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GPU-accelerated three-dimensional phase-field simulation of dendrite growth in a nickel-based superalloy

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ABSTRACT

The microstructure formation of a nickel-based superalloy during solidification in three dimensions was investigated using the phase-field method. To accelerate the large-scale phase-field simulation, a parallel computing approach was developed using the graphic processing unit (GPU), and the limitation of insufficient GPU memory was circumvented by employing an asynchronous concurrent algorithm. The performance of the GPU-based parallel computing method was tested and the results demonstrate that a maximum performance of 774.292 GFLOPS (giga floating-point operations per second) can be obtained using a single NVIDIA GTX1080 GPU. In simulations of isothermal solidification, the microstructure evolution of a single and multiple dendrites under different undercooling levels was shown in detail. During the solidification, the dendrite tip growth velocity and fraction solid were recorded and then analyzed. In simulations of directional solidification, the formation of primary dendrite arms under different temperature gradients was investigated, and the simulated microstructure was in good agreement with experimental observations. Additionally, the distribution of primary dendrite arm spacing was quantitatively analyzed by Voronoi tessellation. Finally, simulation of polycrystalline growth in directional solidification was conducted to study the dendrite competitive growth. The unusual overgrowth phenomenon was observed in the initial growth stage, while as the solidification process proceeded, the dendrites with small inclination angles were more likely to overgrow the dendrites with large inclination angles.

1. Introduction

Nickel-based superalloys have been widely used in aeronautic and industrial gas turbines over the past several decades. The performance of the superalloy parts is strongly related with their microstructural characteristics, such as dendrite morphology, dendrite arm spacing. To optimize the mechanical properties of superalloy castings, it is essential to understand how the processing conditions can affect the dendrite microstructure evolution during solidification. In the past forty years, considerable progress in dendrite growth research has been made through both experimental and theoretical studies [1–4].

The phase-field method has proven to be a powerful tool to simulate complex phase interface changes in phase transitions, especially in alloy solidification [5–7]. In the phase-field model, an order parameter is introduced to represent different phases, and explicit tracking of the interface can be avoided, which makes reconstruction of the liquid solid interface much easier. However, the interface thickness is strictly constrained when obtaining quantitative simulation results according to the thin-interface limit of the phase-field model [8]. This means the computational grid size and time increment need to be rather small. Therefore, to simulate a typical scale of dendrite growth in three dimensions, a large amount of calculation is needed. To overcome the problem of massive computation, many efforts have been made to improve the computing technologies, including cluster computing using MPI [9] and adaptive mesh refinement (AMR) algorithm [10,11]. Nevertheless, these computing techniques are either limited by the number of CPU cores or are too tricky to implement in three-dimensional simulations.

Recently, GPU-based parallel computing technology has emerged as a powerful tool in scientific computation owing to the GPU's massive computation capacity and high memory bandwidth. Researchers have successfully employed GPU computing in a variety of numerical simulations, including molecular dynamics simulations [12], computational fluid dynamics simulations [13], and other engineering applications. In the last few years, there have been attempts [14–22] to apply GPU parallel computing algorithm to phase-field simulations of dendrite growth. In one of

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the earliest works on phase-field simulation using GPU, Kim [14] developed a program to simulate two-dimensional ice crystal growth, and achieved a ninefold speedup compared to the case of using a CPU. Yamanaka et al. [15] extended the phase-field computation algorithm to three dimensions on a GPU, and achieved the performance of 170 GFLOPS for 576^3 computational grids using a single NVIDIA TESLA C1060 GPU. For multi-GPU computing, Shimokawabe [17] reported the phase-field computing performance of 1.017 PFLOPS using 4000 GPUs on the TSUBAME 2.0 supercomputer. As for GPU implementation of multi-dendrite growth simulation, Takaki [18,19] and Tourret [20,21] simulated two- and three-dimensional multi-dendrite competitive growth in directional solidification. Sakane et al. [22] developed a multi-GPU computing scheme that coupled the phase-field method with the lattice Boltzmann model to simulate dendrite growth in a melt flow. However, multi-GPU supercomputers are not available to many researchers, and the implementation of large-scale three-dimensional phase-field computing on a single GPU is still a problem.

In the present work, a phase-field model for solidification in binary alloy is summarized, and the specific implementation is presented. An algorithm is developed for three-dimensional phase-field simulations of multi-dendrite growth using a GPU. The details of reducing memory access latency using GPU shared memory and local registers are explained. However, when performing large-scale phase-field simulations, the shortage of GPU memory emerges as a knotty problem. The common solution is the implementation of multi-GPU computation or the usage of a GPU with a larger GPU memory, such as NVIDIA P100 GPU. However, both of the above GPU devices are currently too expensive for many researchers. Here, we put forward an asynchronous concurrent data transfer and computing algorithm, which overcomes the limitation of insufficient GPU memory, and we successfully carried out large-scale phase-field simulations on a single GPU device. Finally, three-dimensional simulations of dendrite growth in a nickel-based superalloy during the isothermal and directional solidification process are performed using the phase-field model, and the results are quantitatively analyzed.

2. Model description

2.1. Phase-field model

In this study, in order to simplify the computation, the multi-component superalloy was simplified as a pseudo-binary alloy using Raghavan's approach [23]. Further, a quantitative three-dimensional phase-field model [7] for binary alloys was employed to simulate the dendrite growth in nickel-based superalloy. The formulated model could simulate both isothermal and non-isothermal dendrite growth. In isothermal solidification with a constant cooling velocity, the temperature is uniform in the simulation domain and is expressed as:

$$T = T_0 + R_c \cdot t \tag{1}$$

where T_0 is the initial temperature, R_c is the cooling rate and t is time. In directional solidification, the temperature is assumed to follow the frozen temperature approximation, which is expressed as:

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

where T_0 is the temperature at $z = 0$ and $t = 0$, G is the temperature gradient and V_p is the pulling velocity aligned with the z-axis.

The time-dependent equations of the phase-field variable ϕ ($\phi = 1$ in solid and $\phi = -1$ in liquid) and dimensionless solute concentration U in three dimensions are given as:

$$\begin{aligned}\tau A^2(\vec{n})\frac{\partial\phi}{\partial t} &= \frac{\partial}{\partial x}\left(|\nabla\phi|^2 A(\vec{n})\frac{\partial A(\vec{n})}{\partial\phi_x}\right) + \frac{\partial}{\partial y}\left(|\nabla\phi|^2 A(\vec{n})\frac{\partial A(\vec{n})}{\partial\phi_y}\right)\\ &+ \frac{\partial}{\partial z}\left(|\nabla\phi|^2 A(\vec{n})\frac{\partial A(\vec{n})}{\partial\phi_z}\right) + \nabla\cdot\left(A(\vec{n})^2\nabla\phi\right) + \phi\\ &- \phi^3 - \lambda(1-\phi^2)^2(U+\theta)\end{aligned} \tag{3}$$

$$\begin{aligned}\left[\frac{1+k-(1-k)\phi}{2}\right]\frac{\partial U}{\partial t} &= \nabla\cdot\left(D_l\frac{1-\phi}{2}\nabla U + \frac{1}{2\sqrt{2}}(1+(1-k)U)\frac{\partial\phi}{\partial t}\frac{\nabla\phi}{|\nabla\phi|}\right)\\ &+ \frac{1}{2}[1+(1-k)U]\frac{\partial\phi}{\partial t}\end{aligned} \tag{4}$$

with the dimensionless undercooling θ and solute concentration U being:

$$\theta = \frac{T - T_M - mc_\infty}{|m|c_\infty(1/k-1)} \tag{5}$$

$$U = \frac{1}{1-k}\left[\frac{c/c_\infty}{k(1+\phi)/2 + (1-\phi)/2} - 1\right] \tag{6}$$

where T_M is the melting temperature of the pure solvent, m is the liquidus slope, k is the partition coefficient, c_∞ is the value of c far from the interface that equals the initial concentration of the alloy, and D_l is diffusion coefficient in the liquid. The coupling constant λ is defined as:

$$\lambda = a_1\frac{W_0}{d_0} \tag{7}$$

where $a_1 = 5\sqrt{2}/8$ [7], W_0 is the interface thickness, and $d_0 = \Gamma/[|m|c_\infty(1/k-1)]$ is the chemical capillary length, with Γ being the Gibbs–Thomson coefficient. According to thin interface analysis [7,24], the relaxation time τ is constructed to eliminate the kinetic effect. In isothermal solidification, $\tau = \tau_0[1+(1-k)U]$, and in directional solidification $\tau = \tau_0[1-(1-k)\theta]$, with the $\tau_0 = a_2\lambda W_0^2/D_l$, and $a_2 = 47/75$ [7].

The crystalline anisotropy [8][24] defined by $A(\vec{n})$ in Eq. (3) is given as:

$$A(\vec{n}) = 1 - 3\varepsilon_4 - 4\varepsilon_4\frac{(\phi_x)^4 + (\phi_y)^4 + (\phi_z)^4}{(\phi_x^2+\phi_y^2+\phi_z^2)^2} \tag{8}$$

where ε_4 denotes the amplitude of anisotropy strength, and ϕ_x, ϕ_y, ϕ_z denotes the partial derivatives of ϕ in the x, y, z directions. In order to simulate multi-dendrite growth with different orientations, an extra crystal orientation field $p(x,y,z)$ is used, which is defined as $p(x,y,z) = i$ in the ith dendrite and $p(x,y,z) = 0$ in the liquid phase. The value of $p(x,y,z)$ is the index of crystal orientation array, which contains three Euler angles (α, β, γ) to describe the misoriented grain. The following coordinate transformation is used to convert the original coordinate system (x,y,z) to the new one $(\bar{x},\bar{y},\bar{z})$:

$$\begin{pmatrix}\bar{\phi}_x\\ \bar{\phi}_y\\ \bar{\phi}_z\end{pmatrix} = \begin{bmatrix}1 & 0 & 0\\ 0 & \cos\alpha & \sin\alpha\\ 0 & -\sin\alpha & \cos\alpha\end{bmatrix}$$
$$\begin{bmatrix}\cos\beta & 0 & \sin\beta\\ 0 & 1 & 0\\ -\sin\beta & 0 & \cos\beta\end{bmatrix}\begin{bmatrix}\cos\gamma & \sin\gamma & 0\\ -\sin\gamma & \cos\gamma & 0\\ 0 & 0 & 1\end{bmatrix}\begin{pmatrix}\phi_x\\ \phi_y\\ \phi_z\end{pmatrix} \tag{9}$$

The transformed $\bar{\phi}_x, \bar{\phi}_y, \bar{\phi}_z$ is used in substitution of ϕ_x, ϕ_y, ϕ_z in Eq. (8) to calculate the anisotropy of a misoriented dendrite.