Phase-field simulation of the columnar-to-equiaxed transition in alloy solidification

Arnoldo Badillo, Christoph Beckermann *

Department of Mechanical and Industrial Engineering, 2412 Seamans Center, University of Iowa, Iowa City, IA 52242 1527, USA

Abstract

The columnar-to-equiaxed transition (CET) in directional solidification of alloys is simulated using the phase-field method. The method relies on the solution of a solute conservation equation and an equation for the propagation of the phase field on the scale of the developing microstructure. A parametric study is performed to investigate the effects of the applied temperature gradient and pulling speed, the seed spacing and nucleation undercooling for the equiaxed grains, and the crystalline anisotropy strength on the CET. The results qualitatively agree with a previously developed analytical model of the CET. At relatively high pulling speeds, a mixed columnar–equiaxed structure is found to be stable over a range of temperature gradients. Furthermore, the CET depends sensitively on the anisotropy strength. The simulations also reveal the presence of primary spacing adjustments during purely columnar growth due to nucleation of seeds, and deactivation of seeds by solutal interactions from nearby growing grains.
© 2006 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

1. Introduction

The columnar-to-equiaxed transition (CET) in the grain structure of metal alloy castings has fascinated researchers in the solidification area for more than 50 years [1]. The CET is usually assumed to occur when the advance of the columnar front is blocked by equiaxed grains that grow in the constitutionally undercooled liquid ahead of the columnar dendrites. Based on this idea, Hunt [2] developed an analytical model that predicts the CET during directional solidification as a function of the applied temperature gradient, the solidification speed, and the nucleation undercooling and number density of equiaxed grains. This model has been extended and improved by several researchers [3–5]. A simulation model that relies on the solution of averaged conservation equations that are coupled to nucleation and growth laws has been presented

by Beckermann and co-workers [6,7]. More complex models have followed the nucleation and growth of each individual grain (e.g., Refs. [8–12]). By predicting the size, orientation, and shape of each grain, the location of the CET in a casting can be inferred directly from the appearance of the calculated grain structure. These studies rely on the same type of dendrite tip growth models for the evolution of the grain envelopes as the previous modeling studies [2–7]. A solute diffusion equation is not solved, and the motion of the solid–liquid interface on a microscopic scale is not resolved.

With recent advances in computational power, direct microstructure simulation techniques hold some promise for modeling the CET. Spittle and Brown [13], Nastac [14], and Dong and Lee [15] have applied so-called coupled cellular automaton finite difference (CA-FD) methods to simulate the CET in metal alloy castings. In this class of methods, the solid–liquid interface is tracked directly on the numerical grid and its motion is determined from the numerical solution of a solute diffusion equation on a microscopic scale. Grain envelopes are

---

not considered and no use is made of separate dendrite tip growth models. While the CA-FD methods produce realistic-looking dendritic growth patterns and have resulted in much insight into the CET, some questions remain regarding their accuracy. Independence of the results on the numerical grid size is rarely demonstrated. Furthermore, the CA-FD techniques often rely on relatively arbitrary rules for incorporating the effects of crystallographic orientation while propagating the solid–liquid interface. For example, in the most recent and advanced study using a CA-FD technique [15], the strength of the surface energy anisotropy is not even specified. It is now well accepted that dendritic growth of crystalline materials depends very sensitively on the surface energy anisotropy [16,17].

The phase-field method has also become a popular technique for the direct numerical simulation of microstructure evolution in solidification [18]. However, progress in modeling solidification of alloys using the phase-field method has been relatively slow. The first fully quantitative phase-field model that allows for unequal solute diffusivities in the liquid and solid was only developed in 2001 [19]. This model has been extended by Ramirez et al. [20] to account for coupled heat and solute diffusion and by Echebarria et al. [21] to directional alloy solidification with an applied temperature gradient. Recently, Ramirez and Beckermann [22] used this phase-field model to study free dendritic growth of alloy dendrites. These studies clearly demonstrate that the phase-field method allows for accurate and fully grid-independent simulations of alloy solidification on the scale of the microstructure.

The objective of the present study is to perform direct numerical simulations, in two spatial dimensions, of the CET in alloy solidification using the phase-field model of Refs. [20,21]. The phase-field model equations are briefly summarized in the next section. The numerical procedures are explained in Section 3. Section 4 presents the results of numerous simulations where the CET is studied as a function of the applied temperature gradient and pulling speed, the equiaxed grain nucleation undercooling and number density, and the crystalline anisotropy. In addition, the results are compared to the original CET model of Hunt [2]. The conclusions of the study are summarized in Section 5.

2. Phase-field model

The phase-field model employed here allows for the simulation of microstructural patterns during the solidification of dilute binary alloys. It has been derived and extensively validated by Ramirez et al. [20] and Echebarria et al. [21]. The model neglects the solute diffusivity in the solid, and all material properties are assumed constant. It reduces to the sharp interface equations in a thin interface limit where the width of the diffuse interface is smaller than the radius of curvature of the interface but larger than the real width of a solid–liquid interface, and when kinetic effects are neg-

ligible. The anti-trapping current concept of Karma [19] is applied to recover local equilibrium at the interface and eliminate interface stretching and surface diffusion effects that arise when the solute diffusivities are unequal in the solid and liquid.

Let ϕ represent the phase field, where $\phi = 1$ in the bulk solid phase and $\phi = -1$ in the bulk liquid phase. The phase field varies smoothly between these bulk values within the diffuse interface region. The anisotropic and dimensionless forms of the phase-field and species equations, for a vanishing kinetic effect, are given in two-dimensional form, respectively, by [20,21]

$$[1 + (1 - k)U]a_{\mathrm{s}}(\hat{n})^2 \frac{\partial \phi}{\partial t} = \vec{\nabla} \cdot (a_{\mathrm{s}}(\hat{n})^2 \vec{\nabla}\phi)$$
$$+ \partial_x \left(\left| \vec{\nabla}\phi \right|^2 a_{\mathrm{s}}(\hat{n}) \frac{\partial a_{\mathrm{s}}(\hat{n})}{\partial(\partial_x \phi)} \right)$$
$$+ \partial_y \left(\left| \vec{\nabla}\phi \right|^2 a_{\mathrm{s}}(\hat{n}) \frac{\partial a_{\mathrm{s}}(\hat{n})}{\partial(\partial_y \phi)} \right)$$
$$+ \phi - \phi^3 - \lambda(1 - \phi)^2(U + \theta),$$

$$(1)$$

$$\left(\frac{1 + k}{2} \right) \frac{\partial U}{\partial t} = \vec{\nabla} \cdot \left(\tilde{D} \frac{1 - \phi}{2} \vec{\nabla}U + \vec{j}_{\mathrm{at}} \right)$$
$$+ \frac{1}{2} \frac{\partial}{\partial t} \{\phi[1 + (1 - k)U]\},$$

$$(2)$$

where $\hat{n} = -\vec{\nabla}\phi / \left| \vec{\nabla}\phi \right|$ is the unit vector normal to the interface, $a_{\mathrm{s}}(\hat{n}) = 1 + \varepsilon \cos(4\phi)$ is a function that describes the surface energy anisotropy, $\phi = \arctan(\partial_y \phi / \partial_x \phi)$ is the angle between the direction normal to the interface and the horizontal axis, ε is a dimensionless parameter that characterizes the anisotropy strength, k is the partition coefficient, x and y are the spatial coordinates, and t is time. In the present study, the crystal axes are always aligned with the coordinate axes. The anti-trapping current $\vec{j}_{\mathrm{at}}$ is given by [19]

$$\vec{j}_{\mathrm{at}} = \frac{1}{2\sqrt{2}} [1 + (1 - k)U] \frac{\partial \phi}{\partial t} \frac{\vec{\nabla}\phi}{\left| \vec{\nabla}\phi \right|}$$

$$(3)$$

which is non-zero only inside the diffuse interface region.

The time and length scales used to non-dimensionalize equations (1) and (2) are $\tau_0 = (d_0^2/D)a_2\lambda^3/a_1^2$ and $W_0 = d_0\lambda/a_1$, which represent a relaxation time and a measure of the interface width, respectively. Here, d_0 is the chemical capillary length and D is the solute diffusivity in the liquid phase. The dimensionless solute diffusivity is given by $\tilde{D} = D\tau_0/W_0^2$ and λ is a dimensionless coupling parameter, which is chosen as $\lambda = \tilde{D}/a_2$ to simulate kinetics-free growth ($a_1 = 0.8839$, $a_2 = 0.6267$) [23]. The coupling constant λ is the only free parameter and the results should be independent of λ when they are converged. Decreasing λ corresponds to decreasing the diffuse interface width, since $\lambda = a_1 W_0/d_0$.