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Experimental Verification of Finite Element Simulation of Curvature-Driven Grain Growth in Al-Foil

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Abstract. Experimental results on grain boundary properties and grain growth that are obtained from Electron Backscattered Diffraction (EBSD) technique are compared with the Finite Element simulation results of an Al-foil with a columnar grain structure. The starting microstructure and grain boundary properties are implemented as an input for the three-dimensional grain growth simulation. In the computational model, minimization of the interface energy is the driving force for the grain boundary motion. The computed evolved microstructure is compared with the final experimental microstructure, after annealing at 550 °C. Good agreement is observed between the experimentally obtained microstructure and the simulated microstructure. The constitutive description of the grain boundary properties was based on a 1-parameter characterization of the variation in mobility with misorientation angle.

1 Introduction

Computational modeling and experimental characterization can be linked to study the interface properties and microstructural evolution of materials. However, new experimental data is needed for the comprehensive understanding of the kinetics of grain evolution. Grain boundary energy and mobility can be extracted with the measurement of the geometry of triple junctions between grain boundaries [1]. These experimental results on grain boundary properties that are obtained from EBSD technique can be used to simulate the topological changes in grain boundary motion.

Simulation [2, 3], theory [4], and the experimental observation [5] of grain boundary evolution of three-dimensional microstructures have been studied by several authors in the literature. A new technique for three-dimensional grain growth simulations was introduced by Kuprat [6]; this method utilizes gradient-

weighted moving finite elements (GWMFE) [7] combined with algorithms for performing topological reconnections on the evolving mesh [8]. In this model, minimization of the interface energy is the main driving force for the grain boundary motion. Interface motion is assumed to obey a linear equation ($v=\mu\kappa$) where μ is reduced mobility, v is the velocity, and κ is the curvature of the grain boundary. An important verification of the model is that the expected power law dependence of growth kinetics is obtained [9]. The gradient in mobility has a major effect on the growth process. In this paper, the orientation dependence of the boundary mobility is introduced in order to break the symmetry in GWMFE simulations. With the same simulation technique, both normal and abnormal grain growth in three-dimensions can be studied.
In the following section, a brief summary of experimental details is presented. This is followed by results from GWMFE simulation, then comparison with annealing experiment, and ending with a discussion and conclusion.

2 Experimental Procedure

The samples, which have 1x1cm^2 lateral dimensions and 120 μm thickness, were cut from 99.98% pure Al foil. The starting microstructure was polycrystalline and annealed conventionally in a horizontal tube furnace at a temperature of 550 °C for 9 hours in a N_2 environment. Under these conditions, a thin oxide layer is always present on the foil surfaces which prevents thermal grooves from forming along grain boundaries. After annealing, the specimen was quickly removed from the furnace and quenched under water, then mounted on a glass slide. The sample was then electro-polished at room temperature for 60 seconds with a solution of 730 ml ethanol, 100 ml ethylene glycol monobutylether, 78 ml perchloric acid, and 90 ml distilled water. A strong cube texture, {100}<001>, was observed after the annealing, with a small number of grains deviating from cube texture. In order to locate the scanning area, microhardness indents were used. A second annealing for 20 minutes at 550° C, under the same conditions, was performed to generate the final microstructure.
A secondary electron image was recorded from the surface of the crystal and the grain morphology obtained by applying the Gabor Wavelet [10] image-processing algorithm, which detects the boundaries. The orientation information was extracted from EBSD patterns using standard EBSD methods. EBSD scans were performed in beam control mode on the Al foil on an XL-40 Philips FEG Scanning Electron Microscope. A 52 mm diameter phosphor scintillation screen was used to observe the EBSD patterns, and the working distance (sample surface to gun tip) was fixed throughout the data acquisition process. Scan areas of 800x800 μm^2 with a three-μm step size were used. It is important to note that the scan size was chosen so as to minimize the possible errors and accurately measure orientation in the scan plane [11].

3 Simulation Details

To simulate the grain structure evolution, an area of 400x400 μm^2 was chosen from the scanned experimental microstructure. It is assumed that the grains are columnar in nature and as such, their boundaries are perpendicular to the surface [12]. Hence, the area is extruded in the third direction to create the three dimensional mesh. In the initial configuration, the microstructure consists of 26 grains which were used to construct a three-dimensional finite element mesh of 4328 tetrahedral elements in which the mesh lines conformed to the grain boundaries. Each grain is meshed independently and combined with LAGRIT [13] mesh generation software. The initial lattice orientation for each grain is then assigned based on the EBSD measurements. The total volume of the structure is kept constant during the simulation and exterior boundaries are assumed to be quasi periodic. The GWMFE method minimizes the function, $\int(v-\mu\kappa)^2 dA$ over all possible values of dx/dt values, where A is the surface area, x is the vector containing coordinates of all interface nodes, and t is the explicit time. All other details related to GWMFE method can be found in reference [6]. The GWMFE method solves an ordinary differential equation, where computational time scales with the number of tetrahedral elements in the simulation box. In an SGI-O2/R10000, our simulations took approximately 10 minutes of CPU time.

Anisotropy of the model is introduced by a single parameter dependence in the grain boundary mobility. In the calculations, the relative mobility in columnar Al-foil depends on misorientation angle and is low for small misorientations but undergoes a sharp transition to high mobilities between ten and fifteen degrees misorientation. [12]. It is assumed that capillarity is the only driving force for boundary migration. We should also note that relative mobility values are calculated based on the low angle boundaries and all high angle boundaries are considered to behave similarly. The local equilibrium condition at triple junctions is determined by the grain boundary energies. Relative boundary energies and mobilities were extracted through a statistical/multiscale analysis [14] and are given in Table 1 for the pre-annealed microstructure. The variation in energy was not considered in these simulations, however. The first column in Table 1 indicates the relative grain boundary mobility. The second column denotes the grains that have an interface with the relative mobility value in the initial microstructure.

4 Results

The simulated results of microstructure evolution show large differences between isotropic and anistropic dependence in terms of grain morphology. It was found that when starting with identical initial microstructures, varying the mobility dependence caused significant differences in the final microstructure. Isotropic (i.e., mobility is constant and equal at all boundaries) and anisotropic simulation results are contrasted in Fig 1. In the isotropic case, Fig 1c, the final microstructure has

preserved the larger grains, but the smaller grains have disappeared, as would be expected from having fewer than six sides. In contrast to the simulation with isotropic properties, examination of the experimental microstructure, Fig 1b, reveals that four sided grain number 16 did not disappear after annealing. Additionally, some of the small grains (number 13 and 20) shrank but preserved their identities. In addition to these grains, there are also some important topological changes in the final annealed structure. Grains numbered 8, 10, 19 vanished completely, and numbers 21, 22, 25 coalesced into grain number 21. As shown in Fig 1d, for the case of anisotropic simulation [15], grain topology is correctly predicted except for the grain number 8.

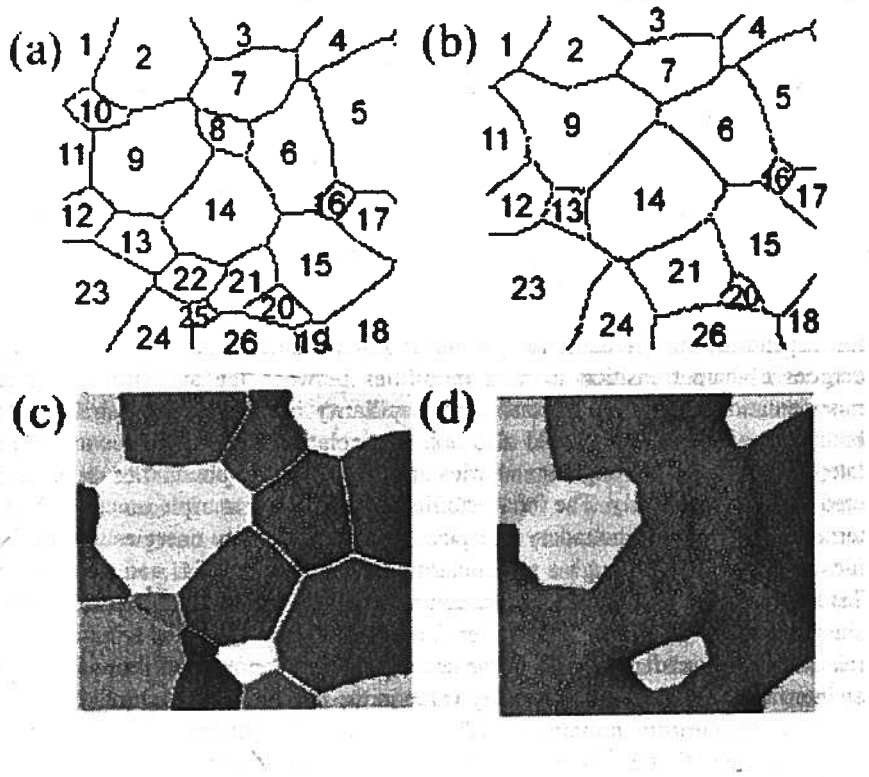

Fig. 1. Comparison of experiment and predicted grain morphology: Experimentally obtained microstructure (a) before annealing (500 μm by 500 μm), (b) after annealing, and simulated final microstructure (top view) with (c) isotropic properties (d) anisotropic properties.

Table 1. Experimentally measured relative mobility values of each grain interface.

Relative mobility values	Grain numbers for each grain interface
0.03239	3-4 4-7 5-17 7-4 9-8 11-9 25-21
0.00355	2-9 5-6 5-16 7-9 13-23 15-21 19-20 19-26
0.037287	2-7 4-6 6-16 9-13 12-13 21-26 25-26
0.0239	2-10 3-7 6-14 15-16 15-19 25-24
0.029	6-8 7-8 12-9 13-14 15-18 16-17 19-18
0.005728	6-15
0.00934	6-7
0.0107	9-10 15-20 23-24
0.05033	24-26
0.254698	14-21
0.282448	14-9
0.404045	1-2 1-10 1-11 8-14 13-22 14-15 14-22 22-21
0.8279	22-25 23-22 24-22

5 Discussions and Conclusion

The comparison between the experiment and computed results provides important details related to grain evolution. A strong similarity is observed between growth experiments and anisotropic three-dimensional GWMFE simulations. It is clear from the simulation results that anisotropy in the grain boundary energy and mobility has a major effect on growth process and the growth is driven by these parameters. Combining the three dimensional grain growth simulations results with experimental outputs will provide a computational tool for the discovery of some new methods to design meso-structures.

Absolute grain boundary mobility values were measured by Gottstein et. al. in Aluminum bi-crystals and reduced mobilities of order 10^{-8} to 10^{-7} $m^2.s^{-1}$ for two similar types of high angle boundary and various purities were obtained [16]. For curvatures about 100 μm^{-1} (i.e., boundary interface between grain 1 and 2) suggest migration rates of approximately $v=A\kappa=5.10^{-8}$ 100 = 5 $\mu m.s^{-1}$. These migration rates are high when compared to the estimated migration rates in the experiment (0.1 $\mu m.s^{-1}$). We note, however, that the purity of the material used in the bi-crystal experiments was significantly higher than that in our experiments. For the comparison of simulation times with experiment, these values can be used to estimate the migration distance during the annealing at various temperatures.

We conclude that the present simulation method verified the experimentally determined microstructure. The simulation model was an idealized grain growth case, and future extensions may be made to systems that are more complex and these further studies should foster a more comprehensive understanding of grain

growth. Extension of this work to a five-parameter dependence of grain boundary energy and mobility is in preparation.

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