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Grain growth in anisotropic systems: comparison of effects of energy and mobility

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Abstract

Grain growth in systems of anisotropic grain boundary energy and mobility is investigated by computer simulations in a two-dimensional textured polycrystalline system. The energy and mobility are allowed to depend on both grain boundary inclination and misorientation. Mobility anisotropy alone does not significantly change the growth kinetics or statistical distributions of misorientation, grain size and number of grain edges, even though grain shapes evolve in a self-dissimilar fashion where the aspect ratio of grains and inclination distribution of grain boundaries are time dependent. Energy anisotropy, however, causes significant deviation of grain growth kinetics, misorientation and edge-distributions from the ones observed in isotropic systems. Moreover, misorientation distribution is skewed towards low energy (special) boundaries. Size distributions are similar in all cases. Mobility anisotropy influences grain growth kinetics only when energy is also anisotropic. Variation of misorientation distribution with time plays the key role in determining the grain growth behavior.

Keywords: Grain growth; Anisotropic systems; Theory; Modeling; Phase field models

1. Introduction

Grain growth is an important phenomenon that influences a variety of physical and mechanical properties of polycrystalline materials. It has been studied for decades using a variety of theoretical and experimental approaches [1–7]. When the motion of grain boundary is driven by its curvature, it is commonly assumed that the migration speed of a small segment of the boundary can be written in the form:

$$v = M\kappa_\gamma \tag{1}$$

where M is the grain boundary mobility, and κ_γ is the local weighted-mean curvature of the boundary. Although grain growth has been analyzed mostly in the isotropic limit, where $\kappa_\gamma = \gamma\kappa$ (κ is the local mean curvature and γ is the boundary energy per unit area) and both M and γ are taken to be constant, it is well known that both the energy and mobility of grain boundaries can be strongly anisotropic, i.e., dependent on grain boundary mis-

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orientation and inclination [1]. From experimental studies [1,8] as well as computer simulations [9,10] it has been shown that energy and mobility anisotropy could alter dramatically the grain growth behavior. Since grain boundary mobility can vary by several orders of magnitude while grain boundary energy (excluding low angle boundaries) varies typically by a factor of two or three[1,11,12], there have been predictions that mobility anisotropy would play a dominant role over energy anisotropy in determining the kinetics and microstructural evolution during grain growth [13]. However, in polycrystalline materials individual segments described by Eq. (1) are interconnected into a two-dimensional (2D) or three-dimensional (3D) network whose dynamic evolution might have different characteristics as compared to a single isolated segment. To analyze the more general polycrystalline case, we have recently performed a computer simulation study of grain growth in two dimensions using a generalized phase field model where misorientation and inclination dependence of grain boundary mobility were taken into account [14,15]. It was found that although the growth/shrinkage rate of an individual grain with triple junctions is strongly affected by the presence of mobility anisotropy, the growth behavior of a polycrystalline aggregate is isotropic-like, i.e. the growth exponent of the average grain area deviates only slightly from unity and the size, edge and misorientation distributions are all time-independent and similar to those observed in isotropic systems.

The main objective of this paper is to investigate and compare the effects of energy anisotropy vs. mobility anisotropy on the kinetics and morphological evolution of grain growth. Grain boundary energy anisotropy is incorporated into the phase field model developed previously for the study of mobility anisotropy [14–16]. In the following sections, we first describe the simulation method, with particular emphasis on the description of energy and mobility anisotropy. Then in Section 3 we present the major results obtained with anisotropy in (a) mobility, (b) energy and (c) both mobility and energy during grain growth in 2D single-phase textured polycrystalline systems. The results are compared with their counterparts in isotropic systems. Finally, the major findings and conclusions are summarized in Section 4.

2. Phase field model

The phase field approach has been successfully applied in computer simulations of pattern formation in many different disciplines. Typical examples in materials research include dendrite formation during solidification [17], multi-phase and multi-domain microstructural evolution during various solid-state phase transformations and grain growth [18]. For grain growth the phase field methods have been developed along two independent routes: (a) the one proposed by Chen et. al. [19,20] where an arbitrary single phase polycrystalline microstructure is described by many non-conserved order parameter fields ($\eta_1,\eta_2,\ldots,\eta_p$) with each of them representing a specific crystallographic orientation of grains and their degree of crystallinity, and (b) the one proposed by Kobayashi et al. [21] and independently by Luck [22] where the microstructure is characterized by two order parameters with one describing the degree of crystallinity and the other describing the crystallographic orientation of each individual grain. In this paper we generalize the first approach by taking into account the dependence of grain boundary energy and mobility on inclination and misorientation to study the relative contributions of energy and mobility anisotropy to the kinetics and statistical distributions and morphological evolution during grain growth.

In contrast to the sharp interface approach where the microstructure is described by mathematically sharp interfaces of zero thickness, the phase field methods characterize an arbitrary polycrystalline microstructure using continuum field variables (called order parameters) which change continuously across grain boundaries. For this reason, the phase field models are often referred to as diffuse-interface models. The spatio-temporal evolution of the order parameters which describe the microstructural evolution during grain growth are given by Ginzburg-Landau type kinetic equations:

$$\frac{\mathrm{d}\eta_i}{\mathrm{d}t} = -L\frac{\delta F}{\delta \eta_i} \tag{2}$$

where L is the kinetic coefficient that characterizes the grain boundary mobility and F is a free energy functional that can be written in the following form:

$$F = F_0 + \int_V \mathrm{d}^3 r[f_0(\eta_1,\eta_2,\ldots,\eta_p) + \frac{k}{2}\sum_{i=1}^{p}|\nabla\eta_i|^2] \quad (3)$$

where $f_0(\eta_1,\eta_2,\ldots,\eta_p)$ is the free energy density and k is the gradient energy coefficient, which together determine the width and energy of the grain boundary.

The exact form of the free energy density function $f_0(\eta_i)$ is not important as long as it provides the correct topology for the free energy functional, which contains a large number of energetically degenerate potential wells at the points in the η space located at $(\eta_1,\ldots,\eta_p) = (\pm 1,\ldots,0),\ldots,(0,\ldots,\pm 1)$, where it is assumed that $|\eta_i| = 1$ inside the ith grain type (grain with a particular spatial orientation) and 0 otherwise. A simple function that satisfies these requirements can be written in the form [19]:

$$f = \sum_{i=1}^{p}\left(-\frac{a_1}{2}\eta_i^2 + \frac{a_2}{4}\eta_i^4\right) + \frac{a_3}{2}\sum_{i=1}^{p}\sum_{j>i}\eta_i^2\eta_j^2 \quad (4)$$

where a_1, a_2, a_3 are positive constants.

If we assume the kinetic coefficient L and the gradient energy coefficient k to be constant, the above equations describe grain growth in isotropic systems. A number of attempts have been made to introduce anisotropy of grain boundary properties into this formalism. For example, in the phase field models of antiphase domain motion and solidification, anisotropy has been introduced by using a set of order parameters based on the underlying crystal symmetries [23,24]. Since a general description of the complicated structure of a grain boundary is still lacking, application of this approach to the description of grain boundaries remains a difficult challenge. On the other hand, a simple phenomenological approach with anisotropic expressions for L and k has been successfully applied to describe surface energy and mobility anisotropy in modeling crystal growth [17,25]. A similar method is used in the current paper to describe grain boundary energy and mobility anisotropy.

To determine the detailed forms of L and k we need to know how the grain boundary energy and mobility vary with misorientation and inclination. These functions could be obtained in principle from a number of sources including direct experimental measurements, analytical models or computer simulations, although due to the complexity of the problem, a general theory of the misorientation and inclination dependence of grain boundary energy and mobility is still lacking. In a simple dislocation model, the energy of a low angle tilt boundary between two cubic crystals in the case of small misorientation ($\theta \leq 20°$) has been obtained as a function of misorientation and inclination [26]:

$$E(\theta,\phi) = E_0\frac{\theta}{\theta_m}\left(1-\ln\left(\frac{\theta}{\theta_m}\right)\right)(|\sin(\phi)| + |\cos(\phi)|) \quad (5)$$

where inclination φ of the grain boundary is measured relative to the symmetric-tilt inclination (see Fig. 1), θ_m is the misorientation angle for which energy is maximum, and E_0 is a constant. The validity of such a form for grain boundary energy as a function of misorientation has been supported by a variety of experimental observations [1].

As shown in the analysis of Cahn and Hilliard [27], there exists a simple relationship between the

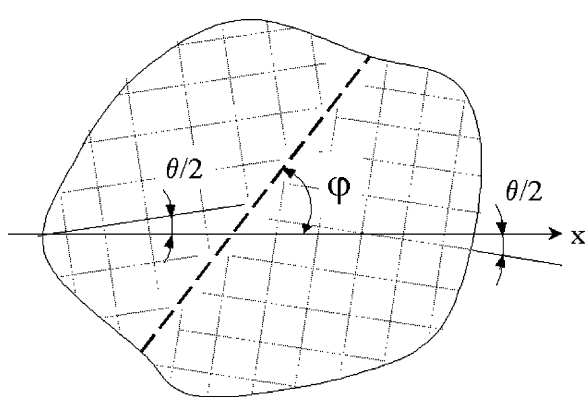

Fig. 1. Schematic drawing of a tilt grain boundary between two cubic crystals with misorientation θ and inclination φ. Note that inclination is measured from the symmetric-tilt reference.

gradient coefficient k in the free energy functional and the grain boundary energy, i.e. $k \propto E_{gb}^2$. Thus, to satisfy the criteria of differentiability of k [28], the inclination dependence of (5) has been modified with a simple differentiable form that satisfies the requirements of periodicity, namely: $E(\theta,\phi) = E_0[(\theta)/(\theta_m)](1-\ln([(\theta)/(\theta_m)]))(1-\delta_E\cos(4\phi))$. This form is similar to the one used in simulations of crystal growth [17,25]. Here δ_E is a phenomenological parameter which controls the degree of anisotropy with respect to inclination. We define the anisotropy ratio as the ratio of the largest to the smallest grain boundary energy at a fixed misorientation θ_0: $r = \max(E(\theta_0,\phi))/\min(E(\theta_0,\phi))$. In a more general case one can consider the inclination dependence to be an n-fold symmetric function: $(1-\delta_E\cos(n\phi))$.

It should be noted, however, that simply taking $k \propto E_{gb}^2$ will alter the grain boundary thickness and, thus, may affect the results of the simulation. It is easily shown that the thickness of a grain boundary in the phase field approach [28] is: $l \sim \sqrt{k/(\Delta f)_{max}}$ (where $(\Delta f)_{max}$ is the maximum height of the barrier in the free energy density between two minima at $f(\eta_i^0)$ and $f(\eta_j^0)$, where η_i^0 and η_j^0 are the equilibrium long range order parameters describing grains i and j) and grain boundary energy is given by $E_{gb} \sim \sqrt{k \cdot (\Delta f)_{max}}$ [28]. In the simulations, by changing both k and $(\Delta f)_{max}$ simultaneously and keeping the ratio $k/(\Delta f)_{max}$=constant one can simulate boundaries of the same thickness but of different energies. We use the following notation: $l^{(0)}$-desired boundary thickness, $k^{(0)}$, $(\Delta f)^{(0)}_{max}$-a certain choice of values for gradient coefficient and barrier height that gives $l^{(0)}$, and $E_{gb}^{(0)}$-corresponding value for the grain boundary energy. Then the relative value of the barrier height corresponding to the energy E_{gb} is:

$$(\Delta f)_{max} = \frac{E_{gb}}{E_{gb}^{(0)}}(\Delta f)_{max}^{(0)} \quad (6)$$

For a free energy density of the form (4), changes in the height of the barrier can be accomplished by varying the coefficient a_3.

In contrast to the grain boundary energy, mobility anisotropy is more difficult to characterize analytically, due in part to limited experimental information. In our model, we take a grain boundary mobility characterized by a kinetic coefficient L of the form:

$$L(\theta,\phi) = L_0 f(\theta)(1-\delta_L\cos(n\phi)) \quad (7)$$

where $f(\theta)$ is a monotonically increasing function of misorientation and n represents the symmetry of the grain boundary mobility with respect to inclination.

One advantage of this formulation is that by varying δ_E and δ_L one can easily change the degree of anisotropy in energy and mobility to investigate effects of their interplay on grain growth. To determine the sensitivity of the simulation results to the particular form of the misorientation dependence of the mobility, two extreme cases for $f(\theta)$ have been considered: (1) a slowly increasing function $\propto\theta(1-\ln(\theta))$ and (2) a rapidly increasing function $\propto\theta^5$. The former has taken the same form as the energy dependence on misorientation given by the Read–Shockley model [26] and the latter is similar to the one proposed by Huang and Humphreys [29] based on experimental observations of subgrain growth in aluminum. It was found that the behavior of the system (including kinetics and statistical distributions) is insensitive to the particular form of the mobility function used.

With the approximations for grain boundary energy and mobility introduced above, the simulation results are most relevant to the evolution of textured systems where only small misorientations are present and there are no singularity points in both grain boundary energy and mobility functions (i.e., no cusped extreme for special boundaries). However, it was found recently in both phase field modeling and Monte Carlo simulations using grain boundary energy and mobility data obtained from the molecular dynamics simulations, that the presence of special boundaries does not change the general features of the kinetics as well as morphological evolution during the grain growth process [30].

3. Results and discussion

To evaluate the relative effects of energy and mobility anisotropy described by Eqs. (5) and (7) on grain growth, we first investigated the shape of

a shrinking island grain in an infinite matrix using different values of δ_E and δ_L [14]. It was found that a relatively large mobility anisotropy ($L_{max}/L_{min} = 19$) and small energy anisotropy ($E_{max}/E_{min} = 1.1$) provided by $\delta_L = 0.9$ and $\delta_E = 0.05$ have comparable effects on the steady-state shape of the shrinking island grain (see Fig. 2a and b). Under these conditions, in fact, a quasi-eightfold shape is obtained as a result of the interplay between the fourfold energy and mobility functions (with $n = 4$ in Eq. (7)) (Fig. 2c). Therefore, the values for the phenomenological parameters δ_E and δ_L are taken to be $\delta_E = 0.05$ and $\delta_L = 0.9$ in all our simulations ($\delta_L/\delta_E = 18$), which provides a base for the comparison between the effects of energy and mobility anisotropy.

Similar conclusions can be obtained using Eq. (1). When energy is anisotropic the expression for the weighted-mean curvature in two dimensions (which is the case in our studies) can be written as $\kappa_\gamma = (\gamma + [(d^2\gamma)/(d\phi^2)])\kappa$, where φ is the inclination angle. It can be clearly seen that in contrast to the case with mobility anisotropy, the local boundary velocity is now determined not only by the boundary energy but also by its second derivative with respect to inclination. Therefore, using the same expressions for the energy and mobility as in the computer simulations, one can show that the same aspect ratio of a shrinking grain (in the self-similar mode) can be achieved when

$$\frac{(1 + 15\delta_E)\kappa_{min}{}^E}{(1 + 15\delta_E)\kappa_{max}{}^E} = \frac{(1 + \delta_E)\kappa_{min}{}^L}{(1-\delta_L)\ \kappa_{max}{}^L} \qquad (8)$$

where $\kappa^{L(E)}_{min(max)}$ is the minimum (maximum) curvature of the shrinking grains with grain boundary energy (mobility) anisotropy. Assuming the ratios of curvatures to be approximately the same in both cases we get the value of $\delta_L/\delta_E = 15$ which is in a good agreement with the results of the computer simulations.

The computer simulations of grain growth in polycrystalline materials were performed on a 1024×1024 square grid with 36 order parameters, η_i, which describes 36 possible grain orientations. The simulations were started from an isotropic polycrystalline microstructure containing approximately 4000 grains, which was obtained from nucleation and growth of crystals from the liquid phase in an isotropic system. To enhance the effect on the shapes of individual grains, the mobility function has been chosen to be twofold symmetric with respect to grain boundary inclination ($n = 2$ in Eq. (7)). It should be noted that in the case of $n = 4$, the simulation results are very similar in terms of both kinetics and statistics of the morphological evolution. Concerning the two particular forms of $f(\theta)$ employed, it was found that the kinetics and statistics of grain growth obtained are very similar, both qualitatively and quantitatively. Thus, in the results presented below we will disregard the particular expression used for the misorientation dependence of grain boundary mobility.

We start our analysis with the discussion of the fundamental question of self-similarity, which requires all statistical distributions to be time-inde-

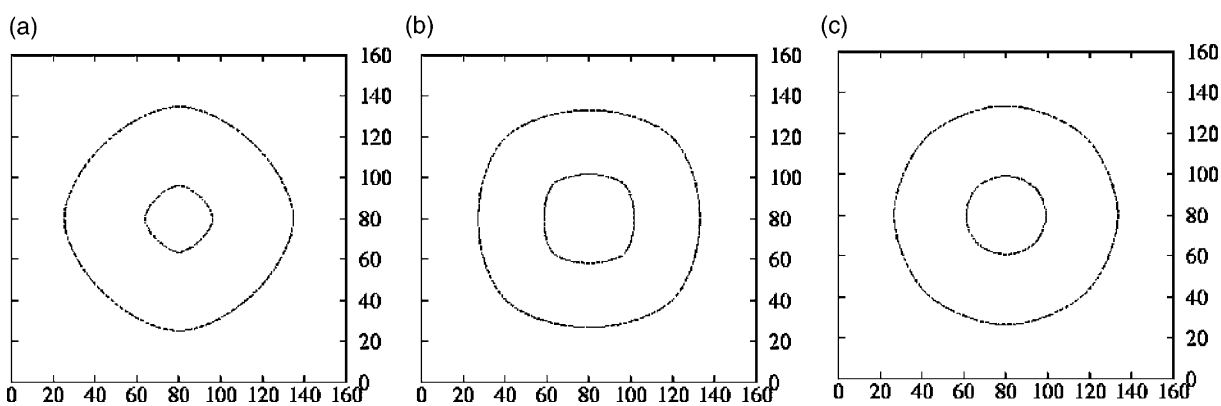

Fig. 2. Shrinkage of a single island grain with (a) mobility anisotropy $L_{max}/L_{min} = 19$, (b) energy anisotropy $E_{max}/E_{min} = 1.1$(c) both energy and mobility anisotropy, using the anisotropy parameters from (a) and (b).

pendent. As long as the self-similarity argument is preserved, it can be shown that average grain area increases linearly with time, as it does in isotropic systems, irrespective of the anisotropy of both energy and mobility of grain boundaries [31]. If at least one of the distribution functions becomes time-dependent, however, the self-similarity argument is no longer valid and a different time dependence should be expected [16].

3.1. Inclination distribution

Fig. 3 presents the typical microstructures obtained from the same initial condition (Fig. 3a) during grain growth in systems with isotropic grain boundary properties (Fig. 3b), anisotropic mobility (Fig. 3c) and anisotropic energy (Fig. 3d). It is readily seen that both energy and mobility anisotropy may significantly change the shapes of grains. For example, in the case of twofold mobility anisotropy used in the simulations, grains become horizontally elongated. When grain boundary energy is anisotropic, with a fourfold symmetry employed in this study, there is an increased number of grain boundaries with vertical and horizontal inclinations, which have lower energies as compared to other boundary orientations. Note that these results were obtained in the small misorientation limit (i.e. $\theta \leq 5°$). Therefore, the shape anisotropy is caused primarily by the inclination dependence of grain boundary energy and mobility. When larger misorientation angles are included, the shape anisotropy should become less significant, because the inclination of a grain boundary is measured in the local coordinate system defined with respect to symmetrical-tilt inclination which may form an arbitrary angle with the global coordinate system.

To analyze the microstructural changes quantitatively, we plot the inclination distribution, which is the fraction of grain boundary length of certain inclination. It can be seen that in both cases (see Fig. 4) the inclination distribution strongly deviates from that of the isotropic system which is a constant and independent of the boundary orientation. However, as will be seen later, in systems with only mobility anisotropy, the kinetics and distributions of size, edge and misorientation are similar to the ones observed in the isotropic case (time-invariant) even though grain shape and inclination distribution change with time. This indicates that self-similarity, which requires all the statistical distributions be time-invariant, is only a sufficient rather than a necessary condition for the average grain area to increase linearly with time [16].

Even though the above observation is obtained for the small range of misorientations, the conclusion of the time-dependent inclination distribution should be valid for the case of arbitrary misorientation as well. When the range of misorientations becomes larger, there will be more grain boundaries, whose local coordinate system deviates from the global one (reference frame), leading to more isotropic grain shapes. However, all the boundaries, whose inclination strongly deviate from their minimum value in the local coordinate system (i.e. their symmetrical-tilt inclination, which has the lowest energy or mobility) will tend to align with the orientation of the symmetrical-tilt boundary. Therefore, this should result in a change of the inclination distribution during microstructural evolution.

3.2. Misorientation distribution

Phenomena such as clustering and texturing have been reported frequently during grain growth [1]. These phenomena are indications of time-dependent misorientation distributions and hence non-self-similar behavior of the systems. Results of our simulations are presented in Fig. 5. The simulations were started with a uniform misorientation distribution, which provides an equal probability to find grain boundaries of any misorientation angles. The distributions shown in Fig. 5 represent a particular moment in time ($t = 0.6$) during the microstructural evolution. As expected, the distribution in the isotropic case is time-invariant because all the boundary properties are independent of misorientation. When mobility is anisotropic, however, a similar result is obtained. This invariance is in contrast to the previous predictions [10] concerning misorientation dependence of grain boundary mobility suggesting that boundaries with high mobilities disappear at faster rates.

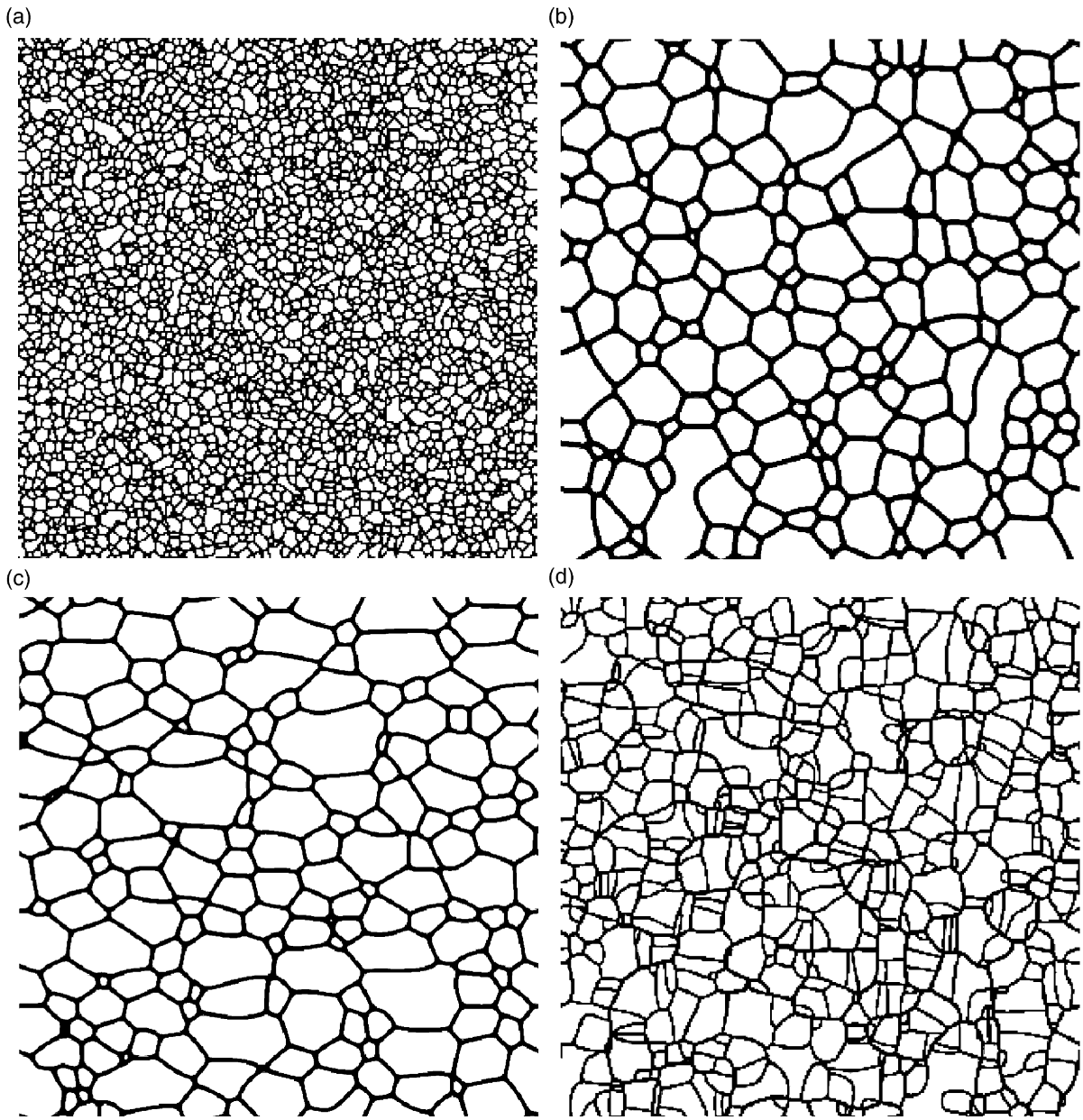

Fig. 3. Typical microstructures obtained from computer simulation of grain growth in various systems: (a) initial microstructure, (b) isotroopic, (c) twofold mobility anisotropy, (d) fourfold energy anisotropy.

When grain boundary energy is anisotropic, however, the fraction of low angle boundaries (which are also low energy boundaries) increases significantly as the grains grow (Fig. 5), suggesting that high angle (high energy) boundaries disappear at a faster rate. Even though only a particular moment in time is shown in Fig. 5, this behavior continues throughout the entire simulation and no stationary stage is observed. These results clearly demonstrate the difference in the effects of energy

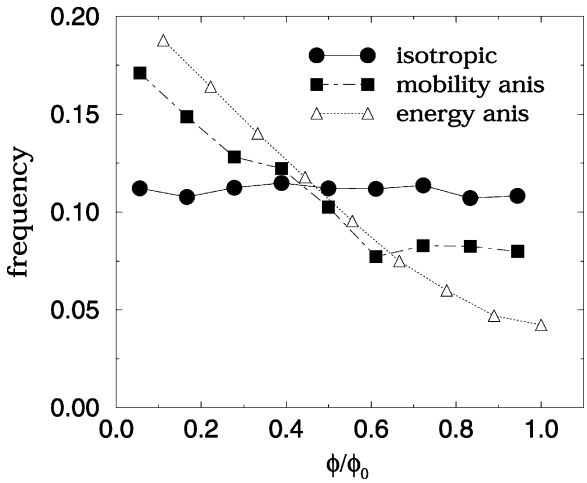

Fig. 4. Inclination distributions at intermediate stage of evolution. φ_0 is the inclination angle which corresponds to half-period of inclination dependence, i.e. $\varphi_0 = 45°$ for a fourfold function and 90° for a twofold function.

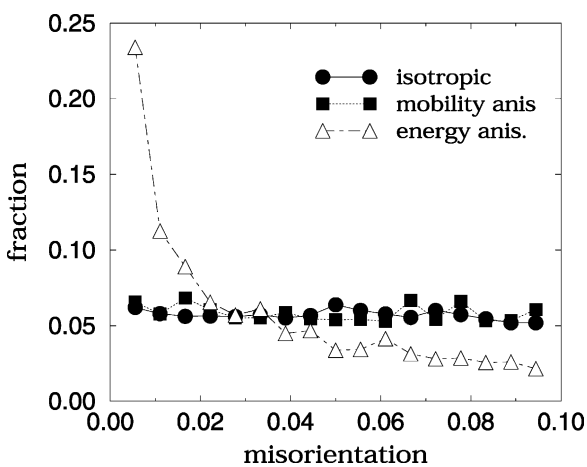

Fig. 5. Misorientation distribution in various systems at intermediate stage of evolution.

and mobility anisotropy on grain growth. The energy anisotropy results in a strongly time-dependent misorientation distribution while the mobility anisotropy has no effect on the misorientation distribution.

The different effects of energy anisotropy and mobility anisotropy on the misorientation distribution can be understood in the following manner. When grain boundary mobility is anisotropic and energy is not, the direction of boundary motion is determined by its curvature. Due to the randomness in the system, a disppearing grain has an equal probability to be bounded by boundaries with high and low mobility. Moreover, after disappearance of a boundary there is an equal probability to form new boundaries with either high or low mobility. Therefore, grain coarsening with mobility anisotropy only is unlikely to change the misorientation distribution. The situation is different when grain boundary energy is anisotropic. In this case, the total free energy of the system can be reduced not only by simply reducing the overall grain boundary area but also by changing the types of boundaries. Since both high and low energy boundaries have the same mobility, the high energy boundary should disappear faster, resulting in the steepest reduction in total free energy of the system which is the most favorable path of evolution according to Eq. (2). As will be seen later, mobility does have an influence on the variation of misorientation distribution with time and hence on grain growth kinetics when grain boundary energy is anisotropic.

Note that when grain boundary energy is anisotropic, the system has another choice to reduce the total energy by grain rotation. This is true in particular for textured grains with small grain sizes. However, in the current formulation of the phase field model, grain rotation is not allowed.

3.3. Aspect ratio evolution

As has been illustrated qualitatively in Fig. 3, both energy and mobility anisotropy (inclination dependence) could have a strong effect on grain shapes. To analyze this effect quantitatively, we calculate the average mean linear intercept (MLI) in different directions and compare their growth rates. Fig. 3 shows that individual grains have their shapes bounded by boundaries of low energy or mobility inclinations and the MLI is the shortest in the directions normal to these inclinations. Correspondingly, the MLI is longest in the directions normal to the inclinations of high energy or mobility. In the twofold symmetry case the shortest MLI, $d_{\min}$, and the largest MLI, $d_{\max}$, are in the vertical, '*y*', and horizontal, '*x*', directions, respectively, and in the fourfold symmetry case in the *y*

(x) and 45° directions, respectively, for the small misorientation angles considered. Fig. 6 shows the ratio of d_{max}/d_{min} as a function of time. The simulations were started from an isotropic microstructure where the ratio is equal to unity. Again, in the isotropic system the ratio is time-invariant and equal to unity, indicating that there is no preferred orientation in the system. However, when the boundary mobility and energy are anisotropic, d_{max}/d_{min} is, in general, time-dependent and self-similarity does not hold anymore. The time period shown in the Fig. 3 reflects a 10-fold increase in the grain size.

It is interesting to note that in the system with mobility anisotropy grains continue to change their shapes (elongate) throughout the entire course of evolution. However, as it will be shown later, the grain growth kinetics is very similar to that obtained for the isotropic case, even though the evolution is no longer self-similar. In addition, analyzing the evolution of the MLI distributions in the case of mobility anisotropy, it was found that distributions of both d_{min} and d_{max} are more or less time independent, suggesting that breaking of self-similarity occurs in the simplest possible fashion through the changes of the grain shapes [16].

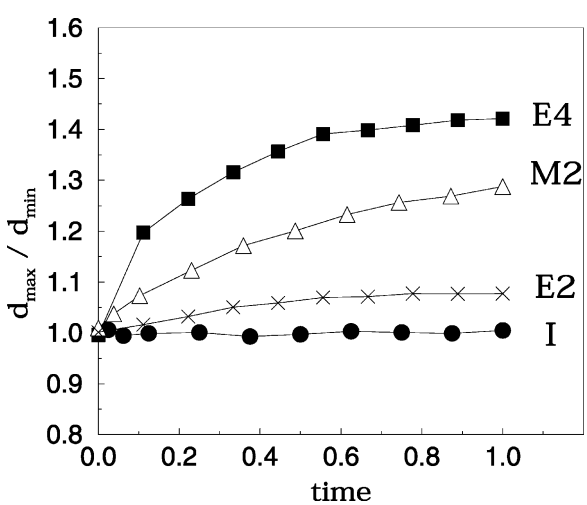

Fig. 6. Time dependence of ratio of MLI in the directions of high energy/mobility to the MLI in the direction of low energy/mobility. I-isotropic system; E2 system with twofold energy anisotropy; E4-system with fourfold energy anisotropy; M2-system with twofold mobility ansiotropy.

3.4. Size and edge distributions

The fractions of grains with different sizes and different number of edges are usually analyzed in the studies of grain growth. In this study, the grain size distribution is obtained by examining the frequency of occurrence of grains with an area A normalized by the average grain area $\langle A \rangle$. Simulation results for three different cases with: (a) anisotropic mobility; (b) anisotropic energy and (c) anisotropic mobility and energy are presented in Fig. 7. For comparison, the size and edge distri-

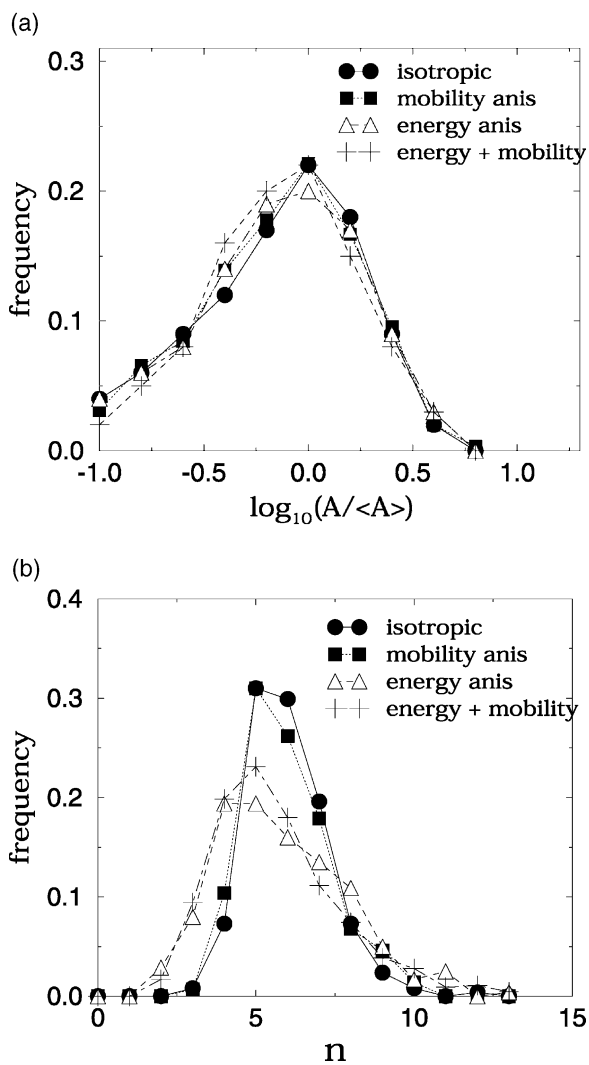

Fig. 7. Comparison of (a) size and (b) edge distributions in different systems.

butions obtained for an isotropic system are also presented. As shown in Fig. 7, the size distribution is similar in all cases, and the major difference is in the edge distributions. Similarly to our previous results [15], edge distributions in systems with mobility anisotropy are found to be almost identical to the one in isotropic systems. However, significant differences are observed when grain boundary energy is anisotropic. For example, the fraction of few sided grains ($n < 6$) is significantly larger as compared to the other cases.

The increase in the fraction of few sided grains could be attributed to the changes in the constraints at the grain boundary junctions. Such changes include energetically stable vertices with more than three boundaries at a junction as well as triple junctions meeting at the angles, that strongly deviate from 120°. For example, there is a possibility of having *T-shaped* triple junctions, which produce ladder-like structures with four-sided grains (see Fig. 3d). These plate-like grains appear similar to annealing twins that are observed in FCC alloys with low stacking fault energy (such as Cu, Cu–Zn and austenitic stainless steel). This result is in contrast to the cases with isotropic grain boundary energy where only triple junctions are stable and the constraint of space filling results in the requirement of $\langle n \rangle = 6$, where $\langle n \rangle$ is the average number of edges for a single grain in a 2D polycrystalline system. If a system consists of quadruple- or multi-junctions in addition to triple junctions, the average number of edges, $\langle n \rangle$ should be less than six. For example, if the dominant junctions are quadra-junctions, $\langle n \rangle$ should be ~4.

3.5. Grain growth kinetics

The growth of the average grain area is usually approximated by a simple power law $\langle A \rangle^m - \langle A_0 \rangle^m = \alpha t$, where m is the grain growth exponent. Results obtained form the simulations are shown in Fig. 8. The curves are normalized so that the initial growth rates are identical in all four cases. In agreement with the classical theories of grain growth, $m = 1$ (linear growth) is obtained for the isotropic case. When grain boundary mobility alone is anisotropic, the growth behavior is identical to the one observed in the isotropic case.

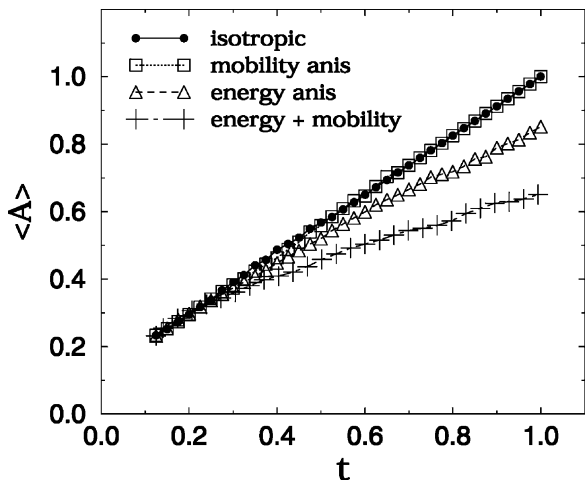

Fig. 8. Time dependence of the average grain area in various systems. Curves are normalized so that they have the same initial slope

According to our theoretical analyses [16], this is a consequence of the time-invariant misorientation distribution (see Fig. 5).

When the boundary energy is anisotropic, the growth is no longer linear. The best fit to the simple power law gives the growth exponent $m = 1.35$. Note that the best fit to the simple power law will depend on the time interval considered in the simulations because fitting to grain growth at different stages may result in different values of the growth exponent. For example, the growth exponent obtained from fitting to early stage growth data ($t \sim 0.3$) is significantly larger (about 1.8) than the one obtained from fitting to later stage data. This is because the relative energy difference of the grain boundaries becomes smaller and smaller as the microstructure evolves and eventually the system will reach asymptotically the isotropic limit where only low energy boundaries are left. Therefore, the value of m should decrease continuously and asymptotically approaching unity. For the same reason, the average number of edges of grains also asymptotically approaches the value of 6.

3.6. Grain growth with both energy and mobility anisotropy

To study the interplay between grain boundary energy and mobility anisotropy during grain

growth, we investigated the grain growth kinetics when both energy and mobility are anisotropic. The simulation results are shown in Figs. 7 and 8. These results are obtained with fourfold symmetry in both energy and mobility functions and the anisotropy parameters have been chosen as $\delta_E = 0.05$ and $\delta_L = 0.9$. It is shown that the size and edge distributions are similar to those obtained with only energy anisotropy. However, the growth exponent deviates even further from the linear growth obtained in the isotropic case (Fig. 8), i.e. $m \approx 1.8$. The reason why the growth exponent is larger than the one obtained in the case with only energy anisotropy is that in the current case higher energy boundaries have higher mobilities as well, which accelerated the elimination of high energy boundaries. When the high-energy boundaries have lower mobilities, the anisotropy in mobility will slow down the variation of misorientation distribution with time and reduce the deviation of the growth kinetics from linear growth.

4. Summary

In an attempt to understand and predict the interplay between grain boundary energy and mobility anisotropy and their effect on grain growth kinetics and morphological evolution, a systematic computer simulation study has been performed on the basis of generalized phase field approach. Simulations are done in textured systems with small range of grain orientations.The major conclusions can be summarized as follows:

- It is shown that there are several occasions where the self-similarity is violated; however, only under certain circumstances does lack of self-similarity change the grain growth kinetics and statistical distributions. In other words, self-similarity is only a sufficient rather than a necessary condition for linear grain growth kinetics. For example, when only boundary mobility is anisotropic, the growth rate of the average grain area as well as several major statistical distributions (size, edge, and misorientation distributions) are time independent, even though grain growth is no longer self-similar (inclination distribution becomes time-dependent).
- When the grain boundary energy is anisotropic, it was found that the misorientation distribution, the grain growth exponent and the average number of edges of grains all become time dependent. In particular, the misorientation distribution shifted significantly towards the small misorientation angles, which are the low energy boundaries. Similarly, if a large misorientation range is considered, misorientation distribution will be shifted towards low energy special boundaries. Variation of the misorientation distribution during grain growth results in significant deviation of the growth kinetics from the linear growth found in an isotropic system.
- Mobility anisotropy influenced the grain growth exponent only when the energy was also anisotropic. When higher energy boundaries also have higher mobilities, the mobility anisotropy accelerates the misorientation distribution variation with time and makes the growth exponent deviate even further from the isotropic case as compared with the case with only energy anisotropy.

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