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Effect of grain boundary energy anisotropy on highly textured grain structures studied by phase-field simulations

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Abstract

Two-dimensional phase-field simulations were performed of grain growth in highly textured materials with equal fractions of two texture components, denoted as α and β grains, and assuming two values of the grain boundary energies, namely σ_{low} for the boundaries between grains of a different texture component and σ_{high} for boundaries between grains of a similar orientation, resulting in microstructures with alternating α and β grains and stable quadruple junctions. For different magnitudes of the anisotropy in grain boundary energy $R = \sigma_{high}/\sigma_{low}$, the occurrence of the different types of triple and quadruple junctions and the distributions of the normalized grain size, the number of faces per grain, the normalized grain boundary length per grain and the dihedral angles at grain boundary junctions were investigated.

Keywords: Grain growth; Phase-field modeling; Textured microstructure

1. Introduction

In order to predict various macroscopic properties of polycrystalline materials, characterization of the microstructural characteristics is an essential step [1–4]. For instance, the average grain size plays an important role in determining the yield strength [1,2] of a material. The evolution of grain structures has been simulated frequently and has been quantitatively characterized by means of the average grain size, the grain size distribution, and the number of faces and their distribution [5–7] for isotropic grain boundary properties. Grain growth in anisotropic systems has been simulated based on a Monte Carlo Potts model [8,9] and using the phase-field method [10]. In previous studies, the role of anisotropy in grain boundary energy and mobility in determining the grain size distribution, the distribution of the number of faces per grain, and the misorientation distribution of the grain boundaries was evaluated. It was assumed that the crystallographic orientations were randomly assigned. Recently, it was also shown that the characteristics of triple- and higher-order junctions are important microstructural features in anisotropic systems in the context of grain topology and the misorientation distribution of grain boundaries [11].

Highly textured materials are also widely used [12,13]. Grain growth of textured materials has been investigated in terms of the distributions of the grain sizes and crystallographic orientations [14,15]. Moreover, Cahn, Holm and Srolovitz have analyzed the stabilities of trijunctions and quadrijunctions in conserved and non-conserved 2-D two-phase microstructures as a function of the ratios between the grain boundary energies of the different types of interfaces [16,17], where a system with two texture components can be considered as a non-conserved two-phase system. Their study shows that quadruple junctions can

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become stable for a high degree of anisotropy in grain boundary energy. Different from triple junction dihedral angles, quadruple junction dihedral angles are thermodynamically not fixed, but can vary within a certain range depending on the ratios of the grain boundary energies. They are therefore expected to affect the grain growth behavior and grain boundary network topology considerably. However, in general, the microstructural characteristics of highly textured materials and the effect of the degree of anisotropy in grain boundary energy in these systems have not been studied extensively. Moreover, very little attention has been paid so far to characterize the different possible types of vertices and the distribution of dihedral angles in highly anisotropic systems.

In this paper, we present a systematic study of the role of degree of anisotropy in grain boundary energy in determining the occurrence of different types of vertices, the dihedral angle distribution, and the distributions of the number of faces, grain boundary length and grain size in highly textured materials for microstructures with two texture components. The grains belonging to the two different components will be labeled respectively as α and β grains. We will consider the case where $\sigma_{\alpha\beta} = \sigma_{low} \leqslant \sigma_{\alpha\alpha} = \sigma_{\beta\beta} = \sigma_{high}$ with $\sigma_{\alpha\beta}$, $\sigma_{\alpha\alpha}$ and $\sigma_{\beta\beta}$ the interfacial energy of the boundaries between α grain-β grain, α grain-α grain and β grain-β grain, respectively, for which quadruple junctions have been predicted to coexist with triple junctions and even become the majority junction type within certain ranges of the degree of anisotropy [16]. This situation is less common than the opposite case where $\sigma_{\alpha\beta} > \sigma_{\alpha\alpha} = \sigma_{\beta\beta}$ for the classical metallic systems (Al, Ni, Cu, etc., alloys) with a simple face-centered or body-centered cubic structure. However, in more complex non-cubic structures, such as monoclinic zirconia [18] and ferroelectric $Cd_{1-x}Zn_xTe$ (CZT) [19], where multiple twin systems may exist, mosaic-like grain structures with only two texture components and quadruple junctions where almost perfect twin boundaries (with extremely low energy) and low-angle boundaries meet, were observed. The case where $\sigma_{\alpha\beta} > \sigma_{\alpha\alpha} = \sigma_{\beta\beta}$ has been studied before [14,17,20] and it was found that the topological characteristics are quite similar to those of isotropic systems since only triple junctions can be stable. The grain growth kinetics can, however, deviate strongly from those observed for isotropic grain structures. Depending on the initial fractions of the α and β texture components and their initial spatial distribution, the steady-state parabolic growth regime as derived for isotropic grain growth [21–23] may not be obtained.

For the simulated microstructures, we will verify five of the findings in Refs. [16,17]:

1. For isotropic grain growth ($\sigma_{low} = \sigma_{high}$), quadrijunction or higher grain junctions are unstable and unlikely ever to form. Even though they form, they decompose immediately.
2. The $q_{\alpha\beta\alpha\beta}$ type of quadrijunction becomes stable when $R(= \sigma_{high}/\sigma_{low}) \geqslant \sqrt{2}$. When $\sqrt{2} \leqslant R \leqslant \sqrt{3}$, $q_{\alpha\beta\alpha\beta}$ quadrijunctions and trijunctions coexist. Although $t_{\alpha\alpha\alpha}$ and $t_{\beta\beta\beta}$ trijunctions can be stable, $t_{\alpha\alpha\beta}$ and $t_{\alpha\beta\beta}$ trijunctions are thermodynamically more favorable.
3. When $\sqrt{3} < R$, $t_{\alpha\alpha\alpha}$ and $t_{\beta\beta\beta}$ trijunctions become unstable. For $\sqrt{3} < R < 2$, $t_{\alpha\alpha\beta}$ and $t_{\alpha\beta\beta}$ trijunctions coexist with $q_{\alpha\beta\alpha\beta}$ quadruple junctions.
4. Only $q_{\alpha\beta\alpha\beta}$ quadrijunctions are stable when $R \geqslant 2$.

Following the notation of Refs. [16,17], $t_{\alpha\alpha\beta}$ is a triple junction where 2α and 1β grains coexist and a similar notation is used for the three other kinds of triple junctions. $q_{\alpha\beta\alpha\beta}$ is a quadruple junction where two α and two β grains meet according to a checkerboard pattern. Other kinds of quadruple junctions have been shown to be unstable [16,17].

Furthermore, the distributions of grain sizes, average number of faces per grain, dihedral angles and grain boundary length per grain will be characterized and the findings will be related to the stability of (a) particular type(s) of junctions. Since it is extremely complex to determine and classify uniquely dihedral angles in 3-D systems, 2-D simulations were performed. Although some of the phenomena present in 3-D systems may not be present in 2-D systems, the 2-D simulations can already provide useful insights. They may also represent grain growth behavior in thin films, as that observed for the monoclininc zirconia or $Cd_{1-x}Zn_xTe$ (CZT) thin films. Moreover, the results from our 2-D simulations can be interpreted based on the analytical theory of Cahn [16] which was also constructed for 2-D systems.

2. Phase-field model and numerical solution

We adopted the multi-order parameter phase-field grain growth model of Ref. [5]. According to Ref. [5], a single-phase material is represented by a set of non-conserved order parameters, which are a continuous function of time and space:

$$\eta_1(\mathbf{r}, t), \eta_2(\mathbf{r}, t), \ldots, \eta_Q(\mathbf{r}, t) \tag{1}$$

Each grain is represented by a unique non-conserved order parameter. The temporal and spatial evolution of the order parameters is described by the time-dependent Ginzburg–Landau equation:

$$\frac{\partial \eta_i(\mathbf{r}, t)}{\partial t} = -L \frac{\delta F}{\delta \eta_i(\mathbf{r}, t)} \tag{2}$$

where the kinetic constant L is related to the grain boundary mobility and the free energy F is a function of the order parameter values and their gradients:

$$F = \int_V \left[\sum_i^Q \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \sum_i^Q \sum_{i \neq j}^Q \theta_{ij} \eta_i^2 \eta_j^2 + \frac{\kappa}{2} \sum_i^Q (\nabla \eta_i)^2 \right] dV \tag{3}$$