Coupled Modeling of Gas and Shrinkage Microporosity with a Gas-Liquid-Solid Multi-Phase-Field Model

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Abstract: One of the most important types of defects that form during solidification is microporosity. There are two types of microporosity, gas porosity and shrinkage porosity. Gas porosity is caused by the gas element supersaturation originating from the difference in solubility between liquid and solid while shrinkage porosity is due to the volume difference between liquid and solid combined with restricted feeding during the last stage of solidification. Due to the difference in formation mechanism, there is a convention that gas and shrinkage porosities are examined separately. However, the two types of porosity can be coupled, i.e., both gas supersaturation and shrinkage flow can contribute simultaneously to the formation of porosity. As a model to incorporate both mechanisms is lacking, we developed a gas-liquid-solid multi-phase-field model to fill the gap. This model contains two core components: a quantitative multi-phase-field model describing the motion of different interfaces, which can reduce to the sharp interface model in the thin-interface limit; and a diffuse interface model of two-phase flows to introduce the shrinkage flow and the motion and deformation of the gas bubbles. A lattice Boltzmann method is used to solve the phase-field model and calculate the shrinkage flow. It is expected our model can provide a unified approach to study gas and shrinkage porosity and shed a new sight on the porosity formation.

Keywords: Phase Field; Lattice Boltzmann; Solidification microporosity; Shrinkage flow.

1 Introduction

Microporosity is one of the most serious solidification defects that can considerably reduce mechanical properties of casting parts during solidification. Thus, understanding the formation and growth of porosity is vital to optimize the materials performance [1].

The microporosity defects can be summarized into two types based on the formation mechanism: gas porosity and shrinkage porosity. Gas porosity is caused by the gas element supersaturation originating from the difference in solubility between liquid and solid while shrinkage porosity is due to the volume difference between liquid and solid combined with restricted feeding during the last stage of solidification [2]. Due to the difference in formation mechanism, gas and shrinkage porosities are investigated separately in numerical modeling. Carslon and Beckermann [3] proposed a dimensionless Niyama criterion to predict shrinkage pore volume fraction. The key of the criterion is the critical pressure drop combined with continuity equation and Dracy's law. Sun [4] developed a multiphase-field model for the solid-liquid-gas system present in gas porosity formation during solidification. Gas supersaturation acts as the driving force for bubble growth, Hele-Shaw flows are adopted to study the evolution of microstructure and the bubble motion. However, it is difficult to solve the Hele-Shaw flows equations. Recently, the lattice Boltzmann (LB) models, having the merits of simple algorithm and high parallel computational efficiency, have received great attention in the fields related to solidification. Zhang et al. [1] used a multiphase-field lattice-Boltzmann model to describe the complex multiphase interaction during solidification. The dendrite growth, bubble growth, motion and deformation, melt flow, and partition of both alloy solute and dissolved gas species are taken into account. The driving force for bubble growth is pressure difference between bubble, liquid and gas-liquid interface. Melt flow, e.g., shrinkage flow can decrease the liquid pressure. However, a constant pressure in liquid is used in their model.

Indeed, both gas supersaturation and shrinkage flow have influence on simultaneously the formation and growth of porosity [5]. Therefore, it is necessary to develop a coupled modeling of gas and shrinkage porosities to describe the growth, motion, and deformation of porosity in the solidification process of real metals.

2 Modeling procedure

Sharp-interface equations

The system is assumed that there are three components: a gas atom from which the bubble is composed, the other two are metal atoms, e.g., hydrogen dissolved in an Al-Cu melt. The sharp-interface equations for solid-liquid-gas system are given by

Liquid:

$$\frac{\partial C_l^{Cu}}{\partial t} = D^{Cu}\nabla^2 C_l^{Cu} \tag{1}$$

$$\frac{\partial C_l^{H}}{\partial t} = D^{H}\nabla^2 C_l^{H} \tag{2}$$

Solid-liquid interface:

$$C_l^{Cu}\left(1-k^{Cu}\right)\boldsymbol{u}_i\cdot\boldsymbol{n}_{sl} = -D^{Cu}\boldsymbol{n}_{sl}\cdot\nabla C_l^{Cu}\big|_l \tag{3}$$

$$C_l^{H}\left(1-k^{H}\right)\boldsymbol{u}_i\cdot\boldsymbol{n}_{sl} = -D^{H}\boldsymbol{n}_{sl}\cdot\nabla C_l^{H}\big|_l \tag{4}$$

$$T = T_m + m^{Cu} C_l^{Cu} - \Gamma \kappa_{sl} - \frac{\boldsymbol{u}_i \cdot \boldsymbol{n}_{sl}}{\mu_k} \quad (5)$$

Gas-liquid interface:

$$C_l^{Cu} \boldsymbol{u}_i \cdot \boldsymbol{n}_{gl} = -D^{Cu} \boldsymbol{n}_{gl} \cdot \nabla C_l^{Cu} \big|_l \quad (6)$$

$$\left(1 - C_l^H\right) \boldsymbol{u}_i \cdot \boldsymbol{n}_{gl} = -D^H \boldsymbol{n}_{gl} \cdot \nabla C_l^H \big|_l \quad (7)$$

$$C_{l,i}^H = \beta \boldsymbol{u}_i \cdot \boldsymbol{n}_{gl} + C_{eq}^H \left(1 + \frac{\sigma \kappa_{gl}}{\rho R T}\right) \quad (8)$$

where subscripts g, l, and s denote the gas, liquid, and solid, respectively, and subscripts sl and gl denote the solid-liquid and gas-liquid interfaces, respectively. D is the mass diffusivity, $\boldsymbol{u}_i$ is the interface velocity, $\boldsymbol{n}$ is the unit normal to the interface and pointing into the liquid, k is the partition coefficient, T is the interface temperature, m is the liquidus slope, Γ is the Gibbs-Thomson coefficient, κ is the local curvature of the interface, μ_k is the kinetic coefficient at the solid-liquid interface, β is the chemical kinetic at the gas-liquid interface, $C_{l,i}$ is the liquid concentration at the interface, C_{eq}^H is the equilibrium solubility of the gas species in the liquid and calculated by Sievert's law, ρ is the density, and R is the universal gas constant.

Phase-field model

A quantitative multi-phase-field model is constructed, which can reduce to the sharp interface model in the thin-interface limit and a diffuse interface model of two-phase flows to introduce the shrinkage flow and the motion and deformation of the gas bubbles.

Assuming equal densities and surface tensions among phases, a complete model for porosity formation in alloy solidification with flow in liquid can be written by [4]

Phase-field:

$$\tau\left(\phi_g,\phi_l,\phi_s\right)\frac{\Gamma_g}{\rho_l} = \nabla^2\phi_g + \frac{2}{3}\left[-2\phi_g\left(1-\phi_g\right)\left(1-2\phi_g\right) + \phi_l\left(1-\phi_l\right)\left(1-2\phi_l\right) + \phi_s\left(1-\phi_s\right)\left(1-2\phi_s\right)\right] + 8\lambda\left[\frac{\partial g_g}{\partial \phi_g}\left(\frac{C_l^H - \left(C_{eq}^H\right)^0}{1-\left(C_{eq}^H\right)^0} - \theta_g\right) - \frac{\partial g_s}{\partial \phi_g}\left(\frac{C_l^{Cu} - \left(C_l^{Cu}\right)^0}{(1-k)\left(C_l^{Cu}\right)^0} + \theta_s\right)\right] \quad (9)$$

$$\tau\left(\phi_g,\phi_l,\phi_s\right)\frac{\partial \phi}{\partial t} = \nabla^2\phi_s + \frac{2}{3}\left[-2\phi_s\left(1-\phi_s\right)\left(1-2\phi_s\right) + \phi_g\left(1-\phi_g\right)\left(1-2\phi_g\right) + \phi_l\left(1-\phi_l\right)\left(1-2\phi_l\right)\right] + 8\lambda\left[\frac{\partial g_g}{\partial \phi_s}\left(\frac{C_l^H - \left(C_{eq}^H\right)^0}{1-\left(C_{eq}^H\right)^0} - \theta_g\right) - \frac{\partial g_s}{\partial \phi_s}\left(\frac{C_l^{Cu} - \left(C_l^{Cu}\right)^0}{(1-k)\left(C_l^{Cu}\right)^0} + \theta_s\right)\right] \quad (10)$$

$$\tau\left(\phi_g,\phi_l,\phi_s\right) = \begin{cases} \frac{1}{2}\left(\frac{1-C_l^H}{1-\left(C_{eq}^H\right)^0} + \frac{C_l^{Cu}}{\left(C_l^{Cu}\right)^0}\right) + \frac{1}{2}\left(\frac{C_l^{Cu}}{\left(C_l^{Cu}\right)^0} - \frac{1-C_l^H}{1-\left(C_{eq}^H\right)^0}\right)\frac{\phi_s-\phi_g}{\phi_s+\phi_g} & \text{if } \phi_l \neq 1 \\ \frac{1}{2}\left(\frac{1-C_l^H}{1-\left(C_{eq}^H\right)^0} + \frac{C_l^{Cu}}{\left(C_l^{Cu}\right)^0}\right) & \text{if } \phi_l = 1 \end{cases} \quad (11)$$

$$\phi_s + \phi_l + \phi_g = 1 \quad (12)$$

Species:

$$\frac{\partial}{\partial t}\left[\left(\phi_l + k\phi_s\right)C_l^H\right] + \phi_l \boldsymbol{u}_l \cdot \nabla C_l^H = \nabla \cdot \left(D_l^H \phi_l \nabla C_l^H\right) - \left(1-r_p\right)C_l^H\left(\frac{\Gamma_g}{\rho_l}\right) - r_p C_g^H\left(\frac{\Gamma_g}{\rho_l}\right) + \nabla \cdot \left[\frac{W}{\sqrt{2}}\left(C_g^H - C_l^H\right)\left(\frac{\Gamma_g}{\rho_l}\right)\frac{\nabla\phi_l}{|\nabla\phi_l|}\left(-\frac{\nabla\phi_l}{|\nabla\phi_l|}\cdot\frac{\nabla\phi_g}{|\nabla\phi_g|}\right)\right] - \nabla \cdot \left[\frac{W}{\sqrt{2}}\left(1-k^H\right)C_l^H\frac{\partial\phi_s}{\partial t}\frac{\nabla\phi_l}{|\nabla\phi_l|}\left(-\frac{\nabla\phi_l}{|\nabla\phi_l|}\cdot\frac{\nabla\phi_s}{|\nabla\phi_s|}\right)\right] \quad (13)$$

$$\frac{\partial}{\partial t}\left[\left(\phi_l + k\phi_s\right)C_l^{Cu}\right] + \phi_l \boldsymbol{u}_l \cdot \nabla C_l^{Cu} = \nabla \cdot \left(D_l^{Cu} \phi_l \nabla C_l^{Cu}\right) - \left(1-r_p\right)C_l^{Cu}\left(\frac{\Gamma_g}{\rho_l}\right) - \nabla \cdot \left[\frac{W}{\sqrt{2}}\left(1-k^{Cu}\right)C_l^{Cu}\frac{\partial\phi_s}{\partial t}\frac{\nabla\phi_l}{|\nabla\phi_l|}\left(-\frac{\nabla\phi_l}{|\nabla\phi_l|}\cdot\frac{\nabla\phi_s}{|\nabla\phi_s|}\right)\right] - \nabla \cdot \left[\frac{W}{\sqrt{2}}C_l^{Cu}\frac{\Gamma_g}{\rho_l}\frac{\nabla\phi_l}{|\nabla\phi_l|}\left(-\frac{\nabla\phi_l}{|\nabla\phi_l|}\cdot\frac{\nabla\phi_g}{|\nabla\phi_g|}\right)\right] \quad (14)$$

where ϕ is order parameter to distinguish the phases. The superscript 0 denote equilibrium values. τ is the relaxation time. W is width of interface. $\Gamma_g = \frac{\partial \phi_g \rho_g}{\partial t} + \nabla \cdot \left(\phi_g \rho_g \boldsymbol{u}_g\right)$ is mass transfer rate per unit volume.

Lattice Boltzmann method

The multi-relaxation-time (MRT) scheme is implemented in the LB model to simulate the liquid-gas flows. The MRT LB equation is written as [6]

$$f_i\left(\boldsymbol{x} + \boldsymbol{e}_i \Delta t, t + \Delta t\right) - f_i\left(\boldsymbol{x}, t\right) = -\left(\mathbf{M}^{-1}\boldsymbol{\Lambda}\mathbf{M}\right)_{ij}\left(f_j - f_j^{eq}\right) \quad (15)$$

$$i, j = 0, 1, \ldots, 8$$

where f_i is the density distribution function and f_i^{eq} represents its equilibrium distribution function. $\boldsymbol{x}$ is the spatial position $\boldsymbol{e}_i$ represents the discrete velocities along the ith direction and Δt represents the time step in the LB model. $\mathbf{M}$ and $\mathbf{M}^{-1}$ are orthogonal transformation matrices and the corresponding inverse matrix.

The density distribution function $\boldsymbol{f}$ and its equilibrium function $\boldsymbol{f}^{eq}$ can be transformed from the velocity space into the moment space via $\boldsymbol{m}=\mathbf{M}\boldsymbol{f}$ and $\boldsymbol{m}^{eq}=\mathbf{M}\boldsymbol{f}^{eq}$, respectively. The MRT LB equation becomes

$$\boldsymbol{m}^* = \boldsymbol{m} - \boldsymbol{\Lambda}\left(\boldsymbol{m} - \boldsymbol{m}^{eq}\right) + \Delta t\left(\mathbf{I} - 0.5\boldsymbol{\Lambda}\right)\boldsymbol{S} \quad (16)$$

The streaming process of the liquid-gas particles is given as

$$f_i\left(\boldsymbol{x} + \boldsymbol{e}_i \Delta t, t + \Delta t\right) = f_i^*\left(\boldsymbol{x}, t\right) \quad (17)$$

where f^* can be obtained by $\boldsymbol{f}^* = \mathbf{M}^{-1}\boldsymbol{m}^*$.

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