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A lattice Boltzmann study on dendritic growth of a binary alloy in the presence of melt convection

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A B S T R A C T

A multi-relaxation-time (MRT) lattice Boltzmann (LB) based model is utilized to simulate the dendritic growth with melt convection in solidification of alloys. It models melt convection by the MRT-LB equation and solute transport by a conservation equation with a pseudo-potential function. The D2Q9 lattice vectors are proposed to describe interface advancement in the liquid-solid transition. Effects of undercoolings, interface curvature and preferred growth orientation are incorporated into the model implicitly. After model validation, dendritic growth under several conditions of pure diffusion and melt convection was numerically investigated, and the solidification entropies were proposed to quantitatively characterize the solidification system. The result shows that the growth behavior, microstructure formation and solute segregation are significantly influenced by melt convection. The solidification entropies reflecting complexity of the solidification system are useful to characterize dendritic growth and solute segregation. This work offers a potential solution for studies of microstructure evolution in solidification of alloys.

1. Introduction

As the most commonly observed microstructure in solidification of metallic materials, dendritic morphologies are closely associated with the mechanical integrity of castings. The dendritic growth is known to be always accompanied by solute transfer and melt convection which may significantly influence microstructure evolution, solute segregation and final properties of castings. Formation of dendritic morphology with melt convection for alloys is much more important than that in pure diffusion condition. Advance in the scientific understanding of dendritic growth with melt convection is of great applicable value for the fabrication of innovative alloys and better castings. There is a great demand for numerical studies of dendritic growth with melt convection. The interactive mechanisms between dendritic growth and melt convection are of great importance in both academic researches and engineering applications.

A considerable amount of numerical studies have been devoted to investigating the dendritic growth with melt convection for decades [1–3]. In the last decades, the lattice Boltzmann (LB) method rapidly emerged as a powerful and indispensable method for modeling complex systems with fluid flows [4–6]. Massive notable researches based on the LB method have been done to study phase transition and microstructure evolution in solidification of metals and alloys [7–9]. The LB method was originated from Ludwig Boltzmann's kinetic theory, which is different from conventional modeling techniques solving the Navier-Stokes equations. It describes the objective fluid system as a collection of microscopic pseudo-particles streaming and colliding on lattices using the Eulerian description. Through the evolution of particles, macroscopic behaviors of the system are modeled, which entitles the LB method to be a mesoscopic bridge connecting microscales and macroscales. As the LB method is kinetic-based, the LB models have several distinctive advantages in modeling innovation, simulation fidelity and computational efficiency [10]. For such intrinsic advantages, the LB models have been therefore coupled with other simulation techniques to model the interaction of phase transition.

Miller et al. [11,12] firstly proposed a phase field (PF) model fitting into the LB framework for anisotropic liquid-solid phase transition, studied the interaction between phase transition and melt convection, and simulated free dendritic growth of a pure metal with moderate buoyancy convection as well as cellular growth with shear flows. Subsequently, Medvedev and Kassner [13,14] combined the PF method and the LB scheme to simulate dendritic growth with liquid flows from a supercooled melt. The

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Nomenclature

C	concentration
c	lattice speed
c_s	lattice sound speed
D	diffusion coefficient
$\mathbf{e}_\alpha$	discrete velocity
f	phase fraction
f_α, f_β	distribution function
F_s	total solid fraction
G_{lattice}	geometrical factor
j_x	mass flux
K	curvature
k_p	partition coefficient
$\mathbf{M}$	transformation matrix
$\mathbf{m}$	moments
m_α	element of moments
m_l	liquidus slope
N_s	seed number
$p()$	probability function
p_{xx}	stress tensor
q_x	energy flux
$\mathbf{S}$	relaxation matrix
$s_0, s_1, \ldots$	relaxation times
S_c	concentration entropy
S_s	solidification entropy
T	temperature
$\mathbf{u}$	velocity
V	pseudo-potential
w_α	weight coefficient
F_α	discrete body force
ϵ_1	energy anisotropy
ϵ_2	kinetic anisotropy
γ	Gibbs-Thomson coefficient
μ_k	kinetic coefficient
ν	shear viscosity
ρ	density
θ	interface orientational angle
θ_p	preferred growth angle
ζ	bulk viscosity

Subscripts

α, β	components
a	average value
c	solutal value
i	interface value
l	liquid value
r	curvature value
s	solid value
t	thermal value

phase-transition part of their problem was modeled by the PF approach, whereas the melt convection was computed by a single-relaxation-time based LB model [13,14]. Selzer et al. [15] numerically studied the influence of melt convection on dendritic growth of a Ni-Cu alloy by using the 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 the melt convection which drives the heat and mass transfer during solidification. Chakraborty and Chatterjee [16] developed an enthalpy-based hybrid LB technique for simulating convection-diffusion phenomena during phase-transition processes, fitting into a thermodynamically consistent manner for non-isothermal systems. After that, the enthalpy-LB model was extended to study the conduction dominated phase change and transport phenomena during solidification [17,18]. The models relying on a level-set and volume-of-fluid tracking procedure with piecewise linear interface reconstruction are also usually used to study dendritic growth in solidification [19,20]. In these models, the growth velocity is constructed to account for both the thermal and solutal balance at the interface. However, the balance conditions are not explicitly satisfied [21] and the reconstruction of distance function is needed to maintain the diffusion interface.

The cellular automaton (CA) method is another widely used modeling technique to study microstructure evolution in solidification of metals and alloys. Historically, the LB method is originated from the lattice gas automaton which is an advanced CA technique. It is therefore natural to combine the CA and LB models to simulate dendritic growth with and without melt convection. Sun and co-workers proposed a CA-LB coupled model to reveal underlying interactions between dendritic growth and melt flows including forced flows and buoyant convection [22,23]. In the model, a single-relaxation-time LB scheme was used to account for solute transport governed by convection and diffusion. It demonstrated the quantitative, numerically stable and computationally efficient capabilities of the LB-based model. Felicelli et al. extended the CA-LB coupled models to study dendritic growth in three-dimension [24,25]. After that, Jelinek et al. developed a large-scale parallel CA-LB model incorporating solute diffusion, heat transfer, melt convection and phase change [26]. The model was then used to numerically study the two-dimensional dendritic solidification under forced convection, showing very good scalability.

The numerical studies on dendritic growth by the PF-LB, the Enthalpy-LB, and the CA-LB methods have proved that the LB method is an efficient numerical tool to reveal correlation between fluid flows, heat transfer and phase transition in solidification. The LB-based models provide significantly improved computational efficiency in the simulation of dendrite growth of metals and alloys [11,22]. Recently, a multi-relaxation-time (MRT) based LB model was proposed to study the three dimensional dendritic growth and bubble formation of alloys [27,28]. It provides an evidence that the MRT-LB based technique is an alternative solution with good numerical stability to study dendritic growth of alloys. However, the effect of melt convection on dendritic growth has not been considered in the model. As melt convection is unavoidable in solidification of alloys, it is very important to have a deep understanding of dendritic growth with melt convection.

The present work is aiming to studying dendritic growth of binary alloys and explore dominant factors affecting microstructure formation in solidification. We attempt to explain the influencing mechanism of several conditions on morphological evolution by a well-defined solidification entropy. Considering the CA models are usually more computationally efficient than the PF models, we combine the CA and the LB techniques into a convenient and efficient scheme to model dynamics of dendritic growth associated with melt convection. The solute conservation equation with the convective term is adopted to account for the mass transport in solidification. The melt convection is described by the multi-relaxation-time (MRT) LB model for its numerical stability. A scheme fitting into the LB framework is utilized to track the advancement of liquid/solid interface and describe the evolution of dendritic morphology. After model verification by simulating the single free dendritic growth, the model is used to study the evolution of multiple dendritic growth under several conditions