



A new front-tracking method to model anisotropic grain & phase boundary motion in rocks

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Microstructures of rocks play an important role in determining the rheological properties and usually help to reveal the processes that lead to their formation. Several processes can be active during the formation of a rock and they may be active simultaneously or in series. Some processes change the microstructure significantly and may obliterate any fabrics that indicate the previous history of the rocks. One of these processes is grain boundary migration (GBM). During static recrystallization, GBM may produce a foam texture that completely overprints any earlier rock fabrics and GBM actively influences the rheology of a rock, via its influence on grain size and lattice defect concentration. Much of the theory on GBM derives from material sciences and in particular metallurgy but these theories cannot easily be transferred to geological materials due to the complexity of geological grain boundaries. Experiments on natural rocks have given insight into GBM in rocks, but their interpolation is seriously hampered by the extrapolation and scaling over many orders of magnitude from laboratory to natural conditions and scales. Numerical modelling is a new and promising alternative that overcomes most of these problems. Numerical models have the additional advantage that single parameters of one process can be singled out and their influence on the microstructure can be investigated.

We present here a new front-tracking method to simulate GBM. Generally, all changes of a microstructure tend to minimize the internal free energy of a system. The new method moves boundaries along the energy gradient towards a lower total energy state of the system. The energy gradient can be calculated as needed and might be limited to (an)isotropic boundary energies but may also include metamorphism, melt-

ing, reaction energies, surface energies, pressure etc.. Three examples are included in this paper where we simulate crystal growth of grains with isotropic and anisotropic boundary energy functions in a liquid (melt) and grain growth in a system with a melt present, again with isotropic and anisotropic boundary energy functions.