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Competitive grain growth during directional solidification of a polycrystalline binary alloy: Three-dimensional large-scale phase-field study

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ABSTRACT

Competitive grain growth during the directional solidification of a polycrystalline binary alloy is investigated by performing systematic three-dimensional large-scale phase-field simulations with the GPU supercomputer TSUBAME2.5 at the Tokyo Institute of Technology. Contrary to two-dimensional investigations, in which an unusual growth of unfavorably oriented (UO) grains has been observed frequently in preference to favorably oriented (FO) ones, the grain selection in the present three-dimensional simulations follows essentially the Walton and Chalmers model, in which FO grains are predominant. The UO dendritic grains persist for longer times than the UO cellular grains, and the FO dendritic grains remain smaller than the FO cellular ones. The change in the number of grains follows a power law, with an exponent that is much lower than that of the Kolmogorov's model describing a purely geometrical growth selection.

1. Introduction

Columnar structures form by the competitive growth of multiple grains in an undercooled melt under a temperature gradient, which develop from randomly nucleated seeds on a chill surface [1]. The widely accepted Walton and Chalmers (WC) selection model for the competitive growth of columnar grains [2] suggests that favorably oriented (FO) grains, whose preferred growth angle relative to the temperature gradient direction is small, grow preferentially relative to unfavorably oriented (UO) grains, which are characterized by a larger preferred growth angle. This selection process has been observed by Esaka et al. using an in-situ investigation of the directional solidification of a succinonitrile–acetone alloy [3]. Gandin et al. [4] have confirmed that the columnar grain growth follows the WC model during the directional solidification of an Inconel x750 superalloy. The authors have also shown that the solid seeds that have nucleated on the chill surface are randomly oriented and follow a Mackenzie distribution [5], and the crystal orientation distribution becomes narrow and the most probable orientation becomes small as the distance from the chill surface increases. Similar results have been reported by Ardakani et al. [6]. However, in recent directional solidification experiments on a bicrystal alloy, an unusual grain selection, inconsistent with the WC model, has been observed, in which UO grains were preferred to FO grains at converging grain boundaries (GBs) [7–9]. In order to clarify the mechanism underpinning this selection, two-dimensional (2D) [10–12] and three-dimensional (3D) [13] phase-field simulations have been performed, which indicate that the lateral migration of FO dendrites at converging GBs is the key factor causing unusual grain selection in both 2D and 3D models. Importantly, there are differences in the frequencies of occurrence of unusual grain selection between the 2D and 3D simulations. Specifically, the unusual selection is more common in 2D than in 3D [13]. Hence, 3D investigation is required for a thorough understanding of grain selection processes. It should be noted that, to date, this unusual selection has been investigated in bicrystal systems. Although it has been recently reported that such unusual selection can also occur during the growth of polycrystals [14], the investigation was conducted in a 2D system. Therefore, it is necessary to carry out 3D investigation of grain selection in polycrystals.

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In this study, we perform comprehensive phase-field simulations to investigate the competitive growth of 3D columnar grains during the directional solidification of a polycrystalline binary alloy. The phase-field method [15–18] solves the free-boundary problem of solid–liquid interface and can therefore accurately account for the grain selection caused by the competitive growth of multiple dendrites. However, high computational cost is a serious issue in phase-field simulations. To overcome this problem, we performed parallel computations using multiple graphic processing units (GPUs) on the GPU-rich supercomputer TSUBAME2.5 at the Tokyo Institute of Technology [18–24].

2. Numerical simulations

2.1. Model

A quantitative phase-field model for isothermal solidification in a dilute binary alloy [25] is applied to the directional solidification. The model is identical to that reported previously [13,20]. Time evolution equations at a temperature T, phase-field ϕ ($\phi=1$ in a solid and $\phi=-1$ in a liquid), and nondimensional supersaturation u are

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

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

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

Eq. (1) represents the frozen temperature approximation, where T_0 is the reference temperature at $z=0$ and $t=0$, G is the temperature gradient, z is the coordinate along the temperature gradient direction, V_p is the pulling velocity, and t is the time. In the phase-field equation, Eq. (2), $u'=(z_T-V_p t)/l_T$ denotes the additional supersaturation associated with the directional solidification, 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, m is the liquidus slope, and z_T is the coordinate in the G direction with an origin at $u=-1$. $\tau(\nabla\phi)=\tau_0 a_s(\nabla\phi)^2$ and $W(\nabla\phi)=W_0 a_s(\nabla\phi)$ are the phase-field relaxation time and interface thickness, respectively, for a crystalline anisotropy $a_s(\nabla\phi)=1-3\varepsilon_4+4\varepsilon_4(\phi_{,x}{}^4+\phi_{,y}{}^4+\phi_{,z}{}^4)/|\nabla\phi|^4$ with the anisotropic strength ε_4. Here, $\phi_{,i}$ is the spatial derivative of ϕ with respect to the i direction. λ^* is a coupling constant associated with the thermodynamic driving force given by $\lambda^*=a_1 W_0/d_0$, with $a_1=0.88388$ and the chemical capillary length $d_0=k\Gamma/(|m|(1-k)c_0)$, where Γ is the Gibbs–Thomson constant. Polynomials $f(\phi)$ and $g(\phi)$ are given as to be $df(\phi)/d\phi=-\phi+\phi^3$ and $dg(\phi)/d\phi=(1-\phi^2)^2$, respectively. The nondimensional supersaturation 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 in the solid, respectively. We followed the Kim–Kim–Suzuki model [26] and used the relations $k=c_s{}^e/c_l{}^e=c_s/c_l$. The concentration c is given by $c=c_s\,(1+\phi)/2+c_l\,(1-\phi)/2$. In the solute diffusion equation, Eq. (3), j_{AT} represents the anti-trapping current, given by $j_{AT}=-(1-kD_s/D_l)/(2\sqrt{2})W_0[1+(1-k)u](\partial\phi/\partial t)\nabla\phi/|\nabla\phi|$, in which D_s and D_l are the diffusion coefficients in the solid and in the liquid, respectively. J is the fluctuating current [27] and $q(\phi)$ is an interpolating function given by $q(\phi)=[kD_s+D_l+(kD_s-D_l)\phi]/(2D_l)$.

2.2. Parallel GPU calculations and computational conditions

Directional solidification simulations of Al–3 wt% Cu (i.e. Al–0.013 at. fract. Cu) were performed in a domain with a size of $768\times768\times1149.75\ \mu m^3$, as shown in Fig. 1. The temperature gradient, G, was set along the z-direction, and five different temperature gradient, $G=10$, 20, 50, 100, and 200 K/mm, under a pulling velocity $V_p=100$ m/s, were used to investigate the growth conditions ranging from dendritic to cellular growth. The simulations were started from 64 seeds with $3\Delta x$ radius with a random crystal orientation and a random distribution on the bottom surface ($z=0$). The preferred growth direction $\langle100\rangle$ of the seeds is defined by the Euler angles φ, θ, and ψ, which are the rotational angles around the x-, z'-, and x"-axes, respectively [19]. Three sets of initial seeds (Cases 1, 2, and 3) were used for each of the five different values of G (Information for the three sets of seeds are found in Tables S1–S3 in the supplementary data). Therefore, 15 simulations in total were performed. The angles between the z-axis and the $\langle100\rangle$ direction, θ_z ($0^\circ<\theta_z<54.74^\circ$), for three sets of 64 seeds are shown in Fig. 2, where the horizontal axis indicates the seed number in increasing order of θ_z. The material and simulation parameters are summarized in Table 1 [20]. For both ϕ and u, periodic boundary conditions were imposed along the x- and y-directions, and zero Neumann conditions were applied along the z-direction. Initially, the computational domain was filled with liquid Al–3 wt% Cu. In the initial conditions, the nondimensional supersaturation at the bottom surface ($z=0$) was set to $u=-0.3$, which corresponds to $T_0=922.39$ K in Eq. (1).

Table 1
Material and simulation parameters [20].

Quality	Symbol	Value
Initial concentration	c_0	0.013 at. frac.
Pulling velocity	V_p	100 μm/s
Temperature gradient	G	10, 20, 50, 100, and 200 K/mm
Mesh size	Δx	0.75 μm (fine grid)
Interface thickness	W_0	$\Delta x/0.8=0.9375$ μm
Diffusion coefficient in liquid	D_l	3×10^{-9} m^2/s
Diffusion coefficient in solid	D_s	3×10^{-13} m^2/s
Partition coefficient	k	0.14
Anisotropic strength	ε_4	0.02
Gibbs–Thomson constant	Γ	0.24×10^{-6} Km
Liquidus slope	m	−620 K/at. frac.
Melting temperature of pure Al	T_m	933.25 K
Time increment	Δt	2.6785716×10^{-5} s

The spatio-temporal large-scale simulations were performed using multiple-GPU parallel computations, carried out on the GPU-rich supercomputer TSUBAME2.5 at the Tokyo Institute of Technology [18,22,23]. As shown in Fig. 1, to reduce the computational cost, coarse grids were used for the liquid region, with a size ($\Delta x_{coarse}=\Delta y_{coarse}=\Delta z_{coarse}=1.5$ μm) that was twice as large as the one used for the fine grids describing the solid/liquid coexistence region ($\Delta x=\Delta y=\Delta z=0.75$ μm). Meshes consisting of $1024\times1024\times1024$ and $512\times512\times256$ grid points were used for the fine and coarse grids, respectively. These meshes were divided into $1\times16\times8$ and $1\times16\times1$ subdomains, respectively, and each subdomain was assigned to a single GPU. Consequently, 144 GPUs were used in the parallel computation. The fine and coarse grids were connected by linear interpolation. A moving-frame algorithm was used and the dendrite/cell tip positions were constrained to remain below the 900-lattice point position. After 1×10^6 steps, the computational domain was shifted by one mesh in the z-direction for every period $\Delta z/(V_p\Delta t)$. The computations with a total time steps of 5×10^6 and a time increment $\Delta t=2.67857\times10^{-5}$ s were performed for each of the 15 simulations, which corresponds to a total time $t=133.9$ s and a pulling distance of 13.4 mm. The total run time of the 144 GPUs (NVIDIA K20X) parallel nodes on the TSUBAME2.5 supercomputer was about 5.2 days.

3. Results

Figs. 3 and 4 show the time slices of the solid-liquid interface (isosurface of $\phi=0$) in bird's-eye and top views, respectively (videos are

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