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A Diffuse-Interface Lattice Boltzmann Method for the Dendritic Growth with Thermosolutal Convection

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Abstract. In this work, we proposed a diffuse-interface model for the dendritic growth with thermosolutal convection. In this model, the sharp boundary between the fluid and solid dendrite is firstly replaced by a thin but nonzero thickness diffuse interface, which is described by the order parameter, and the diffuse-interface based governing equations for the dendritic growth are presented. To solve the model for the dendritic growth with thermosolutal convection, we also developed a diffuse-interface multi-relaxation-time lattice Boltzmann (LB) method. In this method, the order parameter in the phase-field equation is combined into the force caused by the fluid-solid interaction, and the treatment on the complex fluid-solid interface can be avoided. In addition, four LB models are designed for the phase-field equation, concentration equation, temperature equation and the Navier-Stokes equations in a unified framework. Finally, we performed some simulations of the dendritic growth to test the present diffuse-interface LB method, and found that the numerical results are in good agreements with some previous works.

AMS subject classifications: 74N05, 76D05, 80A20

Key words: Dendritic growth, diffuse interface, lattice Boltzmann method, phase-field method.

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1 Introduction

Dendritic growth, as a complicated phase transition process coupling with melt flow, heat and solute transfer, is usually observed in both nature and engineering. To reveal the underlying mechanism of morphological evolution and to improve the properties of materials during the solidification process, the problem of dendritic growth has been investigated extensively from experimental and numerical perspectives [1–5].

With the development of computer science and scientific computing, the numerical simulation has become a powerful and important tool in the study of the solidification processes, and a large number of mathematical models and numerical methods have been developed for the dendritic growth, for instance, the cellular automation method [6, 7], enthalpy method [8, 9], level-set method [10] and phase-field method [11, 12]. The phase-field method with an order parameter introduced to distinguish different phases, has been widely used to investigate dendritic growth [13, 14] for its thermodynamically self-consistence and needless of explicit interface-tracking. In the early works [15–18], however, the phase-field method is only adopted for the dendritic growth with pure diffusion, and the effects of thermal convection, solutal convection and melt flow are usually considered separately. For instance, the thermal dendritic growth and solutal dendritic growth with melt flow in [15], three-dimensional thermal dendritic growth with melt flow in [16,18], and the thermosolutal dendritic growth with pure diffusion in [17]. Moreover, the Navier-Stokes (NS) equations for flow field are solved by some traditional computational fluid dynamics approaches, which may also bring some difficulties in treating fluid-solid interaction and complex boundary conditions.

In the past three decades, the mesoscopic lattice Boltzmann (LB) method, as a popular kinetic-theory based numerical approach, has become an efficiently numerical tool in the simulation of complex fluid flows [19–22] and nonlinear systems [23, 24], such as the multiphase and multicomponent flows [25, 26], phase transitions [27–29] and fluid flows in porous media [21, 30]. Compared to the traditional computational fluid dynamics approaches, the LB method has some distinct features, including the simplicity in coding, easy implementation of complex boundary conditions, and fully parallel algorithms [21]. Considering the advantages of the phase-field and LB methods, some phase-field LB models for the dendritic growth have been developed [31–37]. However, in the most of previous works on phase-field LB models [32–34, 37], the LB method is only used to simulate melt flows as well as heat and solute transfer, and other techniques are adopted to solve the phase-field equation, such as the normal finite difference methods in [32–34] and Para-AMR algorithm in [37]. To develop an efficient computational model in a unified LB framework, Cartalade et al. [31, 38] proposed an anisotropic LB model for the dendritic growth with interfacial anisotropy, and the streaming is modified to achieve the relaxation time in the phase-field equation. However, the supersaturation equation was tediously reformulated to overcome some difficulties in their work. Sun et al. [35, 39] extended the anisotropic LB model to study thermal dendritic growth in the presence of melt flow, in which the multi-relaxation-time (MRT) LB model is applied to