
On the importance of 3D microstructure for the prediction of microstructural evolution

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Abstract

Conventional metallurgy is based on thermomechanical processes. During these processes, strain and temperature induce microstructural evolution including grain boundary migration, recovery and recrystallization mechanisms. Although these mechanisms have been observed and studied for a long time, they are yet to be fully understood. Therefore, it is of particular interest to have a numerical model that can predict the final microstructure of a given material under specific stress and temperature conditions. To achieve this, it is necessary to couple two models: one that predicts microstructure evolution caused by deformation and another that predicts evolution induced by temperature.

The models are used in a decoupled way which allow to study microstructural evolutions during strain followed by annealing. Special care should be given to the simulation data transfer between the two models. To give quantitative prediction of microstructural evolutions, such a numerical procedure should be finely calibrated against experimental data.

This study focuses on the microstructural evolution of pure aluminium (99.999 %) during deformation followed by annealing. The experimental data acquired during the deformation step is used to calibrate a numerical routine of crystal plasticity finite element method (CPFEM) simulations. Then the experimental data acquired during the annealing step is used to calibrate a phase field model.

The main focus of this study is to determine which experimental data is necessary to input to the model and how the transfer of data can be done most efficiently. A major question is

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if a 2D description of the microstructure is sufficient or if it is necessary to describe the full 3D microstructure.

For the experimental part of the study, an *in situ* scanning electron microscope (SEM) tensile test coupled with Electron Backscattered Diffraction (EBSD) analysis is firstly conducted at room temperature. Lithography is performed on the sample to define a region of interest and create a speckle on the surface which is used for digital image correlation (DIC). The tensile test is performed by imposing the crosshead displacement. This displacement is periodically interrupted to acquire secondary electron images for the DIC. Less frequently, the crosshead displacement is stopped and the sample is unloaded in order to perform EBSD analysis without being impacted by relaxation. The sample is previously characterized by laboratory-based diffraction contrast tomography (LabDCT). This provides a spatially resolved 3D orientation map, which can be used to numerically reconstruct the real microstructure.

The same sample is then submitted to an *in situ* SEM annealing test coupled with EBSD analysis. The sample is heated to the desired temperature and then cooled to 50°C to prevent microstructural evolution during the EBSD scan. This can be done as many times as desired.

The comparison between the numerical and experimental microstructural evolutions during strain enables fine calibration of the CPFEM simulations and verification of the model's ability to accurately reproduce lattice reorientation and energy accumulation resulting from plastic deformation. Similarly, the comparison between the numerical and experimental microstructural evolutions during annealing enables fine calibration of the phase field model and verification of the model's ability to accurately reproduce grain boundary migration and eventually recrystallization.

Comparison between numerical results performed only using 2D microstructure from EBSD and 3D microstructure from LabDCT is performed to assess whether full microstructural characterization is needed in order to achieve satisfying results.