



Phase-field modeling of microstructure evolution during solidification in presence of gas bubble



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ABSTRACT

The microstructure evolution during solidification of pure Aluminum metal with gas bubble nucleation and growth is modeled and simulated by the phase-field method. Interface microstructure formation in the presence of gas bubble is simulated to investigate the interaction between gas bubble and microstructural evolution, and also a pressure correction equation is implemented to study the effect of pressure difference between the bubbles and melts. Results indicate that pressure difference between gas bubble and the liquid melt can significantly affect the gas atoms diffusion near the gas–liquid interface, which will lead to the bubble growth velocity change. These simulation results are in agreement with experimental observations.

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1. Introduction

There has been an increasing use of aluminum castings in transportation vehicles to save weight, improve fuel economy, and reduce emissions. Despite the maturity of the aluminum casting industry, to achieve the mechanical integrity required for automobile components of the future requires innovative approaches to the design of alloys [1–5]. One of the critical factors that limit the mechanical properties is the formation of porosity in Al-castings. Two types of porosity are common: gas and shrinkage-driven pores. Hydrogen is always present in foundries, being easily formed from the reduction of atmospheric moisture and other products of combustion. Liquid aluminum readily dissolves hydrogen and, even if the melt is degassed, porosity can occur as the result of the large difference in hydrogen solubility between the liquid and solid states. Gas-driven pores are prototypically spherical, and the roundness of the pores depends on the hydrogen gas pressure when they form and also the impingement of phases that are already solid. Porosity related defects are a major cause of casting rejection and rework in the casting industry [6–8]. The porosity formation and its influence upon the subsequent microstructure development during solidification of an Al–6 wt.% Sn alloy was investigated by using X-ray imaging and directional solidification and X-ray computed tomography techniques [9], the growing porosity induces abnormal macro-segregation of Sn above the pores, which is attributed to mass transportation caused by local

variations in thermal and solution concentration. The evolution of porosity during re-melting of near-eutectic casting Al alloys has been investigated in-situ using X-ray micro-focus radiography [10]. During re-melting process, gas bubbles float out of the melt quickly when the liquid melt interface passes through them. The presence of microporosity and oxides is very detrimental to the mechanical properties, in particular to the fatigue resistance to crack initiation and growth. Therefore, there is a need to understand the phenomena and to predict the porosity present in the castings to avoid defects. Despite experimental investigations [9–13], several models have been developed in the past to determine the pore size and the pore volume fraction both deterministically and stochastically [6–8,14,15]. Important ones among these are Darcy's law coupled with conservation laws, diffusion controlled growth models, Cellular Automata models with stochastic approach to nucleation, First-principle calculations, molecular dynamics simulations and finite element method. These models essentially aim at predicting the porosity fraction and the maximum size of the pore in an averaged manner. Recently, phase-field method has been employed to study the porosity formation problem [16–19], but these attempts are mainly dealing with the microporosity shape change under different conditions, the interaction between gas bubble growth and solidifying still need further modeled and investigated. In this paper, a phase-field model for gas bubble growth during solidification in pure metal is proposed, and a pressure correction term is introduced into the model to study the pressure effect on gas bubble growth, and finally the gas bubble nucleation and growth during columnar dendrite formation is simulated and discussed.

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2. Phase-field model and simulation method

The total free energy density of the system with gas bubble nucleation and growth during pure metal solidifying can be expressed as:

$$f_{\text{total}} = f_{\phi}(\phi, T) + f_c(\eta, C_{\text{gas}}) + \frac{\kappa_{\phi}}{2}(\nabla\phi)^2 + \frac{\kappa_{\eta}}{2}(\nabla\eta)^2 + \frac{\kappa_c}{2}(\nabla C_{\text{gas}})^2 + f_{\text{inter}} \quad (1)$$

where η is the phase parameter introduced to identify the gas phase and liquid phase and ϕ is the phase parameter to identify the solid phase and liquid melt. C_{gas} represents the concentration the gas.

The chemical free energy for solid phase f_{ϕ} is assumed [20] to be

$$f_{\phi}(\phi, T) = \frac{1}{4}\phi^2(1-\phi)^2 - \frac{1}{6}\phi^2(3-2\phi)m(T) \quad (2)$$

and the chemical free energy for gas bubble and liquid phase f_c is

$$f_c(\eta, C_{\text{gas}}) = h(\eta)f_b + (1-h(\eta))f_m + Wg(\eta) \quad (3)$$

where f_b and f_m represents the free energy of bubble and liquid phase, respectively. The interpolation function and double-well function are given as $h(\eta) = \eta^2(3-2\eta)$ and $g(\eta) = \eta^2(1-\eta)^2$. Based on the thermodynamic theory, we write the free energy of bubble and liquid phase in terms of enthalpic and entropic as

$$f_m = \frac{C_{\nu}E_{\text{formation}}^{\nu} + C_{\text{gas}}G_{\text{gas}} + C_{\nu}k_B T \ln C_{\nu} + C_{\text{gas}}k_B T \ln C_{\text{gas}}}{\Omega} \quad (4)$$

$$f_b = \frac{C_{\text{gas}}E_{\text{sublimation}}^{\text{gas}} + C_{\nu}k_B T \ln C_{\nu} + C_{\text{gas}}k_B T \ln C_{\text{gas}}}{\Omega} \quad (5)$$

where G_{ν} and G_{gas} denotes the per unit volume Gibbs energy of an atom lattice with vacancies and gas atoms and with all sites are occupied by gas atoms, respectively. $E_{\text{formation}}^{\nu}$ and $E_{\text{sublimation}}^{\text{gas}}$ are the vacancy formation energy and gas atom sublimation energy. We choose G_{gas} as the reference energy.

A pressure correction to the thermodynamic description can be used to take into account the pressure dependence of the free energy. The Gibbs free energy functions are usually assessed for a constant standard pressure. But this assumption is incorrect when describing gas phases apart from the free atmosphere, as for growth of the gas bubble. Hydrostatic pressure as well as shrinkage of the matrix phase can lead to significant changes in melt pressure. For that reason, an analytical term needs to be added to the conventional function as a correction, so the free energy of gas phase can be rewritten as [16]

$$f_b = f_b(C_{\text{gas}}, T, p_0) + \int_{p_0}^p v dp = f_b(C_{\text{gas}}, T, p_0) + \int_{p_0}^p \frac{RT}{p} dp = f_b(C_{\text{gas}}, T, p_0) + RT \ln \frac{p}{p_0} \quad (6)$$

We consider the interaction energy between phase parameter and gas atom concentration as,

$$f_{\text{inter}} = \omega\theta(\phi) \cdot C_{\text{gas}} \quad (7)$$

where $\theta(\phi) = \phi^2(1-\phi)^2$ which ensuring the interaction only exists at the phase boundaries, ω is a constant to determine the interaction factor.

The phase parameter η and ϕ can be solved by the Allen–Cahn evolutions

$$\frac{\partial\eta}{\partial t} = -M_{\eta} \frac{\delta F_{\text{total}}}{\delta\eta} \quad (8)$$

$$\frac{\partial\phi}{\partial t} = -M_{\phi} \frac{\delta F_{\text{total}}}{\delta\phi} \quad (9)$$

$$\frac{\partial C_{\text{gas}}}{\partial t} = M_c \frac{\delta F_{\text{total}}}{\delta C_{\text{gas}}} \quad (10)$$

$$\frac{\partial T}{\partial t} = k\nabla^2 T - \frac{\partial \xi}{\partial t} \quad (11)$$

Eqs. (8)–(11) are non-dimensionalized and solved by the typical Finite Difference method with periodic boundary conditions to study the effect of pressure inside the gas bubble evolution behavior during the solidification process. All the simulations are carried out in a 300×300 zone, and non-dimensionalized parameters using in the simulations are: grid size $dx = dy = 0.25$, time step $dt = 0.08$, $M_{\eta} = 0.1$, $M_{\phi} = 0.1$, $M_c = 0.06$, $W = 0.04$, $\omega = 0.1$, $k = 1.5$, $\kappa_{\phi} = 0.5$, $\kappa_{\eta} = 0.5$, $\kappa_c = 1.0$.

3. Results and discussions

3.1. Directional solidification with a fixed gas bubble

First we consider the solidifying process with a fixed volume gas bubble in presence to investigate the effect of pre-existing gas bubble on the dendrite formation. As shown in Fig. 1, when the evaluating dendrite tip encounters with the gas bubble, the microstructural formation process is very different comparing with the free dendrite evolution as shown in the right part of the simulation zone. The tip of the primary dendrite is split by the gas bubble and leads to the further progression of two independent tips in this 2-dimensional case, and the side-branching is also enhanced and disturbed by the bubble as shown in Fig. 1(c). These simulation results are in good agreement with experimental observations during the interface microstructure in the presence of bubbles during directional solidification in SCN-DCB-gas system [21], as shown in Fig. 1(d). In general, pre-existing bubbles often strongly influence the interface pattern selection and microstructure evolution.

3.2. Directional solidification with an evolving gas bubble

As discussed above, fixed bubbles in presence interfaces can strongly affect the microstructural evolution. In this section, we continue to consider the evolution processes of a single gas bubble during the directional solidification. In order to reduce the nucleation time of solid phase, we put a nucleus in the system initially (see Fig. 2(a)). The morphology evolution of the solid–liquid interface microstructures with an evolving gas bubble is shown in Fig. 2. As time evolving, concentration of hydrogen in the liquid exceeds the super-saturation limit as dictated by the Sieverts law [22], and pores begin to grow from the pre-existing bubble, and the solid phase will be pinned when it meets the gas bubble interface. On the other hand, the gas bubble is trapped by the solid–liquid interface. The growth of solid phase along the gas bubble interface is much faster than the solid–liquid interface which is much far away from the bubble. Due to the instability of solid–liquid interface, the growth of solid phase in different directions is more remarkable, which subsequently results in the creation of cells and dendrites with radial patterns. The gas bubble is also deformed due to the interaction between the gas bubble and dendritic interface. These results are very similar to the experimental observations [21]. This gas bubble evolving is the result of the large difference in hydrogen solubility between the liquid melt and solid states. When aluminum melt containing dissolved hydrogen is cooled into the two-phase region, hydrogen is partitioned between the solid and liquid phases. With the concentration level increasing in the liquid, the diffusion of gas atoms is enhanced, which makes gas bubbles grow with time evolution.

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