Quantitative phase-field model coupled with lattice Boltzmann method for simulations of practical alloy systems

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ABSTRACT

Understanding of formation process of solidification microstructure in alloys is one of very important issues in the field of metallurgy because features of solidification microstructures such as size and morphology of dendrites directly determine the quality of as-cast materials. The alloy solidification process is essentially a multi-physics problem in which solute diffusion, thermal diffusion and fluid dynamics are involved. Phase-field model [1] has been developed as a powerful computational tool for simulating the solidification microstructure within the framework of the diffuse interface by which one can avoid explicitly tracking the position of interface. This model has been applied to simulation of solidification microstructure including the fluid dynamics. However, it has been well known that standard phase-field models suffer from abnormal interface effects which result in inaccuracy of the simulation results. This serious problem was solved in so-called quantitative phase-field model which is developed based on thin-interface asymptotics. In particular, we have recently demonstrated the variational derivation of quantitative phase-field model for isothermal solidification in a dilute binary alloy [2]. In this study, this variational derivation is extended to non-isothermal solidification in multi-component alloys, that is a multi-physics problem consisting of multi-component solute diffusion and thermal diffusion. Furthermore, we attempt to develop highly accurate and computationally cost-effective approach for simulation of solidification microstructure under the fluid flow by coupling the quantitative model with lattice Bolzmann method [3,4]. These recent progresses in quantitative modelling are presented in this talk.

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