

**SIMULATING MICROSTRUCTURE EVOLUTION OF
REALISTIC 3D ALUMINUM ALLOY POLYCRYSTAL
DURING LARGE PLASTIC DEFORMATION AT
ELEVATED TEMPERATURE**

By

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ABSTRACT

To expand the usage of aluminum alloys, it is desirable to lower the cost of aluminum forming, which means getting the desired material properties efficiently. Since macro scale material behaviors are determined by the microstructural features such as grain shape, grain size distribution, and grain orientation distribution, it is desirable to obtain a better understanding and control of the microstructural feature evolution during large deformation processing. The focus of this work is to simulate texture evolution, and to capture the non-homogeneous deformation within grains of Al6061 polycrystals during large plastic deformation at elevated temperatures.

A crystal elasto-viscoplastic constitutive model is developed that considers not only the twelve compact slip systems, but also the extra twelve non-compact slip systems that become active at elevated temperatures. A modified Voce-Kocks hardening model is used to represent the strain hardening by dislocation entanglement and softening by recovery.

The model is implemented into a multiscale finite element formulation. The implementation involves both the integration of the constitutive model as well as derivation and implementation of the associated consistent tangent. The finite element implementation allows for periodic boundary conditions on the fluctuation field which reduces the effect of the boundary conditions in a multiscale perspective.

An automatic procedure for generating 3D periodic finite element meshes of polycrystals with statistically representative microstructural features has been developed. A modified Potts type Monte Carlo simulation is used to generate polycrystals with periodicity (to allow scale-linking). Then the grain shape, grain size distribution and orientation distribution of the generated polycrystal models are checked against experiment observations to make sure that they are statistically representative. A method referred to as the Boundary Cubes (BC) method was developed and implemented to extract geometry topology information. Finally, the topology information is input into a 3D mesher to generate a finite element mesh with controllable mesh size. Special steps were taken to make sure that the generated mesh

is periodic with matching mesh entities on opposite model faces.

The model is then calibrated, and a simulation on a small polycrystal is performed to demonstrate the method. The results are compared against experiment observations at several scales for calibration and validation. From macroscale tensile tests reported in the literature on a nearby alloy, and from compression tests on the alloy of interest, the model parameters in the constitutive model are calibrated. Tests on simple microstructures are performed to see the effect of the boundary conditions. A simulation of a large deformation of a 17 grain (45 region) polycrystal was carried out, and the evolution of the microstructure, including grain shape and orientation, is compared to experimental observations. The non-homogeneous deformations in the grains and the intragranular variation in the orientations that develops is studied.