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3D grain boundary migration

J.K. Becker and P.D. Bons

Institut fuer Geowissenschaften, Universitaet Tuebingen, Tuebingen, Germany (becker@jkbecker.de)

Microstructures of rocks play an important role in determining rheological properties and help to reveal the processes that lead to their formation. Some of these processes change the microstructure significantly and may thus have the opposite effect in obliterating any fabrics indicative of the previous history of the rocks. One of these processes is grain boundary migration (GBM). During static recrystallisation, GBM may produce a foam texture that completely overprints a pre-existing grain boundary network and GBM actively influences the rheology of a rock, via its influence on grain size and lattice defect concentration.

We here present a new numerical simulation software that is capable of simulating a whole range of processes on the grain scale (it is not limited to grain boundary migration). The software is polyhedron-based, meaning that each grain (or phase) is represented by a polyhedron that has discrete boundaries. The boundary (the shell) of the polyhedron is defined by a set of facets which in turn is defined by a set of vertices. Each structural entity (polyhedron, facets and vertices) can have an unlimited number of parameters (depending on the process to be modeled) such as surface energy, concentration, etc. which can be used to calculate changes of the microstructre.

We use the processes of grain boundary migration of a “regular” and a partially molten rock to demonstrate the software. Since this software is 3D, the formation of melt networks in a partially molten rock can also be studied. The interconnected melt network is of fundamental importance for melt segregation and migration in the crust and mantle and can help to understand the core-mantle differentiation of large terrestrial planets.