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An enthalpy method for modeling eutectic solidification

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ABSTRACT

This paper presents a new micro-scale model for solidification of eutectic alloys. The model is based on the enthalpy method and simulates the growth of adjacent α and β phases from a melt of eutectic composition in a two-dimensional Eulerian framework. The evolution of the two phases is obtained from the solution of volume averaged energy and species transport equations which are formulated using the nodal enthalpy and concentration potential values. The three phases are tracked using the β-phase fraction and the liquid fraction values in all the computational nodes. Solutal convection flow field in the domain is obtained from the solution of volume-averaged momentum and continuity equations. The governing equations are solved using a coupled explicit–implicit scheme.
The model is qualitatively validated with Jackson–Hunt theory. Results show expected eutectic growth pattern and proper species transfer and diffusion field ahead of the interface. Capabilities of the model such as lamella width selection, division of lamella into thinner lamellae and the presence of solutal convection are successfully demonstrated. The present model can potentially be incorporated into the existing framework of enthalpy based micro-scale dendritic solidification models thus leading to an efficient generalized microstructure evolution model.

1. Introduction

Solidification of industrial alloys generally proceeds through the formation of single phase primary crystals such as dendrites or poly-phase structures such as eutectics. Dendrites evolve in presence of varying temperature and concentration fields and grow in a branched tree-like fashion, whereas eutectic solidification is governed by an invariant point in a phase diagram. For the latter, the corresponding microstructures are characterized by simultaneous growth of two solid phases from the liquid in a coupled manner. Eutectic alloys have low melting point and excellent casting behavior [1] and hence casting alloys often have eutectic or near-eutectic composition. Desired orientation of the two solid phases may be obtained by suitable control of the applied heat flux which also creates the potential for formation of high strength composites directly through casting.

Due to the importance of eutectic alloys, various analytical and computational models have been developed for studying eutectic solidification. The well-known theory of Jackson and Hunt [2] describes steady-state eutectic growth and relates the lamellar spacing to the undercooling at the interface for a known value of growth velocity. Simultaneous growth of the lamellae occurs at an optimum lamellar spacing which corresponds to the minimum value of undercooling. This spacing

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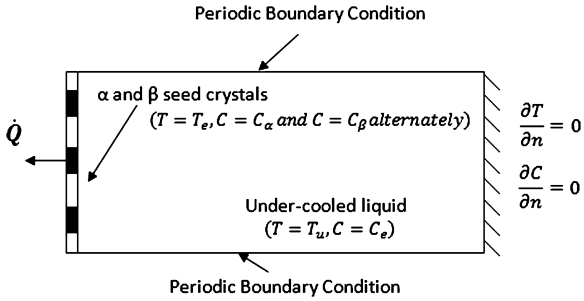

Fig. 1. Schematic diagram of the problem domain.

signifies the equilibrium between the curvature undercooling which increases with reduced lamellar spacing and the constitutional undercooling which increases with higher spacing.

Computational modeling of eutectic solidification is challenging due to the presence of higher number of phases and dynamics of the triple junction. Several microstructural models address dendritic growth and pattern formation during solidification [3–5], among which the phase-field method has been widely used for computational study of eutectic growth [6–12]. In this method, a phase-field parameter is defined to differentiate between two separate phases, the evolution of which is based on thermodynamic and kinetic principles. The phase-field method eliminates the requirement of explicit tracking of the interface and has the capability to handle complex interfaces and topology changes. The methodology has shown potential in resolving multiple phases and complexities associated with eutectic solidification. Although phase-field models have successfully predicted a range of realistic phenomena such as selection of optimum lamella spacing, formation of instability and tip splitting, the main drawback is that it is computationally intensive as the interfacial region needs extremely fine grids to solve strongly nonlinear and coupled equations. To increase the accuracy at the interface length scale, Hoyt et al. [13] have shown that the phase field method coupled with atomistic simulation models such as molecular dynamics and Monte Carlo can be applied for simulation of binary alloy solidification such as eutectic growth. Previously, Kassner and Misbah [14,15] have used boundary integral method to investigate the transition between symmetric lamellar growth and asymmetric tilted growth. Recently, the level set method has also been used for modeling eutectic solidification [16].

The enthalpy method [17,18] is one of the most popular techniques for simulation of solidification. In this method, the latent heat value of each node in the computational domain is used to track the solidification interface. Evolution of this latent heat is governed by the energy equation and the temperature–solutal coupling according to the phase diagram. This allows the computation of the solidification interface position and motion without resorting to any variable transformation. Traditionally, the enthalpy method has been used for studying macro-scale solidification of pure metals [19] and alloys [18,20]. Later, this method was adapted for computation of dendritic solidification at the micro-scale level [21,22]. Recently, this method has also been extended to develop generic models for studying the interaction of melt flow with solidification of dendrites [23,24].

In the present work, a computational model for eutectic solidification is developed based on the enthalpy technique. This is the first time that enthalpy method is being attempted for modeling eutectic microstructure. New features are incorporated in the enthalpy method to account for the three-phase nature of eutectic solidification. For resolving the solid phases, a β-phase fraction parameter g_β is defined. The relevant properties and the governing equations are modified to be a function of g_β in addition to that of liquid fraction f_l. An additional feature of the model is the incorporation of fluid flow in the domain as a result of solutal buoyancy, which is attempted in very few models reported in literature.

The paper is structured in the following manner. First, the generalized enthalpy-based formulation of the governing equations is described. Subsequently, the numerical implementation of the model is discussed. In the results section, the eutectic growth pattern and the resulting solute diffusion field are shown and the predictions computed by the present model are compared with results from the theory given by Jackson and Hunt [2]. Finally, additional results are presented to demonstrate the various features and capabilities of the model, such as lamella width selection, lamella splitting and solutal convection.

2. Problem description

As a model problem, the growth of adjacent α and β phases from under-cooled binary alloy melt of eutectic composition in a two-dimensional rectangular domain is considered. A schematic of the computational domain is shown in Fig. 1. Heat is extracted from one side of the domain and adiabatic boundary conditions for temperature and solute concentration fields are specified on the opposite side. The other two sides of the domain have periodic boundary conditions. There is no externally imposed flow. Convection occurs as a result of the density difference between the two constituent elements and depends on the variation of species concentration in the domain. The process of solidification is initiated by introducing seed crystals for the α and β phases along the heat extraction side of the domain.