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Phase field study of the tip operating state of a freely growing dendrite against convection using a novel parallel multigrid approach

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ABSTRACT

Alloy dendrite growth during solidification with coupled thermal-solute-convection fields has been studied by phase field modeling and simulation. The coupled transport equations were solved using a novel parallel-multigrid numerical approach with high computational efficiency that has enabled the investigation of dendrite growth with realistic alloy values of Lewis number $\sim 10^4$ and Prandtl number $\sim 10^{-2}$. The detailed dendrite tip shape and character were compared with widely recognized analytical approaches to show validity, and shown to be highly dependent on undercooling, solute concentration and Lewis number. In a relatively low flow velocity regime, variations in the ratio of growth selection parameter with and without convection agreed well with theory.

1. Introduction

In the shaped casting industry the growth behavior of dendrites in a solidifying alloy controls the as-cast microstructure and has a strong influence on final component mechanical properties. Cast structures in practice, even in simple binary alloys, are complex and rarely conform to easy classification as homogeneously columnar or equiaxed, and frequently present complex cellular/dendritic patterns that vary from place to place. There has been significant effort to better understand the underlying physics controlling the shape, length scale and solute redistribution processes occurring at a growing dendrite tip in an attempt to control the factors that determine final cast microstructure [1–5]. Both analytical and numerical approaches have been developed, but despite the well-known strong influence of liquid movement and convection on final microstructure in practice, only a small number of recent studies have begun to account for its influence on the prior, more developed thermal-solute approaches.

The operating state of a growing dendrite can be defined by the tip radius R_{tip} and the tip velocity v_{tip}. By assuming the tip to be a parabola (in 2-D) or a paraboloid of revolution (in 3-D) with parabolic tip radius R_p and the steady dendrite is isothermal with the solid at the melting temperature, Ivantsov [6] proposed the most widely quoted relationship for dendrite operating state for a purely thermally-controlled growing dendrite, comprising the relationship between external imposed undercooling $\Delta = (T_m - T_\infty)/(L/C_p)$ and the thermal Peclet number at the tip $Pe_T = R_p v_{tip}/(2\alpha)$ as $\Delta = Iv(Pe_T)$, where T_m is the melting temperature, T_∞ is the temperature of the undercooled melt, L is the latent of fusion, C_p is the specific heat, α is the thermal diffusivity and $Iv(x) = \sqrt{\pi x}\exp(x)erfc(\sqrt{x})$ is the Ivantsov function (in 2-D). Ivantsov's theory

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predicted that for a given undercooling, there were infinite pairs of (R_{tip}, v_{tip}) for the solution of the linked expression since only their product (Peclet number) could be determined. While convenient, this implication is in conflict with experiment where R_{tip} and v_{tip} are invariant for a fixed undercooling. Two subsequent approaches were then developed by the introduction of a *selection constant* defined as σ^*. The *marginal stability* theory was developed by Langer and Muller-Krumbhaar [7] and involved another relationship between the tip radius and velocity given as $R_p^2 v_{tip}/(d_0\alpha) = (1/\sigma^*)^2$ where d_0 is the material thermal capillary length. Drawing on a stability analysis [8] based on the allowable shape of a perturbed, non-flat solid–liquid interface, they proposed $\sigma^* = 1/(2\pi)$. Ben-Jacob et al. [9,10] and Kessler et al. [11,12] developed other approaches that allowed for anisotropic surface energy to give a single, paired solution for R_p and v_{tip}, deduced from the fastest growing mode of perturbed solid–liquid interface, which led to an expression similar to the one given by Langer and Muller-Krumbhaar [7] i.e. $R_p^2 v_{tip} =$ constant. Kessler and Levine [13] extended this idea and found that the dendrite tip shape computed in this way generally displays a cusp (non-zero slope) at the tip and at a unique (R_p, v_{tip}) pair; the cusp reduces to a smooth shape with zero slope at the tip, which is called the *microscopic solvability* condition. Further numerical experiments revealed that the selection constant σ^* was dependent on the strength of the surface anisotropy ε i.e. $R_p^2 v_{tip} = f(\varepsilon)$. Nevertheless, experimental validation of these increasingly complicated analytical/numerical approaches has been difficult since they rely on controlling stable and well-characterized growth conditions, generally far from the more dynamic conditions expected in practice [14].

The extension of the *microscopic solvability* theory to binary alloys, where both solute and thermal diffusion are important, was performed by Lipton, Glicksman and Kurz (LGK) [15] and Lipton, Kurz and Trivedi (LKT) [16]. These approaches are also characterized by the use of a selection constant σ^* (σ^*_{LGK} and σ^*_{LKT} will be used for the LGK and LTK theories respectively):

$$\sigma^* = \frac{d_0}{R_p Pe_T[\xi_T + 2\xi_c Le(\frac{Mc_\infty}{1-(1-k)\Delta_C})]} \tag{1}$$

where $M = |m|(1-k)/(L/C_p)$ is the scaled dimensionless liquidus slope, m is the actual liquidus slope from the phase diagram, k is the solute partition coefficient, $Le = \alpha/D$ is the Lewis number, D is the solute diffusivity in liquid, c is the solute concentration and c_∞ is the equilibrium solute concentration. $\Delta_C = (c_{tip} - c_\infty)/((1-k)c_{tip})$ is the dimensionless solutal undercooling and c_{tip} is the solute concentration at dendrite tip. For the LGK theory, both ξ_T and ξ_c are unity but for the LKT theory:

$$\xi_c = 1 + \frac{2k}{1-2k-\sqrt{1+\frac{1}{\sigma^*(Pe_c)^2}}} \tag{2}$$

and

$$\xi_T = 1 - \frac{1}{\sqrt{1+\frac{1}{\sigma^*(Pe_T)^2}}} \tag{3}$$

The overall undercooling is then given by:

$$\Delta T = \frac{L}{C_p}\Delta_T + \frac{k\Delta T_0 \Delta_c}{1-(1-k)\Delta_c} + \frac{\Gamma}{R_p} \tag{4}$$

where the three terms on the right correspond to thermal, solutal and capillary undercooling, respectively. $\Delta T_0 = |m|c_\infty(1-k)/k$ is the equilibrium freezing range corresponding to c_∞ and Γ is the Gibbs–Thomson coefficient. $\Delta_T = (T_{tip} - T_\infty)/(L/C_p)$ is the dimensionless thermal undercooling. Eqs. (1) and (4) together uniquely determine the tip radius and tip velocity.

Convection in the melt – almost always significant in practice – has long been realized to have a profound effect on dendritic growth [17]. But it is presently unclear how the preceding theories (LGK and LKT) for binary alloys may remain valid or how they might be modified when convection is present. Ananth and Gill [18] and Saville and Beaghton [19] studied the motion of the freezing front between a needle-shaped crystal and a supercooled liquid for situations where there is forced convection aligned along the crystal growth. Analysis was conducted by modeling the transport problem for a pure material solidifying as a paraboloid of revolution in an infinite undercooled melt. The imposed external undercooling could be characterized by the thermal Peclet number Pe_T, the flow Peclet number $Pe_f = R_{tip}v_\infty/2\alpha$ (where v_∞ is the imposed external flow velocity) and the Prandtl number $Pr = \upsilon/\alpha$ (ratio between kinematic viscosity and thermal diffusivity) i.e. $\Delta = \Delta(Pe_T, Pe_f, Pr)$. Through a so-called *linear solvability* analysis, Bouissou and Pelce [20] considered the stability of this solution, and found that the ratio of the selection parameters with convection (σ^*) and without convection (σ_0^*) could be characterized by a dimensionless parameter χ_e:

$$\frac{\sigma_0^*}{\sigma^*} = 1 + b\chi_e^{11/14} \tag{5}$$

where b is a numerical constant,