

Mesoscale Simulation of Texture Evolution in Particle Containing Aluminum Alloys

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Keywords: Recrystallization, Deformation substructure, Monte Carlo, particle stimulated nucleation, random texture

Abstract. Mesoscale simulations of hot deformation and recrystallization were carried out in single crystals, bicrystals and tri-crystals of aluminum with or without hard particles using a coupled finite element – Monte Carlo approach. The hard particles were located either inside a single crystal, or at the grain boundary in a bicrystal or at the triple in a tri-crystal. The deformation simulations captured the formation of high misorientation and localized stored energy in the vicinity of the hard particle. Recrystallization simulations captured the nucleation and growth of “random” texture components at the particle-metal interface during recrystallization following hot deformation. The effect of the amount of prior deformation and particle location within the microstructure on recrystallization texture and kinetics are described.

Introduction

When aluminum alloys containing micrometer-sized hard non-deformable particles are subjected to thermo-mechanical processing, distinct localized deformation zones form near the particles where the stored energy of deformation and crystallographic orientation are different from those in regions far away from the particle. Recrystallized nuclei form from these deformation zones when the deformation substructure is further annealed. This phenomenon known as particle stimulated nucleation (PSN) may result in nuclei orientations that are significantly different from those in the absence of hard particles [1]. Uninterrupted growth of these nuclei may significantly weaken other texture components that develop in particle-free regions. In a polycrystalline alloy containing coarse particles, the recrystallization texture component introduced by PSN depends upon the initial orientation of the grain, the microstructural location where the particle is situated, the particle shape and the amount of deformation.

Recently [2], Ferry and Humphreys carried out careful experiments of PSN using single crystals of aluminum containing hard silicon particles. By choosing a stable orientation such as Goss that is highly stable in plane strain compression due to slip on two (111) type planes that are equally inclined to the compression axis, the lattice rotations about the transverse direction (TD) in the vicinity of a coarse, non-deformable particle was predicted on the basis of a “slip shadowing” effect which is due to the blocking of slip in one set of (111) planes is near the particle. Subsequent recrystallization anneal resulted in the formation of a set of nuclei from the hard particles whose orientations corresponded to the highest TD rotations found near the particles. The above experimental observations were captured by a mesoscale model based on a coupled finite element – Monte Carlo technique developed by the authors [3]. The present work is an extension of the above mesoscale model to the hot deformation and recrystallization of bicrystals and tri-crystals of aluminum containing hard particles on grain boundaries and triple lines. The focus of this investigation is to capture the effect of prior deformation and microstructural location of the hard particle on the orientations of the particle stimulated nuclei.

Computational Approach

The mesoscale computational approach used in this investigation consists of three different steps. The first step is to use a finite element technique based on crystal plasticity to capture the distributions of stored energy and crystallographic orientation at various microstructural locations during hot deformation. The second step involves the extraction of the deformation substructure in each volume element based on the stored energy output. For this purpose it is assumed that the stored energy of deformation in a given volume element is equal to the surface energy per unit volume of the subgrains within the volume element. In order to calculate this quantity it is necessary to calculate the mean subgrain size in the element and the mean misorientation among subgrains in the element. The mean subgrain size is assumed to be a constant for all elements, and the element-to-element variation in the mean subgrain misorientation is calculated from the corresponding stored energy of deformation. The orientations of the subgrains are assumed to be randomly distributed about the orientation of the element given by the finite element simulation. The final step involves the evolution of the deformation substructure using a Monte Carlo technique. A detailed description of the computational approach for the above three steps is not provided here. The interested reader is referred to the recently published articles that describe the above methodology [4-6].

Computations

The hot deformation and recrystallization simulations were carried out for three different starting materials- single crystals, bicrystals and tri-crystals of aluminum. The single crystal orientations were either Cube or S or Copper. The bicrystals were made up of combinations of the above three orientations consisting of S-Cube, S-Copper and Copper-Cube. A tri-crystal consisting of Copper, S and Cube was also used in the simulations. The hard particle was in the form of a sphere which was positioned at various microstructural locations. In the case of the single crystal the hard particle was kept in the body center of the crystal. For bicrystals, the particle was positioned at the center of the grain boundary that formed at the mid-thickness plane. In the case of the tri-crystal the particle was at center of the triple line formed by the three crystal orientations. The samples were deformed in plane strain compression with or without the hard particle to a true strain of up to 0.4, and a temperature of 400C and at a strain rate of 0.1 s⁻¹. Deformation substructures were extracted for each of the above cases, and the evolution of the substructure during subsequent annealing was simulated using the Monte Carlo technique.

Results and Discussions

Single Crystal. Simulations of deformation and recrystallization clearly illustrate the formation of recrystallization nuclei from the deformation zones around the hard particles. Figure 1 shows the temporal evolution of microstructure during annealing of a Cube-oriented single crystal containing a hard particle in the form of contour plot of the rotation angle of the axis-angle pair representing the orientation of each site.

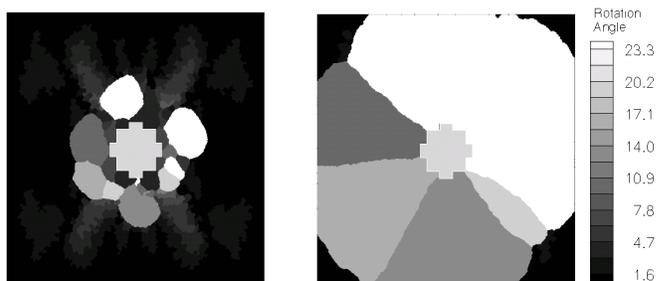


Fig.1 Temporal evolution of crystal orientations during recrystallization of a hot deformed Cube-oriented crystal with hard particle

Note that the nuclei orientations that form near the particle are significantly different from the near-cube orientations away from the particle. Therefore the particle stimulated nuclei (PSN) grow freely by consuming the rest of the matrix.

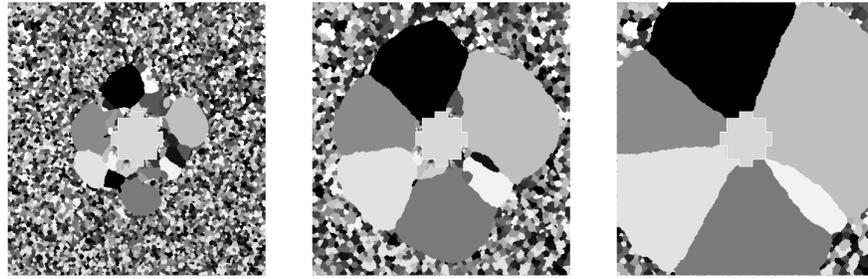


Fig 2. Temporal evolution of deformation substructure in Fig.1 above.

Figure 2 shows the same microstructures shown in fig.1 in the form of a contour plot of the site identification number that has a unique for each crystallographic orientation. In the absence of the hard particle, the material does not recrystallize since the deformation of the cube grain occurs without the development of locally large misorientations. In this case the substructure evolves through uniform subgrain growth as shown in figure 2.

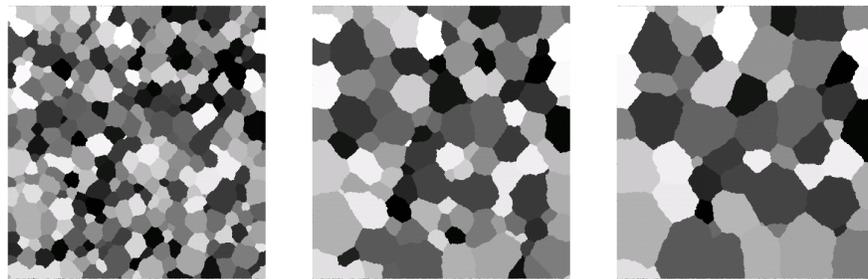


Fig. 3 Temporal evolution of deformation substructure during annealing of Cube-oriented crystal

The distribution of the stored energy of deformation after hot deformation is shown in Fig. 4 for the Cube oriented single crystal with and without the hard particle. In the absence of the particle, the stored energy is uniformly distributed in the crystal. However, for the crystal containing hard particle, locally high values of stored energy are found near the particle-matrix interface. The PSN nuclei are clearly associated with these high stored energy regions.

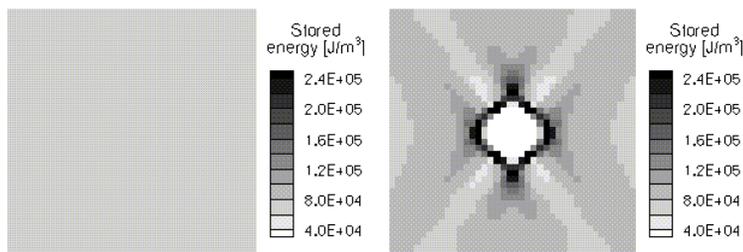


Fig. 4 Stored energy distribution after hot deformation ($\epsilon=0.4$) for the cube-oriented single crystal without (left) and with (right) hard particle

The strong influence of hard particle on nucleating recrystallized grains was also observed for the S and Copper oriented single crystals.

Bicrystals. In the case of bicrystals, the stored energy of deformation in the two crystal orientations is quite different across the grain boundary. Hence in the absence of the hard

particle, nucleation by strain induced boundary migration (SIBM) occurs during annealing of the deformation substructure, leading to recrystallization. The stored energy distribution after hot deformation of the S-Cube bicrystal with and without the hard particle is shown in Fig. 5.

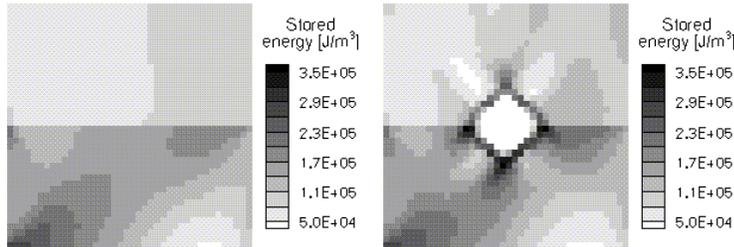


Fig. 5 Stored energy distribution in the S-Cube bicrystal after hot deformation ($\epsilon=0.4$)

The Cube grain situated at the top is seen to contain on an average a lower stored energy compared to the S oriented grain in the bottom. In the presence of the hard particle there exists a high stored energy region at the interface between the particle and the metal, although the overall stored energy difference between the S and the Cube regions is still maintained. The occurrence of nucleation by SIBM in the particle-free S-Cube bicrystal is shown in Fig. 6



Fig. 6. Temporal evolution of crystallographic orientations during annealing of hot deformed S-Cube bicrystal in the absence of hard particle

The lower stored energy in the Cube compared to S drives the interface downward so that S is consumed by the Cube. However, a couple of stray grains with high misorientation are formed in the Cube that grow and consume the Cube. However, these stray orientations probably originated due to end effects and should be disregarded.



Fig. 7 Temporal evolution of crystallographic orientations during annealing of hot deformed S-Cube bicrystal containing hard particle

In the presence of a hard particle, nucleation occurs both by SIBM and PSN as shown in Fig. 7. While the Cube orientation migrates downward by SIBM to consume the S in regions far away from the hard particle, PSN occurs in regions close to the particle resulting in the formation of grains that are significantly misoriented away from Cube. Here again, there are probably some stray nucleation associated with end effects, especially close to the right edge. Similar competing nucleation events were observed for the S-Copper and Copper-Cube bicrystals. The evolution of crystal orientations in the case of the S-Copper bicrystal is shown in Fig. 8. In the absence of

hard particle, columnar grains are observed while in the presence of the particle both columnar and equiaxed grains are observed.

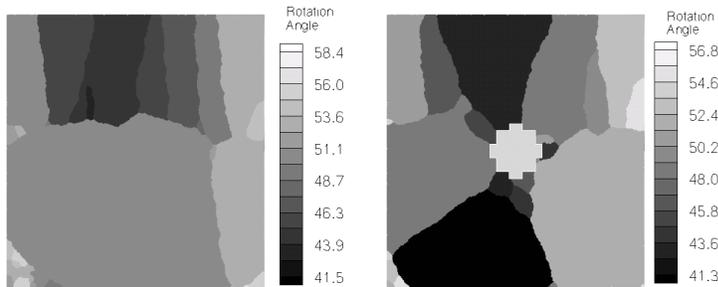


Fig. 8 Crystal orientations and grain microstructure in hot-deformed ($\epsilon=0.4$) and recrystallized S-Copper bicrystal without hard particle (left) and with hard particle (right).

Tri-crystals. The recrystallization behavior of tri-crystals is quite similar to that of bi-crystals in the sense that both SIBM and PSN mechanisms of nucleation operate simultaneously. The distribution of stored energy in the S-Cube-Copper tri-crystal with and without hard particle is shown in Fig. 9.

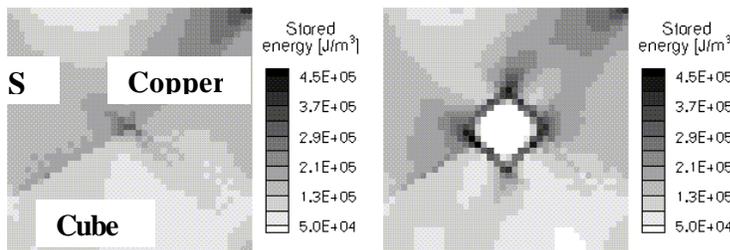


Fig. 9 Stored energy distribution in the S-Cube-Copper tri-crystal after hot deformation ($\epsilon=0.4$)

As in the case of the bicrystal, there is higher stored energy in the vicinity of the hard particle. The stored energy within the Cube is still on an average lower than in S and Copper. However, the stored energy difference is not clear along some segments of the Cube-Copper interface. The crystal orientations after annealing the hot-deformed tri-crystal with and without the hard particle are shown in Fig. 10. In the absence of hard particle nucleation occurs essentially by SIBM mechanism driven by stored energy differences across the S-Cube, S-Copper and Cube-Copper boundaries. However, when the hard particle is present, there are some nuclei that form in the vicinity of the particle resulting in the formation of certain new orientations in the fully recrystallized microstructure. For example, the orientation indicated by dark gray in the lower right hand side is caused by PSN and is absent in the particle-free tri-crystal.

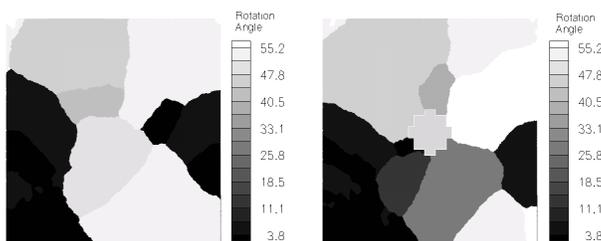


Fig. 10 Grain orientations after annealing the hot-deformed S-Cube-Copper tri-crystal without (left) and with (right) hard particle

Recrystallization Kinetics. While in single crystals free of hard particles recrystallization after hot deformation is very difficult or sluggish because of lack of misorientations in the deformation substructure, bi-crystals and tri-crystals do recrystallize quite easily even in the absence particles because of nucleation by SIBM mechanism. When hard particles are present, both SIBM and PSN are operating.

Therefore, it is interesting to compare the recrystallization kinetics of bicrystals and tri-crystals with and without the PSN mechanism. Careful comparisons of the recrystallization kinetics indicate that the presence of hard particles did not increase the recrystallization kinetics of bicrystals and tri-crystals for a prior deformation of $e=0.4$. The recrystallization kinetics appeared to be more sensitive to prior deformation than the presence or absence of hard particles. In fact, at lower deformations ($e=0.1$ and $e=0.2$) where PSN was found to be less effective, the particle-free system appeared to recrystallize faster than the particle-containing system. The reasons for the above effects are being analyzed.

Summary

A coupled finite element – Monte Carlo mesoscale technique was used to simulate the evolution of recrystallized microstructure and texture in hot-deformed single crystals, bicrystals and tri-crystals of aluminum with and without hard particles. The simulations captured the PSN mechanism operating in particle containing systems. PSN resulted in the formation of recrystallization texture components that were significantly different those in particle-free systems. No significant enhancement in recrystallization kinetics was observed in bicrystals and tri-crystals in the presence of particles. The reasons for such a behavior are being analyzed.

Acknowledgements

Research sponsored by the Office of Basic Energy Sciences, US Department of Energy, under contract DE-AC05-00OR22725 with UT-Batelle, LLC. The submitted manuscript has been authored by a contractor of the US Government under contract no DE-AC05-00OR22725. Accordingly, the US Government retains a non-exclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for US Government purposes

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