analysed by ICP-MS display a typical CM composition, but Tarda shows less depletion of moderately volatile elements. Deviations for Ca, Sr, Ba, Na, Rb, and Cs in the pre-rain samples Aguas Zarcas #3a and 3b suggest that these elements were mobile within the parent body. The metal-rich lithology of Aguas Zarcas #4 displays no systematic enrichment in siderophile elements, but peculiar enrichments of refractory elements, most significantly for Zr, Hf, W, Ir, and some heavy REE. The enrichment of Ca, Sr, Mn, and Mg esp. in Tarda #1 reflects the high abundance of carbonates. Unlike for Tarda and some Aguas Zarcas samples, the Flensburg CM-related composition was not affected by intense aqueous alteration.

Lecture

Topic: 1.4 Multi-scale, dynamic interactions of minerals with fluids: From the shallow subsurface to the deep Earth

Boron isotope fractionation in subducting oceanic crust

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The boron stable isotope ratio is employed to investigate fluid-rock interaction processes in subducting slabs and the slab–mantle interface. Two groups of subduction-related rocks were collected from Syros (Greece): the first group includes high-pressure metamorphic (HPM) rocks, which are interpreted as metamorphosed oceanic crust. They are characterized by prograde mineral assemblages; the second group of samples were collected from reaction zones, which formed in a high-pressure mélange zone and are characterized by the metasomatic formation of hydrous minerals (tourmaline, white mica, glaucophane) and secondary omphacite during exhumation.

Tourmaline and mica show the highest B contents, but in mica-free samples, glaucophane and omphacite control the boron budget. Boron isotope ratios of whole rocks, white mica, glaucophane and omphacite were determined at FIERCE by LA-MC-ICPMS. Published data for tourmaline in these samples are also available.

Group–1 HPM rocks show an average $\delta^{11}\text{B}$ value of $0 \pm 5 \text{‰}$ (4 samples), which is higher than predicted from oceanic-crust dehydration modelling. This may suggest that published models strongly overestimate boron isotope fractionation in subduction zones, likely caused by erroneous assumptions on the B speciation in dehydration fluids. For the boron isotope fractionation among coexisting minerals we found the following: tourmaline–white mica $+13.4 \text{‰}$ (3 samples); tourmaline–glaucophane: $+11 \pm 4 \text{‰}$ (2); tourmaline–omphacite: $+15 \pm 5 \text{‰}$ (5). These values suggest that boron shows the same coordination to oxygen (i.e. tetrahedral) in white mica, glaucophane and omphacite, which contrasts with the dominantly trigonal coordination of B in tourmaline.

Poster

Topic: 3.1 Novel isotopic insights into high-temperature geochemical processes

Kinetic zinc isotope fractionation in olivine phenocrysts records magma evolution history of intra-plate basalts

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Zinc isotope systematics of basaltic magmas have been widely used as novel proxies for terrestrial mantle heterogeneity induced by recycled crustal materials [1-2]. The influence of mineral-melt isotope disequilibrium during magma differentiation on Zn isotopic composition of basaltic melts, nonetheless, has received limited attention. No quantitative constraint has yet been given for the diffusion-driven Zn isotope fractionation between olivine crystals and melts. Here we present high-precision zinc isotope data ($\delta^{66}\text{Zn}_{\text{JMC-Lyon}}$) for a series of olivine phenocrysts separated from intra-plate basalts from the Jiaodong Peninsula in Eastern China, together with in-situ trace element analysis. Olivine phenocrysts have Zn isotopic compositions which are too light in comparison with the host basaltic melts to be explained by equilibrium isotope fractionation at magmatic temperatures. Instead, the decrease of $\delta^{66}\text{Zn}$ values with decreasing Mg# and increasing Zn contents in olivine phenocrysts suggests diffusion-driven kinetic fractionation during olivine crystallization. The data is well-fitted with a diffusion model in which Zn diffuses from surrounding melt into olivine crystals due to the large chemical gradient with a kinetic Zn isotope fractionation factor β_{Zn} of 0.07. It is suggested that diffusion-induced isotope disequilibrium during olivine crystallization may drive Zn isotopic composition of the residual melt toward heavier values by utilizing the fractional crystallization model. Thus, kinetic effects between phenocryst and melt must be considered when applying zinc isotope systematics of any basaltic magma to probe the source heterogeneity.

[1] Liu et al., 2016, *EPSL* 444, 169–178. [2] Beunon et al., 2020 *Earth-Sci. Rev.*, 103174

Lecture

Topic: 3.1 Novel isotopic insights into high-temperature geochemical processes

Experimental investigation of Zn isotope fractionation during sulfur-bearing magma degassing

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Moderately volatile metal elements like Zn may be efficiently transported into the gas phase during magma ascending, and during vaporization may fractionate elements and their isotopes between gas and liquid [1-2]. The effect of major volatile elements like S in the melt on the volatilization process of Zn has not yet been investigated systematically. Here we present an experimental approach to test the effect of S on the evaporation of Zn by comparing the chemical and isotopic compositions of silicate glasses that were formed from both, S-bearing and S-free melts in a $f(\text{O}_2)$ -controlled gas mixing system at 1 bar.

Two series of evaporation experiments (S-bearing and S-free) were conducted with a temperature gradient of 1200-1400 °C, a $\log f(\text{O}_2) = -13.2$ to -0.68 (at air), and a time duration from 10 to 30 min. The results indicate that the volatility of Zn increased with decreasing $f(\text{O}_2)$ and increasing temperature during evaporation, while the isotope fractionation factor remained constant. Besides, the presence of S in the silicate melt seems to have a strong effect on the volatilization of Zn, resulting in less Zn remaining and larger Zn isotopic fractionations under highly reduced conditions. Our experiments reveal that the presence of major volatile elements such as S or Cl may have critical impact on the degassing of moderately volatile metal elements, resulting in a poor correlation with their 50% condensation temperatures.

[1] Sossi et al., 2020 *GCA* 288, 316–340. [2] Renggli and Klemme (2020) *JVGR* 400, 106929.

Lecture

Topic: 8.1 Geosciences and Waste Management

Thermodiffusion of Solutes in Nanoporous Materials

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Thermodiffusion describes the motion of solutes along a temperature gradient, also called the Soret effect. With respect to the geological disposal of high-level radioactive wastes, a better understanding of the thermodiffusion of solutes in geomaterials is essential for the evaluation of radionuclide migration for scenarios of early canister failure during the thermal phase of the repository. In nanoporous (geo)materials (e.g., clay rocks, cementitious materials), the interaction of ions with mineral surfaces plays an important role for the motion of ions, but its theoretical understanding is still incomplete. In this work, we investigated the thermodiffusion of charged tracers in saturated nanoporous silica using complementary experiments and simulations. The fluxes of potassium tracers in the porous solid under different external temperature gradients were determined by through diffusion experiments. To reveal the mechanisms of thermodiffusion of nanoconfined ions, a coupled thermal-electrochemical model was developed to analyze the different contributions to the ion flux. Our model shows that the gradient of the surface charge density induced by the applied temperature field leads to electrophoretic ionic mobility, which significantly promotes ionic transport compared to the classical thermophoretic motion. This study improves the understanding of the underlying mechanisms that govern the transport of solutes in nanoporous geomaterials under an external temperature gradient.

Lecture

Topic: 1.2 Methods in Geochemistry and Mineralogy

Future trends of in-situ beta decay dating

Thomas Zack

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The field of mass spectrometry has seen an impressive boost with the commercialization of an older idea of sandwiching a reaction cell between two mass filters, a configuration dubbed MS/MS. This allows controlled reactions between ions within an ICP-MS instrument and reaction gases, with the aim of reducing or even eliminating isobaric interferences. Rather established now is the example of eliminating $^{87}\text{Rb}^+$ on m/z of 87 by reacting the desired $^{87}\text{Sr}^+$ with gases such as N_2O or SF_6 to $^{87}\text{Sr}^{16}\text{O}^+$ or $^{87}\text{Sr}^{19}\text{F}^+$, leaving the Rb-ion behind. This allows Rb-Sr dating from transient signals, in particular when coupled to a laser ablation system, currently the most commonly utilized “in-situ beta decay dating” tool.

Within the field of in-situ Rb-Sr dating, particular attention is given to develop primary reference material for the scientific community. Here I will demonstrate that more emphasis should be spent on better characterizing suitable reference material (e.g., with the help of isotope dilution TIMS and MC-ICP-MS) rather than trying to “matrix-match” every possible target material. Furthermore, I am calling for a paradigm shift when dealing with Rb-Sr data from the classical isochron approach towards single spot dating, allowing e.g. detrital and age zonation studies.

Besides Rb-Sr dating, with the same technique it has been demonstrated that other exciting beta decay schemes are accessible to in-situ dating, specifically K-Ca, Re-Os and Lu-Hf. Progress was and will be possible by systematically studying ion-molecule reactions from a wide spectrum of reactive gases and gas mixes, such as CH_4 and H_2+SF_6 .

Lecture

Topic: 10.3 Geoscientific museums and collections in the area of responsibility between science and public relations

From the museum into the field and back – The digital link between museum objects and their origin

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Museums act on the interface between public and science and hence are in the best position to communicate scientific topics. We implement this by using our objects as translators: with classic exhibitions as traditional way of museum education. Complementing such classic educational tools, digital offerings are of increasing importance and widely implemented in museums today. Such facilities (e. g. museum apps, virtual tours, multitouch screens or displays etc.) are very attractive for younger guests or technophile visitors in general and hence help to improve the image of the institution, to attract further visitors and to awake interest in geoscientific topics. Digital offerings may provide additional or newest information in an understandable and easily accessible way. Within the scope of a granted project, we develop a tailor-made museum app for the Mineralogical Museum at the University of Bonn. Conventional applications usually give additional information about objects, provide short movies, audio sequences, etc. We go beyond this and use the app to link exclusive objects with their place of origin, guiding our visitors digitally from the museum into the field. Our guests will get the opportunity to explore different exciting geological sites across the country and to get in touch with the wide variety of geoscientific topics. We achieve this by implementing photogrammetric and laser-scanned 3D models of outstanding locations. The project is a cooperation with the mobile database of OutcropWizard and the project 30 Geotope³ – Germany's most beautiful geosites in 3D, both developed at the Institute of Geosciences at the University of Bonn.

Lecture

Topic: 1.5 Fundamentals and applied aspects of nucleation and crystal growth

From Understanding to Tailoring: Molecular Simulations unravel Crystal Nucleation and Growth

Dirk Zahn

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Modern approaches of molecular dynamics simulations have paved the way to the in-depth understanding of crystal formation from solution. This starts from the characterization of precursor solutions and the elucidation of molecular recognition during solute-solute or solute-substrate association. Efficient sampling techniques further enable the analyses of crystallite evolution from solute complexes to ordered nuclei, be it via straight or multi-step mechanisms. Using a small series of showcase systems, we demonstrate the combination of different modelling techniques to investigate redox reactions or proton transfers at the precipitate-solvent interface. From this, the role of different solvent scenarios including redox-potential and pH may be analyzed at the molecular level of detail. Likewise, we exemplify the in-depth understanding of (anti-)nucleation agents and growth-controlling additives as control factors of structural evolution including polymorphic form, crystallite size and shape.

Poster

Topic: 5.5 Deciphering past climates and biogeochemical cycles with geochemical proxy archives

Crystallization conditions of authigenic quartz from salt of the Zechstein basin inferred from their triple oxygen isotope composition

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The triple oxygen isotope composition of authigenic quartz allows reconstructing formation temperature and isotopic composition of the fluid with which the quartz had equilibrated [1]. We studied authigenic quartz grains from salt deposits of the Zechstein evaporitic basin to estimate the formation temperature and $\delta^{18}\text{O}$ of the saline brine. Chemically purified authigenic quartz was analyzed by means of high precision laser fluorination isotope ratio mass spectrometry.

In the triple oxygen isotope space, additional (compared to $\delta^{18}\text{O}$ only) information is gained about the equilibrium conditions during crystallization or diagenesis of the quartz. The coexisting fluid deviated from modern ocean water composition in that it was enriched in $\delta^{18}\text{O}$ in order to account for a valid equilibration temperature. By assuming the mineralizing fluid was fractionated evaporitic water, it is possible to reconstruct the diagenetic environment in which the quartz formed. Utilizing the calibration of [2], the diagenetic temperature and local water $\delta^{18}\text{O}$ value can be determined by high precision analysis of authigenic quartz minerals (pseudo-single-phase thermometer).

[1] Pack, A. and Herwartz, D. (2014) The triple oxygen isotope composition of the Earth mantle and understanding $\Delta^{17}\text{O}$ variations in terrestrial rocks and minerals, *Earth and Planetary Science Letters* **390**: 138-145.

[2] Sharp, Z.D., Gibbons, J.A., Atudorei, V., Pack, A., Sengupta, S., Shock, E.L., and Knauth, L.P. (2016) A calibration of the triple oxygen isotope fractionation in the $\text{SiO}_2\text{-H}_2\text{O}$ system and applications to natural samples, *Geochimica et Cosmochimica Acta* **186**: 105-119.

Lecture

Topic: 9.1 Dynamics of ore-forming processes: constraining mechanisms of metal enrichment

Towards quantitative understanding of volatile and metal release from magmas

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Porphyry-type Cu-Au-Mo deposits form by ore metal sulfide precipitation from magma-derived fluids. For the efficient generation of such deposits, a magmatic fluid phase simultaneously rich in ore metals and SO₂ is required. Silicate melt inclusions from volcanic rocks distributed along strike in the Southern Volcanic Zone of the Andes show that the availability of S and Cl rather than ore metal abundances control magmatic ore fertility. In addition to magma degassing, magmatic sulfides are often invoked in models assessing magma fertility. They may limit ore-forming potential by sequestering chalcophile metals in lower-crustal magma reservoirs, or they may promote ore formation if their metal and sulfur budget later get recycled into a magmatic fluid phase.

I used new experimental data for S and Cl in combination with published values to construct empirical models to predict their fluid/melt partition coefficients in *P-T*-compositional space. These were combined with the best available models for anhydrite and sulfide saturation and metal partitioning between sulfides and silicate melt to assess volatile and metal extraction from magmas during ascent and differentiation in the crust. The results show that sulfide-assisted metal pre-enrichment and transport is a testable hypothesis via silicate melt inclusion studies in arc volcanics because magmatic sulfides will typically break down before fluids rich enough in Cl to pick up their Cu budget can form. On the other hand, magmatic anhydrite saturation is predicted to be common and play an important role in ore genesis by regulating the supply of sulfur to the ore-forming hydrothermal system.

Lecture

Topic: 10.2 Geoethics – fostering ethical perspectives in Geosciences

a_Ponte, bridging geosciences and society

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Science is not good, not bad, or neutral. It is socially built by the subject who operates the research object based on subjectivity (individual and collective). The reduction of reality to a single narrative creates conflicts of interest and sustains games of knowledge and power, leading to a depoliticization of the scientific debate. Considering narrative dispute as being concrete and symbolic, geoscientific researchers must question themselves: our science supports which narrative? Whose interests does it serve? In the context of negationism (e.g. Flat-Earth movement), it is urgent to communicate and disseminate critical geoscientific knowledge, addressing socially relevant topics in accessible language, contributing to the public debate. On this ground, a_Ponte, an online collaborative platform, was born in 2019. With the aim of geoscientific outreach based on geoethical principles, the content produced and disseminated brings light to our role in the construction and management of the Earth System. Given this, a_Ponte exists as a means of circulating materials and ideas (as blog posts, magazines, online talks, training courses, and participation in podcasts and events) through a website (available in Portuguese, English and Spanish) and social media. The topics cover broad themes in geosciences from a decolonial perspective, drawing horizons outside the episteme of Eurocentric-colonial knowledge, questioning privileged spaces and geopolitical boundaries. After all, whoever dominates the discourse consequently possesses the world expressed and implied by it. Finally, it is expected that the actions proposed there promote a reflection on our role in building a more just, equitable and environmentally sustainable society.

Poster

Topic: 5.2/4 Palaeomagnetic, rock magnetic and cyclo-stratigraphic approaches applied to sedimentary sequences - dating and environmental reconstructions

Downhole logging data and its suitability for cyclostratigraphy and time series analysis

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Extensive borehole logging datasets are being gathered for commercial and scientific purposes, but studies exploring their full potential through applying time series analysis remain sparse. Typically, fast available logging data are relatively complete and may contain valuable paleoenvironmental information related to, amongst other signals, orbital forcing. Here, we briefly summarize the most relevant properties of borehole logging data and pitfalls in the context of time series analysis and cyclostratigraphy. In comparison to interpretation of data from core- or outcrop analysis, it is important to be aware of potential issues such as the effect of variation in borehole diameter and the influences of drilling fluids, and that presented logs may consist of merged results logged in several depth sections.

Lecture*Topic:* 2.3 Uniformitarianism of crustal processes**Closing an Archean ocean over 350 Mill. years – the Age-Hf isotope record of granitoids from the Limpopo Belt and adjacent Pietersburg Block****Armin Zeh¹, Maria Kirchenbaur²**¹KIT, Germany; ²Gottfried Wilhelm Leibniz University Hannover, Germany

The Limpopo Belt in southern Africa represents a high-grade gneiss terrane located between the Kaapvaal Craton to the south and the Zimbabwe Craton to the north, and is subdivided into 3 zones: (i) Northern Marginal Zone (reworked part of the Zimbabwe Craton), (ii) Southern Marginal Zone (reworked part of the Pietersburg Block, forming the northern edge of the Kaapvaal Craton), (iii) Central Zone (a polymetamorphic gneiss terrane in between). Results of combined U-Pb dating and Hf isotope analyses of zircon grains from ca. 30 granitoids (TTG's, sanukitoids, biotite granite, hybride granites) from the Pietersburg Block, Southern Marginal Zone and Central Zone indicate that most granitoids were formed periodically during the Meso- to Neoproterozoic between 2.97 and 2.62 Ga (from south to north), and plot on a unique crustal array with $^{176}\text{Lu}/^{177}\text{Hf} = 0.002$. This array and the geological-geographic background suggest emplacement of granitoids from different sources (slab melting, enriched mantle wedge and minor crust) over a period of ca. 350 Ma, most likely during successive closure of wide oceanic basin (>10.000 km^[1]) located between the Zimbabwe and proto-Kaapvaal Craton. Opening of this basin started ca. 70 Ma earlier, as suggested by Hf model ages of ca. 3.05 Ga, and closure by continent collision occurred at 2.62 Ga. We note that the derived timing for Archean ocean formation and closure is similar to that of modern Wilson cycles (ca. 340 Ma^[2]).

^[1] Zeh, A. & Kirchenbaur, M. 2022. *Precambrian Research* **373**, 106631. ^[2] Granot, R. 2016. *Nature Geosciences* **9**, 701-705.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Rare Earth and Yttrium in tissues and shells of mussel from the Danube River and its tributaries

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Due to their numerous applications in various high-technology products, Rare Earths and Yttrium (REY) have become microcontaminants of freshwater systems. Nevertheless, their biogeochemical behaviour, especially their uptake by aquatic organisms is still poorly understood.

Here, we report REY concentrations in the shells of four different mussel species, and in the tissue and shells of three *Anodonta anatina* mussels, and in the respective ambient water from the Danube River and some tributaries. The shells were grouped according to their sizes and meticulously cleaned, while the soft tissues were dissected and lyophilized. All samples were acid-digested and preconcentrated prior to ICP-MS measurements. Analytical quality was monitored by using certificated reference materials JLS-1 and BCR-668 for shells and tissues samples, respectively.

A size dependency of the REY concentration was only observed for *Corbicula* shells, corroborating the previous observations at the Rhine River. Shale-normalized REY patterns are similar for all shells and tissues and slightly MREY-enriched. Compared with the 0.2 µm-filtered ambient water, the biological samples show REY concentrations that are between three to five orders of magnitude higher, revealing significant bioaccumulation of REY. The observed preferential uptake of LREY relative to HREY is due to more stable complexation of HREY with dissolved ligands. Despite significant anthropogenic Gd enrichments in ambient water, there are no positive Gd anomalies in the biological samples, suggesting biounavailability of Gd based contrast agents.

Poster

Topic: 9.4 Chemical sediments and mineral deposits in basins: archives of paleoclimatic, hydrogenetic, biogenic, hydrothermal, and diagenetic, processes throughout Earth's history

The Shahejie Formation in the Dongpu Depression, Bohai Bay Basin, China: Geochemical investigation of the origin, deposition and preservation of organic matter in a saline lacustrine environment during the Middle Eocene

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A new set of geochemical, petrographical and mineralogical data on important petroleum source rocks from Eocene Shahejie Formation in the Bohai Bay Basin, Eastern China is presented to investigate organic matter precursor material, thermal maturity and paleoenvironment during deposition of the Es_3^U , Es_3^L , Es_3^M and Es_4^U members. Different maturity parameters determine early mature to peak oil mature stages and maturity increase with burial depth. Alginite is the predominant maceral, whereas vitrinite and inertinite are rare. Studied shales and marlstones were deposited under episodic PZA as revealed by aryl isoprenoids. Bottom water conditions were anoxic most of the time except for Es_3^M . A fairly uniform biomarker composition displayed in Es_4^U indicates relatively stable hypersaline lake conditions with a shallow chemocline based on the high Gammacerane Index >0.6 and abundant aryl isoprenoids. Salinity changed during deposition of Es_3^L according to variable C_{24} Tet-related parameters and evaporite minerals content. The aquatic algal organisms, i.e. haptophyte algae, diatoms and bryophytes which are reflected by abundant nC_{37-39} alkanes, a variable sterane pattern, and other biomarkers, were flourishing during Es_3^L . Small concentration of specific PAHs, i.e. retene, cadalene, fluoranthene, indeno[1,2,3-cd]pyrene and benzo[ghi]perylene in Es_3^L , may be attributed to limited terrigenous input. Es_3^M was deposited in a normal lacustrine environment under rather low salinity conditions with substantial input of organic matter derived from algae. During Es_3^U , saline lake conditions were re-established accompanied by algal and microbial input, especially cyanobacteria as deduced from MMAs and 2α -MeHs, methanogens from abnormally abundant phytane, PMI, squalane, and methanotrophs from 3β -MeHs.

Lecture

Topic: 6.1 Earth surface processes in extremely water-limited environments

Calcium sulphate-rich wedges in the subsurface indicating salt dynamics in alluvial-fan deposits from the Atacama Desert

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Subsurface wedges are common geomorphological structures in periglacial environments typically associated with polygonal patterned grounds on the surface. Their presence is an indicator for cryogenic processes in the subsurface resulting in vertically laminated sequences from which the wedges are formed. Similar geomorphological features occur in arid to hyperarid environments, such as in the Atacama Desert, where haloturbation processes are assumed to control subsurface-wedge formation. X-ray diffraction and x-ray fluorescence analyses of wedges from the central Atacama Desert revealed various calcium-sulphate phases accompanied by clastic minerals in the laminae sequences. Calcium-sulphate phases in the wedges are thus thought to be potential drivers for salt dynamics and wedge-growth activity. In combination with varying water availability, these salt dynamics lead to significant volumetric changes in the deposits due to phase transitions of calcium-sulphate phases, as well as dissolution and (re)precipitation of salts from infiltrating solutions. As water is scarce in the Atacama Desert, geochronological data of calcium-sulphate wedges is essential to resolve wedge-growth phases and episodes of local moisture supply, indispensable for using the wedges as palaeoclimate archives. We applied post-infrared infrared stimulated luminescence (post-IR IRSL) dating to coarse-grain feldspars extracted from a calcium-sulphate wedge outcropped on the Aroma fan in the Central Depression of the Atacama Desert. Our post-IR IRSL results from two wedge subsamples showed a widespread equivalent-dose distribution indicating multiple phases of wedge formation. Equivalent-dose distributions and palaeodoses based on the minimum age model revealed the most recent wedge-growth activities at 10.6 ± 2.2 ka and 7.9 ± 1.8 ka.

Lecture

Topic: 7.2 Living Earth – geobiological perspectives on an evolving planet

Duckweeds as quasi-hyperaccumulators of rare earths and the bioavailability of Gd-based contrast agents

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Duckweeds are widespread macrophytes in lentic waters. These small, fast-growing aquatic plants receive increasing attention as potential food supplement, which makes detailed knowledge of their chemical composition highly important.

The rare earths and yttrium (REY) are pivotal of many enabling technologies causing a constantly growing release of REY into the environment. However, little is known about their transfer from the geosphere into the biosphere. As duckweeds retrieve their elements primarily from ambient water, they are excellent objects for related studies.

We present data for all REY (and some other elements) in naturally grown duckweeds and ambient waters in their habitat. Some of the waters show shale-normalised (_{SN}) REY patterns with pronounced positive Gd anomalies which originate from Gd-based contrast agents (Gd-CAs) applied in magnetic resonance imaging.

Rare earths and yttrium concentrations in the duckweeds strongly exceed those in ambient water and correlate closely with Mn (but not Ca), possibly indicating a common uptake mechanism. The REY_{SN} patterns of the duckweeds are fractionated relative to both shale and ambient water, with larger distribution coefficients for light compared to heavy REY, probably due to stronger complexation of heavy REY with dissolved ligands. None of the duckweeds displays any anthropogenic Gd_{SN} anomaly, regardless of its presence or absence in ambient water.

Our findings show that duckweeds have a strong bioaccumulation potential and are quasi-hyperaccumulators of REY and further corroborate the conservative behaviour of Gd-CAs in the environment.

Poster

Topic: 5.6 Natural archives as recorders of past climate and environmental conditions – processes, methods and applications

Insights into the skeletal growth of massive corals from the central Belize Barrier Reef (Central America): Results from high-resolution skeletal density variations in *Orbicella faveolata*

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Massive reef-forming corals (Scleractinia) are biological and palaeoclimatological archives, based on their skeletal growth chronology that is characterized by annual density bandings (analogue to dendrochronology). A limitation in coral sclerochronology is the quantification of skeletal density due to the need of precise analytical techniques. This study deals with the application of two-dimensional grid-scanning gamma densitometry (²⁴¹Americium-radiation beam technique) to quantify skeletal density fluctuations at higher spatiotemporal (intra-annual) resolution. An advantage of this method is a reduction of local influences along the coral growth axis (e.g., pore spaces, calyx architecture), comparative to previous one-dimensional track selection techniques with gamma densitometry. The widespread Atlantic coral *Orbicella* (ex *Montastraea*) *faveolata* was used as a representative massive coral species. A colony from the central Belize Barrier Reef (BBR, Central America) was analysed, yielding 1005 calibrated density values corresponding to a skeletal growth period of 38 years (1962-1999 CE). An average of 27.6±3.5 measurements per growth increment translates into a roughly biweekly resolution for selected grid point rows. The colony shows a long-term decline in skeletal density, accompanied by reduced rates in carbonate accretion. This implies limited capability for skeletal formation in *O. faveolata* corals within the central BBR. Annual density bandings are likely connected to intra-annual fluctuations in δ¹³C isotope composition, suggesting a relationship to their mixotrophic lifestyle with a carbon uptake either by heterotrophic feeding and/or photosynthetic activity of their endosymbiotic zooxanthellae. However, combined data suggest a more complex influence of environmental and biological controls on skeletal density variations in the present coral.

Poster

Topic: 4.2 Advances in Geochronology: From present techniques to future applications

Formation and deformation of Triassic skarn (Uppermost Unit, Crete/Greece)

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The nappes of the Uppermost Unit of Crete are counted among the most enigmatic constituents of the Eastern Mediterranean. U-Pb dating of zircons separated from felsic metavolcanics of the deepest Preveli nappe yielded Triassic emplacement ages at 237.3 ±1.8, 241.5 ±1.2 and 242.1 ±1.2 Ma. U-Pb dating of andradite-grossular of subvolcanic skarn yielded the same age at 239.3 ±2.3 Ma. The skarn is dominated by hydrous phases (ferri-actinolite, hydro-grandite, epidote), which developed at T = 400 – 450 °C in a rift-related setting due to fluid-assisted metasomatic reactions between limestone and mafic veins. Thus, U-Pb dating of skarn grandite allows dating the complementary record of hydrothermal activity related to the cooling of the causative melt. Early Cretaceous subduction caused deformation under epidote-blueschist facies conditions at T = 360 ±40 °C and P >1.0 GPa. An ³⁹Ar-⁴⁰Ar age of 125 ±10 Ma obtained from synkinematic ferri-winchite is interpreted to reflect the time of Eohellenic HP-LT metamorphism. During subduction, the differential stress was >300 MPa. Under these conditions, the garnet strain was accommodated not only by fracturing, but also by strain-induced grain boundary migration and subgrain formation. Thus, crystal plastic deformation of garnet is possible at temperatures far below the threshold temperature (ca. 500 °C) commonly reported for dislocation creep.

The new ages obtained from the Preveli nappe suggest the Uppermost Unit of Crete to be derived either from the peri-Rhodope domain of the Internal Hellenides or from the Pontides of northern Turkey.

Funding by DFG (Zu 73-34) is acknowledged.

Poster

Topic: 4.5 Tectonic Systems (TSK Open Session)

Rheological inversion and mullion formation of a composite sill under bulk constriction (Odenwald, Germany).

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We present new data from a composite sill, which intruded at deep structural levels (ca. 18 km depth) into quartzmonzodiorite of the southern Odenwald. Zircon and titanite of the quartzmonzodiorite yielded similar U-Pb ages at 344.3 ± 0.6 and 343.2 ± 2.1 Ma, respectively, reflecting fast cooling ($\geq 76^\circ\text{C}/\text{m.y.}$) until the solidus was attained at ca. 680°C . Under these conditions, the quartzmonzodiorite was cut by a spessartite sill, which yielded a U-Pb titanite age at 342.0 ± 1.0 Ma. Fast migration of contact melt into shrinkage cracks of the sill resulted in thin felsic veins.

Bulk constriction at $T = \text{ca. } 660^\circ\text{C}$ led to (1) subvertical prolate grain-shape fabrics, (2) increase of the sill's dip, (3) doubling of the sill's thickness, (4) mullions with cusps pointing into the host, and (5) boudinage of the felsic veins. The shape of the mullions, the boudinage of the felsic veins and the sigmoidal foliation/lineation indicate that the mafic sill was incompetent and the felsic material of host and veins was competent. This inversion in rheology can be explained by phase-boundary diffusion that was more effective in the fine grained mafic sill than in the coarse grained felsic host.

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