GPU-accelerated 3D phase-field simulations of dendrite competitive growth during directional solidification of binary alloy

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Abstract. Phase-field method has emerged as the most powerful numerical scheme to simulate dendrite growth. However, most phase-field simulations of dendrite growth performed so far are limited to two-dimension or single dendrite in three-dimension because of the large computational cost involved. To express actual solidification microstructures, multiple dendrites with different preferred growth directions should be computed at the same time. In this study, in order to enable large-scale phase-field dendrite growth simulations, we developed a phase-field code using multiple graphics processing units in which a quantitative phase-field method for binary alloy solidification and moving frame algorithm for directional solidification were employed. First, we performed strong and weak scaling tests for the developed parallel code. Then, dendrite competitive growth simulations in three-dimensional binary alloy bicrystal were performed and the dendrite interactions in three-dimensional space were investigated.

1. Introduction

Control and prediction of columnar solidification structure are very important in casting and solidification. The columnar structure is formed through the competitive growth of multiple dendrites with different preferred growth directions. Walton and Chalmers competitive growth model is well accepted for the selection of growing multiple dendrites [1]. However, recently, an unusual competitive growth phenomenon, which cannot be explained by the conventional Walton and Chalmers model, have been reported [2-5]. The detailed mechanisms behind the new selection are not known except for the two-dimensional cases [6-8].

Phase-field method is the most powerful numerical tool for simulating dendrite growth. However, because the phase-field method is a diffuse interface model and fine numerical meshes are required to accurately express dendrite morphology, most phase-field simulations of dendrite growth performed so far are limited to two-dimension (2D) or single dendrite in three-dimension (3D). To express actual solidification structures, multiple dendrites with different preferred growth directions should be computed at the same time in 3D. Therefore, it is critical to develop a high-performance computational scheme for phase-field simulation [9]. In our previous study, we enabled very-large-scale phase-field simulations of dendrite growth during directional solidification of binary alloy [10]. In the computation, the number of meshes and time steps were approximately 4,000^3 and four million,
respectively. Although it was quite a large computation, the results were qualitative and the pulling time for directional solidification was not enough.

The objective of the present study is to develop a 3D phase-field code using multiple graphics processing units (GPUs) with a quantitative phase-field method for binary alloy solidification [11] and moving frame algorithm for directional solidification, and to investigate the dendrite interactions in 3D space.

The organization of this paper is as follows: First, we specify the quantitative phase-field model for the simulation of dendrite growth during the directional solidification of a dilute binary alloy. Next, we describe parallel computation using multi-GPUs and show strong scaling and weak scaling results for a developed code. Then, we describe the simulation of 3D dendrite competitive growth of binary alloy bicrystal and consider the simulation results.

2. Phase-field model

Here, we employed a quantitative phase-field model developed by Ohno and Matsuura [11] for dilute binary alloy solidification. In this model, the phase-field variable \( \phi \) is defined as \( 1 + \phi \) for solids and \( 1 - \phi \) for liquids. According to the mixture rule, the local concentration \( c \) is defined as

\[
c = \frac{\phi c_s + (1 - \phi) c_l}{2},
\]

where \( c_s \) and \( c_l \) are the concentrations in the solid and liquid phases, respectively. We assume the relation \( c_s^e = k c_l^e \) between the equilibrium concentrations of solid \( c_s^e \) and liquid \( c_l^e \) at a temperature \( T_0 \), where \( k \) is the partition coefficient.

The dimensionless supersaturation \( u \) is defined as

\[
u = \frac{c - c_s^e}{c_s^e - c_l^e}.
\]

Introducing the frozen temperature approximation during directional solidification [12], the temperature \( T \) is given as

\[
T = T_0 + G (z - V_p t),
\]

where \( G \) is temperature gradient along \( z \) axis, \( V_p \) is pulling speed, \( T_0 \) is the temperature at \( z = 0 \) and \( t = 0 \), and \( t \) is the time.

The time-evolution equation of the phase-field variable \( \phi \) is expressed as

\[
\tau [1 - (1 - k) u'] \frac{\partial \phi}{\partial t} = \nabla [W^2 \nabla \phi] + \frac{\partial}{\partial x} \left[ W \frac{\partial W}{\partial \phi_x} \nabla \phi \right] + \frac{\partial}{\partial y} \left[ W \frac{\partial W}{\partial \phi_y} \nabla \phi \right] + \frac{\partial}{\partial z} \left[ W \frac{\partial W}{\partial \phi_z} \nabla \phi \right] - \frac{\partial f(\phi)}{\partial \phi} - \lambda' \frac{\partial g(\phi)}{\partial \phi} (u + u'),
\]

where \( \phi_x = \partial \phi/\partial x, \phi_y = \partial \phi/\partial y, \) and \( \phi_z = \partial \phi/\partial z \). \( \tau = \tau_0 a_s^2 \) is the inverse mobility and \( W = W_0 a_s^2 \) is interface thickness. The anisotropy function \( a_s \) is expressed as

\[
a_s(\nabla \phi) = a(1 - 3 \zeta) \left[ 1 + \frac{4 \zeta}{1 - 3 \zeta} \left( \frac{\partial \phi}{\partial x} \right)^4 + \left( \frac{\partial \phi}{\partial y} \right)^4 + \left( \frac{\partial \phi}{\partial z} \right)^4 \right],
\]

where \( \zeta \) is the anisotropy parameter. The interpolating functions \( f(\phi) \) and \( g(\phi) \) are selected as \( \partial f(\phi)/\partial \phi = -\phi + \phi^3 \) and \( \partial g(\phi)/\partial \phi = (1 - \phi^2)^2 \), respectively. \( \lambda' \) is associated with the thermodynamic driving force expressed as \( \lambda' = a W_0 / d_0 \), where \( a_s = 0.8839 \) and \( d_0 \) is the capillary length defined as \( d_0 = k \Gamma / |\nabla (1 - k) c_s^e| \) with the Gibbs-Thomson coefficient \( \Gamma \), liquid slope \( m \), and
the initial alloy concentration \( c_\infty \). In equation (3), \( u' \) is added by introducing the frozen temperature approximation and is expressed as

\[
u' = \frac{z - V_p t}{l_T}, \quad (5)
\]

where \( l_T \) is the thermal length defined by \( l_T = |\mathbf{n}|(1 - k)c_\infty/(Gk) \). The dendrite crystal orientations, which express preferred growth direction of each grain, are expressed by the coordinate transformation of \( \phi_x = \partial \phi / \partial x \), \( \phi_y = \partial \phi / \partial y \), and \( \phi_z = \partial \phi / \partial z \)[7].

The diffusion equation is expressed as

\[
\frac{1 + k - (1 - k)\phi}{2} \frac{\partial u}{\partial t} = \nabla \left[ D_s q(\phi) \nabla u - j_{AT} \right] + \frac{1 + (1 - k)u}{2} \frac{\partial \phi}{\partial t} + \nabla \cdot J,
\]

where the interpolating functions \( q(\phi) \) is given as \( q(\phi) = [ k D_s + D_l + (D_s - D_l) \phi ]/(2 D_l) \), where \( D_s \) and \( D_l \) are the diffusion coefficients of the solid and liquid phases, respectively. The antitrapping current term \( j_{AT} \) is added to remove all the spurious effects at the interface and enable quantitative simulations independent of the interface thickness. \( j_{AT} \) is expressed as

\[
j_{AT} = -a(\phi)W_0 \left[ 1 + (1 - k)u \right] \frac{\partial \phi}{\partial t} \nabla \phi,
\]

where we set \( a(\phi) = [ 1 - k D_s/D_l ]/(2\sqrt{2}) \). The side branching is expressed by introducing a fluctuating current \( J \) of the Gaussian random number with the variance of \( 2D_l F_0^2 q(\phi) [ 1 + (1 - k)u ]/(\Delta t \Delta x^2) \), where \( F_0^2 \) is the constant noise magnitude, \( \Delta t \) is the time increment, and \( \Delta x \) is the lattice size [13].

Equations (3) and (6) are discretized by using the normal finite difference method. The time is discretized by the first-order forward difference method. For the Laplacians in equations (3) and (6), the isotropic discretization using the nearest and next-to-nearest neighbors and the second-order central difference approximations are used respectively.

3. Parallel computation using multi-GPUs

In the following computations, we employ the TSUBAME2.5 supercomputer at Tokyo Institute of Technology. The TSUBAME2.5 has 1408 compute nodes, each of which are equipped with three NVIDIA Tesla K20X GPU accelerators and two Intel Xeon X5670 central processing units (CPUs). Therefore, the TSUBAME2.5 can be called a GPU rich supercomputer.

**Figure 1.** Domain decomposition and boundary data exchange between distributed GPUs.
The GPU code is written in compute unified device architecture (CUDA), and message passing interface (MPI) is used for the inter-node communication. Figure 1 shows the image of domain decomposition and boundary data exchange between distributed GPUs. The whole domain is decomposed along the $y$ and $z$ directions, and the decomposed subdomains are assigned to each GPU. Because the domain used in the following simulations is not wide in the $x$-direction, the 2D domain decomposition shows higher computational efficiency than the 3D domain decomposition.

The connection process of the boundary data is as follows: First, one GPU sends the boundary data to a CPU. Next, the boundary data is exchanged between CPUs in the distributed neighbor subdomain by MPI. One CPU then sends the received boundary data to the GPU. This process is performed in every step.

Figure 2 and 3 shows the results of strong scaling and weak scaling for developed code running on the multiple GPUs in single precision. The strong scaling tests were executed for $3^{512}$ and $3^{1024}$ meshes. In figure 2, the performance increases linearly with increase in the number of GPUs for both of $3^{1024}$ and $3^{512}$ domains. However, the good linearity breaks down at 512 GPUs for $3^{512}$ meshes. Therefore, from these results, we determine the number of GPUs that show the best performance. In addition, it can be observed that the performance is higher for $3^{1024}$ than $3^{512}$ meshes. This is the same as previous study [14]. The weak scaling tests were performed by fixing 128 $3^{m}$ meshes for each GPU. From figure 3, we can observe good linearity with increasing GPU number.

4. Computational conditions

Figure 4 shows the computational and initial conditions for the directional solidification of Al–Cu binary alloy bicrystal. Initially, all domains were filled with liquid Al-3wt%Cu (0.013 at. frac.), and seeds were placed regularly on the bottom as shown in top view. To simulate bicrystal competitive growth, seeds with two different preferred growth directions $\theta$ are prepared. As shown in figure 4, the favorably and unfavorably oriented (FO and UO) seeds are placed on the left and right, respectively. The FO seed has $\theta = 0^\circ$ or grows toward heat flow direction, which is parallel to the $z$-direction, and the UO seeds have $\theta = 10^\circ$ and $30^\circ$. Here, secondary arms of the dendrites grow to the $x$ and $y$ directions. The domain is meshed into $n_x \times n_y \times n_z = 512 \times 2048 \times 1536$, and a periodic boundary condition in the $x$-direction and zero flux boundary condition in the $y$-direction are imposed. The temperature gradient $G$ along the $z$-direction was set to 5.0 K/mm. The pulling velocity was also fixed to $V_p = 100 \mu m/s$. The other parameters are as follows: $D_0 = 3 \times 10^{-9}$ m$^2$/s, $D_s = 3 \times 10^{-13}$ m$^2$/s, $k = 0.14$, $\zeta = 0.02$, $\Gamma = 0.24 \times 10^{-6}$Km, $m = -620$ K/at. frac., $W_0 = 0.625 \times 10^{-6}$ m, $\Delta t = 1.18 \times 10^{-5}$s, and $\Delta x = \Delta y = \Delta z = 0.5 \times 10^{-6}$m. The directional solidification is modeled by the moving frame algorithm to reduce the computational domain, where the computational domain shown in figure 4 tracks the dendrite tips to keep the enough diffusion layers in front of the dendrite tip.
5. Computational results and discussion

Figures 5 and 6 show the time slices during the simulations with the crystal orientation $\theta = 10^\circ$ and $\theta = 30^\circ$, respectively. Here, the isosurfaces with $\phi = 0$ are expressed with different colors for the two crystal orientations. After starting the simulations, the bottom of the domain is covered with the solid phase, and many dendrites initiate and grow upwards with selection. At that time, as shown in figures 5(a) and 6(a) the FO dendrites grow faster than the UO dendrites. Especially, the FO dendrites located at the grain boundaries grow faster than the other dendrites. Figure 6(a) shows that the side arms of the FO dendrites at the grain boundary overhang the UO dendrites side because the growth speed of UO dendrites with $\theta = 30^\circ$ is much slower than the FO dendrites. Even in figures 5(e) and 6(e) at 1,000,000 steps, the dendrite selections in FO grain occur and the equilibrium growth condition is not achieved. The UO dendrites migrate to left with dendrite growth, and are blocked by the FO dendrites at the grain boundary. Figure 6(d) shows that the UO dendrite goes into the space between the FO dendrites at that time. This phenomenon cannot be expressed by 2D simulations. The new dendrites of the UO dendrites with $\theta = 30^\circ$ are initiated by the branching as shown by the red circle in figure 6. On the other hand, for the UO dendrites with $\theta = 10^\circ$, the dendrite initiations cannot be observed until one million steps. Therefore, we need much longer computation time to investigate the dendrite competitive phenomena at the grain boundary as performed in 2D simulations [7]. The 384 GPUs are used for these computations and the computation time was about 12 hours. Therefore, it can be concluded that the present 3D simulations can be continued with reasonable computational time.

6. Conclusions

In this study, we developed a 3D phase-field code using multi-GPUs with a quantitative phase-field method for binary alloy solidification and moving frame algorithm for directional solidification. Then, we simulated the dendrite competitive growth during the directional solidification of a binary alloy bicrystal, and demonstrated that the 3D phase-field simulations can be performed within reasonable computational time. It will be a powerful simulation tool for predicting solidification microstructures.
Figure 5. Dendrite morphologies at (a) 200,000, (b) 400,000, (c) 600,000, (d) 800,000, and (e) 1,000,000 steps for the case of the UO dendrite with $\theta = 10^\circ$.

Figure 6. Dendrite morphologies at (a) 200,000, (b) 400,000, (c) 600,000, (d) 800,000, and (e) 1,000,000 steps for the case of the UO dendrite with $\theta = 30^\circ$. 

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