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Two-dimensional phase-field study of competitive grain growth during directional solidification of polycrystalline binary alloy

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ABSTRACT

Selections of growing crystals during directional solidification of a polycrystalline binary alloy were numerically investigated using two-dimensional phase-field simulations. To accelerate the simulations, parallel graphics processing unit (GPU) simulations were performed using the GPU-rich supercomputer TSUBAME2.5 at the Tokyo Institute of Technology. Twenty simulations with a combination of five sets of different seed orientation distributions and four different temperature gradients covering dendritic and cellular growth regions were performed. The unusual grain selection phenomenon, in which the unfavorably oriented grains preferentially grow instead of the favorably oriented grains, was observed frequently. The unusual selection was more remarkable in the cellular structure than in the dendritic structure.

1. Introduction

In casting, solidification is usually initiated from the chilled mold surface. A fine equiaxed structure is first formed on the mold surface, followed by the development of a columnar structure [1–3]. Controlling and understanding the growth of the columnar structure is very important because size, morphology, and crystallographic orientations of the columnar structure have a great influence on the ingot surface quality. The columnar structure is formed from grains composed of multiple dendrites or cells. The grain selection was modeled by Walton and Chalmers [4]: the grains with a small angle between the ⟨100⟩ direction in the cubic metal and the heat flow direction keep growing, while the grains with a large angle grow behind the ones with the small angle, and hence, their growth will be blocked by the ones with the small angle. Fig. 1 schematically illustrates the Walton and Chalmers model [5,6], in which we consider two types of grains: favorably oriented (FO) and unfavorably oriented (UO) along the heat flow direction. Because the growth velocity of UO dendrites, V_{UO}, is higher than that of FO dendrites, V_{FO}, the tip undercooling of the UO dendrite, ΔT_{UO}, is larger than that of FO dendrites, ΔT_{FO}. Hence, the UO dendrite tips lag behind the FO dendrite tips [7]. Accordingly, at the converging grain boundary (GB), the FO dendrites block the growth of UO dendrites, and at the diverging GB, the UO dendrites cannot grow along the heat flow direction because of growth suppression by the branching FO dendrites. Consequently, UO grain growth is stopped by the FO grain at both types of GB [8,9]. This model has been widely accepted in studies on the formation of columnar structures.

Recently, an unusual grain selection phenomenon that cannot be explained by the Walton and Chalmers model has been reported in studies on the directional solidification of a bicrystal Ni-based super alloy [10–12]. Specifically, overgrowth of UO grains over FO grains at the converging GB in a bicrystal condition was observed. Hereafter, this overgrowth phenomenon is referred to as "unusual overgrowth," and "unusual grain selection" is used for the phenomenon where the UO grain overgrows the FO grain regardless of GB type, i.e. converging and diverging. To clarify the unusual overgrowth mechanism, Li et al. performed two-dimensional (2D) phase-field simulations during directional solidification of binary alloy bicrystals [13]. They concluded that the solute interaction around the tips of GB dendrites is a key to the occurrence of the unusual overgrowth. Furthermore, they have confirmed the occurrence of the unusual overgrowth by in-situ observation of a transparent alloy [14]. We also performed detailed and systematic investigations of the unusual overgrowth based on

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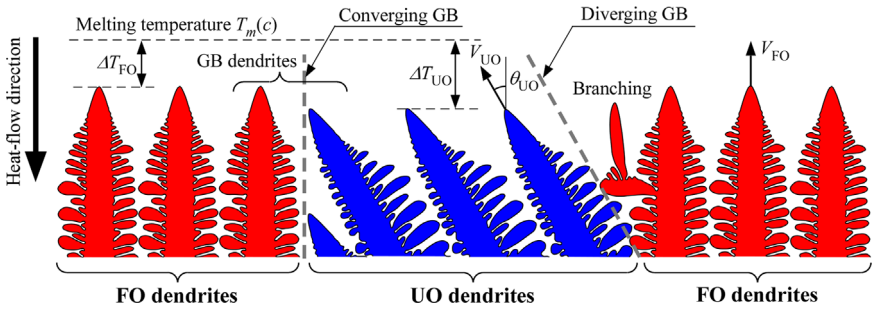

Fig. 1. Dendrite competitive growth model.

large-scale 2D phase-field simulations and reached the following conclusions [15,16]: the unusual overgrowth is a universal phenomenon occurring in metallic materials, the differences in the diffusion layers in front of the FO and UO dendrites at the converging GB had a dominant effect on the unusual overgrowth, and overgrowth occurs when the spacing between the FO dendrite at the GB and the next FO dendrite is approximately equal to a critical minimum spacing. Tourret and Karma also performed a systematic 2D phase-field study on the competitive growth in the bicrystal [17]. It is important to point out that detailed analyses of the unusual overgrowth have been performed only for bicrystal alloys until now. Although the occurrence of the unusual selection was also observed in our recent 3D phase-field simulation of a polycrystal alloy [18], the details of the competitive growth in polycrystal systems such as frequency of the occurrence of the unusual grain selection have not yet been examined.

In this study, in order to investigate the competitive growth phenomena in the 2D polycrystal in detail, we performed systematic phase-field simulations of the polycrystal growth during the directional solidification of a binary alloy. Although the actual competitive growth is a 3D phenomenon, 2D study before the 3D study is essential for the fundamental understanding of the polycrystal competitive growth. Note that this investigation requires significant computational cost even in 2D, because the selections take place over a long time in a large system. To increase the computational speed, we performed a parallel computation using multiple graphics processing units (GPUs) using the supercomputer TSUBAME2.5 at the Tokyo Institute of Technology [16,18–24].

2. Phase-field model and computational conditions

2.1. Quantitative phase-field model

In this study, we simulated the directional solidification of a binary alloy in a 2D system. Here, we extended the quantitative phase-field model for isothermal solidification in a dilute binary alloy developed by Ohno and Matsuura [25] to handle the directional solidification [26] of a polycrystal [18]. The details of the model are discussed in Ref. [15], and here, only the important points are briefly discussed.

The directional solidification in a binary alloy can be described by three variables, temperature T, phase-field ϕ ($\phi=1$ in solid and $\phi=-1$ in liquid), and nondimensional supersaturation u. The time evolution equations of these variables are given in a 2D system as follows:

$$T(y)=T_0+G(y-V_p t), \tag{1}$$

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

$$\frac{1}{2}\left[1+k-(1-k)\phi\right]\frac{\partial u}{\partial t}=\nabla\left[D_l q(\phi)\nabla u-j_{AT}\right]+\frac{1}{2}\left[1+(1-k)u\right]\frac{\partial\phi}{\partial t}-\nabla\cdot J. \tag{3}$$

Here, we employed a frozen temperature approximation, Eq. (1), where T_0 is the reference temperature at $y=0$ and $t=0$, G is the temperature gradient, y is the coordinate along the heat flow direction, V_p is the pulling velocity, and t is the time. u' in Eq. (2) denotes the additional supersaturation for the directional solidification and is defined as $u'=(y-V_p t)/l_T$, where $l_T=|m|(1-k)c_0/(kG)$ is the thermal length, k is the partition coefficient, c_0 is the initial concentration in the liquid, and m is the slope of the liquidus. $\tau(\nabla\phi)=\tau_0 a_s(\nabla\phi)$ and $W(\nabla\phi)=W_0 a_s(\nabla\phi)^2$ are the phase-field relaxation time and interface thickness, respectively, and $a_s(\nabla\phi)=1-(3\varepsilon_4+4\varepsilon_4(\phi_{,x}{}^4+\phi_{,y}{}^4)/|\nabla\phi|^4)$ represents the crystalline anisotropy with the anisotropic strength ε_4. Here, $\phi_{,i}$ is the spatial derivative of ϕ with respect to the i direction. We chose $df(\phi)/d\phi=-\phi+\phi^3$ and $dg(\phi)/d\phi=(1-\phi^2)^2$. λ^* is a coupling constant 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 defined by $d_0=k\Gamma/(|m|(1-k)c_0)$ with the Gibbs–Thomson constant Γ. u is defined as $u=(c_l-c_l^e)/(c_l^e-c_s^e)$, where c_l is the concentration in the liquid, and c_l^e and c_s^e are the equilibrium concentrations in the liquid and solid, respectively, at a temperature T_0. We followed the Kim–Kim–Suzuki (KKS) model [27] and used the relations $k=c_s^e/c_l^e=c_s/c_l$. Then, the concentration c is given as $c=c_s(1+\phi)/2+c_l(1-\phi)/2$. In Eq. (3), j_{AT} is an antitrapping current expressed as $j_{AT}=-(1-kD_s/D_l)/(2\sqrt{2})W_0[1+(1-k)u](\partial\phi/\partial t)\nabla\phi/|\nabla\phi|$ using the diffusion coefficients in the solid, D_s, and liquid, D_l. J is the fluctuating current [26] and $q(\phi)$ is an interpolating function expressed as $q(\phi)=[kD_s+D_l+(kD_s-D_l)\phi]/(2D_l)$.

The polycrystal is expressed using the single phase-field variable introducing the additional parameter expressing the crystal orientation and by performing the coordinate transformation of the gradient of ϕ [15,18]. Eqs. (2) and (3) were discretized based on the standard finite difference method. The moving-frame algorithm was employed to reduce the computational cost.

2.2. Computational conditions

Fig. 2 shows the computational domain and the initial conditions. The computational domain size was set to $L_x\times L_y=8192\Delta x\times 1536\Delta y=6.144\ \text{mm}\times 1.152\ \text{mm}$ with a square mesh size of $\Delta x=\Delta y=0.75\ \mu\text{m}$. For both ϕ and u, the periodic boundary condition was set to the left and right ends, and the zero Neumann conditions were applied to the top and bottom ends. The heat flow direction, i.e., the temperature gradient direction, was set to the y-direction. Initially, the computational domain was filled with the liquid Al–3 wt%Cu. Seventeen solid seeds with $3\Delta x$ radius were distributed on the bottom at an interval of $481.9\Delta x$ from the