PUBLISHABLE FINAL ACTIVITY REPORT

DIGIMAT PROJECT (Contract no NMP3-CT-2006-017105)

Multiscale modeling of recrystallization in metals based on a digital material framework

The project is focused on producing and demonstrating a model for deformation and recrystallization of polycrystalline metals using techniques based on 3D digital microstructures. Important components include plastic deformation with newly developed constitutive relations, and simulation of subsequent recrystallization with detailed examination of the early stages that lead to nucleation of new grains.

1 Main results

• A “DigiMicro” software has been developed for constructing, visualizing and analyzing 3D microstructures. Two formats are available : Voronoï tessellations and voxels.
• Meshing methods that conform to microstructural features, as in polycrystals, with a good quality.
• Software developed that permits parallelized calculation of : meshing of polycrystal microstructures, large deformation of microstructures, and recrystallization of microstructures.
• Elastic-viscoplastic crystal plasticity models of deformation in the context of large deformations. Account is taken for the evolution of different types of dislocations. Comparisons to experimental data (work hardening, calorimetry) have been made to validate the model. A non local dislocation-based model has been developed as well, and is able to represent size effects.
• A constitutive relation (force-velocity) for dislocation motion has been obtained from the numerical solution of the 2D continuum theory of dislocations. The interaction of dislocations with solute atoms can be included.
• A level set approach for the description of grain boundary migration and nucleation phenomena has been developed within the same finite element software as the one used for the modelling of plastic deformation. Grain and subgrain boundary motion have been described with a phase field model as well.
• A level set method for simulating the migration of low angle grain boundaries based on their actual dislocation structure has been developed and verified for symmetric and asymmetric tilt boundary types. Further developments have looked at the role of extrinsic dislocations on the effective mobility value of the boundaries.
• The mechanism of grain boundary migration for low angle grain boundaries has been studied with the ultimate goal of developing an analytical model. A first approach is a continuum dislocation dynamics method based upon the level set method. A second approach consists in performing very large molecular dynamics simulations of the migration of low angle grain boundaries. The latter simulations are of a scale that they can be used to validate the larger scale level-set calculations.
• Comparisons have been made between Monte Carlo and level set methods for the simulation of recrystallization and grain growth.
• Diffraction experiments have been performed at the ESRF Synchrotron facility to characterize 3D polycrystalline microstructures non-destructively.
• In situ diffraction experiments have been performed to study the recovery and recrystallization (grain growth) during heat treatment of Al-0.5%Mg.

• Analysis of a wide range of grain boundary mobility data, both experimental and theoretical, has been performed with the aim of developing constitutive relations for grain boundary properties.
• An exact extension from 2D to 3D of the famous von Neumann-Mullins law describing grain growth has been derived. This approach provides an exact expression for the capillarity-driven growth (or shrinkage) of every grain in a polycrystalline body. The work has been published in the journal Nature. This new theory is fundamental to any work on microstructural evolution of interface networks. Tests have been performed on microstructures that have been discretized with tetrahedral meshes. Results show very good agreement with the theory.

2 Main issues

• Constitutive relations for plastic hardening : many choices exist for incorporating the effect of dislocation interactions. They lead to different evaluations of stored energy, and hence have an impact on the modelling of recrystallization.
• The introduction of subgrain structures into calculations corresponds to the problem of how to predict cell and subgrain development. This remains a challenge.
• In continuum theory of dislocations, the proper description of combining effects of dislocations and grain boundaries remains an issue.
• In devising constitutive relations for grain boundary properties, need to include the influence of boundary normal on energy and mobility.
• Using the level-set method simulation of full 3-d dislocation dynamics of grain boundary migration, insurmountable difficulties have been encountered, when dealing with dislocation reactions in grain boundaries.
• Reconstruction of 3D samples from synchrotron measurements proved to be much more difficult than initially anticipated, in particular due to the presence of orientation gradients within grains.