Interfacial evolution of a spherical particle in a uniaxial straining flow*

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The growth behavior of a spherical particle in undercooled melt, affected by uniaxial straining flows, is studied. The analytical solution obtained by the matched asymptotic expansion method shows that the uniaxial straining flow effect results in higher local growth rate near the surface where the flow comes in and lower local growth rate near the surface where the flow goes out, and that the uniaxial straining flow causes an initially spherical particle to evolve into an oblate spheroid.

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1. Introduction

Pattern formation of interface microstructures is a fundamental problem in materials science and engineering.[1] During the past decades, many experiments and numerical simulations have been performed to study the effect of fluid convection on the interface morphology and a deep understanding of metal solidification and its precise control has been gained.[2−10] However, since fluid convection is complicated and the nonlinear system of the coupling of the growth of spherical particles with the convective flow has no exact general analytical solution available, the theoretical investigation of the morphological evolution of interface microstructures in convective melt has been greatly hindered and the interface morphology of spherical particles has not been expressed analytically.[11−16] In fact, the relative fluid velocity near a particle can be approximated and decomposed into the superposition of two parts: one is the uniform straining flow past through the particle and the other is the linear flow.[6,10] In the present paper, we study the effect of the fluid convection induced by the uniaxial straining flow on the interface morphology of the particle in the undercooled melt. By using the matched asymptotic expansion method,[12−16] we obtain the approximate analytical solution for the solidification system of the particle in the undercooled melt to show the morphological evolution and growth velocity of the interface of the particle affected by the uniaxial straining flow.

2. Theoretical model

We consider the morphological evolution of a spherical particle growing in the undercooled melt affected by the uniaxial straining flow. It is assumed that the melt is an isotropic incompressible Newtonian fluid. The temperature far from the particle is $(T_\infty)_D$, the undercooling of the melt is $\Delta T = (T_M)_D - (T_\infty)_D$, where $(T_\infty)_D < (T_M)_D$, $(T_M)_D$ is the equilibrium melting temperature, the subscripts 'D' represent the dimensional quantities. $(T_{\rm L})_D$ and $(T_{\rm S})_D$ denote the dimensional temperatures in the liquid and solid phases, respectively, $(\boldsymbol{U})_D$ and $(P)_D$ denote the dimensional convective velocity and pressure,

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respectively. $T_{\rm L}$ and $T_{\rm S}$ denote the dimensionless temperatures in the liquid and solid phases, respectively, $\boldsymbol{U}$ and P denote the dimensionless convective velocity and pressure, respectively. We adopt the initial radius of the spherical particle r_0 as the length scale, the characteristic velocity of the interface V as the velocity scale and r_0/V as the time scale and $\Delta HV^2/(c_p\Delta T)$ as the pressure scale. The scale of the temperature field is taken as $\Delta H/(c_p\rho_{\rm L})$, where ΔH is the latent heat per unit volume, c_p is the specific heat and $\rho_{\rm L}$ is the density in the melt. In the spherical coordinates whose origin is at the centre of the sphere, the dimensionless interface of the particle is written as $r = R(\theta,\varphi,t)$ and the dimensionless governing equations for the particle growth contain the continuity equation, the momentum equation, and the thermal conduction equations

$$\boldsymbol{\nabla}\cdot\boldsymbol{U} = 0, \tag{1}$$

$$\varepsilon\left(\frac{\partial \boldsymbol{U}}{\partial t} + (\boldsymbol{U}\cdot\boldsymbol{\nabla})\boldsymbol{U}\right) = -\boldsymbol{\nabla}P + Pt\boldsymbol{\nabla}^2\boldsymbol{U}, \tag{2}$$

$$\varepsilon\left(\frac{\partial T_{\rm L}}{\partial t} + (\boldsymbol{U}\cdot\boldsymbol{\nabla})T_{\rm L}\right) = \boldsymbol{\nabla}^2 T_{\rm L}, \tag{3}$$

$$\varepsilon\lambda_{\rm S}\frac{\partial T_{\rm S}}{\partial t} = \boldsymbol{\nabla}^2 T_{\rm S}, \tag{4}$$

where $\varepsilon = \Delta T/(\Delta H/(c_p\rho_{\rm L}))$, $Pt = \upsilon/\kappa$, $\lambda_{\rm S} = \kappa_{\rm T}/\kappa_{\rm S}$, in which υ is the kinematical viscosity, $\kappa_{\rm T}$ and $\kappa_{\rm S}$ are the thermal diffusivities in the liquid and solid phases, respectively. It is assumed that the densities in the liquid and solid phases are equal, and the buoyancy effects are neglected.

At the interface, the total mass conservation condition, the tangential non-slip condition, the thermal equilibrium condition, the Gibbs–Thomson condition, and the energy conservation condition hold, i.e.,

$$T_{\rm L} = T_{\rm S} = 2\varepsilon\Gamma K - \varepsilon E^{-1}MU_{\rm I}, \tag{5}$$

$$\varepsilon U_{\rm I} = (k\boldsymbol{\nabla}T_{\rm S} - \boldsymbol{\nabla}T_{\rm L})\cdot\boldsymbol{n}, \tag{6}$$

where $U_{\rm I}$ is the local interface velocity of the interface, K the local mean curvature at the interface, $\Gamma = \gamma(T_M)_D/(r_0\Delta H\Delta T)$, γ is the isotropic surface energy, $k = k_{\rm S}/k_{\rm L}$, $k_{\rm L}$ and $k_{\rm S}$ are, respectively, the heat conduction coefficients in the liquid and solid phases, $E = \Delta T/(T_M)_D$, $M = V/(\mu(T_M)_D)$, μ is the kinetics coefficient.

The far-field temperature condition and the convection-driven condition are, respectively, as $r\to\infty$,

$$T_{\rm L}\to -\varepsilon,\quad \boldsymbol{U}\to\boldsymbol{U}_\infty, \tag{7}$$

where $\boldsymbol{U}_\infty$ is

$$\boldsymbol{U}_\infty = Pe\left(x\boldsymbol{e}_x - \frac{1}{2}y\boldsymbol{e}_y - \frac{1}{2}z\boldsymbol{e}_z\right).$$

Here, x, y, and z are the rectangular coordinates, Pe is defined as the Peclet number, $Pe = \beta r_0/V$, with β being a constant.

Finally, the initial condition holds, in which the initial condition for the interface is $R(\theta,\varphi,0) = 1$ at time $t = 0$.

3. Asymptotic solution

We separate the entire space region into two subregions: one is the inner region near the interface of the sphere, and the other is the outer region far from the interface. For small parameter ε, we seek the regular expansion solution (called inner solution) in the inner region and the outer solution in the outer region, and then we match them to obtain the uniformly valid asymptotic solution in the entire region.

In the inner region, when $\partial/\partial t = O(1)$, we derive the regular expansion solution of the form as $\varepsilon\to 0$

$$\begin{aligned}\{\boldsymbol{U},P,R\} &= \{\boldsymbol{U}_0,P_0,R_0\} + \varepsilon\{\boldsymbol{U}_1,P_1,R_1\} + \cdots,\\ \{T_{\rm L},T_{\rm S}\} &= \varepsilon\{T_{\rm L0},T_{\rm S0}\} + \varepsilon^2\{T_{\rm L1},T_{\rm S1}\} + \cdots,\end{aligned} \tag{8}$$

in which each order term is expanded into the spherical harmonics series. Substituting Eq. (8) into Eqs. (1)–(7) and equating the terms of like powers of ε, we derive the equations and boundary conditions and initial conditions for each order term in Eq. (8). For the leading order terms, we have the solution $\boldsymbol{U}_0 = (u_0, v_0, w_0)$ that has the three components

$$\begin{aligned}u_0 &= Pe\left[x - \frac{5R_0^3x(2x^2-y^2-z^2)}{4r^5}\right.\\ &\quad\left.\times\left(1-\frac{R_0^2}{r^2}\right) - \frac{R_0^5x}{r^5}\right],\\ v_0 &= -\frac{1}{2}Pe\left[y + \frac{5R_0^3y(2x^2-y^2-z^2)}{2r^5}\right.\\ &\quad\left.\times\left(1-\frac{R_0^2}{r^2}\right) - \frac{R_0^5y}{r^5}\right],\\ w_0 &= -\frac{1}{2}Pe\left[z + \frac{5R_0^3z(2x^2-y^2-z^2)}{2r^5}\right.\\ &\quad\left.\times\left(1-\frac{R_0^2}{r^2}\right) - \frac{R_0^5z}{r^5}\right],\end{aligned} \tag{9}$$

$$P_0 = -\frac{5\,{\rm Pr}\,PeR_0^3(2x^2-y^2-z^2)}{2r^5} + {\rm const}, \tag{10}$$

$$T_{\rm L0} = -1 + \frac{b_0(t)}{r},$$

$$T_{\rm S0} = -\frac{2\Gamma}{R_0} - E^{-1}M\frac{{\rm d}R_0}{{\rm d}t}, \tag{11}$$

where

$$b_0(t) = \frac{(R_0 - 2\Gamma)R_0}{R_0 + E^{-1}M},$$
$$\frac{\mathrm{d}R_0}{\mathrm{d}t} = \frac{R_0 - 2\Gamma}{R_0(R_0 + E^{-1}M)}. \quad (12)$$

When initial radius r_0 is taken to be larger than the critical radius of a nucleus $R_* = 2\gamma T_M/(\Delta H \Delta T)$, the leading order approximation of the interface R_0 which obeys the initial condition for the interface is expressed, in the implicit function form, as

$$t = \frac{1}{2}(R_0^2 - 1) + (2\Gamma + E^{-1}M) \times \left[(R_0 - 1) + 2\Gamma \ln\left(1 + \frac{R_0 - 1}{1 - 2\Gamma}\right)\right]. \quad (13)$$

For the first order terms, we have the solution

$$T_{\mathrm{L1}} = \frac{a_{0,0}}{r} + \frac{a_{2,0}}{r^3}\mathrm{P}_2(\cos\theta) + \frac{a_{2,2}}{r^3}\mathrm{P}_2^2(\cos\theta)\cos 2\varphi + T^*_{\mathrm{L1}}, \quad (14)$$

$$T_{\mathrm{S1}} = b_{0,0} + b_{2,0}r^2\mathrm{P}_2(\cos\theta) + b_{2,2}r^2\mathrm{P}_2^2(\cos\theta)\cos 2\varphi + T^*_{\mathrm{S1}}, \quad (15)$$

$$R_1 = h_{0,0} + h_{2,0}\mathrm{P}_2(\cos\theta) + h_{2,2}\mathrm{P}_2^2(\cos\theta)\cos 2\varphi, \quad (16)$$

where $\mathrm{P}_l^m(\cos\theta)$ is the adjoint Legendre polynomial of order m and degree l,

$$T^*_{\mathrm{L1}} = \frac{r}{2}\frac{\mathrm{d}b_0(t)}{\mathrm{d}t} - \frac{Pe}{2}\left(\frac{r}{4} - \frac{5R_0^3}{8r^2} - \frac{R_0^5}{4r^4}\right) \times b_0(t)\mathrm{P}_2(\cos\theta) - \frac{3Pe}{2}\left(-\frac{r}{24} + \frac{5R_0^3}{48r^2} + \frac{R_0^5}{24r^4}\right) \times b_0(t)\mathrm{P}_2^2(\cos\theta)\cos 2\varphi,$$
$$T^*_{\mathrm{S1}} = \frac{\lambda_{\mathrm{S}}r^2}{6}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{b_0(t)}{R_0}\right),$$
$$a_{0,0} = \frac{2\Gamma + b_0(t)}{R_0}h_{0,0} - E^{-1}MR_0\frac{\mathrm{d}h_{0,0}}{\mathrm{d}t} - \frac{R_0^2}{2}\frac{\mathrm{d}b_0(t)}{\mathrm{d}t},$$
$$b_{0,0} = \frac{2\Gamma}{R_0^2}h_{0,0} - E^{-1}M\frac{\mathrm{d}h_{0,0}}{\mathrm{d}t} - \frac{\lambda_{\mathrm{S}}R_0^2}{6}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{b_0(t)}{R_0}\right),$$

$$h_{0,0} = \frac{(R_0 - 2\Gamma)}{3R_0(R_0 + E^{-1}M)}\int_1^{R_0}\frac{E^{-1}M(6\Gamma - 6\omega + k\lambda_{\mathrm{S}}\omega)\omega^3 + (2k\lambda_{\mathrm{S}}\Gamma - 3\omega)\omega^4}{(\omega - 2\Gamma)^2(\omega + E^{-1}M)}\mathrm{d}\omega, \quad (17)$$

with $h_{0,0}$ satisfying the differential equation

$$\frac{\mathrm{d}h_{0,0}}{\mathrm{d}t} = -\frac{1}{R_0^2}\Re(R_0, 0)h_{0,0} + \frac{R_0}{(R_0 + E^{-1}M)}\left(\frac{k\lambda_{\mathrm{S}}R_0}{3}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{b_0(t)}{R_0}\right) - \frac{\mathrm{d}b_0(t)}{\mathrm{d}t}\right), \quad (18)$$

where

$$\Re(R_0, l) = \frac{R_0 - 2\Gamma - (l+2)(lk + l + 1)\Gamma}{R_0 + (lk + l + 1)E^{-1}M} - \frac{E^{-1}MR_0}{R_0 + (lk + l + 1)E^{-1}M}\frac{\mathrm{d}R_0}{\mathrm{d}t}, \quad (19)$$

$$a_{2,0} = -\frac{5Pe}{16}R_0^4 b_0(t) - E^{-1}MR_0^3\frac{\mathrm{d}h_{2,0}}{\mathrm{d}t} + (b_0(t) - 4\Gamma)R_0h_{2,0},$$
$$b_{2,0} = -\frac{E^{-1}M}{R_0^2}\frac{\mathrm{d}h_{2,0}}{\mathrm{d}t} - \frac{4\Gamma}{R_0^4}h_{2,0},$$
$$h_{2,0} = \frac{5PeR_0^2(R_0 + (2k+3)E^{-1}M)^c}{16(R_0 - 2\Gamma)^b} \times \int_1^{R_0}\frac{(\omega - 2\Gamma)^b}{(\omega + (2k+3)E^{-1}M)^{c+1}}\mathrm{d}\omega, \quad (20)$$

with

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

and $h_{2,0}$ satisfying the differential equation

$$\frac{\mathrm{d}h_{2,0}}{\mathrm{d}t} = \frac{1}{R_0^2}\Re(R_0, 2)h_{2,0} + \frac{5Peb_0^{(}t)}{16(R_0 + (2k+3)E^{-1}M)}, \quad (21)$$

$$a_{2,2} = (b_0(t) - 4\Gamma)R_0h_{2,2} - E^{-1}MR_0^3\frac{\mathrm{d}h_{2,2}}{\mathrm{d}t} + \frac{5Pe}{32}R_0^4b_0(t),$$
$$b_{2,2} = -\frac{4\Gamma}{R_0^4}h_{2,2} - \frac{E^{-1}M}{R_0^2}\frac{\mathrm{d}h_{2,2}}{\mathrm{d}t},$$
$$h_{2,2} = -\frac{1}{2}h_{2,0}, \quad (22)$$

and $h_{2,2}$ satisfying the differential equation

$$\frac{\mathrm{d}h_{2,2}}{\mathrm{d}t} = \frac{1}{R_0^2}\Re(R_0, l)h_{2,2} - \frac{5PeR_0b_0(t)}{32(R_0 + (2k+3)E^{-1}M)}. \quad (23)$$

Therefore, we obtain the regular expansion solution (8) and the dimensionless interface and local growth

rate interface velocity,

$$R = R_0 + \varepsilon h_{0,0} + \varepsilon h_{2,0} \mathrm{P}_2(\cos\theta) + \varepsilon h_{2,2} \mathrm{P}_2^2(\cos\theta)\cos 2\varphi + \cdots . \quad (24)$$

$$\frac{\partial R}{\partial t} = \frac{\mathrm{d}R_0}{\mathrm{d}t} + \varepsilon \frac{\mathrm{d}h_{0,0}}{\mathrm{d}t} + \varepsilon \frac{\mathrm{d}h_{2,0}}{\mathrm{d}t} \mathrm{P}_2(\cos\theta) + \varepsilon \frac{\mathrm{d}h_{2,2}}{\mathrm{d}t} \mathrm{P}_2^2(\cos\theta)\cos 2\varphi + \cdots . \quad (25)$$

The solution in Eq. (8) does not satisfy the initial condition. The reason for this is that we made the presumption of $\partial/\partial t = O(1)$, then the solution for the temperature field is valid only in the time interval $[O(\varepsilon), +\infty]$. In a way similar to that for Chen's analysis,[14,16] by introducing the time inner variable $\tau = t/\varepsilon$ and solving a classical initial-boundary value problem in the sense of time, we prove that the obtained solution satisfies the required initial condition.

In the outer region, the solution of Eq. (8) does not satisfy the vanishing condition at the far field. By introducing the outer variable

$$\bar{x} = \sqrt{\varepsilon}(1 - Pet)x,$$
$$\bar{y} = \sqrt{\varepsilon}(2 + Pet)y/2,$$
$$\bar{z} = \sqrt{\varepsilon}(2 + Pet)z/2,$$

we seek the outer solution for the temperature field to match the 'inner' regular expansion solution in Eq. (8). It can be proved that the solution of Eq. (3) which obeys the far field condition (7) and the initial condition at time $t = t$ may be taken as the regular expansion solution in Eq. (8). Consequently, we obtain the uniformly valid asymptotic expansion solution for the growth of the spherical particle. According to the theory of solidification, the momentum transport and energy transport occur mainly within the region near the interface, regular expansion solution (8) determines the temperature distribution and the evolutions of morphology and velocity of the interface.

It is seen from Eqs. (24) and (25) that the growth of the spherical particle contains two parts: one is the symmetrical growth that is not influenced by the uniaxial straining flow, in which the term $\varepsilon h_{0,0}$ is due to the change of temperature in the melt; the other is the non-symmetrical growth that is influenced by the uniaxial straining flow. The solution for the shape of a growing particle in a uniaxial straining flow is a function of θ and φ. The third and fourth terms correspond to the change of coming and outgoing flows, respectively. Affected by the uniaxial straining flow, the interface shape of the spherical particle will be distorted. On the planes $\varphi = \pm\pi/4, \pm 3\pi/4$, the fourth term vanishes and the transform occurs. The fourth term attains its maximum when $\varphi = 0$ (i.e., on the cross section of the oxz plane), and it reaches its minimum when $\varphi = \pm\pi/2$. For the uniaxial flow that is outgoing near the equatorial plane and incoming near the poles, when $\mathrm{d}R_0/\mathrm{d}t > 0$, we have $\mathrm{d}h_{2,0}/\mathrm{d}t > 0$ and $\mathrm{d}h_{2,2}/\mathrm{d}t < 0$. We illustrate the shape evolution with the following data: $\beta = 0.5$, $\Gamma = 0.1$, $\Delta T = 400$, $\lambda_{\mathrm{S}} = 0.01$, $E = 0.01$, $M = 0.03$, $\varepsilon = 0.15$, and $k = 1$. Figure 1 shows the shape evolution of a particle growing in a uniaxial straining flow on the cross section of the oxz plane ($\varphi = 0$). It implies that the energy transfer rate is higher near the poles and lower near the oxz plane of the equatorial plane and the particle grows soon into a prolate shape on the cross section of the oxz plane. It is consistent with the results on the cross section of interface shape evolution made by Noh *et al.*[10] However, across the transform planes of $\varphi = \pm\pi/4, \pm 3\pi/4$, the situation on the cross section of the oyz plane is contrary to that on the cross section of the oxz plane. Figure 2 shows the shape evolution of a particle growing in a uniaxial straining flow on the cross section of the oyz plane ($\varphi = \pm\pi/2$).

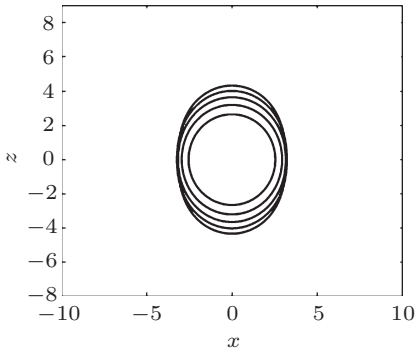


Fig. 1. Cross sections of interface shape evolution of a particle in the uniaxial straining flow when $\varphi = 0$, at time $t = 10, 15, 20, 25, 30$ (from inside to outside).

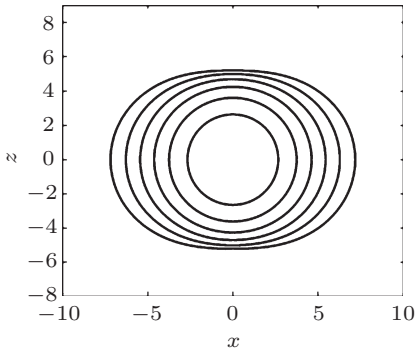


Fig. 2. Cross sections of interface shape evolution of a particle growing in the uniaxial straining flow when $\varphi = \pi/2$ at time $t = 10, 15, 20, 25, 30$ (from inside to outside).

It implies that the energy transfer rate is higher near the *oyz* plane of the equatorial plane and lower near the poles and then the growth velocity near the *oyz* plane of the equatorial plane is higher than that near the poles, and the particle grows quickly into an oblate shape on the cross section of the *oyz* plane. This is the case that Noh *et al.*[10] neglected in their simulations.

4. Conclusion

By using the method of matched asymptotic expansion, we studied the growth behaviour of a spherical particle in the undercooled melt, affected by a uniaxial straining flow. The resulting asymptotic solution for the interface shape of a particle growing in the uniaxial straining flow is a function of both azimuth angle and polar angle. The asymptotic solution shows that the uniaxial straining flow has a significant effect on the growth of the spherical particle and that the uniaxial straining flow effect results in higher local growth rate near the surface where the flow is incoming and lower local growth rate near the surface where the flow is outgoing, and that the initially spherical particle evolves into an oblate spheroid.

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