International Journal of Heat and Mass Transfer 104 (2017) 607–614

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Effect of interface anisotropy on growth direction of tilted dendritic arrays in directional solidification of alloys: Insights from phase-field simulations

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ARTICLE INFO

Article history:
Received 27 May 2016
Accepted 29 August 2016

Keywords:
Directional solidification
Phase-field simulation
Tilted growth

ABSTRACT

We investigate the effect of interfacial anisotropy on the growth direction selection during directional solidification of alloys by using the thin-interface phase-field model. A convergence study with respect to the coupling constant λ is carried out for the tilted growth of dendritic arrays with different values of anisotropic to choose proper λ in simulations. The influence of the artificial noise at the interface on the growth direction selection is discussed. By analyzing the data from two-dimensional phase-field simulations, we discuss the dependence of the coefficients f and g in DGP law (Deschamps et al., 2008) on anisotropic strength ε_4 for a wide range of misorientation angle Θ_0 in order to extend the DGP law. Results confirm that the coefficient f can be expressed as $f(\Theta_0, \varepsilon_4) \equiv \alpha(\varepsilon_4)\chi(\Theta_0)$, where $\alpha(\varepsilon_4)$ is an increasing function of ε_4 and $\chi(\Theta_0)$ solely depends on Θ_0 with a constant coefficient β. Meanwhile, $g(\varepsilon_4)$ is a decreasing function of ε_4, which can be modeled by a power-law function. Moreover, we comment on the influence of the pulling velocity on the growth direction selection for a wider range of the pulling velocity.

1. Introduction

Directional solidification of alloys has been a well-accepted paradigm for the investigation of competitive effects and the pattern formation resulting from the morphological instability in non-equilibrium systems for many years [1,2]. In this generic experiment, the alloy sample is pulled at a constant pulling velocity V_p through a fixed temperature gradient G. When the pulling velocity exceeds a critical velocity, the initial planar interface becomes unstable, as described by the well-known Mullins–Sekerka instability [3], giving rise to cellular or dendritic arrays. The competition between two specific directions determines the growth direction of dendritic arrays: the thermal gradient direction that is defined at a macroscopic level from the experimental set-up and the preferred crystalline orientation that is determined at a microscopic level by the grain orientation [4]. Once the two specific directions differ, the growth direction of dendritic arrays approaches to the preferred crystalline orientation from the thermal gradient direction as well as the dramatic changes of interfacial morphologies as the pulling velocity is increased [4–15]. The tilted growth of dendritic arrays and their growth direction selection have received much attention due to the dramatic influence on the mechanical properties of the casting products. Understanding the mechanism of the growth direction selection in directional solidification is crucial for controlling growth patterns and optimizing the mechanical properties of alloys casting for a wide range of applications, especially the grains competition and selection [13–15].

Because the thermal gradient varies slightly near the dendritic tip, the slow solute diffusion process dominates the selection of the growth direction while the thermal gradient does not play an important role in that. The solute diffusion is restricted by the Gibbs–Thomson relation with the anisotropic surface tension, yielding

$$c_l/c_l^0 = 1 - (1-k)d_0\kappa[1 - 15\varepsilon_4\cos 4(\psi - \Theta_0)] - (1 - k)(z - V_p t)/l_T, \quad (1)$$

where c_l is the concentration at the liquid side of the interface, $c_l^0 = c_\infty/k$ the concentration on the liquid side of a growing steady-state planar interface, c_∞ the average solute concentration, k the partition coefficient, d_0 the capillary length, κ the interface curvature, Θ_0 the misorientation angle that is defined as the angle

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.08.096
0017-9310/

between the preferred crystalline orientation and the thermal gradient direction, ψ the angle between the interface normal and the thermal gradient, $l_T = D_l/V_p$ the thermal length, D_l the solute diffusion coefficient, and ε_4 the anisotropic strength of surface tension for cubic crystals. Clearly, ε_4, Θ_0 and V_p are important factors which determine the solute distribution that is dominant in growth direction selection.

Previous experimental finding by Akamatsu and Ihle [7] shows that the growth direction depends on the primary spacing Λ and pulling velocity V_p. Through analyzing a large amount of data from the experiments of thin samples of a succinonitrile-ethylene alloy, Deschamps et al. [8] proposed a scale invariance with respect to the primary Péclet number ($Pe = V_G\Lambda/D_l$, where V_G is the pulling velocity projected on thermal gradient direction), i.e., the DGP law, which yields

$$\Theta/\Theta_0 = 1 - [1 + f(\Theta_0)Pe^g]^{-1}, \tag{2}$$

$$\text{with } f(\Theta_0) = \alpha\left[1 - (\Theta_0/\Theta_m)^\beta\right], \tag{3}$$

where Θ is the angle between the growth direction of dendritic arrays and the thermal gradient direction, representing the real growth direction of the crystal, also known as the tilted angle, f is a function of Θ_0, Θ_m is a constant, α, β and g are fitting parameters. This law presents that the real growth direction is a common nonlinear function of the Péclet number: $\Theta/\Theta_0 \to 0$ when $Pe \to 0$ and $\Theta/\Theta_0 \to 1$ when Pe is relatively large. However, the limitation of the DGP law should not be ignored: it is obtained in experiments of SCN based transparent model alloys. Whether the growth direction of dendritic arrays with higher surface tension anisotropy follows the DGP law is still unclear.

Numerical methods, especially the phase-field method, have been widely used to study the growth direction selection of dendritic arrays in two- and three-dimensional systems [7,9–15]. Predicted results [9] show that the tilted angle increases with the increase of the pulling velocity. Li et al. [10] tested the reliability of the phase-field simulations for the growth direction selection of dendritic arrays in Ni-based alloys, qualitatively reproducing the DGP law in the case of $\Theta_0 = 30^\circ$. Xing et al. [11] investigated the asymmetrical morphologies of dendritic shapes and the role of the misorientation angle on the selection mechanisms of primary spacing. Comparisons between experimental results and phase-field simulations by Ghmadh et al. [12] indicate that three-dimensional simulations are helpful for more accurate quantitative results. Tourret and Karma [13] carried out two-dimensional phase-field simulations for a wide range of misorientation angle, highlighting that the thermal gradient influences the dendritic growth direction through its major influence on the primary spacing. As shown in Eq. (1), the anisotropic strength of surface tension can also influence the growth direction selection and morphologies of tilted dendritic arrays in directional solidification of alloys. Previous numerical simulations [7,11] show that the growth direction rotates to the preferred crystalline orientation as the anisotropic strength is increased. Hence, the dependence of f and g in the DGP law on ε_4 needs to be systematically investigated for a wide range of Θ_0. Understanding this can provide the insight into what alloy and control parameters influence the growth direction selection. However, relevant study is scarce. In the following sections, we examine the dependence of the coefficients f and g in DGP law on anisotropic strength ε_4 through two-dimensional phase-field simulations in order to extend the DGP law into the dendritic growth direction selection of other alloys system. The remainder of this paper is organized as follows. In Section 2, we briefly summarize the thin-interface phase-field model, and a convergence study with respect to the coupling constant λ for different anisotropic strength is carried out. Our results are presented and discussed in Section 3. The role of the artificial noise at the interface on the growth direction selection is investigated. According to the data from numerical simulations, we show the morphological transition and the dependence of f and g in DGP law on ε_4 for a wide range of misorientation angles. The DGP law is extended based on the data analysis. We also discuss the influence of the pulling velocity on the growth direction selection for a wide range of pulling velocity in this section. The conclusions of this study are presented in Section 4.

2. Model descriptions and convergence study

The thin-interface phase-field model [16,17] is adopted here to investigate tilted growth of dendritic arrays with different anisotropic strength in directional solidification. The anti-trapping term is added to recover local equilibrium at the interface and eliminate spurious effects [16]. This model has been successfully used in solidification of alloys under various conditions [11–18]. Detailed derivations and validations of this model can be found in the Ref. [17]. It is proved that this model can provide quantitative results to compare with theoretical solutions. We choose Al-3 wt% Cu as the numerical calculation object, and its properties and parameters as follows: $m = -2.6$ K/wt%, $D_l = 3000$ μm^2/s, $\Gamma = 0.24$ K · μm, and $k = 0.14$. The diffusion in the solid is neglected. Moreover, the latent heat production is neglected, and hence the so-called "frozen temperature approximation" is adopted for the directional solidification

$$T = T_0 + G(z - V_p t), \tag{4}$$

where T_0 is a reference temperature. In this model, the scalar field $\phi(\mathbf{r}, t)$ takes on the values $\phi = 1$ in the solid phase, $\phi = -1$ in the liquid phase and varies continuously across the interface. The solute concentration field $c(\mathbf{r}, t)$ is characterized by a dimensionless supersaturation field $U = ((2kc/c_\infty)/[1 + k - (1 - k)\phi] - 1)/(1 - k)$ with respect to (c_l^0, T_0). The anisotropy function of cubic crystals can be expressed as

$$A(\psi - \Theta_0) = 1 + \varepsilon_4 \cos 4(\psi - \Theta_0) \tag{5}$$

in two-dimensional systems. For Al-3 wt% Cu, experiments show that the anisotropic surface tension is $\varepsilon_4 = 0.0101$ [19]. To study the effect of the anisotropic strength on the growth direction, the range of the anisotropic strength ε_4 is from 0.0075 to 0.05 in our work. $\tau_0 = a_2\lambda W_0^2/D_l$ and $W_0 = d_0\lambda/a_1$ are the time and length scales, respectively, where $a_1 = 0.8839$ and $a_2 = 0.6267$, λ the coupling constant between the phase-field and concentration equations, $d_0 = \Gamma/(|m|(1 - k)c_l^0)$ the capillary length. The interface width is given by W_0, and hence λ is seen as a numerical convergence parameter of this model.

The thermal gradient influences the growth direction selection by its influence on the primary spacing [13]. Given the primary spacing in each simulation, the thermal gradient is irrelevant with the growth direction selection. In previous simulations of directional solidification of Al–Cu alloys [20], the thermal gradient and pulling velocity are chosen as $G = 0.005$ K/μm and $V_p = 10$ μm/s, respectively. In our work, a total of over 420 simulations are carried out to study the anisotropic strength on the growth direction selection for a large range of misorientation angle. To decrease the primary dendrite spacing so as to reduce the computational cost, a relatively large thermal gradient G and pulling velocity V_p are specified, i.e., $G = 0.14$ K/μm and $V_p = 500$ μm/s. Because the growth direction is a function of the Péclet number, for convenience, the primary spacing Λ is given by varying the initial wavelength of the interface. Microstructure instabilities of cell elimination or tertiary branching will be encountered at too low or large primary spacing, respectively. In