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Numerical simulation of dendritic growth in directional solidification of binary alloys using a lattice Boltzmann scheme

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ABSTRACT

A lattice Boltzmann (LB) based model is utilized to simulate three dimensional dendritic growth in directional solidification of alloys. The LB–D3Q19 lattice vectors are used to describe advancement of solid–liquid interface, coupling with a conservation equation for solute transport in solidification. After model validation, the dendritic growth under several conditions of directional solidification was investigated and a solidification entropy was proposed to quantitatively characterize solidification morphologies. The results show that the present model captures tip-splitting occurring at a relative fast solidification rate. Initial thermal undercooling and solute concentration are dominant factors influencing the final microstructure. The solidification entropy reflects complexity of dendritic morphologies and it is useful to characterize dendritic growth in solidification. A design map was proposed to predict dendritic growth with and without tip-splitting, offering potential for simulating dendritic growth and microstructure evolution in solidification of alloys.

1. Introduction

Dendritic growth is a commonly phenomenon encountered in solidification of metals and alloys. It directly influences the heat and mass transfer, macro/micro segregation, microstructure evolution, and subsequently determines final physical properties of castings. Revealing formation mechanisms of dendrites would provide useful information for optimization of materials processes and design of advanced alloys. A considerable amount of numerical research has been devoted to investigate the dendritic growth and microstructure evolution for several decades [1–4]. The directional solidification which can produce simple and uniform microstructure enables us to correlate the formation of microstructure and its characteristic length scales quantitatively with processing parameters [5]. Advance in the scientific understanding of dendritic growth in directional solidification is of great applicable value for the fabrication of innovative alloys and better castings.

In the last decades, the lattice Boltzmann (LB) method has been rapidly emerging as a powerful tool for modeling and simulation of phenomena in complex systems [6–10]. A considerable amount of work based on the LB method has been carried out to research phase transition and microstructure evolution of metals and alloys [11–13]. The LB method is different from conventional modeling techniques for it describes the objective system as a collection of fictitious particles moving on lattices of the discrete computational space. The macroscopic behaviors of the system are modeled by the evolution of particles, which enables the LB method to be a mesoscopic bridge connecting microscales and macroscales. The kinetic-based background provides the LB models several distinctive advantages in modeling innovation, simulation fidelity and computational efficiency [14]. Such intrinsic features of the LB models allow themselves to simulate microstructure evolution with techniques which are used to describe kinetics of dendritic growth. The LB models we aware of were firstly coupled with phase filed (PF) models to study the dendritic growth of metals and alloys [15–18]. Miller and co-works firstly proposed a PF model fitting into the LB framework for anisotropic liquid–solid phase transition [15]. Subsequently, several PF–LB coupled models were proposed to investigate dendritic growth with melt convection [16–19]. Medvedev and Kassner [17,18] developed a PF–LB

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coupled scheme to simulate the growth of dendrites from a supercooled melt, allowing for heat transport by both diffusion and convection. Selzer et al. [19] numerically studied the influence of melt flow on dendritic morphology of a Ni–Cu alloy by a PF–LB coupled model. In these models, the PF method is adopted to describe the liquid–solid transition, while the LB method is employed to model melt convection, heat and mass transfer during solidification.

The cellular automaton (CA) method is another widely used technique in modeling and simulation of dendritic growth. As the LB method is developed from the lattice gas automaton which can be considered as an advanced CA technique, it is very straightforward to combine the CA and the LB methods to simulate dendritic growth. Sun et al. developed a CA–LB coupled model to study dendritic growth of binary alloys with forced flow and natural convection [20,21]. In the model, the CA technique is deployed to track the new interface cells, and the LB method is used to account for solute transport. After that, Felicelli and co-workers extended the CA–LB coupled models to study the three-dimensional dendritic growth [22,23]. Jelinek et al. developed a large-scale parallel CA–LB coupled model and studied the dendritic growth during solidification of a binary alloy [24]. These models can be used to simulate dendrite growth of alloys with significantly improved computational efficiency and large-scale parallelization capability. The numerical studies on dendritic growth by using the PF–LB and the CA–LB models have demonstrated that the LB method is indeed very promising as an efficient numerical tool for the investigation of phase transition during solidification. However, all the above-mentioned studies with the LB methods were mostly focused on free dendritic growth from melts of alloys, and the advancing of solid–liquid interface in these models is described by the PF, the CA or other techniques. Little work has been reported about the application of LB methods to study the dendritic growth in directional solidification. Recently, Sun et al. developed a multi-relaxation-time based LB model to study the three dimensional dendritic growth and bubble formation during directional solidification of alloys [25]. It provides an evidence that the LB based technique is an alternative solution for investigation of microstructure evolution. The microstructure formed in directional solidification can be significantly affected by various processing conditions. As the directional solidification is widely used in the fabrication of technical alloys, it is of great importance to have a deep understand on dendritic growth in the conditions of directional solidification.

The main purpose of this work is to study dendritic growth of binary alloys and explore dominant factors influencing microstructure formation in directional solidification. We attempt to explain the influencing mechanism of several conditions on morphological evolution by a well-defined solidification entropy. As the CA models are usually of higher computational efficiency than the PF models [4], we combine the CA and the LB modeling techniques into a convenient and efficient scheme to describe the growth dynamics of dendrites. The solute conservation equation with a well-defined pseudo-potential is adopted to account for the mass transport in solidification. A LB scheme is utilized to track the advancement of solid–liquid interface and describe the evolution of dendritic morphology. After model validation by simulating the problems of transient diffusion and free growth of dendrites, the model is utilized to study the evolution of dendritic morphologies under several conditions of directional solidification. The effects of initial undercoolings and solute concentrations are subsequently investigated in a systematic way. Finally, a design map is proposed to facilitate the prediction of tip-splitting during dendritic growth of alloys.

2. Mathematical modeling

2.1. Governing equations

2.1.1. Solute conservation

In this work, we focus on growth kinetics of dendrites rather than melt convection on the microstructure evolution. The convective effect of melt flow on solute transport and growth kinetics is therefore neglected for simplicity. For the present solidification system, we take the solute diffusion in both liquid and solid phases into consideration. The solute conservation during dendritic growth is governed by

$$\frac{\partial C(\mathbf{x},t)}{\partial t} = \nabla \cdot [D(\mathbf{x},t)\nabla V(\mathbf{x},t)], \tag{1}$$

where C is solute concentration, D is solute diffusion coefficient, and V is pseudo-potential driving solute transport with $V = C/(f_L + k_p f_S)$. Here, f denotes phase fraction, and k_p is solute partitioning coefficient. The subscripts, L, S and I are used to indicate the solid phase, the liquid phase, and the solid–liquid interface, respectively. Therefore, f_S represents the solid fraction at $(\mathbf{x}, t)$. The concentration and diffusion coefficient at the solid–liquid interface, C_I and D_I, can be calculated by using their respective values in solid and liquid phases, i.e. $C_I = f_L C_L + f_S C_S$ and $D_I = f_L D_L + k_p f_S D_S$.

We should emphasize that the liquid concentration in an interface cell should increase due to the rejected solute from the solidifying dendrite. However, there is no additional term on the right hand side of Eq. (1) to account for the solute partition during solidification. That is because any change of solid fraction in an interface cell can alter the potential V, which in turn influences the solute concentration according to Eq. (1). Therefore, the concentration change caused by solute partition during the liquid–solid phase transition has been involved implicitly into the solute conservation equation. In addition, the present model allows us to incorporate melt flow into solute transport equation by adding a convertive term. The governing equation for solute transport can be solved on the regular spatial mesh by the finite volume (FV) and the LB methods. In the present work, the FV scheme is used to solve the solute conservation equation. Other details of numerical strategy for simulations by the LB based models, especially the convective effect on microstructure evolution as well as the three dimensional dendritic growth, can be found in our previous work [20,21,25].

2.1.2. Kinetics of growth

In the present model, the dendritic growth is considered to be driven by the total undercooling in the front of solid–liquid interface. The growth speed at the solid–liquid interface is evaluated by the following relation

$$V_g(\mathbf{x},t) = \mu_k \Delta T(\mathbf{x},t), \tag{2}$$

where V_g is growth speed at position $\mathbf{x}$ and time t, μ_k is the interfacial kinetic coefficient, and $\Delta T(\mathbf{x}, t)$ denotes the total undercooling at $(\mathbf{x}, t)$. To describe the interface advancement, Zhu et al. [26] suggested a simple and efficient geometrical factor G_{lattice} fitting into framework of CA method, and connected the growth speed and the increased solid fraction by G_{lattice}. In the present model, the growth kinetics is also modeled by a G_{lattice} for its simplicity and efficiency. However, the lattice neighborhood is described by a LB scheme rather than the CA scheme. The increased fraction of solid phase in an interface cell during each time interval is computed by

$$\Delta f_S(\mathbf{x},t) = \mu_k \Delta T(\mathbf{x},t) G_{\text{lattice}} \frac{1}{c}, \tag{3}$$

where $\Delta f_S(\mathbf{x}, t)$ represents the increment of solid fraction at $(\mathbf{x}, t)$, and c is the lattice speed. For a given discrete system with spatial step Δx and time interval Δt, the lattice speed can be computed