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The effect of the shear flow on particle growth in the undercooled melt

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ABSTRACT

We study the effect of the linear shear flow on particle growth in the undercooled melt by using the method of matched asymptotic expansion. The analytical result shows that the shear effect of flow results in the significant distorted deformation of the interface. Under the combined action of both shear flow and anisotropic surface tension, the lateral interface of the particle is further compressed but the upper interface and lower interface further grow during the early stage after nucleation to form the distorted ear-like shape formation. As a result, the minimum inner diameter decreases to less than two times the critical radius for nucleation and the strength of the particle becomes weaker, and then the particle will split or be broken into several more fine particles. The analytical result provides the prediction of the interface evolution of the particle under the influence of the linear shear flow.

1. Introduction

Convection effects are of fundamental importance in controlling pattern formation of interface microstructures. A great number of experimental and simulation works have shown the effect of solute convection, external forced flows on interface microstructures [1–3]. The external forced flow imposed in the undercooled melt will strongly change the solidification dynamics and then pattern formation of interface microstructures. The upstream flow imposed on the growing crystal enhances the growth velocity of the interface in the upwind direction [4]. The uniform streaming flow results in higher local growth rate near the surface where the flow is incoming [5]. Due to the melt convection induced by stirring, the crystal directly nucleates from the convective undercooled melt and grows up to a large scale [6]. In the uniform streaming flow, an initially spherical particle evolve into a peach-like shape [7]. Liu et al. [8,9] experimentally and numerically investigated the convective effects driven by accelerated crucible rotation on the segregation, interface shape, and morphological instability during crystal growth. Jung et al. [10] investigated the effect of an external time-dependent flow to simulate the industrial Czochralski process for growing silicon crystals. In recent years, these phase selection and grain refinement have been investigated for the perspective of applications. By the centrifugal casting technique, Wang et al. [11] fabricated a nano-composite with the relatively uniform dispersed iron particles in the copper matrix, whose mechanical properties show a significant increase. It has provided strong motivation for the direct calculation of interface evolution and morphology of particle growth. When a forced flow is exerted on the melt, the fully coupled problem of the heat transfer and the fluid flow is hard to solve accurately with numerical and analytical approaches. However, the fluid velocity near the particle can be decomposed into the superposition of the uniform streaming flow and the linear flow. In the paper, we study the effect of a well-defined linear shear flow on particle growth in the undercooled melt. By using the matched asymptotic expansion method, we find the asymptotic solution for temperature fields and shape of the particle in the fully coupled problem. With the analytical solution, we analyze the interface evolution and morphology of the particle growth.

2. The theoretical formation

We consider the evolution and growth of a particle in the convective undercooled melt driven by a linear shear flow. In the Cartesian coordinate system (x_1, x_2, x_3) whose origin is at the center of the particle, the linear shear flow is expressed as

$$S = Px_2\mathbf{i} + 0\mathbf{j} + 0\mathbf{k}, \tag{2.1}$$

where $\mathbf{i}$, $\mathbf{j}$ and $\mathbf{k}$ are the unit vectors of the Cartesian coordinate frame, respectively, P is the constant velocity gradient. The temperature far from the particle is T_∞ ($T_\infty < T_M$, T_M is the solidification equilibrium temperature for the pure substance) to form the undercooled melt of undercooling $\Delta T = T_M - T_\infty$. The anisotropy function is described by a four-fold symmetry system [12]

$$\gamma = \gamma_0[1 + \alpha_4((\sin^4\varphi + \cos^4\varphi)\sin^4\theta + \cos^4\theta)], \tag{2.2}$$

where γ_0 is the dimensional isotropy that gives the average magnitude of surface tension, α_4 is the anisotropy parameter. After we rescale the length scale as made in [13,14], the fluid velocity in the

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liquid phase $\mathbf{U}$, pressure P, temperature in the liquid T_L and temperature in the solid T_S satisfy the dimensionless governing equations [13]

$$\varepsilon\frac{\partial \mathbf{U}}{\partial t}+\varepsilon(\mathbf{U}\times\nabla)\mathbf{U}=-\nabla P+Pt\nabla^2\mathbf{U},\ \nabla\times\mathbf{U}=0,, \tag{2.3}$$

$$\varepsilon\frac{\partial T_L}{\partial t}+\varepsilon(\mathbf{U}\times\nabla)T_L=\nabla^2 T_L,\ \varepsilon\lambda_S\frac{\partial T_S}{\partial t}=\nabla^2 T_S, \tag{2.4}$$

where $\varepsilon=\Delta T/(\Delta H/(c_{pL}\rho_L))$, $Pt=\upsilon/\kappa_L$, $\lambda_S=\kappa_L/\kappa_S$, ΔH is the latent heat per unit volume, c_{pL} is the specific heat and ρ_L is the density in the melt, υ is the kinematical viscosity, κ_L and κ_S are the thermal diffusivities in the liquid and solid phases, respectively. In the spherical coordinates whose origin is at the center of the particle, and the interface of the particle is expressed as $R=R(\theta,\varphi,t)$. At the interface, the total mass conservation condition, the tangential non-slip condition, the thermal equilibrium condition, the Gibbs–Thomson condition and energy conservation condition hold [14]. The flow-driven condition and far-field condition are, as $r\to\infty$,

$$\mathbf{U}\to py\mathbf{i},\ T_L\to-\varepsilon, \tag{2.5}$$

where y is the rectangular coordinate, p is the dimensionless constant velocity gradient, $p=r_0P/V$, where V is the characteristic velocity of the interface. Finally, the initial condition holds, in which the initial condition for the interface is, at time $t=0$,

$$R(\theta,\varphi,0)=1, \tag{2.6}$$

For the sake of simplicity, it is assumed that the densities in the liquid and solid phases are equal, and the buoyancy effects are neglected. The separation or split of a particle into two particles or the interaction between particles does not involve.

3. Asymptotic solution and analysis

For the case of small undercooling parameter ε, $\varepsilon\ll1$, we seek the asymptotic solution of Eqs. (2.1)–(2.6)

$$\mathbf{U}\sim\mathbf{U}_{L0}+\varepsilon\mathbf{U}_{L1}+\cdots,\ P\sim P_{L0}+\varepsilon P_{L0}+\cdots,$$
$$T_L\sim\varepsilon T_{L0}+\varepsilon^2T_{L1}+\cdots,\ T_S\sim\varepsilon T_{S0}+\varepsilon^2T_{S1}+\cdots,\ R\sim R_0+\varepsilon R_1+\cdots \tag{3.1}$$

in which each order approximation is further expanded into a series of spherical harmonics. Substituting (3.1) into Eqs. (2.1)–(2.6) and equating the terms of like powers of ε, we derive the governing equations and boundary conditions and initial conditions for each order approximation, and found the solution for the temperature fields and the interface of the particle.

For the flow field, when it is superimposed additionally on the linear shear flow, the flow field throughout the melt is modified by the additional fluid velocity. After carrying out the differentiation algebra, we have the leading order approximation $\mathbf{U}_{L0}=(u_0,v_0,w_0)$ and P_{L0} in the form of Cartesian rectangular coordinates [15],

$$u_0=-\frac{5p}{2}\frac{R_0^3}{r^5}\left(1-\frac{R_0^2}{r^2}\right)x^2y-\frac{p}{2}\frac{R_0^5}{r^5}y+py,\ v_0=-\frac{5p}{2}\frac{R_0^3}{r^5}\left(1-\frac{R_0^2}{r^2}\right)xy^2-\frac{p}{2}\frac{R_0^5}{r^5}x,$$

$$w_0=-\frac{5p}{2}\frac{R_0^3}{r^5}\left(1-\frac{R_0^2}{r^2}\right)xyz,\ P_{L0}=-\frac{5pPtR_0^3xy}{r^5}\left(1-\frac{R_0^2}{r^2}\right)+const; \tag{3.2}$$

for the temperature fields, the leading order approximation is [13,14]

$$T_{L0}=-1+\frac{R_0(R_0-2\Gamma)}{(R_0+E^{-1}M)}\frac{1}{r},\ T_{S0}=-\frac{2\Gamma+E^{-1}M}{R_0+E^{-1}M}, \tag{3.3}$$

where R_0 satisfies the ordinary differential equation

$$\frac{dR_0}{dt}=\frac{R_0-2\Gamma}{R_0(R_0+E^{-1}M)} \tag{3.4}$$

with the initial condition (2.6), Eq. (3.4) has an implicit solution $t=t(R_0)$,

$$t=\frac{1}{2}(R_0^2-1)+(2\Gamma+E^{-1}M)\left(R_0-1+2\Gamma\ln\frac{R_0-2\Gamma}{1-2\Gamma}\right) \tag{3.5}$$

The leading order approximation influences the first order approximation for the temperature field. By using the method of matched asymptotic expansion, we obtain the uniformly valid asymptotic expansion solution for the particle growth, in which the interface shape function is expressed as

$$\begin{aligned}R={}&R_0-\frac{\varepsilon(R_0-2\Gamma)}{3R_0(R_0+E^{-1}M)}\\&\times\int_1^{R_0}\frac{\omega^2(3\omega^2+6E^{-1}M\omega-6\Gamma E^{-1}M-k\lambda_SE^{-1}M-2k\lambda_S\Gamma)}{(\omega-2\Gamma)(\omega+E^{-1}M)^2}d\omega\\&-\frac{5\varepsilon pR_0^2(R_0+(2k+3)E^{-1}M)^{d_2}}{48(R_0-2\Gamma)^{d_1}}\\&\times\int_1^{R_0}\frac{\omega(\omega-2\Gamma)^{d_1}}{(\omega+(2k+3)E^{-1}M)^{d_2+1}}d\omega P_2^2(\cos\theta)\sin2\varphi\\&-\frac{2\alpha_4\Gamma(R_0-2\Gamma)}{R_0(R_0+E^{-1}M)}\int_1^{R_0}\frac{\omega(\omega+E^{-1}M)}{(\omega-2\Gamma)^2}d\omega\\&+\frac{24\alpha_4(4k+5)\Gamma R_0^9(R_0+(4k+5)E^{-1}M)^{d_4}}{(R_0-2\Gamma)^{d_3}}\\&\times\int_1^{R_0}\frac{(\omega-2\Gamma)^{d_3-1}(\omega+E^{-1}M)}{\omega^9(\omega+(4k+5)E^{-1}M)^{d_4+1}}d\omega P_4(\cos\theta)\\&+\frac{\alpha_4(4k+5)\Gamma R_0^9(R_0+(4k+5)E^{-1}M)^{d_4}}{12(R_0-2\Gamma)^{d_3}}\\&\times\int_1^{R_0}\frac{(\omega-2\Gamma)^{d_3-1}(\omega+E^{-1}M)}{\omega^9(\omega+(4k+5)E^{-1}M)^{d_4+1}}d\omega P_4^4(\cos\theta)\cos4\varphi+O(\varepsilon^2),\end{aligned} \tag{3.6}$$

where $P_n^m(\cos\theta)$ is the associated Legendre polynomial of degree n and order m,

$$\Gamma=\frac{\gamma_0T_M}{r_0\Delta H\Delta T},\ E=\frac{\Delta T}{T_M},\ M=\frac{V}{\mu T_M},\ k=\frac{k_S}{k_L},$$

$$d_1=\frac{2(2k+3)(2\Gamma+E^{-1}M)}{2\Gamma+(2k+3)E^{-1}M},\ d_2=\frac{(2k+3)E^{-1}M+(8k+10)\Gamma}{2\Gamma+(2k+3)E^{-1}M},$$

$$d_3=\frac{9(4k+5)(2\Gamma+E^{-1}M)}{2\Gamma+(4k+5)E^{-1}M},\ d_4=\frac{3(4k+5)E^{-1}M+6(12k+13)\Gamma}{2\Gamma+(4k+5)E^{-1}M},$$

here, μ is the interfacial kinetics coefficient, k_L and k_S are respectively the heat conduction coefficients in the liquid and solid phases.

The approximate solution obtained above are performed on a basis of the order of magnitude analysis, For our asymptotic analysis, the error of the asymptotic solution is of the $O(\varepsilon^2)$ order of magnitude according to the requirement of asymptotic expansion. Therefore, the range of the asymptotic expansion solution in (3.6) holds for the situation that are of the first order of magnitudes. As we see that the value of Prandtl number does not influence the thermal fields in the leading and first order approximations. When we proceed to the second order approximation of