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Simulation of subgrain scale deformation and its effect on recrystallisation

A. Griera (1), M. W. Jessell (1), L. Evans (2)

(1) Laboratoire des Mécanismes et Transferts en Géologie, Université Paul-Sabatier, Toulouse, France, (2) School of Earth Sciences, University of Melbourne, Victoria, Australia (griera@lmtg.obs-mip.fr)

In rocks deforming by crystal plastic mechanisms, a complex substructure of subgrain walls and dislocations develops in the crystals, resulting from the interaction between subgrain-scale heterogeneity of the deformation field, the misorientation of deformed lattice, variations in dislocation densities and interactions with migrating grain boundaries. One key to increasing our knowledge of substructure evolution in minerals is our ability to translate our understanding of the plastic anisotropy of minerals into predictions of the subgrain scale heterogeneities that govern the subsequent evolution within individual grains. However subgrain formation is particularly problematic as the process is mineral specific and even in a single material different process for subgrain formation has been identified.

Until recently, the tools to predict these variations were not available despite the observations in natural and experimentally deformed polycrystals that measured plastic anisotropy and the resulting grain and subgrain heterogeneities. The advent of 2D and then 3D crystal plastic FEM and related techniques allowed us to predict the heterogeneity of the deformation field, and associated variations in lattice orientation.

The objective of this contribution is to describe the conceptual basis for a new numerical scheme for polycrystals deformation based on coupled of Elle modelling platform (Jessell et al 2001) and an N-Site FFT plastic code (Lebensohn, 2001). The FFT code computes a solution of equilibrium equation of elastic and viscoplastic anisotropic 3D polycrystals based on the Fast Fourier Transform (FFT) algorithm. Both codes can be formulated with periodic boundary conditions and regular distribution of discrete nodes, so a direct one to one mapping between the data structures of both codes is

possible. Grain boundary and subgrain structure interaction can be allowed using a Front-Tracking approach similar to the one currently available in Elle (Becker et al., submitted).

Finally, this new numerical scheme opens up the possibility for us to simulate the influence of spatial variation of subgrain scale heterogeneities on the recrystallisation of polycrystals and provides us with a new multi-scale simulation tool to study substructure formation. Verification of the simulations will be performed by comparison with physical in situ experiments where the temporal evolution of the system can be followed (c.f. Piazolo et al., 2004).

References

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