

Modeling the overall solidification kinetics for undercooled single-phase solid-solution alloys. I. Model derivation

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Abstract

Departing from the volume-averaging method, the equiaxed solidification model was extended to describe the overall solidification kinetics of undercooled single-phase solid-solution alloys. In this model, a single grain, whose size is given assuming site saturation, is divided into three phases, i.e. the solid dendrite, the inter-dendritic liquid and the extra-dendritic liquid. The non-equilibrium solute diffusion in the inter-dendritic liquid and the extra-dendritic liquid, as well as the heat diffusion in the extra-dendritic liquid, is considered. The growth kinetics of the solid/liquid interface is given by the solute or heat balance, where a maximal growth velocity criterion is applied to determine the transition from thermal-controlled growth to solutal-controlled growth. A dendrite growth model, in which the nonlinear liquidus and solidus, the non-equilibrium interface kinetics, and the non-equilibrium solute diffusion in liquid are considered, is applied to describe the growth kinetics of the grain envelope. On this basis, the solidification path is described.

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1. Introduction

Rapid solidification of bulk undercooled melts is generally applied to prepare metals in a metastable state and thus gives the potential of forming novel metastable phases and microstructures [1]. Much attention has been paid in previous works to modeling the pattern formation (e.g. dendrite growth [2–12]), microstructure evolution (e.g. grain refinement mechanism [9,13–15]), etc. However, the overall solidification kinetics, including pattern formation and microstructure evolution, and the overall solidification process (e.g. the thermal history upon cooling) has not, to our knowledge, been modeled.

For near-equilibrium solidification (e.g. normal casting), however, such a model of the overall solidification kinetics (called as the equiaxed solidification model) has been studied extensively [16–27]. The original model was proposed by Rappaz and Thévoz (RT) [16,17], who adopted a micro–macroscopic approach [18] to treat the conservation

of global energy from the macroscopic scale and nucleation and dendrite growth from the microscopic scale. In the RT model, nucleation and growth are assumed to occur in a spherical volume-element without mass or species exchange between neighboring grains. A single grain is subdivided into three phases (regions): the solid dendrite (s), the inter-dendritic liquid (l_i) within and the extra-dendritic liquid (l_e) outside the grain envelope, defined as a fictitious spherical surface “stretched” by (or around) the dendrite tip. Note that l_i is assumed to be uniform and its concentration is equal to that of the dendrite tip at each instant or temperature [16]. Using the volume-averaging method [28,29], Wang and Beckermann (WB) [19,20] proposed a more general model, which can be applied to deal with arbitrary geometries, back diffusion in the solid, non-uniform concentration in the inter-dendritic liquid, etc. Following the RT model, three different regions, i.e. s , l_i and l_e , are considered, and a similar idea is used to deal with the growth kinetics of the grain envelope.

Since its inception, the equiaxed solidification model – especially the WB model – has been improved or extended by many authors [21–27]. Nielsen et al. [21] developed a

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model to account for a transition from globular to dendritic growth. Heringer et al. [22] proposed a model of equiaxed growth for the droplet produced by atomization, by tracking the development of growth front between the mushy zone and the undercooled extra-dendritic liquid, i.e. the grain envelope. Gandin et al. [23] extended the WB model to consider the formation of a secondary eutectic structure, starting from the inter-dendritic liquid and finally developing into the undercooled extra-dendritic liquid. Recently, this idea was developed further and a general model for concurrent dendritic, peritectic and eutectic solidification was proposed [24,25]. Departing from the volume-averaging method, the effects of melt convection and grain sedimentation were introduced by Wu and Ludwig [26,27]. Furthermore, application of the equiaxed solidification model to the columnar/equiaxed transition [30–32] and extension of the model to multi-component alloys [33,34] have also been paid much attention.

However, all the above models are only applicable to solidification where the growth velocity is sufficiently small, i.e. the local equilibrium condition is fulfilled at the solid/liquid interface. As such, the interface kinetics and the curvature effect are negligible, and a uniform temperature is generally appropriate (see Refs. [16–21,23–25]). For rapid solidification of undercooled melts, the growth velocity can be so fast that not only the solid/liquid interface but also the bulk undercooled liquid are under local non-equilibrium conditions [7–12,35–40]. On this basis, the assumption of linear liquidus and solidus in the above equiaxed solidification models (except Ref. [21]) may not be reasonable. As mentioned by Gandin et al. [22,24], the thermodynamic calculation of the phase diagram (i.e. the effect of nonlinear liquidus and solidus) should be considered to extend the above equiaxed solidification model into extremely non-equilibrium solidification. In addition, the thermal undercooling, i.e. the difference between the temperature of the dendrite tip and the bath temperature far from the dendrite tip, could be so large in rapid solidification [1–12] that the temperature distribution is actually non-uniform.

As a first step to modeling the overall solidification kinetics of undercooled melts, single-phase solid-solution alloys were chosen. On this basis, the WB model [19,20] was extended further by considering non-equilibrium kinetics both at the solid/liquid interface and in the bulk undercooled liquid, and non-uniform temperature distribution. The application of nonlinear liquidus and solidus was then combined with the current model to produce a detailed classification of the solidification path.

2. The volume-averaging method

2.1. Averaging theorems

For a field property φ in the α phase, φ^α , its derivative over time and space within a reference volume V^α can be given according to the averaging theorems (see, e.g. Beckermann et al. [19,20,28]) as

$$\left\langle \frac{\partial \varphi^\alpha}{\partial t} \right\rangle = \frac{\partial \langle \varphi^\alpha \rangle}{\partial t} - \frac{1}{V^\alpha} \sum_{\beta(\beta \neq \alpha)} \left(\int_{A^{\alpha\beta}} \varphi^\alpha \mathbf{v}^{\alpha\beta} \mathbf{n}^{\alpha\beta} dA \right) \quad (1)$$

$$\langle \nabla \varphi^\alpha \rangle = \nabla \langle \varphi^\alpha \rangle + \frac{1}{V^\alpha} \sum_{\beta(\beta \neq \alpha)} \left(\int_{A^{\alpha\beta}} \varphi^\alpha \mathbf{n}^{\alpha\beta} dA \right) \quad (2)$$

where $A^{\alpha\beta}$, $\mathbf{n}^{\alpha\beta}$ and $\mathbf{v}^{\alpha\beta}$ are, respectively, the area, the outwardly directed normal unit vector and the velocity, of the α/β interface, and $\langle \rangle$ is an averaging operator. The volume average of φ^α over V^α follows as

$$\langle \varphi^\alpha \rangle = \frac{1}{V^\alpha} \int_{V^\alpha} \varphi^\alpha dV^\alpha \quad (3)$$

where γ^α , a phase function, is equal to 1 in the α phase and 0 elsewhere. Analogously, the intrinsic volume average is defined with respect to the volume of the α phase, V^α , as

$$\langle \varphi^\alpha \rangle^\alpha = \frac{1}{V^\alpha} \int_{V^\alpha} \gamma^\alpha \varphi^\alpha dV^\alpha = \langle \varphi^\alpha \rangle / g^\alpha \quad (4)$$

where g^α is the volume fraction of the α phase.

2.2. Conservation equations for mass, species and energy

In a system without melt convection, phase movement and exchange of mass or species with the surrounding environment, the conservation of the total mass of the α phase, the mass fraction of the i th species in the α phase C_i^α and the specific enthalpy of the α phase H^α , respectively, can be expressed as

$$\frac{\partial \rho^\alpha}{\partial t} = 0 \quad (5)$$

$$\frac{\partial (\rho^\alpha C_i^\alpha)}{\partial t} + \nabla \cdot \mathbf{J}_i^\alpha = 0 \quad (6)$$

$$\frac{\partial (\rho^\alpha H^\alpha)}{\partial t} + \nabla \cdot \mathbf{q}^\alpha = 0 \quad (7)$$

where ρ^α , \mathbf{J}_i^α and \mathbf{q}^α are respectively the density, the diffusive flux of the i th species and the heat flux of the α phase.

Integrating Eqs. (1)–(4) with Eqs. (5)–(7) gives the averaged conservation equations:

$$\frac{\partial \langle \rho^\alpha \rangle}{\partial t} = \frac{\partial \langle \rho^\alpha g^\alpha \rangle}{\partial t} = \sum_{\beta(\beta \neq \alpha)} \Gamma_{\alpha\beta} \quad (8)$$

$$\frac{\partial \langle \rho^\alpha C_i^\alpha \rangle}{\partial t} + \nabla \cdot \langle \mathbf{J}_i^\alpha \rangle = \sum_{\beta(\beta \neq \alpha)} (J_{\alpha\beta}^i + J_{\alpha\beta}^j) \quad (9)$$

$$\frac{\partial \langle \rho^\alpha H^\alpha \rangle}{\partial t} + \nabla \cdot \langle \mathbf{q}^\alpha \rangle = \sum_{\beta(\beta \neq \alpha)} (q_{\alpha\beta}^r + q_{\alpha\beta}^q) \quad (10)$$

where the right-hand term of Eq. (8) stands for the exchange rate of the total mass of the α phase due to the movement of the α/β interface and the first right-hand terms (the second right-hand terms) of Eqs. (9) and (10) are, respectively, the mass exchange rate of the i th species and the energy exchange rate due to the movement of the α/β interface (due to diffusion). The second term on the left-hand side of Eq. (9), i.e. $\nabla \cdot \langle \mathbf{J}_i^\alpha \rangle$, describes a macroscopic diffusion, which is actually negligible since its

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