Geophysical Research Abstracts,
Vol. 11, EGU2009-5842, 2009
EGU General Assembly 2009

Deformation and recrystallisation of polycrystalline materials: a numerical approach to predicting microstructure evolution.

A. Griera (1), M. Jessell (1), R. Lebensohn (2), and L. Evans (3)

(1) Université Toulouse III, UMR 5563 UR 154 Laboratoire des Mecanismes et Transferts en Geologie, Toulouse, France (mjessell@lmtg.obs-mip.fr), (2) Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, USA, (3) School of Earth Sciences, University of Melbourne, Victoria, Australia

We present a new numerical scheme to simulate deformation and recrystallization of 2D microstructure of polycrystalline materials. The scheme is based on the coupling of a full-field crystal plasticity code (Lebensohn, 2001) and a recrystallisation code (the Elle modelling platform, www.materialsknowledge.org/elle, Bons et al., 2008).

The crystal plasticity code computes the micromechanical response of a polycrystalline medium deforming by dislocation glide using a Fast Fourier Transform (FFT) algorithm. Based on the evolution of the local misorientation field predicted by the FFT-based model, we have implemented the calculation of the corresponding geometrically-necessary dislocation density field, which in turn is used to drive recrystallization in the aggregate, using the Elle platform. Elle is an open-source code for the simulation of microstructural evolution of rocks during deformation and metamorphism. The modular architecture of the code allows us to efficiently simulate multiple and competitive processes. The code has been verified and validated using simple analytical models of plasticity and grain boundary migration.

The first predictions of dynamic recrystallization of polycrystalline columnar ice are presented. Numerical results are compared with observations from creep experiments of synthetic ice samples. Comparison of numerical predictions with experiments shows that the numerical scheme can simulate the spatial and time evolution of subgrain/grain scale heterogeneities and the recrystallisation of polycrystals.

Results from these simulations can be used to validate homogenization approaches, which it can serve as an input to the development of large-scale models (e.g. ice sheet flow, mantle flow). In the opposite sense, the obtained strain and stress histories from large-scale models can serve as boundary conditions for full-field simulations to predict microstructure evolution quantitatively for specific tectonic settings.

Bons, P., et al., (2008) Microdynamics Simulation. Lecture Notes in Earth Sciences, 106, Springer.
Lebensohn, R. A. (2001) N-site modelling of a 3D viscoplastic polycrystal using Fast Fourier transform. Acta Materialia 49, 2723-2737.