Computational Materials Science 147 (2018) 338–352

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Fast simulations of a large number of crystals growth in centimeter-scale during alloy solidification via nonlinearly preconditioned quantitative phase-field formula

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ARTICLE INFO

Article history:
Received 28 November 2017
Received in revised form 18 January 2018
Accepted 2 February 2018
Available online 22 February 2018

Keywords:
Phase-field
Centimeter-scale simulations
Polycrystalline
Alloy
Solidification

ABSTRACT

Ameliorating the computing efficiency is always of importance in phase-field simulations of material microstructure formation and evolution. Borrowing from the nonlinear preconditioning treatment of diffuse interface models, the usual quantitative phase-field model for a binary alloy has been transformed to make it easier to compute accurately. The transformation yields a new variable whose value changes linearly across the interface. The dependences of simulated results of the nonlinearly preconditioned phase-field formula on the interface grid size and the discretization time step have been examined in detail through numerical experiments, including the growth velocity, the radius and the solute concentration of a steady tip. The results show that the new evolution equations are able to be solved on a computational mesh with interface grids 2–4 times coarser than those used in the conventional method. In combination with the front-tracking method to capture the crystallographic orientation of each crystal, the orientation gradient energy is incorporated into the nonlinearly preconditioned phase-field model, which enables simulations of grain boundary behaviors. The algorithm of the distributed parallel finite element method on an adaptive mesh is applied to further raise the computing efficiency. Simulations of multi-dendrites growth of Al-4 wt.%Cu alloy in undercooled melt cooling down continuously are performed. The results demonstrate that the proposed fast simulation approaches allow quantitative simulations of a large number of dendrites growth on the scale of centimeters or millimeters, respectively in two or three dimensions, just using an ordinary workstation instead of clusters or supercomputers.

1. Introduction

Solidification microstructures of alloys have a crucial influence on the performance of castings [1]. The dendritic crystal is one of the most common microstructural patterns formed during solidification. Its evolution has been investigated in physics and material science for several decades since the classic theory was proposed by Ivantsov [2], who gave an analytical relationship of the operating state of dendritic tip, the growth velocity and the radius, with the undercooling. Recently, inherited from the convenience of the in situ and real-time observations of solidification process on transparent organic alloys [3,4], the synchrotron X-ray radiography has become an effective method to reveal dendrite growth dynamics in metallic alloys [5–7]. These dynamical observations have substantially improved our cognition of the microstructure evolution during solidification of alloys. For the moment, however, the in situ and real-time observations are still limited to quasi-two-dimensional (quasi-2-D) thin samples. Actually, for most of the polycrystalline alloy materials, the collective behavior of a large number of crystals in large-scale three-dimensional (3-D) space is of vital significance in determining the final microstructure selection of castings.

Over the past few decades, as a novel tool to reproduce the microstructure evolution, numerical computing techniques have become a powerful method to explore the underlying mechanism of the solidification microstructure evolution [8–11]. Largely on account of the development in a numerical modelling approach called phase-field method, accompanied by the ever-increasing computational capabilities, great progress has been made in simulations of solidification on the scale of the developing microstructure [1,8,12]. This method employs an auxiliary continuous order parameter to describe the time- and space-dependent phase evolution. The value of this order parameter is constant in the bulk

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https://doi.org/10.1016/j.commatsci.2018.02.003
0927-0256/

liquid and solid phases, while varies sharply but continuously in the interface layer between disparate phases, which makes the location of the interface thus available to be tracked implicitly. Owing to the circumvention of explicitly tracking the interface, the boundary conditions which should be applied to guarantee the individual solutions to transport equations in the bulk phases match properly at the interface are removed. This convenience leads to the phase-field method becoming a prime choice to simulate the complicated interface change in phase transformations, especially during solidification of pure materials and alloys [13–17].

However, owing to the strict constraint on the interface width in phase-field models, the computational gird size and the discretization time step need to be rather small to obtain quantitative simulations [14,16]. This means that an enormous amount of calculation is required to accurately simulate a typical scale of the crystal growth in a large domain, particularly in 3-D space. To overcome this drawback of the massive computation, many researchers have proposed diverse numerical techniques to improve the computational efficiency of phase-field simulations.

The adaptive mesh technique has been demonstrated to be a computationally efficient approach to open a window of large-scale simulations on solidification physics. Using the adaptive mesh procedure, the grid size in the whole domain is not uniform, but changes with the moving phase interface. For instance, in the h-adaptive finite element method [18], the mesh is rather fine across the interface while very coarse in the bulk phases, thus pronouncedly reducing the computing degree of freedom. Utilization of the adaptive mesh algorithm to simulate the microstructure evolution during solidification goes back to the numerical calculation of heat and phase field equations by Schmidt [19]. Two coupled finite element algorithms were proposed to solve the governing equations on time-dependent, locally refined and coarsened adaptive meshes, for modelling the dendrite growth in both of 2-D and 3-D domains [19]. Braun and Murray [20] employed a general-purposed adaptive finite difference approach to solve the phase-field model of pure material solidification with a small undercooling, and good convergence to sharp-interface models had been achieved, which indicated adaptivity in space and time was able to extend the parameter regime used in phase-field simulations. Provatas et al. [21,22] studied the solidification microstructure evolution through solving the phase-field formula proposed by Karma and Rappel [23] on an adaptive mesh using the finite element method. In that calculation, the domain size was enlarged to a scale of millimeters, and the 2-D time-dependent computations were in good agreement with the prediction of the solvability theory for high undercoolings. Lan et al. [24,25] proposed an adaptive finite volume method to expedite computations of phase-field simulations for both equiaxed and columnar dendrite growth, in which the fluid dynamics was coupled. Guo and Xiong [26] presented an algorithm consisting of the adaptive mesh refinement and parallel computing capabilities, to efficiently solve the coupled thermo-solutal phase-field equations in 3-D space, and the simulated results of single and multi-dendrites growth showed that the proposed method could shorten the computing time for about two orders of magnitude.

Besides these numerical algorithms to enhance the computing efficiency and enlarge the simulation scale, the fast-developed high-performance supercomputers have been used extensively. In the past few years, on account of the massive computational capacity, the parallel computing using the graphic processing unit (GPU) has become a powerful tool in numerical computations, and has been also applied in phase-field simulations of dendrite growth. Yamanaka et al. [27] employed a GPU to accelerate the phase-field simulation for dendritic solidification of a binary alloy, and it was confirmed that a real-time 3-D phase-field simulation of the microstructure evolution was able to be realized on a personal desktop computer. When it comes to polycrystalline solidification, Takaki et al. [28,29] and Tourret et al. [30,31] investigated the competitive growth of columnar dendrites in both of 2-D and 3-D large-scale domains, using the GPU-accelerated phase-field simulations. Yang et al. [32] researched the microstructure formation of a nickel-based superalloy during solidification in 3-D by a GPU-based parallel computing approach. These simulations have demonstrated that the GPU-accelerated parallel computing is remarkably high-efficiency and extends phase-field simulations to a scale of millimeters in 3-D. However, the large-scale simulation employing a high-performance computing supercomputer is extremely costly.

Additionally, Glasner [33] has proposed a nonlinear preconditioning method of transforming diffuse interface problems to improve the computing accuracy associated with typical discretization schemes. This method allows coarser girds to be utilized to expedite computation remarkably, which has been used in recent phase-field simulations of columnar crystals growth during directional solidification [30,31,34]. However, the influence of this transformation on the accuracy of simulated results for binary alloys has not been investigated in detail. In this work, the widely used quantitative phase-field model of binary alloys proposed by Karma [16] is preconditioned using the transformation procedure. The accuracy of the nonlinearly preconditioned model with the variation of the grid size and the time step will be examined in 2-D and 3-D simulations, for clarifying the allowable interface grid size and time step which can be used in quantitative phase-field simulations after this transformation. The front-tracking method proposed in our previous work [35] adopted to capture crystal orientations in polycrystalline solidification is extended to including the grain boundary energy, and the method is then combined into the preconditioned phase-field model. Finally, with the distributed parallel adaptive finite element method to solve the phase-field equations, simulations of multi-dendrites growth of Al-4 wt.%Cu alloy under the continuous-cooling condition are carried out in very large domains on the scale of centimeters in 2-D and millimeters in 3-D just using an ordinary workstation, in order to provide a straightforward awareness of the computational capability of the fast simulation schemes proposed in the present work.

2. Model descriptions and numerical implementations

2.1. Nonlinear preconditioning transformation of a phase-field formula

Although the phase-field method has advantages in handling free boundary problems with moving interfaces, the stringent but indispensable limitations on the characteristic interface width and the grid size in the diffuse interface layer are the critical factors imposing restrictions on quantitative simulations in large computational domains. In order to overcome this drawback for diffuse interface models, Glasner [33] proposed a nonlinear preconditioning transformation of the governing equations. The original phase field varying nonlinearly across the interface is transformed to a new variable whose value changes linearly in both interface layer and bulk phases. The key point of the transformation is that it can substantially reduce spatial errors deriving from typical discretization scheme, which allows coarser grids to be used to expedite computing [33]. Moreover, the truncation errors in time can be improved to permit a larger discretization time step. The mathematical detail of the nonlinear preconditioning treatment can be found in Ref. [33], and here we just give a concise introduction.

Considering the following conventional one-dimensional time-dependent phase field equation for a binary alloy with isotropic