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Two-dimensional phase-field simulations of dendrite competitive growth during the directional solidification of a binary alloy bicrystal

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Abstract—We investigated the competitive growth of dendrites at the converging grain boundaries (GBs) of bicrystals during the directional solidification of an Al–Cu alloy by means of two-dimensional phase-field simulations. In particular, the focus was on the recently observed phenomenon of unusual overgrowth during the directional solidification of a Ni-based superalloy, where the favorably oriented (FO) dendrites are overgrown by the unfavorably oriented (UO) ones. The phase-field simulations were accelerated by parallel computations on graphics processing units. The simulation results showed that unusual overgrowth occurs in Al–Cu alloys, indicating that this phenomenon is a common one in metallic materials. It was also concluded that the differences in the diffusion layers in front of the FO and UO dendrites had a dominant effect on the competitive growth of dendrites at the converging GB as well as on the unusual overgrowth. In addition, unusual overgrowth was observed in all the FO dendrites with a spacing that allowed the dendrite array to grow stably without necessitating a change in the number of dendrites. The FO dendrite at the GB is overgrown by the UO dendrite when the spacing between the FO dendrite at the GB and the next FO dendrite is approximately equal to the critical minimum spacing. However, the unusual overgrowth was not observed for UO dendrites with a large inclination angle. In this case, all the UO dendrites are blocked by the FO dendrite at the GB, and the FO dendrites migrate toward the UO dendrites.

Keywords: Dendritic solidification; Directional solidification; Phase-field simulation

1. Introduction

Solidification microstructures have great significance in materials science, as they directly determine the properties of cast materials and correspond to the initial microstructures for several of the production processes that follow casting. With respect to the ingot casting of alloys, the solidification structure can typically be classified as one three types: a small equiaxed structure near the surface (i.e. a chill structure), a columnar structure, and an equiaxed structure in the central zone of the ingot [1–3]. During casting, randomly oriented solid seeds nucleate on the chill wall and grow in the shape of dendrites, which are typical solidification structures, in the direction of the heat flow. Competitive growth takes place between these dendrites. Frequent collisions occur between the growing dendrites near the wall surface, resulting in the formation of fine equiaxed grains. Subsequently, during the continuous competitive growth of the dendrites, columnar grains are formed. As a result, small equiaxed and columnar structures are formed on the outer surface through the competitive growth of the dendrites, which exhibit different growth directions.

The competitive growth of dendrites has been modeled by Walton and Chalmers [4], who found that favorably oriented (FO) dendrites, for which the angle between the preferred growth direction and the heat-flow direction is small, can keep growing by blocking unfavorably oriented (UO) dendrites, which have a larger inclination angle than that of the FO dendrites [5–7]. The Walton and Chalmers model is accepted as a general competitive-growth model. During dendrite growth under steady-state conditions in the course of directional solidification, the growth velocity of the UO dendrites is higher than that of the FO dendrites [8–12]. This means that the degree of tip undercooling of the UO dendrites is higher than that of the FO dendrites. Therefore, the tips of the UO dendrites lag behind those of the FO dendrites [5,6]. It is for this reason that the Walton and Chalmers model is a reasonable one and has been widely accepted.

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However, an unusual phenomenon has been reported in recent studies on the directional solidification of bicrystals of a Ni-based superalloy, where the UO dendrites preferentially grow over the FO dendrites along converging grain boundaries (GBs) [13–15]. This new phenomenon of overgrowth cannot be explained by the Walton and Chalmers model. According to the Walton and Chalmers model, at converging GBs, secondary arms, which are formed from the FO dendrites and grow towards the UO dendrites, stop the growth of the UO dendrites. On the other hand, it has been observed that the formation of the secondary arms is suppressed by the diffusion of the solute from around the tips of the UO dendrites [13,15].

To elucidate the mechanism underlying the newly observed and unusual phenomenon of overgrowth, Li et al. [16] performed 2-D phase-field simulations of the directional solidification of bicrystals whose properties are similar to those of a Ni-based superalloy. Their simulations showed that solute interaction in front of the dendrite tips is essential for the overgrowth, and, therefore, it occurs only when the pulling velocity for directional solidification is low where the solute interaction is strong. It was also concluded that the new overgrowth occurs independent of the initial spacing of the FO and UO dendrites.

In this study, we investigated in detail the unusual phenomenon of overgrowth at converging GBs by systematically performing 2-D phase-field simulations of the directional solidification of a binary alloy bicrystal; these simulations were similar to those performed by Li et al. [16]. Here, an Al–Cu alloy was used to show that the unusual phenomenon is a common one in metallic materials. Through systematic simulations, the effects of the initial spacing of the FO dendrites, the number of FO dendrites, and the inclination angle of the UO dendrites on the competitive growth behavior at the converging GBs were investigated quantitatively. We used a quantitative phase-field model developed by Ohno and Matsuura for the solidification of a dilute binary alloy [17]. Although the computations were performed assuming a 2-D problem, the computational domain and time were large. Therefore, parallel computations using graphics processing units (GPUs) were employed, and the simulations were performed using the GPU supercomputer TSUBAME2.5 at the Tokyo Institute of Technology [18–20].

2. Numerical simulations

2.1. Phase-field model

Phase-field methods have emerged as the most powerful numerical schemes for studying dendrite solidification [17,21–32]. In this study, we employed a quantitative phase-field model developed by Ohno and Matsuura [17] for the isothermal solidification of a dilute binary alloy to study directional solidification. The advantage of this model is that it can treat solute diffusion in both the solid phase and the liquid phase.

In this model, the phase-field variable, ϕ, is defined as $+1$ for solids and -1 for liquids. The dimensionless supersaturation, u, is defined as

$$u = \frac{c_l - c_l^e}{c_l^e - c_s^e}, \tag{1}$$

where c_l is the solute concentration in the liquid phase. The local concentration, c, is expressed by the mixture rule, $c = \phi c_s + (1-\phi)c_l$, where c_s is the concentration in the solid phase. In a dilute alloy, the relation $k = c_s/c_l$ is satisfied, where k is the partition coefficient, according to the equal chemical potential condition proposed by Kim, Kim and Suzuki (KKS model) [29]. Further, c_l^e and c_s^e are the equilibrium concentrations of the liquid and solid at T_0, respectively. These also have the relation $k = c_s^e/c_l^e$. The temperature, T, is assumed to follow the frozen temperature approximation [33] during directional solidification. That is to say:

$$T(y) = T_0 + G(y - V_p t), \tag{2}$$

where G is the temperature gradient along the y-axis, V_p is the pulling velocity, T_0 is the temperature at $y = 0$ and $t = 0$, and t is the time.

By taking the interface anisotropy into account, the time-evolution equation of the phase-field variable, ϕ, can be expressed as [17,32]:

$$\begin{aligned}\tau\left(\widetilde{\nabla}\phi\right)[1-(1-k)u']\frac{\partial\phi}{\partial t} &= \nabla\times\left[W\left(\widetilde{\nabla}\phi\right)^2\nabla\phi\right] + \frac{\partial}{\partial x}\left[W\left(\widetilde{\nabla}\phi\right)\frac{\partial W\left(\widetilde{\nabla}\phi\right)}{\partial\phi_{,x}}\frac{\partial\phi}{\partial y}\right] \\ &+ \frac{\partial}{\partial y}\left[W\left(\widetilde{\nabla}\phi\right)\frac{\partial W\left(\widetilde{\nabla}\phi\right)}{\partial\phi_{,y}}\frac{\partial\phi}{\partial x}\right] - \frac{df(\phi)}{d\phi} \\ &- \lambda^*\frac{dg(\phi)}{d\phi}(u+u')\end{aligned} \tag{3}$$

where $\phi_{,x} = \partial\phi/\partial x$ and $\phi_{,y} = \partial\phi/\partial y$. $\tau\left(\widetilde{\nabla}\phi\right) = \tau_0 a_s\left(\widetilde{\nabla}\phi\right)^2$ and $W\left(\widetilde{\nabla}\phi\right) = W_0 a_s\left(\widetilde{\nabla}\phi\right)^2$ are the inverse mobility and interface thickness, respectively. The anisotropy function $a_s\left(\widetilde{\nabla}\phi\right)$ is expressed as:

$$a_s\left(\widetilde{\nabla}\phi\right) = \bar{a}(1-3\varepsilon_4)\left\{1 + \frac{4\varepsilon_4}{1-3\varepsilon_4}\frac{\left(\frac{\partial\phi}{\partial\tilde{x}}\right)^4 + \left(\frac{\partial\phi}{\partial\tilde{y}}\right)^4}{\left|\widetilde{\nabla}\phi\right|^4}\right\}, \tag{4}$$

where ε_4 is the anisotropy parameter, and the coordinates $(\tilde{x},\tilde{y})$ are the material coordinates aligned to the $\langle 1\,0\,0\rangle$ direction. The following relation is used for the coordinate transformation between $(\tilde{x},\tilde{y})$ and (x,y):

$$\begin{Bmatrix}\frac{\partial\phi}{\partial\tilde{x}}\\ \frac{\partial\phi}{\partial\tilde{y}}\end{Bmatrix} = \begin{bmatrix}\frac{\partial x}{\partial\tilde{x}} & \frac{\partial y}{\partial\tilde{x}}\\ \frac{\partial x}{\partial\tilde{y}} & \frac{\partial y}{\partial\tilde{y}}\end{bmatrix}\begin{Bmatrix}\frac{\partial\phi}{\partial x}\\ \frac{\partial\phi}{\partial y}\end{Bmatrix} = \begin{bmatrix}\cos\theta_i & \sin\theta_i\\ -\sin\theta_i & \cos\theta_i\end{bmatrix}\begin{Bmatrix}\frac{\partial\phi}{\partial x}\\ \frac{\partial\phi}{\partial y}\end{Bmatrix}. \tag{5}$$

Here, θ_i is the angle between $[1\,0\,0]$ and the x-coordinate for the ith grain. The interpolating functions are chosen as $\mathrm{d}f(\phi)/\mathrm{d}\phi = -\phi + \phi^3$ and $\mathrm{d}g(\phi)/\mathrm{d}\phi = (1-\phi^2)^2$. λ^* is associated with the thermodynamic driving force and is expressed as $\lambda^* = a_1 W_0/d_0$, where $a_1 = 0.88388$ and d_0 is the chemical capillary length. u' is the equivalent nondimensional undercooling resulting from the introduction of the frozen temperature approximation Eq. (2) and is expressed as:

$$u' = \frac{y - V_p t}{l_T}, \tag{6}$$