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Numerical modelling of subgrain scale deformation and recrystallisation: model set-up and integration.

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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 in grains. However subgrain formation is particularly problematic as the process is mineral dependent 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 present a new numerical scheme for polycrystals deformation based on coupled of a full-field crystal plastic code (Lebensohn, 2001) and the Elle modelling platform (Bons et al., 2007). The crystal code computes the micromechanical response that develops in a polycrystalline medium deforming by dislocation using a Fast Fourier Transform algorithm (FFT). From local stress and strain-rate fields computed, the shear-rates or activities of slip modes can be obtained. Geometrically and statically dislocation densities are estimated by means of gradient plasticity theory and spatial gradients of lattice orientation. The numerical code Elle is an efficient tool in modelling multiple and competitive processes, and computes the simulation of recrystallisation and grain growth. Grain boundary motion is performed

using a Front-Tracking approach (Becker, et al., 2007), where Gibbs free energy is minimized. This algorithm allows the incorporation of any relevant driving force such as strain stored energy or surface energy. 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. First results obtained for the simulation of dynamic recrystallisation of polycrystalline ice will be presented. The new numerical scheme is efficient to simulate the influence of spatial variation of subgrain scale heterogeneities on the recrystallisation of polycrystals and provides a new multi-scale simulation tool to study microstructure evolution. 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).

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