

project 1

Linking dislocation and subgrain dynamics: Multiscale modelling and verification by comparison with results from in-situ experiments

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Minerals are for the most part crystalline materials and contain defects: point defects as well as one-, two- and three-dimensional defects such as dislocations. The dynamics of such defects influence directly subgrain scale phenomena such as subgrain boundary development and movement.

In this project Linking dislocation and subgrain dynamics: Multiscale modelling and verification the emphasis lies in the development of a numerical system integrating dislocation dynamics simulations and (sub)grain scale front tracking and Potts simulations using the framework of the existing Elle code. Once this integration is developed it should be possible to simulate the development of a substructure at different scales where dislocation dynamics provide information about the energy and position of tilt and subgrain walls as well as dislocation type and dislocation density at any material point through time. This information will direct feed into the energy equations used to simulated cell development, subgrain nucleation and growth. Transferring information to different scales should give the researcher the opportunity to explore the possibilities and probabilities of nucleation events during recrystallization. Different nucleation theories (see e.g. Doherty et al., 1997) will be tested as well as the different modes of energy accumulation and dissipation during substructure development, subgrain growth and subgrain boundary movement.

In the second phase of the project, modelling results will be compared to selected in-situ experiments of pre-deformed then heated materials observed in 2D and 3D.

Specifically the main aims of this project are:

- Link dislocation dynamics (provided by IP5) and the subgrain level simulation in Elle
- Test of new simulations code against in situ experiments in the SEM and data from 3D experiments performed at the ESRF facility, Grenoble.
- investigate subgrain growth, subgrain boundary movement and nucleation by combined experiment and simulation