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Effect of Anisotropic Interfacial Energy on Grain Boundary Distributions During Grain Growth

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Abstract. Through simulations with the moving finite element program GRAIN3D, we have studied the effect of anisotropic grain boundary energy on the distribution of boundary types in a polycrystal during normal grain growth. An energy function similar to that hypothesized for magnesia was used, and the simulated grain boundary distributions were found to agree well with measured distributions. The simulated results suggest that initially random microstructures develop nearly steady state grain boundary distributions that have local maxima and minima corresponding to local minima and maxima, respectively, of the energy function.

Introduction

It is well known that the properties and area fractions of various grain boundary types in polycrystals have a dramatic effect on macroscopic materials properties. The goal of the present study is to examine the quantitative relation between grain boundary energies and the distribution of grain boundary types that result from grain growth.

In keeping with the prior work, we parameterize the five-dimensional space of grain boundary types using three parameters to describe the lattice misorientation and two parameters to describe the orientation of the grain boundary plane. Of particular interest is the observation that at fixed misorientations, there is significant texture in the distribution of the grain boundary planes and planes with low surface energies appear more frequently [1-3]. Here we use simulation to test the idea that the observed distributions arise because of the grain boundary energy anisotropy. In comparison to the experiments, the simulations are advantageous because they make it possible to monitor the time evolution of the distribution and to independently determine the influence of different grain boundary properties on the development of the distribution.

A moving finite element program, GRAIN3D [4], has been developed with the capability to incorporate anisotropic grain boundary energy and mobility functions into grain growth simulations. We have modified the GRAIN3D code to simulate grain growth with anisotropic grain boundary energy and isotropic mobility.

Procedure

The simulations performed in this study required minor modifications of the GRAIN3D code. Specifically, a new function for calculating grain boundary energy from geometry was introduced. We used a function that is considered to be a reasonable estimate for the observed energy anisotropy of magnesia; the grain boundary energy was assumed to be the sum of the surface energies of the two opposing boundary planes [3]. The surface energy function used is that proposed by Saylor et al. [5].

The area elements in GRAIN3D are linear triangles. Boundaries between grains consist of many triangular elements that approximate smooth surfaces. The grain boundary energy, based on calculations of area and orientation, was computed separately for each individual triangular boundary element.

The same mesh was used to initiate each simulation, and for each simulation the orientation of each grain was assigned randomly. This mesh had been previously produced by isotropic growth of a structure with finer grains and had grain shapes and a size distribution typical of isotropic grain growth. This mesh contained 2758 grains, and a total of sixteen simulations (2758x16 = 41248 grains total) were completed.

Grain boundary types are usually characterized by their macroscopic geometry. For arbitrary boundaries, this includes a minimum of three real parameters to describe grain boundary misorientation and two real parameters to describe the boundary plane with respect to one grain; the reader is referred elsewhere [6] for more details. A five-parameter array was then used to store the total area of each boundary type. Specifically, for our grain boundary distributions we partition the space of Euler angles (misorientation) into equal volume elements and partition the unit sphere (boundary normal vectors) into equal area elements, all angles having a resolution of approximately 10°. We take as limits for Euler space the cube with 0-90° sides, and for the space of boundary normal vectors only those with positive z component, giving 9x9x9x36x9 = 236196 discrete bins. Each triangular element accumulates boundary area in multiple points of the array due to grain boundary symmetries. This array was normalized so as to represent the multiple random distribution (MRD) value of each boundary plane type at all fixed misorientations.

Grain faces generally consist of many triangular elements with similar orientations, thus relatively few distinct grain boundary types are represented by a single grain face. A large number of grains is therefore necessary for statistically reasonable results. We have found that the number of boundary types *not* represented in the simulation becomes nonzero when the total number of grains drops below approximately 10000 and increases steadily thereafter.

Results and Discussion

Steady-state behavior. Both the misorientation distribution and the distribution of boundary planes show steady state behavior after some initial period. We use the distribution of boundary planes, independent of misorientation, to illustrate the onset of steady state behavior. Fig. 1 shows the fraction of grains and the fraction of boundary area as a function of time. Fig. 2 shows (as stereographic projections) the distribution of boundary planes at various times. Fig. 3 shows the maximum and minimum values of the boundary plane distribution as a function of time. It is clear from these plots that a steady state distribution of boundary planes is reached after the number of grains in the sample has decreased by more than about 25-40% (loss of approximately 10000-16000 grains) or, equivalently, after a reduction of total boundary area of more than 10-20%. The distribution exhibits increasing statistical noise after output 20 (11070 grains).

Comparison with measured distributions. The grain boundary distributions from simulations with GRAIN3D are very similar to those measured in previous studies of magnesia [1]. Fig. 4 compares plots of boundary plane distributions for various fixed misorientations obtained with the GRAIN3D simulations with equivalent plots of measured distributions. The success of the simulations in this respect suggests that the energy anisotropy alone may account for the development of anisotropic grain boundary plane distributions. The influence of anisotropic mobility and the initial crystallographic texture will be examined in the future.

Boundary plane distribution. The misorientation distribution function (MDF) did not change significantly during the simulation. However, anisotropic grain boundary energy had a noticeable effect on the distribution of grain boundary planes, Fig. 2-4. In Fig. 5 we have plotted boundary plane distributions for several fixed misorientations along with the energy function. There is a clear

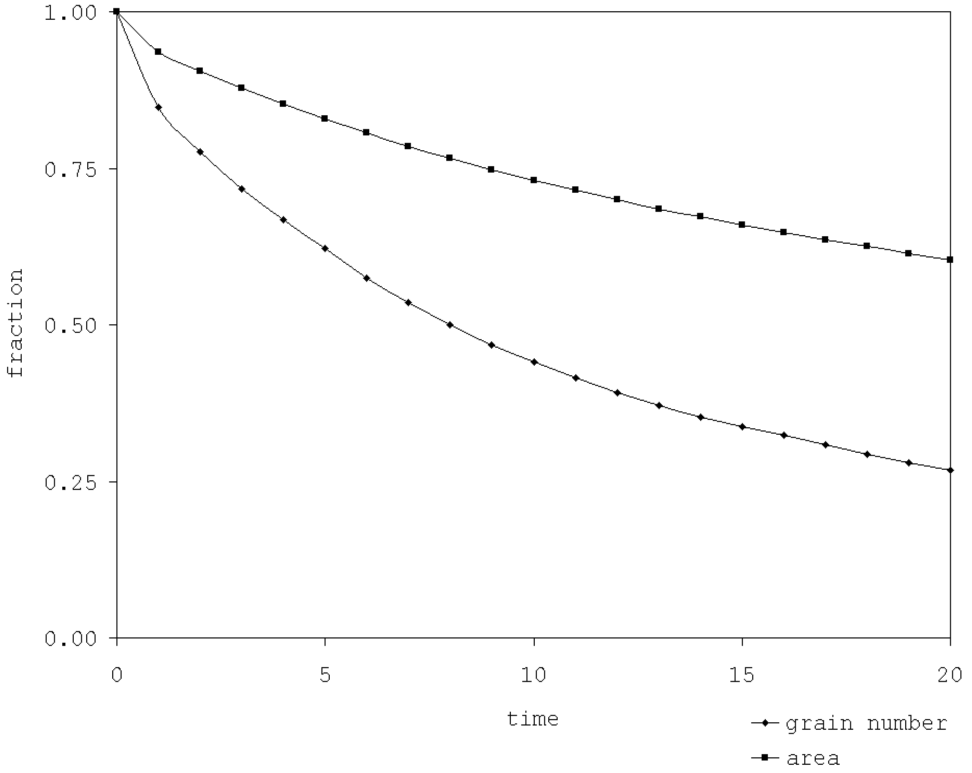
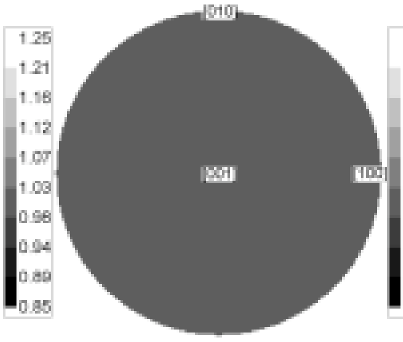


Fig. 1. Relative grain number and boundary area as a function of simulation output time.



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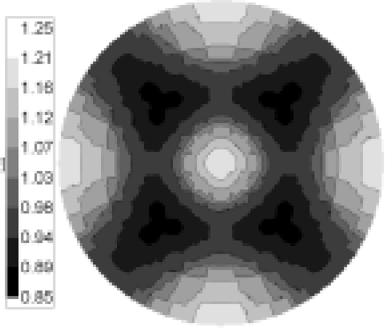

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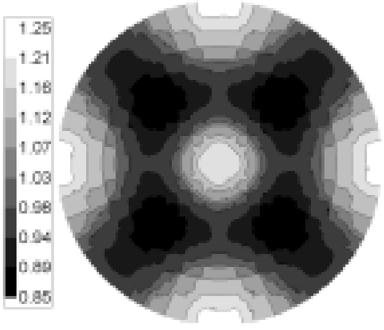

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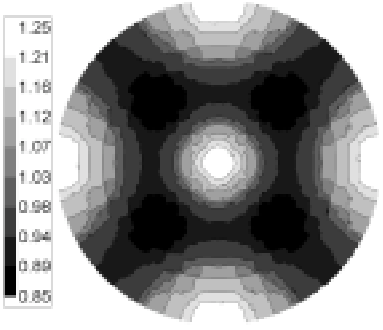

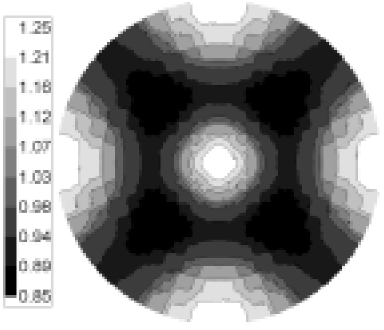

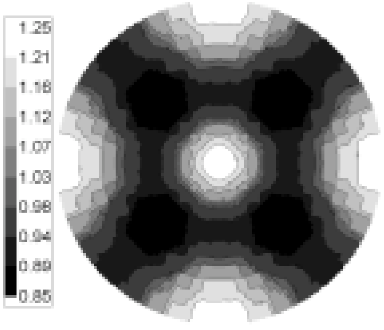

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Fig. 2. Boundary plane distributions averaged over all misorientations. Plots are (001) stereographic projections with [100] pointing right. All scale values in multiples of random distribution (MRD). Simulation output times given below scales correspond to those in Fig. 1.

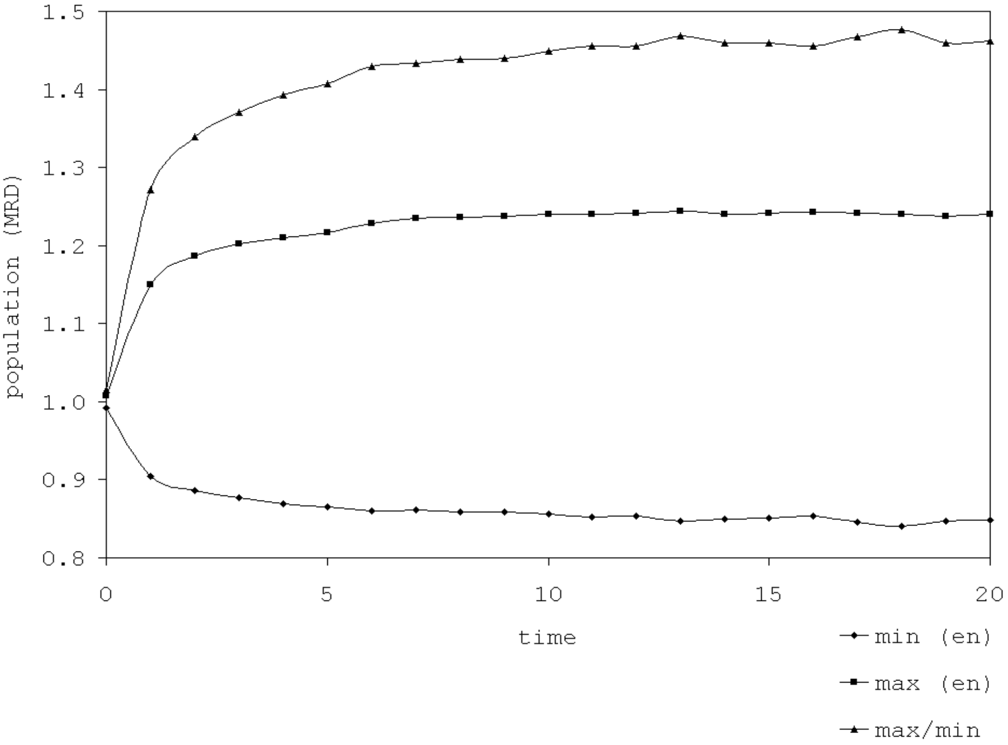
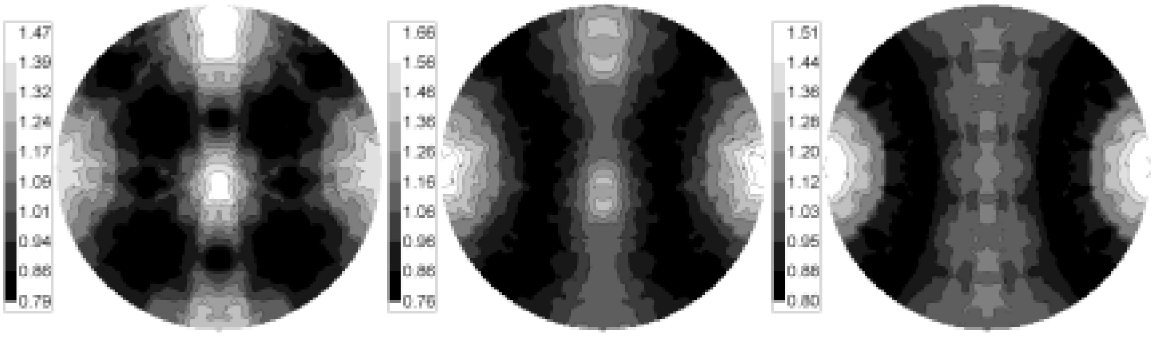
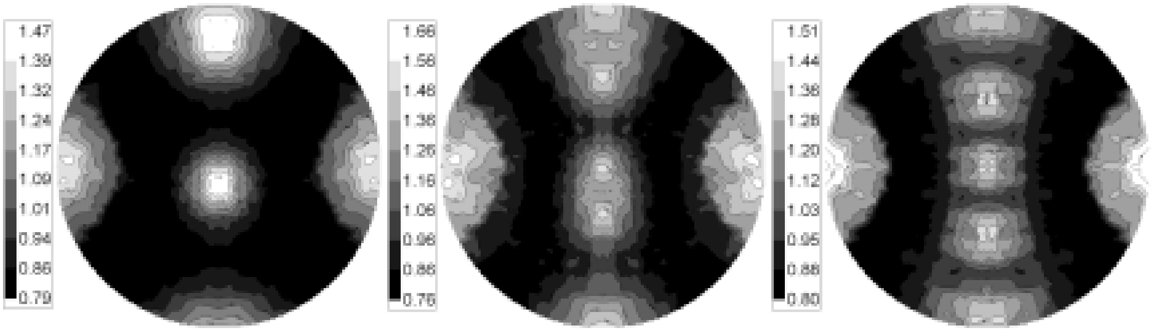


Fig. 3. Plane average extrema as a function of simulation output time.

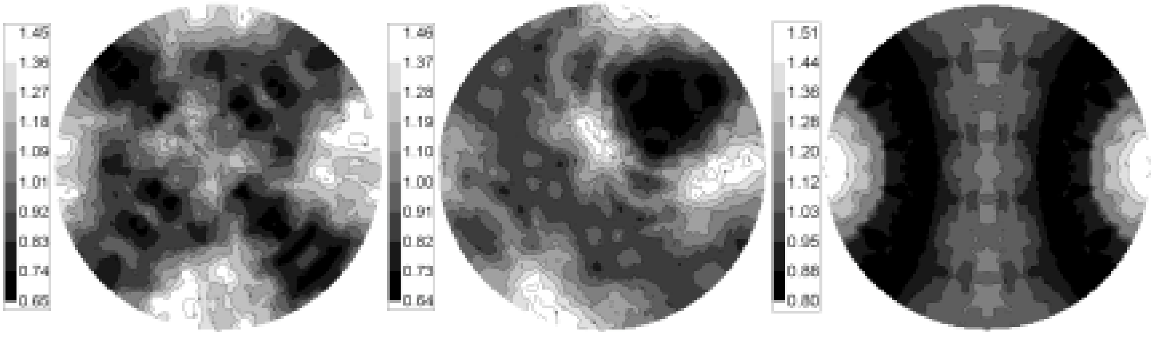


simulated, 25° about [100] simulated, 35° about [100] simulated, 45° about [100]

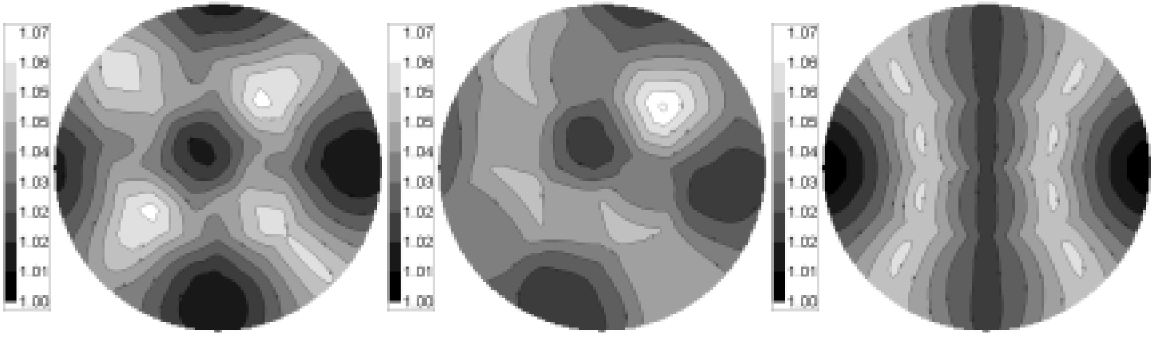


experimental, 25° about [100] experimental, 35° about [100] experimental, 45° about [100]

Fig. 4. Comparison of simulated and measured boundary plane distributions for three different fixed misorientations about [100]. Plots are (001) stereographic projections with [100] pointing right. All scale values in multiples of random distribution (MRD). Simulation output time = 10.



population, 30° about [110] population, 45° about [111] population, 45° about [100]



energy, 30° about [110] energy, 45° about [111] energy, 45° about [100]

Fig. 5. Comparison of simulated boundary plane distributions with maps of the energy function. Plots are (001) stereographic projections with [100] pointing right. Scale values in multiples of random distribution (MRD) for boundary populations and in arbitrary units (min = 1.00) for maps of the energy function. Simulated output time = 10.

inverse relation between energy and population that appears to be linear in most cases. However, for misorientations where the energy function is not everywhere convex, this relation is not linear. Fig. 6 compares energy for a boundary type (relative to the average energy 1.040) with the MRD value from the simulated data. A strictly inverse energy-population relationship would place all points in either the upper left or lower right sections of this plot. We find that only 71% of the boundary types follow this inverse relation. In general, it appears that local maxima in the energy function correspond to local minima in the population, as well as the converse, but a strict inverse relation does not hold. We will present a functional form for this relation in an upcoming publication [7].

Conclusions

We have simulated grain growth with anisotropic energy and isotropic mobility using GRAIN3D. Grain boundary distributions under these conditions appear to reach a steady state after some initial period. The distribution of grain boundary planes for a fixed misorientation appears to be dependent on the energy function for that misorientation, specifically, an inverse relation exists for local extrema.

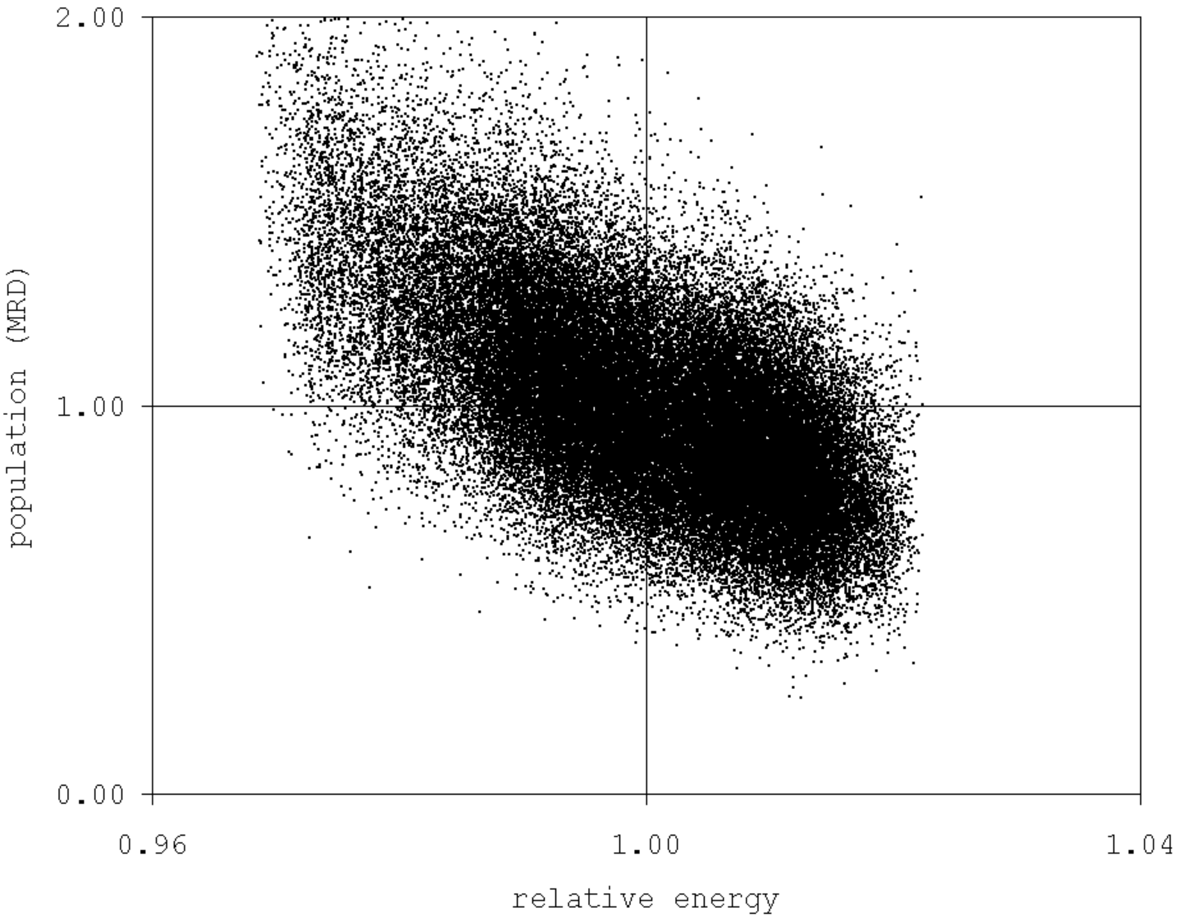


Fig. 6. Plot of population (MRD) and energy (relative to average) for each grain boundary type. The trend confirms inverse behavior for most boundary types but there is significant scatter.

Acknowledgment

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