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Grain growth and grain translation in crystals

Kevin McReynolds [a, *], Kuo-An Wu [b], Peter Voorhees [a]

[a] Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA
[b] Department of Physics, National Tsing Hua University, Hsinchu, 30013, Taiwan, ROC

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ABSTRACT

Grain growth is generally driven to minimize the overall grain boundary energy. However, for low-angle grain boundaries the requirement that lattice planes be continuous across the boundary gives rise to a coupling between the normal motion of the grain boundary and the tangential motion of the lattice. We show through phase-field crystal simulations this coupling in polycrystalline systems can give rise to a rigid body translation of the lattice as a grain shrinks. The process is mediated by significant climb of the dislocations in the boundary and dislocation reactions at the trijunctions. Thus the grain growth process is coupled to vacancy diffusion processes as well as the dynamics of grain trijunctions. Moreover, grain shrinkage can cease because of dislocation behavior near the trijunction, illustrating that this coupling can have an influence on the grain growth process in polycrystals.

1. Introduction

Systems composed of domains of differing crystallographic orientation occur in systems ranging from dusty plasmas to colloidal crystals and polycrystalline materials [1,2]. Grain boundaries are classically understood to move in a way that reduces the total interfacial energy, in a manner similar to soap froths. However, unlike soap froths there can be a coupling between the normal motion of the grain boundary (grain growth) and the tangential motion of the lattice [3–15]. For example, low angle grain boundaries contain a unique constraint that lattice planes must be continuous across the grain boundary except at the dislocations that lie in the boundary. This induces a tangential velocity of the lattice that is proportional to the normal velocity of the grain boundary by the coupling parameter β, which is equal to the misorientation in the small angle limit. This coupling can either induce a stress during motion, or allow the boundary motion to couple to an applied stress. However, this coupling is surprisingly general, since it also occurs at high angle grain boundaries [4,9]. For a circular grain embedded in a single grain, this gives rise to a rotation of the lattice as the grain shrinks [4,16–21]. However, the effects of the coupling in the more general and widely observed case where there are multiple grains and grain boundary trijunctions has not been investigated.

We study the effect of coupling on a system with a circular grain embedded in a symmetric tilt planar grain boundary using the phase-field crystal (PFC) model. The PFC model is uniquely suited to studying nanoscale grain growth because it captures atomic motion over diffusive timescales. Atomic resolution is required to resolve the lattice continuity across the grain boundary and, as we will show, the diffusive timescales are necessary to observe grain growth. The PFC model has been previously used to study phenomena in solid state grain growth. Dislocations form spontaneously in the PFC model to relieve strain (e.g. at low-angle grain boundaries) and move through the crystal via climb and glide mechanisms [22,23]. For low-angle grain boundaries, the grain boundary energy follows the Read-Shockley relationship [16,24,25]. The Asaro-Tiller-Grinfeld instability was studied using the PFC model, and the results were in quantitative agreement with continuum theory [26,27]. The PFC model has also been used to study coupling during grain growth [16,17,28–30], and the results match well with molecular dynamics simulations [9].

For this study, the symmetric tilt geometry was chosen as the worst case scenario for grain rotation according to Cahn and Taylor [3] where the rotation induced by the first matrix grain would be exactly opposed by the rotation induced by the second matrix grain, and grain growth would be arrested due to this geometric frustration. We find that the coupling of the normal grain boundary motion and lattice translation leads to grain growth that is markedly different from that of a simple soap froth. Furthermore, in contrast to the case of an isolated grain, when a grain is embedded at a symmetric planar tilt grain boundary the coupling

* Corresponding author.
E-mail address: k.s.mcreynolds@gmail.com (K. McReynolds).

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between the normal motion of the boundary and the tangential motion of the lattice gives rise to a rigid body translation of the lattice without rotation as the grain shrinks. The process is mediated by significant climb of the dislocations in the boundary, and dislocation interactions at the trijunctions. Since climb is involved, this mechanism for grain growth depends on the self-diffusion process in the bulk crystal. Moreover, we find that grain shrinkage ceases if certain dislocation reactions do not occur at the trijunctions.

2. The phase-field crystal model

We use the dimensionless PFC model that employs the free energy functional [24,25],

$$\mathcal{F} = \int d\vec{r}\left\{\psi\left[-\varepsilon + \left(1+\nabla^2\right)^2\right]\frac{\psi}{2} + \frac{\psi^4}{4}\right\} \tag{1}$$

where $\mathcal{F}$ is the dimensionless free-energy density, ψ is the dimensionless atomic density field defined as time-averaged density of atoms relative to a reference value, and ε is a temperature parameter. The evolution of ψ follows the standard phase-field evolution for a conserved order parameter, with t as the dimensionless time

$$\frac{\partial\psi}{\partial t} = \nabla^2\frac{\delta\mathcal{F}}{\delta\psi} = \nabla^2\left[-\varepsilon\psi + \left(1+\nabla^2\right)^2\psi + \psi^3\right] \tag{2}$$

where the equations have been nondimensionalized by the length scale given by the lattice spacing and time scale related to the lattice spacing and diffusion coefficient [25,31]. The PFC model has roots in classical density functional theory (CDFT). From CDFT the order parameter ψ can be viewed as a dimensionless time-averaged atomic density field. Peaks in ψ can be considered as the positions of the atoms. However, these peaks also occur at lattice sites. As the height of a peak decreases, the vacancy concentration at that site increases until the site disappears. Thus while the average density of the system is conserved, the number of peaks (or lattice sites) in the system is not, since lattice sites can be created and destroyed by physical mechanisms such as dislocation climb. The simplicity of the PFC model allows us to identify the system-independent mechanisms responsible for grain growth in polycrystalline systems.

3. Results and discussion

3.1. System description

The PFC model, Eq. (2), was solved with periodic boundary conditions using $\varepsilon = 0.1$ (a relatively high temperature, close to the solid-liquid phase boundary) unless otherwise stated, the average density $\overline{\psi} = -0.195$, and a hexagonal two-dimensional lattice. The initial density profile is given by the single-mode approximation, which then relaxes over short timescales. The three-grain system consists of circular grain embedded in a symmetric tilt planar grain boundary with a misorientation of $\pm\theta$ between the embedded grain and each of the two outer grains, and a misorientation 2θ of between the two outer grains (Fig. 1). The initial diameter of the embedded grain was set as not more than 60% of the smallest dimension of the rectangular computational domain. The values of θ are limited due to the periodic boundary conditions. Misorientations of 3.4°, 5.2°, and 7.1° were chosen using the method of Mellenthin et al. [32]. The 5.2° system was tested using square meshes with 768^2, 1152^2, and 2304^2 mesh points. The mesh spacing

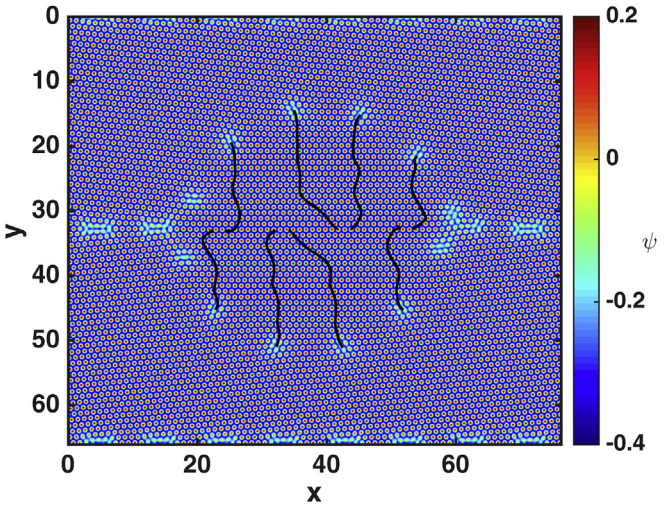

Fig. 1. An example of the density field near the beginning of the simulation for the smallest system size. The lighter areas, those with low density, are where the periodicity of the lattice is interrupted by dislocations. There are peaks in the density field at each lattice point. The black lines indicate the path of the dislocations as the grain shrinks.

was held constant yielding three different system sizes with three different initial sizes of the embedded grain. The mesh spacing varied slightly between the x and y directions because of the periodicity condition but was held constant between system sizes. The 3.4° and 7.1° systems were computed using the 1152^2 system size. The mesh spacing varies slightly between the three different misorientations to maintain periodicity but is kept less than $\sqrt{3}/16$, which is required for numerical accuracy. All distances in this paper are in units of the one-mode lattice parameter, but the system size was set using the equilibrium lattice parameter corresponding the free-energy minimum.

3.2. Grain translation

As the embedded grain shrinks, the dislocations move towards the plane of the planar bicrystal grain boundary in a path that is approximately perpendicular to it (Fig. 1). This maintains the constant average spacing of the dislocations, indicating that the misorientation does not change and therefore no rotation occurs. However, we find that there is rigid body tangential *translation* of the embedded grain (in the $-x$ direction), and that this motion exists in all of the initial conditions employed at $\varepsilon = 0.1$. The translation was significant: over four lattice parameters in the largest system.

If this translation is the result of the coupling described in Section 1, the coupling parameter follows from the slope of the displacement of the embedded grain's lattice (tangential motion) vs. grain size (normal motion) curve and should be equal to the misorientation between the embedded grain and the outer grains. The grain size was measured as half the largest distance between the embedded grain boundaries in a direction perpendicular to the outer planar grain boundaries. Since the motion of the boundary is relatively uniform away from the trijunctions, this captures the normal motion of the entire grain boundary. The rigid body displacement was measured by tracking the location of a density peak in the center of the embedded grain. The relationship between the grain size and displacement is linear, but the coupling parameters are about 5–10% lower than the theoretical values. This difference is a result of a small, fraction of a lattice parameter,