

Large Scale Simulations of Mesoscale Plasticity and Recrystallization of Aluminum Polycrystals

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ABSTRACT

The deformation of polycrystalline aluminum is simulated at the microstructural length scale using a crystal-plasticity based finite element technique. The deformation substructure is extracted from the finite element results, and the evolution of the deformation substructure during subsequent annealing is simulated using a Monte Carlo approach. Both the finite element and the Monte Carlo simulations are implemented for large, three-dimensional domains using the massively parallel computational capabilities at Oak Ridge National Laboratory. The simulations are able to capture for the first time, the formation of a strong Cube component following recrystallization from an initial grain structure containing a small volume fraction of Cube. The microstructural and kinetic aspects of cube texture evolution are discussed.

1. Introduction

The key to the successful production of aluminum sheet for high formability applications is the ability to control the crystallographic texture in the hot band. A strong Cube texture component following hot deformation and coiling is an essential requirement for many applications of aluminum sheet. It has been known for quite some time that the Cube texture component originates from Cube bands that survive the hot deformation process. Careful experiments using slip trace analysis [1] have shown that the stability of Cube during hot deformation is due to slip activity on the $\{110\} \langle 110 \rangle$ non-octahedral slip systems in addition to the usual $\{111\} \langle 110 \rangle$ octahedral slip systems. Recent experiments using aluminum bi-crystals [2] have shown that the stored energy inside the Cube grains is lower than in other deformation components such as S, Copper and Brass. The above experimental results have been captured adequately by recent microstructural deformation simulations based on crystal plasticity concepts [3]. The authors have developed an approach [3, 4] to extract a deformation substructure from the results of the deformation simulations by assuming that the deformation substructure exists in the form of a well-defined subgrain structure, where the local subgrain size and/or the mean misorientation varies according to the stored energy, and evolving the reconstructed subgrains during annealing using a Monte Carlo approach. Although the simulations were able to capture the annealing behavior of deformed bi-crystals [3], the evolution of a strong Cube texture from an initial polycrystalline sample containing very little Cube

component has not been successfully simulated. This paper presents our initial simulations of Cube texture evolution in polycrystals using large scale, three-dimensional simulations of deformation and recrystallization.

2. Mesoscale Simulations

The initial grain structure used in the deformation simulations was generated using a three-dimensional, Monte Carlo simulation of grain growth in a $60 \times 60 \times 60$ simple cubic lattice by considering the first-, second- and third-nearest neighbors of a site for local energy calculations. A random texture was introduced to this grain structure, and four Cube-oriented grains were randomly introduced in the grain structure. The total volume fraction of initial cube was roughly 0.01. The initial grain structure had a total of 412 grains. The deformation was carried out in plane strain compression to a compressive strain of -0.7 and -1.2 at a strain rate of 1.0 s^{-1} . Slip on both octahedral and non-octahedral slip systems was included in the polycrystal deformation calculations. The deformation substructure was extracted using a procedure that has been outlined elsewhere [3, 4]. Each element was assumed to consist of 27 subgrains whose orientations were scattered around the mean element orientation, and the mean misorientation among the subgrains was calculated based on the stored energy of the element. The stored energy within the element was assumed to be proportional to the square of the slip system critical resolved shear stress within the element.

3. Results and Discussion

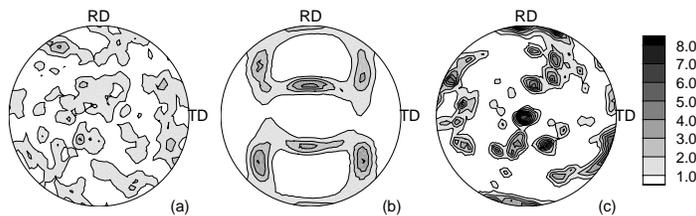


Figure 1: (100) pole figures showing (a) initial texture, (b) deformation texture for $e = -1.2$, and (c) recrystallized texture.

The initial, deformed and recrystallized textures are shown in Fig. 1. The initial texture is random. The deformation texture after a compressive strain of -1.2 is a typical face centered cubic (fcc) rolling texture. The texture after recrystallization shows strengthening of the Cube

component. The stored energy of deformation and the misorientation from the Cube orientation are shown in Fig. 2. Careful analysis revealed that the regions that are close to Cube orientation are surrounded by regions with higher stored energy. The mechanism of Cube nucleation involves the migration of the boundary between the Cube and the surrounding non-Cube regions, leading to the consumption of the non-Cube regions by the Cube regions. In the early stages of growth, some of the migrating boundaries had a misorientation close to $40^\circ \langle 111 \rangle$ thus indicating the presence of near $\Sigma 7$ boundaries. However, during the course of recrystallization, the special boundaries disappeared because of the changing orientation of the surrounding grains.

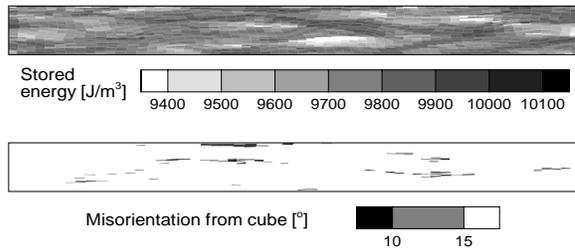


Figure 2: Stored energy of deformation (top) and the misorientation from Cube (bottom) for $e = -1.2$.

The evolution of the Cube component during recrystallization appears to depend upon the amount of deformation. Fig. 3 shows the temporal evolution of the cube for prior deformations of $e = -0.7$ and $e = -1.2$. The Cube fraction initially increases but then drops for $e = -0.7$ while for $e = -1.2$, the Cube fraction increases continuously. It appears that large strains favor stronger Cube fraction after recrystallization.

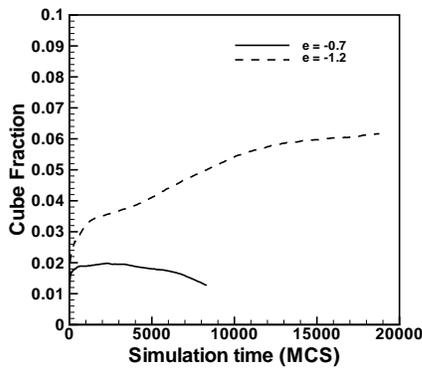


Figure 3: Effect of prior deformation on Cube evolution.

The current simulations involve several simplifying assumptions about the dislocation substructure. However, deformation structures are more complex in commercial alloys containing impurities and second phase particles. A theory that can deal with the evolution of dislocation substructures at the mesoscale for large deformations, and that can be coupled with crystal plasticity simulations, is needed in order to make realistic predictions of recrystallization in commercial alloys.

Acknowledgements

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