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# Effect of anisotropic grain boundary properties on grain boundary plane distributions during grain growth

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**Abstract**

The effects of anisotropic grain boundary properties on the evolution of boundary plane distributions were studied using three-dimensional finite element simulations of normal grain growth. The distribution of boundary planes was affected by energy anisotropy whereas no effect was observed for comparatively larger mobility anisotropy.


*Keywords:* Grain growth; Grain boundaries; Grain boundary energy; Grain boundary mobility; Anisotropy

## 1. Introduction

The distribution of grain boundary types in a polycrystalline material has been shown to affect its bulk properties, e.g. corrosion resistance [1]. Grain boundary populations are specified by the grain boundary character distribution, $\lambda(\Delta g, n)$, which is the relative areas of distinguishable grain boundaries parameterized by their lattice misorientation ($\Delta g$) and boundary plane orientation ($n$) [2]. Previous experimental work has demonstrated that significant texture can appear in grain boundary character distributions and that low energy boundaries occur in these distributions with greater frequency than higher energy boundaries [2,3].

The influence of anisotropic grain boundary properties on grain growth has been examined previously using two-dimensional grain growth simulations [4–7]. The conclusion from each of these studies was that the grain boundary energy anisotropy was more influential than the mobility anisotropy in determining the distribution of grain boundary types. However, two-dimensional simulations are unable to reproduce the topological complexity of three-dimensional systems or to represent the five-dimensional domain of grain boundary character. A number of papers describe three-dimensional grain growth simulations, but these were calculated under the assumption of isotropic grain boundary properties [8–12]. One of these methods (GRAIN3D) was recently used to simulate growth in a system with anisotropic grain boundary energies and successfully reproduced an experimentally observed grain boundary character distribution [13]. The purpose of the present work is to examine the relative effects of anisotropic interfacial energy and mobility on the grain boundary character distribution in materials undergoing normal grain growth in three dimensions.

## 2. Simulations

The simulation results are provided by a three-dimensional finite element model using the code GRAIN3D,

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which is described in detail elsewhere [12,14]. Briefly, GRAIN3D approximates the interfaces in a grain boundary network as a mesh of triangular elements. Nodal velocities are calculated by minimizing a functional that depends on the local geometry of the mesh and the (anisotropic) properties of the grain boundaries. Grain boundary properties are assigned on the basis of the grain boundary character. The interfacial energy $\gamma(\Delta g, \mathrm{n})$ and mobility $M(\Delta g, n)$ functions we use are defined by an interface plane scheme, in which we imagine each boundary to be comprised of the two surfaces bounding the grains on either side of the interface [2]. Taking $n^1$ to be the interface normal pointing into grain one and indexed in the crystal reference frame of that grain, and $n^2$ to be the interface normal pointing into grain two and indexed in the crystal reference frame of that grain, the energy and mobility are assigned in the following way:

$$\gamma = (E(n^1) + E(n^2))/2 \tag{1}$$

$$M = (\mu(n^1) + \mu(n^2))/2 \tag{2}$$

where the functions $E(n)$ and $\mu(n)$ are chosen as

$$E = \alpha\left[\sum_{i=1}^{3}(|n_i| - 1/\sqrt{3})^2\right] + 1 \tag{3}$$

$$\mu = \beta\left[\sum_{i=1}^{3}(|n_i| - 1/\sqrt{3})^2\right] + 1 \tag{4}$$

where $\alpha$ and $\beta$ are positive constants. Minima for either functional then occur with normal vectors of $\langle 1\,1\,1\rangle$ type and maxima with normal vectors of $\langle 1\,0\,0\rangle$ type, as illustrated in Fig. 1. Note that Eqs. (3) and (4) imply cubic crystal symmetry. The choice of cubic symmetry minimizes the number of grain boundaries necessary to produce a statistically significant data set and simplifies the analysis. The form of the energy function is also motivated by experimental observations in Al [15].

The anisotropy of the energy function is controlled by the parameter $\alpha$. With $\alpha = 0$ the function is isotropic and with $\alpha = 0.2957$, the ratio of the minimum to maximum energy is 1/1.25. Similarly, $\beta$ controls the mobility anisotropy; when $\beta = 0$ the mobility is isotropic and when $\beta = 13.60$, the ratio of the minimum to maximum mobility is 1/12.5. Simulations were run for four situations: (1) isotropic energy and mobility, (2) isotropic energy and anisotropic mobility, (3) anisotropic energy and isotropic mobility, and (4) anisotropic energy and mobility.

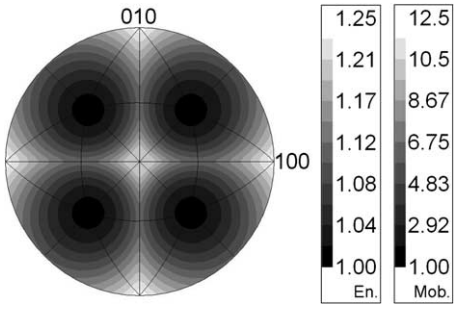


Fig. 1. Energy (En.) and mobility (Mob.) as a function of interface normal vector, [001] stereographic projection. Scale values are in arbitrary units.

The initial microstructure for each simulation was produced from a regular volume-filling tetrahedral mesh of the unit cube. This mesh consisted of 500,000 tetrahedra. Grain centers were assigned randomly to individual tetrahedra with the condition that no grain centers lie in adjacent tetrahedra. After assigning 5000 grain centers, all remaining tetrahedra were assigned to the nearest grain. To produce a relatively equiaxed structure for the simulations, isotropic grain growth was simulated until about half of the grains remained. The mesh that results from this procedure was taken as the starting point for our simulations with anisotropic interfacial properties.

In our simulations, individual grains are represented by collections of tetrahedra, and so any grain boundary is represented by a set of triangular elements. For each triangular element, the lattice misorientation is parameterized by three Euler angles $(\phi_1, \Phi, \phi_2)$ and the boundary orientation is parameterized by two spherical angles $(\phi, \theta)$. We use discrete binning to measure the relative populations of grain boundaries, with the five-dimensional space of boundary types partitioned into bins of equal volume with sizes of $\Delta\phi_1 = \Delta\phi_2 = \Delta\phi = 10^\circ$ and $\Delta\cos\Phi = \Delta\cos\theta = 1/9$. This discretization results in approximately $6.5 \times 10^3$ physically distinct grain boundary types. We assume that making $1.3 \times 10^5$ observations, i.e. 20 times the number of distinct boundaries, will produce sufficiently accurate boundary populations. Although each face separating two grains is represented in GRAIN3D as a number of triangular elements, the orientations of the triangles on each face are usually similar. Therefore, as a lower bound, we assume that each face contributes only one distinct orientation. The average grain is bounded by 13–14 faces, each of which is shared with a neighbor grain, and therefore contributes an average of about 6.5–7 observations. It is therefore necessary to have data from more than 20,000 grains to ensure that the total number of observations is at least 20 times the number of distinguishable boundary types. The results from 20 simulations (51,560 grains initially) have therefore been combined to study each case. The results presented here arise from the analysis of data sets with >20,000 grains.

## 3. Results

The grain boundary plane distributions reached a steady state after a modest amount of growth, as found