Influence of viscosity on the growth of high pressure phases in computer experiments *Poster*

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Introduction

The general aim of the project is the examination of microstructures that develop under HP conditions in computer experiments. Starting point is an interest in the dynamics of HP phase transitions, as for instance the probably catastrophic phase-change event of olivine to spinel in the upper mantle. This is either explained by large overpressure or failure during the development of micro-structures during the growth of the spinel phase. Experimental results on this subject are rare, and do not lead by themselves to a deeper insight into the complicated stress/strain/volume-change/micro-crack relationships of the transition. We developed a central force spring model, where particles can undergo a phase change using parameters of olivine and spinel. The algorithm is capable of simulating the local growth of the mentioned phases on the basis of direction-dependant rate laws.

In the current context newtonian viscosity is added to the previously solely elastic system, since under HP/HT conditions the viscous flow within the material will have a large influence on the distribution of elastic energies, which in turn have an important influence on the driving force of the transition. Thus we are dealing with a visco-elastic system, which will be subjected to time-dependant strain.

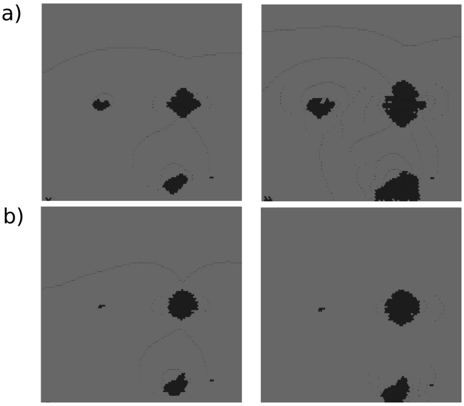

Figure 1: Spinel (black) growing within olivine (grey) in a computer simulation. In run a) the reaction is sluggish due to a low high activation energy. Run b) uses a high activation energy. The resolution is 100 × 100 particles, the system size is 0.5 mm

Mechanism

A solely brittle rock will fracture if a certain yield stress is reached, while a rock that behaves only viscously, deforms like a fluid and will compensate stress by flow. Combining these properties leads to a viscoelastic model, which is elastic for small strain rates but viscous for large ones. Whether or not a rock will fracture or flow depends therefore on the interplay of these properties. In the context of stress-driven rapid phase transitions, this means a large viscous deformation during deformation previous to the reaction, and brittle fracturing during the rapid volume reduction after the reaction started. The system itself is sensitive to the starting conditions, which will be influenced by the reduced differential stresses due to viscous flow. An important role in the development of microstructures plays also the velocity of the transition, since this controls

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the interplay with the latent heat release and the subsequent heat conduction (see Fig. 1).