# Simulation of phase-boundary structures under high pressure 

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The olivine/spinel phase transition is a possible explanation for deep-seated earthquakes in the upper mantle, and is thus a matter of intense empirical as well as computational research. Earthquakes at the transition are either explained by a catastrophic phase-change event due to 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. Riggs and Green (2001) performed high-pressure experiments on germanium olivine and observed rough, fractal grain-boundaries of spinel in olivine. However, they were not able to observe the dynamic evolution of these structures. In order to understand the dynamics of such a process, we developed a central force spring model, where particles can undergo a phase change simulating the olivine-spinel transition. Two approaches are taken into account with regard to the special nature of a dissipative, probably self-organized system: a probabilistic Monte Carlo versus a direct approach. Basis of the simulations are stochastic rate laws for growth and nucleation of new phases in conjunction with a detailed calculation of the free energy change due to shear stress, volume/pressure change and latent heat release. We present the first results of the pressure/volume-change affected structures and their stability over time and space.

References: E. M. Riggs and H. W. Green. Shear localization in transformationinduced faulting: first-order similarities to brittle shear failure. Tectonophysics, 340, 95-107, 2001.

