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RESEARCH ARTICLE

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Steady needle growth with 3-D anisotropic surface tension

Abstract The effect of the anisotropic interfacial energy on dendritic growth has been an important subject, and has preoccupied many researchers in the field of materials science and condensed matter physics. The present paper is dedicated to the study of the effect of full 3-D anisotropic surface tension on the steady state solution of dendritic growth. We obtain the analytical form of the first order approximation solution in the regular asymptotic expansion around the Ivantsov's needle growth solution, which extends the steady needle growth solution of the system with isotropic surface tension obtained by Xu and Yu (J. J. Xu and D. S. Yu, J. Cryst. Growth, 1998, 187: 314; J. J. Xu, Interfacial Wave Theory of Pattern Formation: Selection of Dendrite Growth and Viscous Fingering in a Hele-Shaw Flow, Berlin: Springer-Verlag, 1997).

The solution is expanded in the general Laguerre series in any finite region around the needle-tip, and it is also expanded in a power series in the far field behind the tip. Both solutions are then numerically matched in the intermediate region . Based on this global valid solution, the dependence of Peclet number Pe and the interface's morphology on the anisotropy parameter of surface tension as well as other physical parameters involved are determined. On the basis of this global valid solution, we explore the effect of the anisotropy parameter on the Peclet number of growth, as well as the morphology of the interface.

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1 Introduction

In studying free dendritic growth, the effect of anisotropic interfacial energy on pattern formation and selection bas been an important subject, which has preoccupied many researchers in the field of materials science and condensed matter physics for quite a long time now [1–4]. During the past decades, most theoretical investigations on this subject were focused on the system of 2-D dendritic growth with anisotropy of surface tension, or the system of 3-D axi-symmetric dendritic growth with axial anisotropy of surface tension, neglecting the three dimensionality of the anisotropy of surface tension [5–15]. With these efforts, the effect of the anisotropy of surface tension on the morphology of the steady state, interfacial stability mechanisms and selection of dendritic pattern formation for 2-D systems are now well explored analytically.

A realistic system of dendritic growth is always three dimensional. The anisotropy of surface tension at the interface is also three dimensional. Up to now in literature, there are very few analytical works on dendritic growth in systems with full 3-D anisotropic surface tension. As a consequence, the effects of three dimensionality of anisotropy on the steady state solution as well as the stability mechanisms of dendritic growth are still unclear.

In order to explore the effect of 3-D anisotropic surface tension on the stability mechanisms and the selection condition of dendritic growth, as the first step, it is necessary to study the effect of 3-D anisotropic surface tension on the steady state of dendritic growth. The goal of our effort is to attack this problem.

We obtain the analytical solution in the form of regular asymptotic expansion around Ivantsov's needle growth solution, which extends the work on steady needle growth solution of the system with isotropic surface tension conducted by Xu and Yu [7, 14]. The solution is expended in the general Laguerre series in any finite region around the needle-tip and is also expanded in a power series in the far field behind the tip. Both solutions are then matched in the intermediate region numerically. On the basis of this global valid solution, we explore the effect of the anisotropy parameter on the Peclet number of growth, as well as the morphology of the interface.

The paper is arranged as follows. In Section 2, we formulate the problem in the moving paraboloidal coordinate system; in Section 3, we derive the asymptotic solution in the finite region behind the tip in the form of a general Laguerre series; in Section 4, we derive the solution in the region far away from the tip in the power series; then in Section 5, we match two solutions in the intermediate region numerically; in Section 6, we show the numerical results for various cases; finally in Section 7, we give the discussions and conclusions.

2 Mathematical formulation of the problem of steady needle crystal growth

Let us consider a system of free dendritic growth from a pure substance at the later stage of evolution, when the dendrite is fully developed with a sufficiently long stem. At this stage, the effects of the initial growth conditions as well as the situation at the root in the finite region around the tip on the solution will diminish to a minimum. Thus, for a mathematical model of the steady state of dendritic growth at the later stage, one may consider a needle-like crystal growing with a constant tip-velocity U into an undercooled pure melt with the undercooling temperature $T_\infty < T_{\rm M0}$, where $T_{\rm M0}$ is the melting temperature of a flat interface (refer to Refs. [7, 14]). The full 3-D anisotropic surface tension at the interface between liquid and solid phase is taken into account, so that the needle-like crystal under consideration is non-axisymmetrical. For simplicity, we assume that in the growth system, the mass density ρ, the specific heat $c_{\rm p}$, and other thermal characteristic constants of the solid state are the same as that of the liquid state (the so-called symmetric model); gravity is negligible, so no convection is involved.

As usual, we use the growth speed of dendrite U, as the scale of the velocity, and the thermal length $\ell_{\rm T} = \kappa_{\rm T}/U$ as the length scale, $\ell_{\rm T}/U$ as the time scale and $\Delta H/(c_{\rm p}\rho)$ as the temperature scale, where ΔH is the latent heat per unit volume of the solid.

We adopt the paraboloidal coordinate system moving together with the growing need-crystal (refer to Ref. [14]), which can be defined through the Cartesian coordinate system (x, y, z) by (see Fig. 1):

$$\frac{x}{\eta_0^2} = \xi\eta\cos\theta, \quad \frac{y}{\eta_0^2} = \xi\eta\sin\theta, \quad \frac{z}{\eta_0^2} = \frac{1}{2}(\xi^2 - \eta^2) \tag{2.1}$$

where the constant η_0^2 is to be chosen, so that the steady interface shape satisfies

$$\eta_{\rm s}(0) = 1 \tag{2.2}$$

It is known that this constant is just the Peclet number, Pe_0, of the system with zero surface tension, fully determined by the undercooling T_∞ via the Ivantsov solution. In general, the Peclet number, Pe, is defined as the ratio of the tip radius $\ell_{\rm t}$ and the thermal diffusion length $\ell_{\rm T}$, and is a function of all physical parameters involved in the system, including the anisotropy parameter.

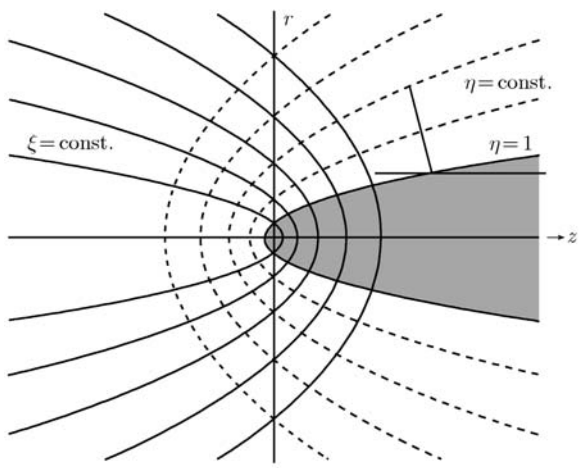

Fig. 1 The paraboloidal coordinate system (ξ, η, θ) for three-dimensional dendrite growth.

The governing equation for three-dimensional dendritic growth can be written in the forms:

(1) In the liquid region:

$$\frac{\partial^2 T}{\partial \xi^2} + \frac{\partial^2 T}{\partial \eta^2} + \left(\frac{1}{\xi} - \eta_0^2\xi\right)\frac{\partial T}{\partial \xi} + \left(\frac{1}{\eta} + \eta_0^2\eta\right)\frac{\partial T}{\partial \eta} + \left(\frac{1}{\xi^2} + \frac{1}{\eta^2}\right)\frac{\partial^2 T}{\partial \theta^2} = 0 \tag{2.3}$$

(2) In the solid region:

$$\frac{\partial^2 T_S}{\partial \xi^2}+\frac{\partial^2 T_S}{\partial \eta^2}+\left(\frac{1}{\xi}-\eta_0^2\xi\right)\frac{\partial T_S}{\partial \xi}+\left(\frac{1}{\eta}+\eta_0^2\eta\right)\frac{\partial T_S}{\partial \eta}+\left(\frac{1}{\xi^2}+\frac{1}{\eta^2}\right)\frac{\partial^2 T_S}{\partial \theta^2}=0 \tag{2.4}$$

The boundary conditions are:

(1) The up-stream far-field condition:

$$T=T_\infty \quad \text{as} \quad \eta\to\infty \tag{2.5}$$

(2) The regularity condition:

$$T_S=O(1) \quad \text{as} \quad \eta\to 0 \tag{2.6}$$

(3) The interface conditions, at $\eta=\eta_s(\xi,\theta)$, we have

(a) the temperature continuity condition:

$$T_L=T_S \tag{2.7}$$

(b) the Gibbs–Thomson condition: The surface tension coefficient can be expressed in the form:

$$\gamma=\gamma_0[1+\hat{\alpha_4}Q_4(\boldsymbol{n})] \tag{2.8}$$

where γ_0 is the coefficient of isotropic surface tension, α_4 is the coefficient of forth fold anisotropic surface tension, $\boldsymbol{n}$ is the unit normal vector of the interface pointing to the liquid phase, and $Q_4(\boldsymbol{n})=(n_x^4+n_y^4+n_z^4)$ is the anisotropic scalar function. The temperature at the interface can be determined by the Herring formula [10, 11]:

$$T_S=T_I=-\varepsilon^2\left[1+\alpha_4\left(\frac{\partial Q_4}{\partial\theta_1^2}+\frac{\partial Q_4}{\partial\theta_2^2}\right)\right]\mathcal{K}_3\{\eta_s(\xi,\theta)\} \tag{2.9}$$

where (θ_1,θ_2) respectively represent the orientation angles of the directions of the two principal curvatures; $\mathcal{K}_3\big\{\eta_s(\xi,\theta)\big\}$ is the local twice mean curvature of the interface $\eta_s(\xi,\theta)$, which is derived as:

$$\begin{aligned}
&\mathcal{K}_3\{\eta_s(\xi,\theta)\}\\
&=-\frac{1}{(\xi^2+\eta_s^2)^{\frac{3}{2}}\left[\xi^2\eta_s^2(1+\eta_s'^2)+\eta_{s,\theta}^2(\xi^2+\eta_s^2)\right]^{\frac{3}{2}}}\\
&\cdot\Big\{\left[(1+\eta_s'^2)(\xi^2+\eta_s^2)\right]\left[-(\xi\eta_s)^2(\eta_s\eta_s'-\xi)\right.\\
&+2\xi\eta_{s,\theta}^2(\xi^2+\eta_s^2)+\xi^2\eta_s\eta_{s,\theta\theta}(\eta_s\eta_s'-\xi)\\
&\left.-\xi\eta_s(\xi\eta_s)'(\eta_{s,\theta}^2+\eta_s\eta_{s,\theta\theta})\right]-2\left[\eta_{s,\theta}\eta_s'(\xi^2+\eta_s^2)\right]\\
&\cdot\left[(\xi\eta_s)'\eta_{s,\theta}(\xi^2+\eta_s^2)+\xi\eta_s(\eta_s\eta_s'-\xi)(\xi\eta_{s,\theta})'\right.\\
&\left.-\xi\eta_s(\eta_s\eta_{s,\theta})'(\xi\eta_s)'\right]+\left[(\xi\eta_s)^2+\eta_{s,\theta}^2(\xi^2+\eta_s^2)\right]\\
&\cdot\left[(\xi\eta_s)''\xi\eta_s(\eta_s\eta_s'-\xi)+\xi\eta_s(\xi\eta_s)'(1-\eta_s'^2-\eta_s\eta_s'')\right]\Big\}
\end{aligned} \tag{2.10}$$

Especially, for the special axi-symmetric case, $\eta_s=\eta_s(\xi)$, we have

$$\begin{aligned}
\mathcal{K}_3\big\{\eta_s(\xi,\theta)\big\}=-\frac{1}{\sqrt{\xi^2+\eta_s^2}}\Bigg[&\frac{\eta_s''}{(1+\eta_s'^2)^{\frac{3}{2}}}-\frac{1}{\eta_s(1+\eta_s'^2)^{\frac{1}{2}}}\\
&+\frac{\eta_s'(\eta_s^2+2\xi^2)-\xi\eta_s}{\xi(\xi^2+\eta_s^2)(1+\eta_s'^2)^{\frac{1}{2}}}\Bigg]
\end{aligned} \tag{2.11}$$

The complete form of Eq. (2.9) in the paraboloidal coordinate system is very complicated. Fortunately, in this investigation, we only need its first order approximation form, which is given in the Appendix. In Eq. (2.9), the interfacial stability parameter ε is defined as:

$$\varepsilon=\frac{\sqrt{\ell_c/\ell_T}}{\eta_0^2},\quad \ell_c=\frac{\gamma_0 c_p\rho T_{M0}}{(\Delta H)^2} \tag{2.12}$$

where T_{M0} is the melting temperature of the flat interface.

(c) the heat balance condition:

$$\left(\frac{\partial}{\partial\eta}-\eta_s'\frac{\partial}{\partial\xi}\right)(T-T_S)-\eta_{s,\theta}\left(\frac{1}{\xi^2}+\frac{1}{\eta_s^2}\right)\frac{\partial}{\partial\theta}(T-T_S)+\eta_0^2(\xi\eta_s)'=0 \tag{2.13}$$

(4) The tip-smoothness condition: at $\xi=0$,

$$\eta_s(0,\theta)=1,\quad \eta_s'(0,\theta)=0 \tag{2.14}$$

The problem under study is how to solve the three unknown functions involved: the temperature fields $T(\xi,\eta,\theta)$, $T_S(\xi,\eta,\theta)$, and the interface shape $\eta_s(\xi,\theta)$.

3 Steady state asymptotic expansion solution away from the root region

It is known that the interfacial stability parameter ε is, in practice, very small, whose numerical magnitude is about 0.1–0.2. Thus, in order to examine the steady perturbation induced by the anisotropic surface tension in the region away from the root of dendrite, one may make the regular perturbation expansion (RPE) around the Ivantsov solution in the limit $\varepsilon\to 0$. Namely, let

$$\begin{cases}T=T(\xi,\eta,\theta)=T_0(\eta)+\varepsilon^2\eta_0^2T_1(\xi,\eta,\theta)+\cdots\\ T_S=T_S(\xi,\eta,\theta)=T_{S0}+\varepsilon^2\eta_0^2T_{S1}(\xi,\eta,\theta)+\cdots\\ \eta_s=\eta_B(\xi,\theta)=1+\varepsilon^2\eta_1(\xi,\theta)+\cdots\end{cases} \tag{3.1}$$

Substitute (3.1) into the system (2.3)–(2.13) and equate coefficients of like powers of ε to zero, then we can successively derive the systems of each order approximation.

3.1 Zeroth-order approximation $O(\varepsilon^0)$

The zeroth order approximation solution is the Ivantsov's solution,

$$\begin{cases} T_0 = T_\infty + \dfrac{\eta_0^2}{2}\mathrm{e}^{\frac{\eta_0^2}{2}}E_1\left(\dfrac{\eta_0^2\eta^2}{2}\right) \\ T_{S0} = 0 \\ \eta_0 = 1 \\ T_\infty = -\dfrac{\eta_0^2}{2}\mathrm{e}^{\frac{\eta_0^2}{2}}E_1\left(\dfrac{\eta_0^2}{2}\right) \end{cases} \tag{3.2}$$

where $E_1(x)$ is the exponential integral function defined as (see Ref. [13]):

$$E_1(x) = \int_x^\infty \frac{\mathrm{e}^{-t}}{t}\mathrm{d}t \tag{3.3}$$

3.2 First order approximation $O(\varepsilon^2)$

In the first-order approximation, we derive that in the liquid phase region

$$L\{T_1\} = \left[\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2} + \left(\frac{1}{\xi} - \eta_0^2\xi\right)\frac{\partial}{\partial\xi} + \left(\frac{1}{\eta} + \eta_0^2\eta\right)\frac{\partial}{\partial\eta}\right]T_1 + \left(\frac{1}{\xi^2} + \frac{1}{\eta^2}\right)\frac{\partial^2 T_1}{\partial\theta^2} = 0 \tag{3.4}$$

while in the solid phase region

$$L\{T_{S1}\} = \left[\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2} + \left(\frac{1}{\xi} - \eta_0^2\xi\right)\frac{\partial}{\partial\xi} + \left(\frac{1}{\eta} + \eta_0^2\eta\right)\frac{\partial}{\partial\eta}\right]T_{S1} + \left(\frac{1}{\xi^2} + \frac{1}{\eta^2}\right)\frac{\partial^2 T_{S1}}{\partial\theta^2} = 0 \tag{3.5}$$

The boundary conditions are

(1) As $\eta \to \infty$,

$$T_1 \to 0 \quad \text{(exponentially)} \tag{3.6}$$

(2) It is hard to determine the asymptotic behavior of the solution at the first space, which specifies whether the solution is growing or decaying as $\xi \to \infty$. However, one may very reasonably assume that the solution cannot grow exponentially, if it grows. Thus, we impose that as $\xi \to \infty$,

$$T_1 \to 0 \quad \text{(or, at most, algebraically grows)} \tag{3.7}$$

(3) As $\eta \to 0$,

$$T_{S1} = O(1), \quad \text{is regular} \tag{3.8}$$

(4) The interface conditions are linearized around the interface of Ivantsov paraboloid ($\eta = 1$), which can be written as:

(a) Temperature continuity condition:

$$T_1 = T_{S1} + \eta_1 \tag{3.9}$$

(b) Gibbs-Thomson condition: The first order approximation of the interface temperature can be derived in the form (Ref. [11], the details of the derivation is given in the Appendix.):

$$T_{S1} = -[K_0 + \hat{\alpha}_4(F_0 + F_4\cos 4\theta)] \tag{3.10}$$

where

$$K_0 = \frac{2+\xi^2}{(1+\xi^2)^{\frac{3}{2}}}, \quad F_0 = \frac{\frac{3}{4}\xi^6 + \frac{3}{2}\xi^4 + 21\xi^2 - 6}{(1+\xi^2)^{\frac{7}{2}}}$$

$$F_4 = \frac{-\frac{15}{4}\xi^6 - \frac{15}{2}\xi^4}{(1+\xi^2)^{\frac{7}{2}}} \tag{3.11}$$

(c) Heat balance condition:

$$\frac{\partial}{\partial\eta}(T_1 - T_{S1}) + (2+\eta_0^2)\eta_1 + \xi\frac{\mathrm{d}\eta_1}{\mathrm{d}\xi} = 0 \tag{3.12}$$

(5) The tip-regularity condition, at $\xi = 0$,

$$\eta_1'(0) = 0, \quad \eta_1(0) = 0 \tag{3.13}$$

Note that Eq. (3.10) is the only inhomogeneous condition in the above system. With the superposition principle, one may separate the solution vector $q_1 \equiv \{T_1, T_{S1}, \eta_{s1}\}$ into three parts:

$$q_1 = q_1^{(\mathrm{iso})} + \hat{\alpha}_4 q_1^{(0)} + \hat{\alpha}_4 q_1^{(4)}$$

Among them, $q_1^{(\mathrm{iso})}$ is the isotropic component of the solution with $\hat{\alpha}_4 = 0$, $\hat{\alpha}_4 q_1^{(0)}$ is the axi-symmetric component of the solution induced by the anisotropy of surface tension, while $\hat{\alpha}_4 q_1^{(4)}$ is the non-axi-symmetric component of the solution induced by the anisotropy of surface tension. These components of the solution are subject to the following simplified Gibbs-Thomson conditions at the interface, respectively:

$$T_{S1}^{(\mathrm{iso})} = -K_0(\xi), \quad T_{S1}^{(0)} = -F_0(\xi)$$
$$T_{S1}^{(4)} = -F_4(\xi)\cos 4\theta \tag{3.14}$$

while other boundary conditions remain unchanged.

The isotropic component of solution $q_1^{(\mathrm{iso})}$ has been obtained by Xu and Yu previously (refer to Ref. [14]). Therefore, the present paper attempts to solve the solutions $\hat{\alpha}_4 q_1^{(0)}$ and $\hat{\alpha}_4 q_1^{(4)}$ only.

3.3 The solution for the temperature field in liquid phase

The solution for Eq. (3.4) can be derived by using separation of variables. Let

$$T_1(\xi, \eta, \theta) = X(\xi)Y(\eta)\cos m\theta \tag{3.15}$$

From Eq. (3.4) it follows that

$$X'' + \left(\frac{1}{\xi} - \eta_0^2\xi\right)X' + \left(\eta_0^2\lambda_1^2 - \frac{m^2}{\xi^2}\right)X = 0 \tag{3.16}$$

$$Y'' + \left(\frac{1}{\eta} + \eta_0^2\eta\right)Y' - \left(\eta_0^2\lambda_1^2 + \frac{m^2}{\eta^2}\right)Y = 0 \tag{3.17}$$

By letting

$$\sigma = \frac{\eta_0^2\xi^2}{2}, \quad X = X(\sigma) \tag{3.18}$$

the equation (3.16) is transformed into the Kummer equation [13]:

$$\sigma X''(\sigma)+(1-\sigma)X'(\sigma)+\left(\frac{\lambda_1^2}{2}-\frac{m^2/4}{\sigma}\right)X=0 \tag{3.19}$$

Furthermore, letting

$$X(\sigma) = \mathrm{e}^{\frac{\sigma}{2}}\sigma^{-\frac{1}{2}}W(\sigma)$$

Eq. (3.19) is transformed in the Wittaker's equation:

$$\frac{\mathrm{d}^2W}{\mathrm{d}\sigma^2} + \left(-\frac{1}{4} + \frac{\kappa}{\sigma} + \frac{1-4\mu^2}{4\sigma^2}\right)W = 0 \tag{3.20}$$

with

$$\kappa = \frac{1+\lambda_1^2}{2}, \quad \mu = \frac{m}{2}$$

which has the two fundamental solutions:

$$W(\sigma) = \mathrm{e}^{-\frac{\sigma}{2}}\sigma^{\frac{1}{2}+\frac{m}{2}}\begin{cases} M\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right) \\ U\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right)\end{cases} \tag{3.21}$$

Here M and U are the confluent hypergeometric functions [13].

Hence, the fundamental solutions of Eq. (3.19) are

$$X(\sigma)=\mathrm{e}^{\frac{\sigma}{2}}\sigma^{-\frac{1}{2}}W(\sigma) = \sigma^{\frac{m}{2}}\begin{cases} M\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right) \\ U\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right)\end{cases} \tag{3.22}$$

Note that function M and U have the following properties:

- $M\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right)$ is regular at $\sigma = 0$;
- $U\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right)$ has a logarithmic singularity

for $m = 0$ and $O(\sigma^{-m/2})$ singularity for $m > 0$ at $\sigma = 0$. Thus, one must choose

$$X(\sigma) = \sigma^{\frac{m}{2}}M\left(\frac{m-\lambda_1^2}{2}, 1+m, \sigma\right) \tag{3.23}$$

On the other hand, as $\sigma \to \infty$, $M\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right)$ grows algebraically only for

$$\frac{m-\lambda_1^2}{2} = -n = 0, -1, -2, \cdots \tag{3.24}$$

For other values of $m-\lambda_1^2/2$, the function $M\left(\dfrac{m-\lambda_1^2}{2}, 1+m, \sigma\right)$ grows exponentially, as $\sigma \to \infty$. From the far field condition of the liquid phase (3.7), one must set $\lambda_1^2/2 = n + m/2$ so that we derive

$$X(\sigma) = \sigma^{\frac{m}{2}}M(-n, 1+m, \sigma) = a_0\xi^m L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right) \tag{3.25}$$

Here, we have denoted $a_0 = \left(\dfrac{\eta_0^2}{2}\right)^{\frac{m}{2}}\dfrac{n!\Gamma(m+1)}{\Gamma(m+n+1)}$ and applied the formula:

$$L_n^{(m)}(\sigma) = \frac{\Gamma(m+n+1)}{n!\Gamma(m+1)}M(-n, 1+m, \sigma) \tag{3.26}$$

where $L_n^{(m)}(x)$ is the m-th order general Laguerre polynomial.

We now return to solve Eq. (3.17). Let

$$\tau = \frac{\eta_0^2\eta^2}{2}, \quad Y = Y(\tau) \tag{3.27}$$

So that Eq. (3.17) is transformed to

$$\tau Y''(\tau)+(1+\tau)Y'(\tau)-\left(\frac{\lambda_1^2}{2}+\frac{m^2/4}{\tau}\right)Y = 0 \tag{3.28}$$

With the new variable $Z(\tau)$ defined as

$$Y(\eta) = \mathrm{e}^{-\frac{\tau}{2}}\tau^{-\frac{1}{2}}Z(\tau) \tag{3.29}$$

Eq. (3.28) can be transformed to the Whittaker equation:

$$Z''(\tau) + \left(-\frac{1}{4} + \frac{\kappa}{\tau} + \frac{\frac{1}{4}-\mu^2}{\tau^2}\right)Z(\tau) = 0 \tag{3.30}$$

where

$$\mu = \frac{m}{2}, \quad \kappa = -\frac{1+\lambda_1^2}{2}$$

Hence, we can obtain the two fundamental solutions of Eq. (3.28):

$$Y(\tau) = \mathrm{e}^{-\tau}\tau^{m/2}\begin{cases} M(1+m+n, 1+m, \tau) \\ U(1+m+n, 1+m, \tau)\end{cases} \tag{3.31}$$

Note that as $z \to \infty$,

$$M(a,b,z) \sim \frac{\Gamma(b)}{\Gamma(a)}\mathrm{e}^z z^{a-b}, \quad U(a,b,z) \sim z^{-a}$$

In the present case, $a = 1 + m + n, b = 1 + m, a - b = n$. It is seen that the two basic solutions of $Y(\eta)$ have the following properties, respectively:

- $Y(\eta) = \mathrm{e}^{-\tau}\tau^{m/2}M\big(n + m + 1, 1 + m, \tau\big)$ vanishes or grows algebraically as $\eta \to \infty$;
- $Y(\eta) = \mathrm{e}^{-\tau}\tau^{m/2}U\big(n + m + 1, 1 + m, \tau\big)$ vanishes exponentially as $\eta \to \infty$.

From the boundary condition (3.6), one must choose

$$Y(\eta) = \mathrm{e}^{-\frac{\eta_0^2\eta^2}{2}}\frac{\eta_0^m\eta^m}{2^{m/2}}U\left(n + m + 1, 1 + m, \frac{\eta_0^2\eta^2}{2}\right) \tag{3.32}$$

Thus, the general solution for the temperature in the liquid region is obtained as:

$$T_1(\xi,\eta,\theta) = \frac{\eta_0^{2m}\xi^m\eta^m}{2^m}\sum_{n=0}^{\infty}\beta_n L_n\left(\frac{\eta_0^2\xi^2}{2}\right) \cdot\frac{\mathrm{e}^{-\frac{\eta_0^2\eta^2}{2}}U\left(n+m+1, 1+m, \frac{\eta_0^2\eta^2}{2}\right)}{\mathrm{e}^{-\frac{\eta_0^2}{2}}U\left(n + m + 1, 1 + m, \frac{\eta_0^2}{2}\right)}\cos m\theta \tag{3.33}$$

where the coefficients β_n are to be determined later.

3.4 The solution for the temperature field in solid phase

The solution for Eq. (3.5) can be derived similarly. Let

$$T_{\mathrm{S}1}(\xi,\eta,\theta) = X(\xi)Y(\eta)\cos m\theta \tag{3.34}$$

The solution for $X(\xi)$ is entirely the same as that obtained for the liquid phase, namely,

$$X(\sigma) = \sigma^{\frac{m}{2}}M(-n, 1 + m, \sigma) = a_0\xi^m L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right) \tag{3.35}$$

The function $Y(\eta)$ is also subject to Eq. (3.17). However, in the solid phase region, we let

$$\hat{\tau} = -\frac{\eta_0^2\eta^2}{2} \tag{3.36}$$

so that Eq. (3.17) is transformed into

$$\hat{\tau}Y''(\hat{\tau}) + (1 - \hat{\tau})Y'(\hat{\tau}) + \left(\frac{\lambda_1^2}{2} - \frac{m^2/4}{\hat{\tau}}\right)Y = 0 \tag{3.37}$$

The form of Eq. (3.37) is completely the same as Eq. (3.19). Hence, its solution, regular at $\hat{\tau} = \eta = 0$, can be found as:

$$Y(\hat{\tau}) = \hat{\tau}^{\frac{m}{2}}M(-n, 1 + m, \hat{\tau}) = b_0\eta^m L_n^{(m)}\left(\frac{-\eta_0^2\eta^2}{2}\right) \tag{3.38}$$

where $b_0 = \left(-\frac{\eta_0^2}{2}\right)^{\frac{m}{2}}\frac{n!\Gamma(m + 1)}{\Gamma(m + n + 1)}$. Thus, the general solution for the temperature in the solid phase is obtained as:

$$T_{\mathrm{S}1}(\xi,\eta,\theta) = \frac{\eta_0^{2m}\xi^m\eta^m}{2^m}\sum_{n=0}^{\infty}\alpha_n \cdot\frac{L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)L_n^{(m)}\left(-\frac{\eta_0^2\eta^2}{2}\right)}{L_n^{(m)}\left(-\frac{\eta_0^2}{2}\right)}\cos m\theta \tag{3.39}$$

where the coefficients α_n are to be determined later.

3.5 The solution of the interface shape function

We expand the interface shape function $\eta_1(\xi,\theta)$ in the following general Laguerre series:

$$\begin{aligned}\eta_1(\xi,\theta) &= \eta_1^{(\mathrm{iso})}(\xi) + \hat{\alpha}_m\eta_1^{(0)}(\xi) + \hat{\alpha}_m\eta_1^{(m)}(\xi,\theta)\\ &= \sum_{n=0}^{\infty}\gamma_n^{(\mathrm{iso})}L_n\left(\frac{\eta_0^2\xi^2}{2}\right) + \hat{\alpha}_m\sum_{n=0}^{\infty}\gamma_n^{(0)}L_n\left(\frac{\eta_0^2\xi^2}{2}\right)\\ &\quad+\hat{\alpha}_m\frac{\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}\gamma_n^{(m)}L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\cos m\theta\end{aligned} \tag{3.40}$$

Thus, the form of the solution derived above contains three sets of unknown constants: $\{\alpha_n, \beta_n, \gamma_n\}$ $(n = 0, 1, 2, \cdots)$, which can be determined by the three boundary conditions (3.9), (3.10) and (3.12).

Once the solution $\eta_1(\xi,\theta)$ is fully determined, one may determine the tip radius as well as the Peclet number with the effect of anisotropic surface tension. As a matter of fact, after linearization, Eq. (2.10) is reduced to

$$\begin{aligned}\mathcal{K}_3\{\eta_{\mathrm{s}}(\xi,\theta,\varepsilon)\} &= -\frac{2 + \xi^2}{(1 + \xi^2)^{\frac{3}{2}}} + \frac{\varepsilon^2}{(1 + \xi^2)^{\frac{1}{2}}}\\ &\quad\cdot\left[\frac{\xi^2(2 + \xi^2) + 4}{(1 + \xi^2)^2}\eta_1 + \frac{1 + 2\xi^2}{\xi(1 + \xi^2)}\eta_1'\right.\\ &\quad\left.+\eta_1'' + \frac{(1 + \xi^2)}{\xi^2}\eta_{1,\theta\theta}\right] + O(\varepsilon^4)\end{aligned} \tag{3.41}$$

Due to $\eta_1(0) = \eta'(0) = 0$, the twice of the mean curvature at the tip can be calculated as:

$$\mathcal{K}_3\{\eta_{\mathrm{s}}(0,\theta,\varepsilon)\} = -2 + 2\varepsilon^2\eta_1''(0,\theta) + O(\varepsilon^4)$$

By the definition of the Peclet number, we derive

$$\begin{aligned}\mathrm{Pe} &= \frac{\ell_{\mathrm{t}}}{\ell_{\mathrm{T}}} = \frac{2\eta_0^2}{-\mathcal{K}_3(0)} + O(\varepsilon^4)\\ &= \frac{\eta_0^2}{1 - \varepsilon^2\big[\eta_1^{(\mathrm{iso})''}(0) + \hat{\alpha}_4\eta_1^{(0)''}(0)\big]} + O(\varepsilon^4)\end{aligned} \tag{3.42}$$

It yields the dependence of the Peclet number of dendrite growth on the anisotropy of surface tension.

3.6 Determination of the unknown constants

By substituting the above obtained solutions (3.39) and (3.40) to the boundary conditions (3.9) and (3.10), one may derive the three sets of algebraic equations for the three sets of unknown constants. The details are given below.

3.6.1 Temperature continuity condition

From Eq. (3.9) it follows that

$$\beta_n = \alpha_n + \gamma_n \tag{3.43}$$

3.6.2 Gibbs-Thomson condition

From Eq. (3.10) it follows that

$$\frac{\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}\alpha_n^{(m)}L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\cos m\theta = -F_m(\xi)\cos m\theta \tag{3.44}$$

It is derived that

- for the component with $m=0$, we have

$$\sum_{n=0}^{\infty}\alpha_n^{(0)}L_n^{(0)}\left(\frac{\eta_0^2\xi^2}{2}\right) = -F_0(\xi) \tag{3.45}$$

- for the component with $m=4$, we have

$$\frac{\eta_0^8\xi^4}{2^4}\sum_{n=0}^{\infty}\alpha_n^{(4)}L_n^{(4)}\left(\frac{\eta_0^2\xi^2}{2}\right) = -F_4(\xi) \tag{3.46}$$

and

$$\sum_{n=0}^{\infty}\alpha_n^{(\text{iso})}L_n^{(0)}\left(\frac{\eta_0^2\xi^2}{2}\right) = -K_0(\xi) \tag{3.47}$$

Noting that the associated Laguerre polynomials $L_n^{(m)}(x)$ $(n=0,1,2,\cdots)$ form the weighted orthogonal set of functions:

$$\int_0^{\infty}x^m\mathrm{e}^{-x}L_n^{(m)}(x)L_k^{(m)}(x) = \begin{cases} 0, & n\neq k \\ \dfrac{(n+m)!}{n!}, & n=k\end{cases}$$

the coefficients α_n can be determined from the following integral:

$$\alpha_n^{(0)} = -\int_0^{\infty}\mathrm{e}^{-x}L_n^{(0)}(x)F_0(\sqrt{2x}/\eta_0)\mathrm{d}x, \quad m=0$$

$$\alpha_n^{(4)} = -\frac{\Gamma(n+1)}{\frac{\eta_0^4}{2^2}\Gamma(n+5)} \cdot\int_0^{\infty}\mathrm{e}^{-x}x^2L_n^{(4)}(x)F_4(\sqrt{2x}/\eta_0)\mathrm{d}x, \quad m=4 \tag{3.48, 3.49}$$

and

$$\alpha_n^{(\text{iso})} = -\int_0^{\infty}\mathrm{e}^{-x}L_n^{(0)}(x)K_0(\sqrt{2x}/\eta_0)\mathrm{d}x \tag{3.50}$$

3.6.3 Heat conservation condition

We now turn to apply the boundary condition (3.12). From Eqs. (3.39) and (3.33), one obtains

$$\begin{aligned}
&\frac{\partial T_{\text{S1}}}{\partial\eta}(\xi,1) \\
&= \frac{m\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\alpha_n^{(m)}\cos m\theta \\
&\quad+\frac{\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}(-\eta_0^2)L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right) \\
&\quad\cdot\frac{nL_n^{(m)}\left(\frac{-\eta_0^2}{2}\right)-(m+n)L_{n-1}^{(m)}\left(\frac{-\eta_0^2}{2}\right)}{-\frac{\eta_0^2}{2}L_n^{(m)}\left(\frac{-\eta_0^2}{2}\right)}\alpha_n^{(m)}\cos m\theta \\
&= \frac{\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}\left[m+2n-2(m+n)\frac{L_{n-1}^{(m)}\left(\frac{-\eta_0^2}{2}\right)}{L_n^{(m)}\left(\frac{-\eta_0^2}{2}\right)}\right] \\
&\quad\cdot L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\alpha_n^{(m)}\cos m\theta
\end{aligned} \tag{3.51}$$

and

$$\begin{aligned}
&\frac{\partial T_1}{\partial\eta}(\xi,1) \\
&= \frac{m\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}\beta_n^{(m)}L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\cos m\theta \\
&\quad+\frac{\eta_0^{2m}\xi^m}{2^m}\left\{\sum_{n=0}^{\infty}\beta_n^{(m)}L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\right. \\
&\quad\cdot\frac{-\eta_0^2\mathrm{e}^{-\frac{\eta_0^2}{2}}U\left(n+m+1,1+m,\frac{\eta_0^2}{2}\right)+2\mathrm{e}^{-\frac{\eta_0^2}{2}}}{U\left(n+m+1,1+m,\frac{\eta_0^2}{2}\right)\mathrm{e}^{-\frac{\eta_0^2}{2}}} \\
&\quad\cdot\left[(n+m+1)(1+n)U\left(n+m+2,1+m,\frac{\eta_0^2}{2}\right)\right. \\
&\quad\left.\left.-(n+m+1)U\left(n+m+1,1+m,\frac{\eta_0^2}{2}\right)\right]\right\}\cos m\theta \\
&= \frac{\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}\Bigg[m-2(m+n+1)-\eta_0^2
\end{aligned}$$

$$+2(n+m+1)(1+n)\frac{U\left(n+m+2,1+m,\frac{\eta_0^2}{2}\right)}{U\left(n+m+1,1+m,\frac{\eta_0^2}{2}\right)}\Bigg]$$
$$\cdot L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\beta_n^{(m)}\cos m\theta$$

In the above we have applied the formulas:

$$a(1+a-b)U(a+1,b,x)=aU(a,b,x)+xU'(a,b,x)$$
$$x(L_n^{(m)})'(x)=nL_n^{(m)}(x)-(m+n)L_{n-1}^{(m)}(x) \tag{3.52}$$

With the notations

$$\begin{cases} a_n=(m+2n)-2(n+m)\dfrac{L_{n-1}^{(m)}\left(\frac{-\eta_0^2}{2}\right)}{L_n^{(m)}\left(\frac{-\eta_0^2}{2}\right)} \\ b_n=-\eta_0^2-2n-m-2 \\ \qquad +2(n+m+1)(n+1)\dfrac{U\left(n+m+2,m+1,\frac{\eta_0^2}{2}\right)}{U\left(n+m+1,m+1,\frac{\eta_0^2}{2}\right)} \end{cases} \tag{3.53}$$

one may write

$$\frac{\partial T_1}{\partial\eta}(\xi,1)=\frac{\eta_0^{2m}\xi^m}{2^m}\left[\sum_{n=0}^{\infty}b_nL_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\right]\beta_n\cos m\theta$$
$$\frac{\partial T_{S1}}{\partial\eta}(\xi,1)=\frac{\eta_0^{2m}\xi^m}{2^m}\left[\sum_{n=0}^{\infty}a_nL_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\right]\alpha_n\cos m\theta \tag{3.54}$$

Thus, from the boundary condition (3.12), we derive

$$\sum_{n=0}^{\infty}b_nL_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\beta_n^{(m)}-\sum_{n=0}^{\infty}a_nL_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\alpha_n^{(m)}$$
$$+(2+\eta_0^2)\sum_{n=0}^{\infty}L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\gamma_n^{(m)}+\sum_{n=0}^{\infty}\Bigg\{mL_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)$$
$$+\left[2nL_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)-2(n+m)L_{n-1}^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\right]\Bigg\}\gamma_n^{(m)}$$
$$=0 \tag{3.55}$$

So that,

$$b_n\beta_n^{(m)}-a_n\alpha_n^{(m)}+(2+\eta_0^2+2n+m)\gamma_n^{(m)}$$
$$-2(n+m+1)\gamma_{n+1}^{(m)}=0,\quad n=0,1,2,3,\cdots \tag{3.56}$$

Combining Eqs. (3.43) and (3.56), we derive that

$$\gamma_{n+1}^{(m)}=g_n\gamma_n^{(m)}+f_n\alpha_n^{(m)},\quad n=0,1,2,\cdots \tag{3.57}$$

where

$$g_n=(n+1)\frac{U\left(n+m+2,m+1,\frac{\eta_0^2}{2}\right)}{U\left(n+m+1,m+1,\frac{\eta_0^2}{2}\right)} \tag{3.58}$$

$$f_n=g_n+\frac{m+n}{m+n+1}\frac{L_{n-1}^{(m)}\left(-\frac{\eta_0^2}{2}\right)}{L_n^{(m)}\left(-\frac{\eta_0^2}{2}\right)}$$
$$-2+\frac{m+1-\frac{\eta_0^2}{2}}{n+m+1} \tag{3.59}$$

Eq. (3.57) is a non-homogeneous difference equation for $\{\gamma_n^{(m)}\}$. For any given initial value $\gamma_0^{(m)}$, the formula (3.57) allows us to generate the sequence:

$$\{\gamma_0^{(m)},\gamma_1^{(m)},\gamma_2^{(m)},\cdots,\gamma_n^{(m)},\cdots\}$$

Thus, the function $\eta_1^{(m)}\left(\gamma_0^{(m)},\xi,\theta\right)$ can be written in the form:

$$\eta_1^{(m)}(\gamma_0^{(m)},\xi,\theta)$$
$$=\frac{\eta_0^{2m}\xi^m}{2^m}\sum_{n=0}^{\infty}\gamma_n^{(m)}L_n^{(m)}\left(\frac{\eta_0^2\xi^2}{2}\right)\cos m\theta \tag{3.60}$$

For the case $m=0$, one may apply the tip condition (3.13), namely

$$\eta_1^{(0)}(\gamma_0^{(0)},0)=\sum_{n=0}^{\infty}\gamma_n^{(0)}=0 \tag{3.61}$$

to determine $\gamma_0^{(0)}$. Once it is done, all the coefficients $\gamma_n^{(0)}(n=0,1,2,\cdots)$ are determined. However, for the case $m=4$, the tip conditions (3.14) are automatically satisfied by any constant $\gamma_0^{(4)}$. Hence, in order to determine the constant $\gamma_0^{(4)}$, one must use the far field condition for $\eta_1(\xi,\theta)$, that is $\eta_1(\xi,\theta)\to 0$, as $\xi\to\infty$.

4 Asymptotic behavior of the needle-like crystal solution as $\xi\to\infty$

The Laguerre polynomial expansion for $\eta_1(\xi,\theta)$ obtained above (3.40) and (3.60) is a convergent eigen-function enpension, valid in the whole interval ($0\leqslant\xi<\infty$). However, this expansion is an alternative series, and the numerical computation of this series at the point $\xi\gg 1$ cannot yield an accurate value of the sum function due to the numerical instability. In fact, the partial summation of the expansion with any large number of terms N, starts to rapidly oscillate when $\xi\gg 1$, as the partial sum becomes dominated by the past term $\gamma_NL_N^{(m)}(\xi^2/2)$ [see Fig. 2(a) and (b)]. In other words, the Laguerre

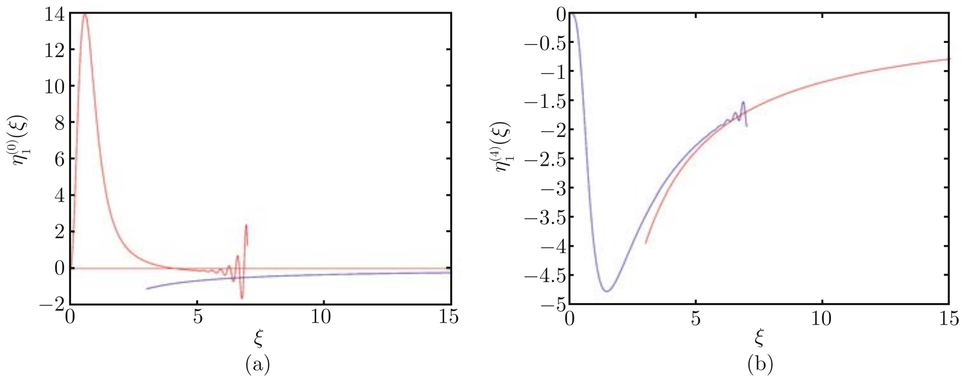

Fig. 2 The interface shape function for the case, $\frac{\eta_0^2}{2} = 0.5$: **(a)** $\eta_1^{(0)}(\xi)$ for $m = 0$; **(b)** $\eta_1^{(4)}(\xi)$ for $m = 4$.

polynomial expansion solution obtained above, numerically, is useful only in a finite region behind the tip ($0 \leqslant \xi \leqslant \xi_{\max}$). To obtain the accurate numerical value of the solution in the region $\xi \gg 1$, one needs to find a different asymptotic form of the solution. For this purpose, we make the following asymptotic expansion for the solution as $\xi \to \infty$:

$$T_1(\xi,\eta,\theta) = \left[\frac{B_1^{(m)}(\eta)}{\xi} + \frac{B_2^{(m)}(\eta)}{\xi^2} + \cdots\right]\cos m\theta$$

$$T_{S1}(\xi,\eta,\theta) = \left[\frac{A_1^{(m)}(\eta)}{\xi} + \frac{A_2^{(m)}(\eta)}{\xi^2} + \cdots\right]\cos m\theta$$

$$\eta_1(\xi,\eta,\theta) = \left[\frac{\hat{C}_1^{(m)}}{\xi} + \frac{\hat{C}_2^{(m)}}{\xi^2} + \cdots\right]\cos m\theta \tag{4.1}$$

By substituting Eq. (4.1) into Eqs. (3.4) and (3.5), one may derive each order approximation of the solution successively.

4.1 Zeroth order approximation $O(\xi^{-1})$

In the zeroth order approximation, we obtain the equations:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\eta^2} + \left(\frac{1}{\eta} + \eta_0^2\eta\right)\frac{\mathrm{d}}{\mathrm{d}\eta} - \left(-\eta_0^2 + \frac{m^2}{\eta^2}\right)\right]\begin{pmatrix} A_1^{(m)} \\ B_1^{(m)} \end{pmatrix} = 0 \tag{4.2}$$

$$X'' + \left(\frac{1}{\xi} - \eta_0^2\xi\right)X' + \left(\eta_0^2\lambda_1^2 - \frac{m^2}{\xi^2}\right)X = 0 \tag{4.3}$$

$$Y'' + \left(\frac{1}{\eta} + \eta_0^2\eta\right)Y' - \left(\eta_0^2\lambda_1^2 + \frac{m^2}{\eta^2}\right)Y = 0 \tag{4.4}$$

with the interface conditions: at $\eta = 1$,

(1)

$$B_1^{(m)}(1) = A_1^{(m)}(1) + \hat{C}_1^{(m)} \tag{4.5}$$

(2)

$$\frac{A_1^{(m)}(1)}{\xi} + \frac{A_2^{(m)}(1)}{\xi^2} + \cdots = -F_m(\xi) \tag{4.6}$$

where

$$F_0 = \frac{\frac{3}{4}\xi^6 + \frac{3}{2}\xi^4 + 21\xi^2 - 6}{(1+\xi^2)^{\frac{7}{2}}}, \quad F_4 = \frac{-\frac{15}{4}\xi^6 - \frac{15}{2}\xi^4}{(1+\xi^2)^{\frac{7}{2}}}$$

The values of $A_1^{(m)}(1)$ follow from the above, which are

$$A_1^{(4)}(1) = \frac{15}{4}, \quad A_1^{(0)}(1) = -\frac{3}{4}$$

(3)

$$\frac{\partial}{\partial\eta}(B_1^{(m)} - A_1^{(m)}) + (1+\eta_0^2)\hat{C}_1^{(m)} = 0 \tag{4.7}$$

Eq. (4.2) is of similar type as that for $Y(\eta)$ in Eq. (3.17). Letting

$$\tau = \frac{\eta_0^2\eta^2}{2} \quad \text{and} \quad F(\eta) = \frac{\mathrm{e}^{-\frac{\tau}{2}}}{\tau^{\frac{1}{2}}}Z(\tau)$$

where $F(\eta)$ represents both $A_1^{(m)}(\eta)$ and $B_1^{(m)}(\eta)$, then Eq. (4.2) is transformed to Eq. (3.30) with $\lambda_1^2 = -1$. Thus, we obtain the solutions

$$F(\eta) = \frac{\eta_0^m\eta^m}{2^{m/2}}\mathrm{e}^{-\frac{\eta_0^2\eta^2}{2}}\begin{cases} M\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\eta^2\right) \\ U\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\eta^2\right) \end{cases} \tag{4.8}$$

Taking into account the far field condition of the liquid phase region and the regular condition at the $\eta = 0$ in the solid phase region, we derive the solutions in the liquid region and solid region, respectively as follows:

$$A_1^{(m)}(\eta) = \hat{A}_1^{(m)}\frac{\eta_0^m\eta^m}{2^{m/2}}\mathrm{e}^{-\frac{\eta_0^2\eta^2}{2}}M\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\eta^2\right) \tag{4.9}$$

$$B_1^{(m)}(\eta) = \hat{B}_1^{(m)}\frac{\eta_0^m\eta^m}{2^{m/2}}\mathrm{e}^{-\frac{\eta_0^2\eta^2}{2}}U\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\eta^2\right) \tag{4.10}$$

where $\hat{A}_1^{(m)}$ and $\hat{B}_1^{(m)}$ are constants to be determined.

To determine the three sets of constants: $\{\hat{A}_1^{(m)}, \hat{B}_1^{(m)}, \hat{C}_1^{(m)}\}$, we apply the interface conditions (4.5)–(4.7). From Eq. (4.6), we obtain

$$\hat{A}_1^{(m)} = -\frac{e^{\frac{\eta_0^2}{2}} 2^{m/2}}{\eta_0^m M\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{\eta_0^2}{2}\right)} A_1^{(m)}(1) \tag{4.11}$$

From Eq. (4.5), we derive

$$\hat{B}_1^{(m)} P_2 = \hat{A}_1^{(m)} Q_2 + \hat{C}_1^{(m)} \tag{4.12}$$

where we have defined

$$\begin{cases} P_2 = \dfrac{\eta_0^m}{2^{m/2}} e^{-\frac{\eta_0^2}{2}} U\left(\dfrac{m}{2}+\dfrac{1}{2}, m+1, \dfrac{1}{2}\eta_0^2\right) \\ Q_2 = \dfrac{\eta_0^m}{2^{m/2}} e^{-\frac{\eta_0^2}{2}} M\left(\dfrac{m}{2}+\dfrac{1}{2}, m+1, \dfrac{1}{2}\eta_0^2\right) \end{cases} \tag{4.13}$$

From Eq. (4.7), we derive

$$\hat{B}_1^{(m)} P_1 - \hat{A}_1^{(m)} Q_1 + (1+\eta_0^2)\hat{C}_1^{(m)} = 0 \tag{4.14}$$

where we have defined

$$\begin{aligned} P_1 &= \frac{\eta_0^m e^{-\frac{\eta_0^2}{2}}}{2^{m/2}} \left[-U\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\right) \right. \\ &\quad \left. -2U\left(\frac{m}{2}-\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\right)\right] \\ Q_1 &= \frac{\eta_0^4 e^{-\frac{\eta_0^2}{2}}}{2^2} \left[-M\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\right) \right. \\ &\quad \left. +(m+1)M\left(\frac{m}{2}-\frac{1}{2}, m+1, \frac{1}{2}\eta_0^2\right)\right] \end{aligned} \tag{4.15}$$

In terms of formulas (4.11)–(4.14), and making some organizations, one may derive

$$\hat{C}_1^{(m)} = -\frac{2R+(m+1)S}{\eta_0^2 - 2R} \hat{A}_1^{(m)}(1) \tag{4.16}$$

where the following notations are used:

$$R = \frac{U\left(\frac{m}{2}-\frac{1}{2}, m+1, \frac{\eta_0^2}{2}\right)}{U\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{\eta_0^2}{2}\right)}$$

$$S = \frac{M\left(\frac{m}{2}-\frac{1}{2}, m+1, \frac{\eta_0^2}{2}\right)}{M\left(\frac{m}{2}+\frac{1}{2}, m+1, \frac{\eta_0^2}{2}\right)}$$

The constants $\hat{B}_1^{(m)}$ then follow from Eq. (4.14). Up to this point, the asymptotic solution in the far field is fully determined.

5 Matching the condition of the RPE with the far field asymptotic solution

Since the asymptotic solution (4.1) is applicable in the far field as $\xi \to \infty$, it can thus yield the accurate numerical value of solution $\eta_1(\xi_{\max}, \theta)$ at $\xi = \xi_{\max} \gg 1$. On the other hand, as it has been demonstrated, the Laguerre expansion solution can be applied in the region $(0 \leqslant \xi \leqslant \xi_{\max})$ with good accuracy, provided $\xi_{\max}$ is not too large. Thus, in order to determine the parameter $\gamma_0^{(m)}$, we may let the Laguerre expansion solution shoot the value of the asymptotic solution (4.1) at $\xi = \xi_{\max}$. In other words, we may choose the value of $\gamma_0^{(m)}$ properly, so that the Laguerre expansion solution can meet the far field asymptotic solution at the intermediate point $\xi = \xi_{\max}$. This procedure is shown in Fig. 2 (a) and (b) for a typical case of $m = 0$ and $m = 4$, respectively. The shape of a typical needle's interface for the case $\eta_0^2/2 = 0.5, \hat{\alpha}_4 = 0.5, \varepsilon = 0.15$ is shown in Fig. 3.

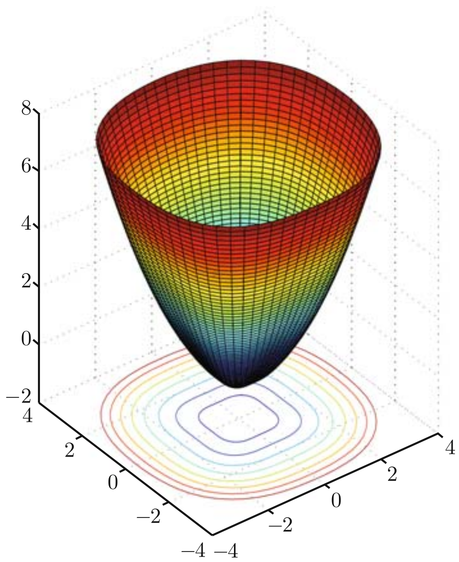

Fig. 3 The shape of 3-D dendrite's tip with $\frac{\eta_0^2}{2} = 0.5$, $\hat{\alpha}_4 = 0.5$, $\varepsilon = 0.15$.

6 Numerical results

We have computed the solutions with various parameters of ε, η_0^2 and $\hat{\alpha}_4$. Our numerical results for the isotropic case $\hat{\alpha}_4 = 0$ recovered the results previously obtained by Xu and Yu [14]. Our numerical results are summarized as follows.

6.1 Variation of Peclet number with the parameters ε and $\hat{\alpha}_4$

The Peclet number of needle crystal growth can be calculated with the formula (3.42). The numerical values of Pe for the case with various parameters ε and $\hat{\alpha}_4$ are shown in Table 1. The numerical values of $\eta_1''(0)$ and $\mathcal{K}_3(0)$ at the tip are computed through the paraboloid-like tip that best fits the solution for the shape of the interface obtained by using the method of least square approximation.

The variations of relative Peclet number $\widehat{\mathrm{Pe}} = \mathrm{Pe}/\mathrm{Pe}_0$ with anisotropy parameter $\hat{\alpha}_4$ for the typical case $\eta_0^2/2 = 0.5$ and $\varepsilon = 0, 0.1, 0.12, 0.15, 0.2, 0.3, 0.4$ are shown in Fig. 4 (a) and (d). Here Pe_0 is the Peclet number for the case of $\varepsilon = 0$. It is seen that the results that we obtained for the case of $\hat{\alpha}_4 = 0$ are consistent with those previously obtained by Xu and Yu [14], that is, the Peclet number decreases as ε increases. However, if $\hat{\alpha}_4$ is not small, the Peclet number increases as ε increases. Particularly, when $\hat{\alpha}_4 \approx 0.2$, as ε increases from 0.2 to 0.4, the relative Peclet number $\widehat{\mathrm{Pe}}$ increases very rapidly.

The variations of the Peclet number Pe with T_∞ for the cases of anisotropic parameters $\hat{\alpha}_4 = -0.5, -0.2, -0.1, 0.1, 0.2, 0.5$ are shown in Fig. 5. It is seen again that the anisotropy parameter $\hat{\alpha}_4$ may significantly affect the Peclet number, especially in the large undercooling regime. When the $\hat{\alpha}_4$ number is negative or positive but small, the Peclet number decreases with increasing ε. However, when the $\hat{\alpha}_4$ number is larger than a certain positive value $\alpha_c \approx 0.2$, the Peclet number will increase as ε increases.

Table 1 The variation of the Peclet number with the parameters ε and $\hat{\alpha}_4$ for the case $\eta_0^2/2 = 0.5$, or $T_\infty = -0.4615$.

$\hat{\alpha}_4$	ε	$\mathcal{K}_3(0)$	Pe
0.5000E+000	0.0000E+000	0.1000E+001	0.1000E+001
0.5000E+000	0.1000E+000	0.7236E+000	0.1382E+001
0.5000E+000	0.1200E+000	0.6124E+000	0.1633E+001
0.5000E+000	0.1500E+000	0.4226E+000	0.2366E+001
0.2000E+000	0.0000E+000	0.1000E+001	0.1000E+001
0.2000E+000	0.1000E+000	0.9854E+000	0.1015E+001
0.2000E+000	0.1200E+000	0.9790E+000	0.1022E+001
0.2000E+000	0.1500E+000	0.9670E+000	0.1034E+001
0.1000E+000	0.0000E+000	0.1000E+001	0.1000E+001
0.1000E+000	0.1000E+000	0.1080E+001	0.9260E+000
0.1000E+000	0.1200E+000	0.1116E+001	0.8960E+000
0.1000E+000	0.1500E+000	0.1184E+001	0.8447E+000
−0.1000E+000	0.0000E+000	0.1000E+001	0.1000E+001
−0.1000E+000	0.1000E+000	0.1281E+001	0.7804E+000
−0.1000E+000	0.1200E+000	0.1416E+001	0.7060E+000
−0.1000E+000	0.1500E+000	0.1685E+001	0.5934E+000
−0.2000E+000	0.0000E+000	0.1000E+001	0.1000E+001
−0.2000E+000	0.1000E+000	0.1389E+001	0.7201E+000
−0.2000E+000	0.1200E+000	0.1581E+001	0.6324E+000
−0.2000E+000	0.1500E+000	0.1976E+001	0.5060E+000
−0.5000E+000	0.0000E+000	0.1000E+001	0.1000E+001
−0.5000E+000	0.1000E+000	0.1740E+001	0.5746E+000
−0.5000E+000	0.1200E+000	0.2146E+001	0.4662E+000
−0.5000E+000	0.1500E+000	0.3064E+001	0.3265E+000

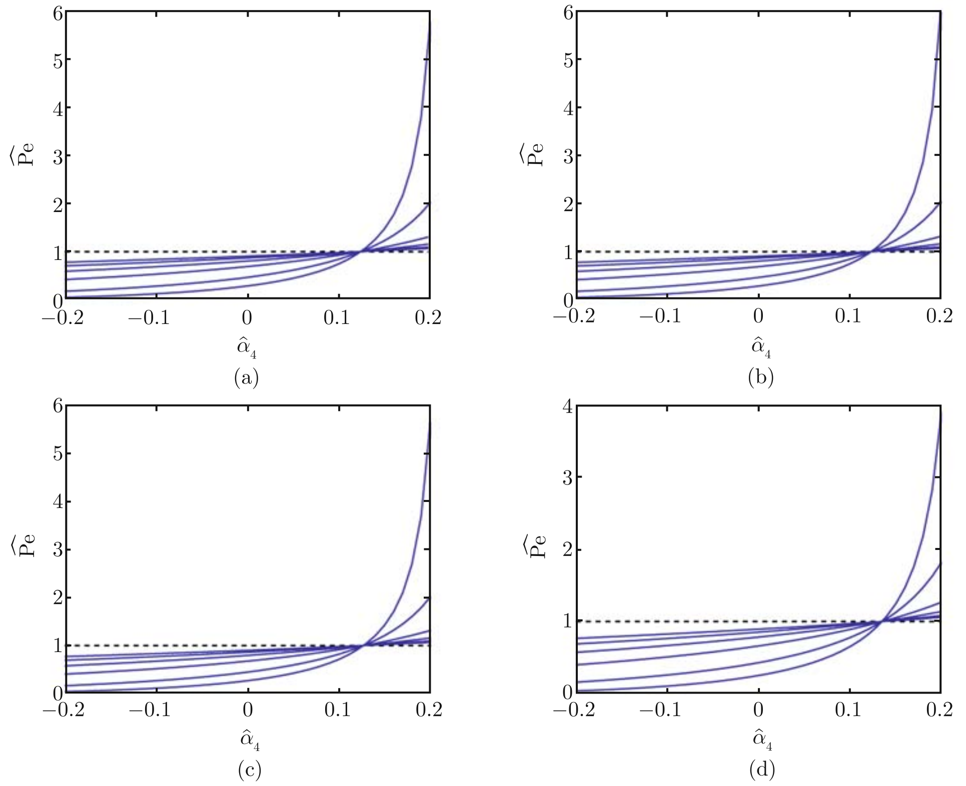

Fig. 4 The variation of relative Peclet number $\widehat{\mathrm{Pe}} = \mathrm{Pe}/\mathrm{Pe}_0$ with $\hat{\alpha}_4$ and $\varepsilon = 0, 0.1, 0.12, 0.15, 0.2, 0.3, 0.4$, from bottom to top on the left side for the cases: **(a)** $\eta_0^2/2 = 0.005$; **(b)** $\eta_0^2/2 = 0.01$; **(c)** $\eta_0^2/2 = 0.05$; **(d)** $\eta_0^2/2 = 0.1$.

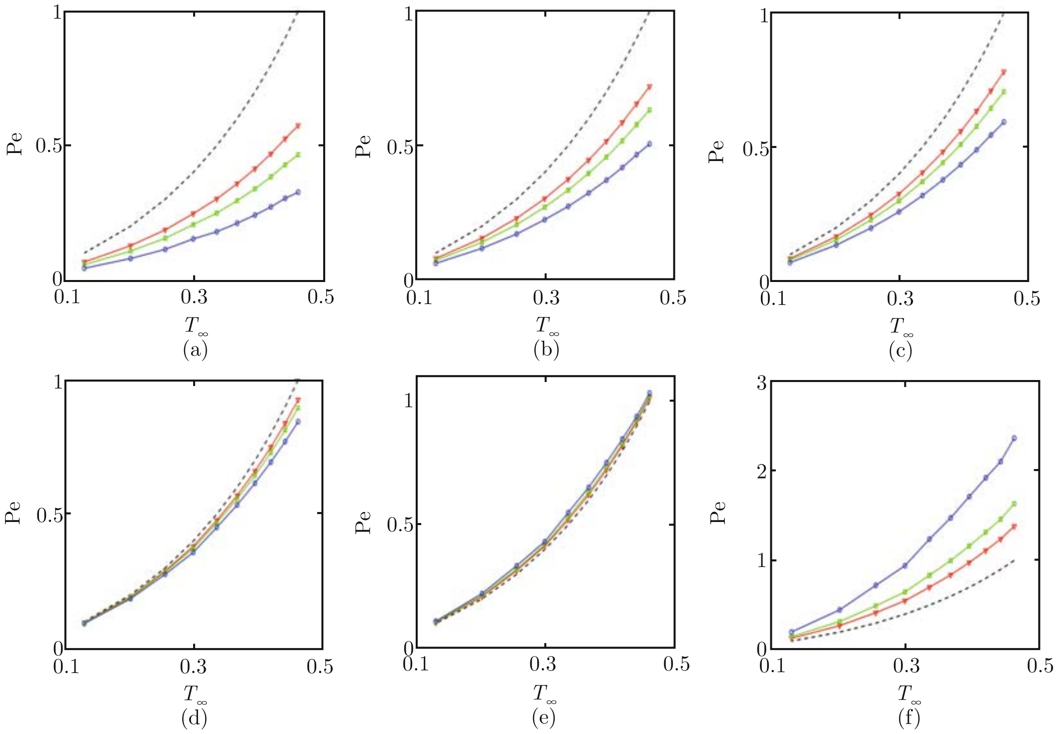

Fig. 5 The variation of Peclet number with T_∞ for the cases of anisotropic surface tension with $\varepsilon = 0$ (*dashed line*), $\varepsilon = 0.1$ (*red line*), $\varepsilon = 0.12$ (*green line*), $\varepsilon = 0.15$ (*blue line*) and **(a)** $\hat{\alpha}_4 = -0.5$; **(b)** $\hat{\alpha}_4 = -0.2$; **(c)** $\hat{\alpha}_4 = -0.1$; **(d)** $\hat{\alpha}_4 = 0.1$; **(e)** $\hat{\alpha}_4 = 0.2$; **(f)** $\hat{\alpha}_4 = 0.5$.

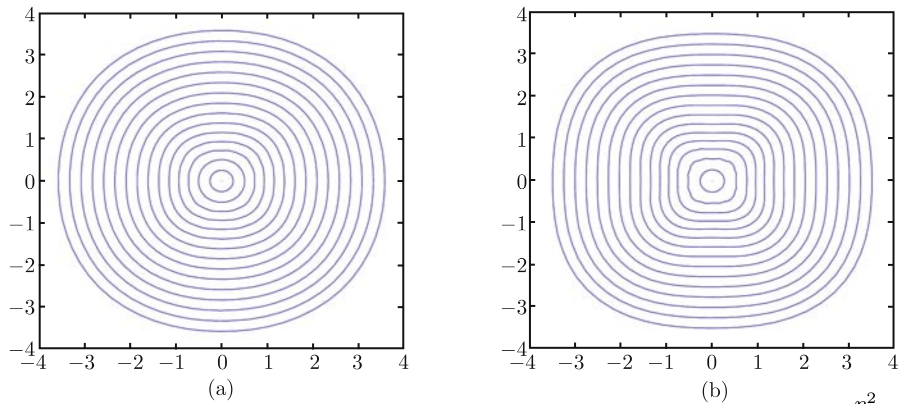

Fig. 6 The contours of needle crystal on (x, y) plane with different coordinates z for the cases of $\frac{\eta_0^2}{2} = 0.5$, $\varepsilon = 0.15$ and **(a)** $\hat{\alpha}_4 = 0.2$; **(b)** $\hat{\alpha}_4 = 0.5$.

6.2 Shape of the cross-section of the needle crystal in (x, y)-plane

The contours of the needle crystal on the (x, y)-plane for the cases $\varepsilon = 0.15, \hat{\alpha}_4 = 0.2, 0.5$ are shown in Fig. 6 (a) and (b), respectively. It is seen that the fourth fold symmetric feature of the interface morphology generated by the anisotropic surface tension in steady state of needle crystal growth can be most clearly seen over a certain region of needle interfaces behind the tip. However, such a feature can only be weakly seen in the region far away from the dendrite's tip. This fact is also consistent with the Gibb-Thomson condition (3.10), which shows that as $\xi \gg 1$, the interface temperature $T_{S1} = \mathcal{O}(1/\xi)$. It can also be seen from the asymptotic expansion form of the solution in the far field (4.1), which shows that as $\xi \gg 1$, the interface shape $\eta_1 = \mathcal{O}(1/\xi)$. The result implies that the correction to Ivantsov's solution induced by the anisotropic surface tension is rather weak in the root region far away from the needle's tip.

7 Discussion and conclusions

In the present paper, we considered the steady needle-like crystal growth with full 3-D anisotropic surface tension with m-th fold symmetry. The uniformly valid asymptotic form of the solution is obtained in terms of the general Laguerre function expansion in the finite region around the tip of needle crystal, which matches with the asymptotic expansion solution in the far field behind the tip. On the basis of the solution, we derive the effect of the anisotropy parameter on the Peclet number Pe and the interface's morphology. The results show that two components of the variation of the interface morphology of the needle crystal are generated due to the presence of the 3-D anisotropy of surface tension: the axi-symmetric component and 4-th fold symmetric component. The numerical computations for the case of $m = 4$ show that a fourth fold symmetric feature of the interface morphology can be most clearly seen over a certain section of the needle interface behind the tip; such feature, however, is rather weak and faint as $\xi \gg 1$ in the far field. One of the most important results derived in this work is that the 3-D anisotropy of surface tension may significantly affect the Peclet number Pe. For example, our numerical calculations for the case of $\eta_0^2/2 = 0.005, \varepsilon = 0.12 - 0.15$ show that, with a small value of anisotropy parameter $\hat{\alpha}_4 = 0.005$, we have the relative Peclet number $\widehat{\mathrm{Pe}} \approx 1$. However, when the anisotropy parameter increases to the value $\hat{\alpha}_4 \approx 0.2$, and $\varepsilon = 0.3 - 0.4$, one has $\widehat{\mathrm{Pe}} = 2 - 6$.

The present paper does not attempt to carry out a stability analysis for the needle solution obtained. The detailed analysis and discussions for the selection and determination of the tip-velocity U_{tip} will be given in future papers.

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Appendix: Gibbs-Thomson condition at the interface with anisotropic surface tension

1 The geometric properties of the interface of needle crystal

We attempt to derive the temperature T_{S} at the interface of needle-like crystal. For the first order approximation, we may assume that the needle shape is the Ivantsov paraboloid, namely, $\eta_{\mathrm{s}} \equiv 1$. Thus, the shape equation can be written in the following parameterized form in the Cartesian coordinate system:

$$\begin{aligned}\boldsymbol{r} &= \boldsymbol{x}(\xi, \theta)\\ &= \eta_0^2\left[\xi\cos\theta\boldsymbol{i} + \xi\sin\theta\boldsymbol{j} + \frac{1}{2}(\xi^2 - 1)\boldsymbol{k}\right]\end{aligned} \tag{A-1}$$

The tangent vectors along the curves ξ = const. and η = const. on the interface can be respectively expressed as:

$$\boldsymbol{x}_\xi = \eta_0^2(\cos\theta\boldsymbol{i} + \sin\theta\boldsymbol{j} + \xi\boldsymbol{k}) \tag{A-2}$$

$$\boldsymbol{x}_\theta = \eta_0^2(-\xi\sin\theta\boldsymbol{i} + \xi\cos\theta\boldsymbol{j}) \tag{A-3}$$

which are orthogonal, namely $\boldsymbol{x}_\xi \cdot \boldsymbol{x}_\theta = 0$. It can be written that along any curve on the interface, $\mathrm{d}\boldsymbol{x} = \boldsymbol{x}_\xi\mathrm{d}\xi + \boldsymbol{x}_\theta\mathrm{d}\theta$ and

$$\begin{aligned}\mathrm{d}s^2 &= \mathrm{d}\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{x} = \eta_0^4(1+\xi^2)\mathrm{d}\xi^2 + \eta_0^4\xi^2\mathrm{d}\theta\\ &= h_\xi^2\mathrm{d}\xi^2 + h_\theta^2\mathrm{d}\theta^2\end{aligned} \tag{A-4}$$

where we introduce the scale factors

$$h_\xi = \eta_0^2\sqrt{1+\xi^2}, \quad h_\theta = \eta_0^2\xi \tag{A-5}$$

The unit vector along the curves ξ = const. and η = const. on the interface are then

$$\boldsymbol{e}_\xi = \frac{1}{h_\xi^2}\boldsymbol{x}_\xi, \quad \boldsymbol{e}_\theta = \frac{1}{h_\theta^2}\boldsymbol{x}_\theta \tag{A-6}$$

On the other hand, as the cross product of $\boldsymbol{x}_\xi$ and $\boldsymbol{x}_\theta$ is

$$\boldsymbol{x}_\xi \times \boldsymbol{x}_\theta = \eta_0^4(-\xi^2\cos\theta\ \boldsymbol{i} - \xi^2\sin\theta\ \boldsymbol{j} + \xi\boldsymbol{k}) \tag{A-7}$$

and

$$|\boldsymbol{x}_\xi \times \boldsymbol{x}_\theta| = \eta_0^4\xi(1+\xi^2)^{\frac{1}{2}} = h_\xi h_\theta \tag{A-8}$$

one may write the outward unit normal to the paraboloid needle interface as:

$$\boldsymbol{n} = \boldsymbol{e}_\eta = -\frac{\boldsymbol{x}_\xi \times \boldsymbol{x}_\theta}{|\boldsymbol{x}_\xi \times \boldsymbol{x}_\theta|} = \frac{\xi\cos\theta\ \boldsymbol{i} + \xi\sin\theta\boldsymbol{j} - \boldsymbol{k}}{(1+\xi^2)^{\frac{1}{2}}} \tag{A-9}$$

The derivatives of $\boldsymbol{n}$ with respect to ξ and η are

$$\boldsymbol{n}_\xi = \frac{\cos\theta\ \boldsymbol{i} + \sin\theta\boldsymbol{j} + \xi\boldsymbol{k}}{(1+\xi^2)^{\frac{3}{2}}} \tag{A-10}$$

$$\boldsymbol{n}_\theta = \frac{-\xi\sin\theta\ \boldsymbol{i} + \xi\cos\theta\boldsymbol{j}}{(1+\xi^2)^{\frac{1}{2}}} \tag{A-11}$$

respectively.

On the other hand, with the angle ϕ between $\boldsymbol{k}$ and $\boldsymbol{n}$, one may write

$$\cos\phi = \boldsymbol{n}\cdot\boldsymbol{k} = \frac{-1}{(1+\xi^2)^{\frac{1}{2}}} \tag{A-12}$$

and accordingly,

$$\sin\phi = \frac{\xi}{(1+\xi^2)^{\frac{1}{2}}} \quad \text{and} \quad \tan\phi = -\xi \tag{A-13}$$

Thus, one may re-write $\boldsymbol{n}$ as follows:

$$\boldsymbol{n} = \sin\phi\cos\theta\ \boldsymbol{i} + \sin\phi\sin\theta\ \boldsymbol{j} + \cos\phi\ \boldsymbol{k} \tag{A-14}$$

From (A-15),

$$\begin{aligned}\boldsymbol{r} &= \boldsymbol{r}(\xi,\theta)\\ &= \eta_0^2\left[\xi\cos\theta\boldsymbol{i}+\xi\sin\theta\boldsymbol{j}+\frac{1}{2}(\xi^2-1)\boldsymbol{k}\right]\end{aligned} \tag{A-15}$$

It may be computed that

$$\begin{aligned}\boldsymbol{x}_{\xi\xi} &= \eta_0^2\boldsymbol{k}\\ \boldsymbol{x}_{\xi\theta} &= \eta_0^2(-\sin\theta\boldsymbol{i}+\cos\theta\boldsymbol{j})\\ \boldsymbol{x}_{\theta\theta} &= \eta_0^2(-\xi\cos\theta\boldsymbol{i}-\xi\sin\theta\boldsymbol{j})\end{aligned} \tag{A-16}$$

which yield the factors

$$\begin{aligned}L &= \boldsymbol{n}\cdot\boldsymbol{r}_{\xi\xi} = -\frac{\eta_0^2}{(1+\xi^2)^{\frac{1}{2}}}\\ M &= \boldsymbol{n}\cdot\boldsymbol{r}_{\xi\theta} = 0\\ N &= \boldsymbol{n}\cdot\boldsymbol{r}_{\theta\theta} = -\frac{\eta_0^2\xi^2}{(1+\xi^2)^{\frac{1}{2}}}\end{aligned} \tag{A-17}$$

The relations $\boldsymbol{x}_\xi\cdot\boldsymbol{x}_\theta = 0$ and $M = 0$ imply that the ξ and θ coordinates are the principal directions. The associated principal curvatures are given by

$$\begin{aligned}\mathcal{K}_\xi &= \frac{L}{h_\xi^2} = -\frac{1}{\eta_0^2(1+\xi^2)^{\frac{3}{2}}}\\ \mathcal{K}_\theta &= \frac{N}{h_\theta^2} = -\frac{1}{\eta_0^2(1+\xi^2)^{\frac{1}{2}}}\end{aligned} \tag{A-18}$$

We shall express the orientation of vector in terms of the spherical angles Φ and Θ. In this way, for the unit normal vector $\boldsymbol{n}$ we have

$$\begin{aligned}\tan\Theta &= \frac{\boldsymbol{n}_y}{\boldsymbol{n}_x} = \tan\theta\\ \tan\Phi &= \frac{\sqrt{\boldsymbol{n}_x^2+\boldsymbol{n}_y^2}}{\boldsymbol{n}_z} = \tan\phi = -\xi\end{aligned} \tag{A-19}$$

It implies that for the normal vector $\boldsymbol{n} = \boldsymbol{e}_\eta$, we have $\Phi = \phi$ and $\Theta = \theta$. This is evident. It is noted that $(\boldsymbol{e}_\xi, \boldsymbol{e}_\theta, -\boldsymbol{n})$ constitute a right-handed orthonormal system as the basis vectors, and the relations

$$\boldsymbol{n}_\xi = \frac{\eta_0^4}{h_\xi^2}\boldsymbol{e}_\xi, \quad \boldsymbol{n}_\theta = \frac{h_\theta}{h_\xi}\boldsymbol{e}_\theta \tag{A-20}$$

and

$$\boldsymbol{e}_\xi\cdot\boldsymbol{n}_\xi = \frac{\eta_0^4}{h_\xi^2}, \quad \boldsymbol{e}_\xi\cdot\boldsymbol{n}_\theta = \boldsymbol{e}_\theta\cdot\boldsymbol{n}_\phi = 0, \quad \boldsymbol{e}_\theta\cdot\boldsymbol{n}_\theta = \frac{h_\theta}{h_\xi} \tag{A-21}$$

hold.

2 The properties of perturbed surfaces

We now consider the surfaces (S) near the paraboloid needle interface determined by the equation:

$$\boldsymbol{X}(\xi,\theta) = \boldsymbol{x}(\xi,\theta)+\varepsilon f(\xi,\theta)\boldsymbol{n}(\xi,\theta) \tag{A-22}$$

where $f(\xi,\theta)$ is a given arbitrary function and $\varepsilon \ll 1$ is a parameter. Then the tangent vector along the curve ξ = const. and η = const. on the surface (S), can be respectively determined as:

$$\begin{aligned}\boldsymbol{X}_\xi &= \boldsymbol{x}_\xi+\varepsilon f_\xi\boldsymbol{n}+\varepsilon f\boldsymbol{n}_\xi\\ \boldsymbol{X}_\theta &= \boldsymbol{x}_\theta+\varepsilon f_\theta\boldsymbol{n}+\varepsilon f\boldsymbol{n}_\theta\end{aligned} \tag{A-23}$$

The normal vector of the surface (S) is determined by the formula:

$$\begin{aligned}\boldsymbol{X}_\xi\times\boldsymbol{X}_\theta &= \boldsymbol{x}_\xi\times\boldsymbol{x}_\theta+\varepsilon[\boldsymbol{x}_\xi\times(f_\theta\boldsymbol{n}+f\boldsymbol{n}_\theta)\\ &\quad +(f_\xi\boldsymbol{n}+f\boldsymbol{n}_\xi)\times\boldsymbol{x}_\theta]+O(\varepsilon^2)\\ &= -h_\xi h_\theta\boldsymbol{n}+\varepsilon\left[h_\xi\boldsymbol{e}_\xi\times\left(f_\theta\boldsymbol{n}+f\frac{h_\theta}{h_\xi}\boldsymbol{e}_\theta\right)\right.\\ &\quad \left.+\left(f_\xi\boldsymbol{n}+f\frac{\eta_0^4}{h_\xi^2}\boldsymbol{e}_\xi\right)\times(h_\theta\boldsymbol{e}_\theta)\right]+O(\varepsilon^2)\\ &= -h_\xi h_\theta\boldsymbol{n}+\varepsilon\left[h_\xi f_\theta\boldsymbol{e}_\theta-fh_\theta\boldsymbol{n}\right.\\ &\quad \left.+f_\xi h_\theta\boldsymbol{e}_\xi-f\frac{\eta_0^4}{h_\xi^2}h_\theta\boldsymbol{n}\right]+O(\varepsilon^2)\\ &= -h_\xi h_\theta\left\{\left[1+\varepsilon\left(\frac{1}{h_\xi}+\frac{\eta_0^4}{h_\xi^3}\right)\right]\boldsymbol{n}\right.\\ &\quad \left.-\frac{\varepsilon f_\theta}{h_\theta}\boldsymbol{e}_\theta-\frac{\varepsilon f_\xi}{h_\xi}\boldsymbol{e}_\xi\right\}+O(\varepsilon^2)\end{aligned} \tag{A-24}$$

One may write

$$\begin{aligned}\boldsymbol{X}_\xi\times\boldsymbol{X}_\theta &= -h_\xi h_\theta\left[(1+\varepsilon f\mathcal{H})\boldsymbol{n}\right.\\ &\quad \left.-\frac{\varepsilon f_\theta}{h_\theta}\boldsymbol{e}_\theta-\frac{\varepsilon f_\xi}{h_\xi}\boldsymbol{e}_\xi\right]+O(\varepsilon^2)\end{aligned} \tag{A-25}$$

where the mean curvature

$$\mathcal{H} = \mathcal{K}_\theta+\mathcal{K}_\xi \tag{A-26}$$

is introduced, and as previously defined,

$$\mathcal{K}_\theta = -\frac{1}{h_\xi}, \quad \mathcal{K}_\xi = -\frac{\eta_0^4}{h_\xi^3} \tag{A-27}$$

The magnitude of the above normal is

$$\begin{aligned}|\boldsymbol{X}_\xi\times\boldsymbol{X}_\theta|^2 &= h_\xi^2h_\theta^2+2\varepsilon h_\xi h_\theta f\left[h_\theta+\frac{\eta_0^4}{h_\xi^2}h_\theta\right]+O(\varepsilon^2)\\ |\boldsymbol{X}_\xi\times\boldsymbol{X}_\theta| &= h_\xi h_\theta\left[1+\varepsilon\frac{f}{h_\xi h_\theta}\left(h_\theta+\frac{\eta_0^4}{h_\xi^2}h_\theta\right)\right]+O(\varepsilon^2)\\ &= h_\xi h_\theta[1-\varepsilon f(\mathcal{K}_\theta+\mathcal{K}_\xi)]+O(\varepsilon^2)\end{aligned} \tag{A-28}$$

So that, the unit normal can be written as

$$\begin{aligned}\boldsymbol{N} &= -\frac{\boldsymbol{X}_\xi \times \boldsymbol{X}_\theta}{|\boldsymbol{X}_\xi \times \boldsymbol{X}_\theta|}\\ &= -\frac{-h_\xi h_\theta\left[(1+\varepsilon f\mathcal{H})\boldsymbol{n}-\frac{\varepsilon f_\theta}{h_\theta}\boldsymbol{e}_\theta-\frac{\varepsilon f_\xi}{h_\xi}\boldsymbol{e}_\xi\right]+O(\varepsilon^2)}{h_\xi h_\theta(1+\varepsilon f\mathcal{H})+O(\varepsilon^2)}\\ &= \left[(1+\varepsilon f\mathcal{H})\boldsymbol{n}-\frac{\varepsilon f_\theta}{h_\theta}\boldsymbol{e}_\theta-\frac{\varepsilon f_\xi}{h_\xi}\boldsymbol{e}_\xi\right]\\ &\quad \cdot(1-\varepsilon f\mathcal{H})+O(\varepsilon^2)\\ &= \boldsymbol{n}-\frac{\varepsilon f_\theta}{h_\theta}\boldsymbol{e}_\theta-\frac{\varepsilon f_\xi}{h_\xi}\boldsymbol{e}_\xi+O(\varepsilon^2) \qquad \text{(A-29)}\end{aligned}$$

The components of the normal vector $\boldsymbol{N}$ along the directions $(\boldsymbol{i},\boldsymbol{j},\boldsymbol{k})$ are

$$\begin{aligned}\boldsymbol{N}_x &= \frac{\xi\cos\theta}{\sqrt{1+\xi^2}}+\frac{\varepsilon f_\theta}{h_\theta}\sin\theta-\frac{\varepsilon f_\xi}{h_\xi}\frac{\cos\theta}{\sqrt{1+\xi^2}}+O(\varepsilon^2)\\ &= \frac{\xi\cos\theta}{\sqrt{1+\xi^2}}\left(1+\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}\tan\theta-\frac{\varepsilon f_\xi}{\xi h_\xi}\right)+O(\varepsilon^2)\\ \boldsymbol{N}_y &= \frac{\xi\sin\theta}{\sqrt{1+\xi^2}}-\frac{\varepsilon f_\theta}{h_\theta}\cos\theta-\frac{\varepsilon f_\xi}{h_\xi}\frac{\sin\theta}{\sqrt{1+\xi^2}}+O(\varepsilon^2)\\ &= \frac{\xi\sin\theta}{\sqrt{1+\xi^2}}\left(1-\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}\cot\theta-\frac{\varepsilon f_\xi}{\xi h_\xi}\right)+O(\varepsilon^2)\\ \boldsymbol{N}_z &= \frac{-1}{\sqrt{1+\xi^2}}-\frac{\varepsilon f_\xi}{h_\xi}\frac{\xi}{\sqrt{1+\xi^2}}+O(\varepsilon^2)\\ &= \frac{-1}{\sqrt{1+\xi^2}}\left(1+\frac{\varepsilon\xi f_\xi}{h_\xi}\right)+O(\varepsilon^2) \qquad \text{(A-30)}\end{aligned}$$

respectively. Thus, we have

$$\begin{aligned}\boldsymbol{N}_x^2 &= \frac{\xi^2\cos^2\theta}{1+\xi^2}+2\frac{\xi\cos\theta}{\sqrt{1+\xi^2}}\frac{\varepsilon f_\theta}{h_\theta}\sin\theta\\ &\quad -2\frac{\xi\cos\theta}{\sqrt{1+\xi^2}}\frac{\varepsilon f_\xi}{h_\xi}\frac{\cos\theta}{\sqrt{1+\xi^2}}+O(\varepsilon^2)\\ &= \frac{\xi^2\cos^2\theta}{1+\xi^2}+2\frac{\xi\cos\theta\sin\theta}{\sqrt{1+\xi^2}}\frac{\varepsilon f_\theta}{h_\theta}\\ &\quad -2\frac{\xi\cos^2\theta}{1+\xi^2}\frac{\varepsilon f_\xi}{h_\xi}+O(\varepsilon^2)\\ \boldsymbol{N}_y^2 &= \frac{\xi^2\sin^2\theta}{1+\xi^2}-2\frac{\xi\sin\theta}{\sqrt{1+\xi^2}}\frac{\varepsilon f_\theta}{h_\theta}\cos\theta\\ &\quad -2\frac{\xi\sin\theta}{\sqrt{1+\xi^2}}\frac{\varepsilon f_\xi}{h_\xi}\frac{\sin\theta}{\sqrt{1+\xi^2}}+O(\varepsilon^2)\\ &= \frac{\xi^2\sin^2\theta}{1+\xi^2}-2\frac{\xi\cos\theta\sin\theta}{\sqrt{1+\xi^2}}\frac{\varepsilon f_\theta}{h_\theta}\\ &\quad -2\frac{\xi\sin^2\theta}{1+\xi^2}\frac{\varepsilon f_\xi}{h_\xi}+O(\varepsilon^2)\end{aligned} \qquad \text{(A-31)}$$

$$\boldsymbol{N}_x^2+\boldsymbol{N}_y^2 = \frac{\xi^2}{1+\xi^2}-2\frac{\xi}{1+\xi^2}\frac{\varepsilon f_\xi}{h_\xi}+O(\varepsilon^2) \qquad \text{(A-32)}$$

$$\sqrt{\boldsymbol{N}_x^2+\boldsymbol{N}_y^2} = \frac{\xi}{\sqrt{1+\xi^2}}\left(1-\frac{1}{\xi}\frac{\varepsilon f_\xi}{h_\xi}\right)+O(\varepsilon^2) \qquad \text{(A-33)}$$

3 Orientation angles

To determine the orientation of the normal of the surface, we calculate

$$\begin{aligned}\frac{\boldsymbol{N}_y}{\boldsymbol{N}_x} &= \tan\theta\left(1-\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}\cot\theta-\frac{\varepsilon f_\xi}{\xi h_\xi}\right)\\ &\quad \cdot\left(1-\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}\tan\theta+\frac{\varepsilon f_\xi}{\xi h_\xi}\right)+O(\varepsilon^2)\\ &= \tan\theta\left(1-\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}\cot\theta-\frac{\varepsilon f_\xi}{\xi h_\xi}\right.\\ &\quad \left.-\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}\tan\theta+\frac{\varepsilon f_\xi}{\xi h_\xi}\right)+O(\varepsilon^2)\\ &= \tan\theta-\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}-\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}\tan^2\theta+O(\varepsilon^2)\end{aligned} \qquad \text{(A-34)}$$

$$\begin{aligned}\frac{\sqrt{\boldsymbol{N}_x^2+\boldsymbol{N}_y^2}}{\boldsymbol{N}_z} &= -\xi\left(1-\frac{1}{\xi}\frac{\varepsilon f_\xi}{h_\xi}\right)\left(1-\frac{\varepsilon\xi f_\xi}{h_\xi}\right)+O(\varepsilon^2)\\ &= -\xi\left(1-\frac{1}{\xi}\frac{\varepsilon f_\xi}{h_\xi}-\frac{\varepsilon\xi f_\xi}{h_\xi}\right)+O(\varepsilon^2)\\ &= \tan\phi+\frac{\varepsilon f_\xi}{h_\xi}+\frac{\varepsilon f_\xi}{h_\xi}\tan^2\phi+O(\varepsilon^2)\end{aligned} \qquad \text{(A-35)}$$

Thus, one may express the orientation of the normal vector through the spherical angles $\Phi=\Phi(\theta,\phi,\varepsilon)$ and $\Theta=\Theta(\theta,\phi,\varepsilon)$, which are determined as:

$$\begin{aligned}\tan\Theta &= \frac{\boldsymbol{N}_y}{\boldsymbol{N}_x} = \tan\theta+\frac{\varepsilon f_\theta\sqrt{1+\xi^2}}{h_\theta\xi}(1+\tan^2\theta)+O(\varepsilon^2)\\ \tan\Phi &= \frac{\sqrt{\boldsymbol{N}_x^2+\boldsymbol{N}_y^2}}{\boldsymbol{N}_z} = \tan\phi+\frac{\varepsilon f_\xi}{h_\xi}(1+\tan^2\phi)+O(\varepsilon^2)\end{aligned} \qquad \text{(A-36)}$$

We make Taylor expansion for he function $\Phi(\theta,\phi,\varepsilon)$ and $\Theta(\theta,\phi,\varepsilon)$ in the limit $\varepsilon\to 0$:

$$\begin{aligned}\Theta &= \Theta^{(0)}+\varepsilon\Theta^{(1)}+\cdots\\ \Phi &= \Phi^{(0)}+\varepsilon\Phi^{(1)}+\cdots\end{aligned} \qquad \text{(A-37)}$$

Then it is derived that

$$\tan\Theta = \tan\Theta^{(0)}+\varepsilon[1+\tan^2\Theta^{(0)}]\Theta^{(1)}+O(\varepsilon^2)$$

and

$$\tan \Phi = \tan \Phi^{(0)} + \varepsilon[1 + \tan^2 \Phi^{(0)}]\Phi^{(1)} + O(\varepsilon^2)$$

Combining the above with (A-36), it follows that

$$\Theta^{(0)} = \theta,\ \Theta^{(1)} = -\frac{f_\theta\sqrt{1+\xi^2}}{h_\theta \xi} = -\frac{f_\theta h_\xi}{h_\theta^2},\ \cdots \quad \text{(A-38)}$$

$$\Phi^{(0)} = \phi,\ \Phi^{(1)} = \frac{f_\xi}{h_\xi},\ \cdots \quad \text{(A-39)}$$

4 Minimum principle of free surface energy

Now consider a given segment of the perturbed needle (V_{B}), whose projection onto the (ξ, θ) plane is $(A) : \big(0 \leqslant \xi < \xi_m; 0 \leqslant \theta < 2\pi\big)$. The boundary of (A) is denoted by (C). The minimum free energy principle under the constant volume constraint leads to the equation

$$\delta G = \delta\mathcal{F} + \delta\mathcal{V} = 0 \quad \text{(A-40)}$$

where (δG) is the variation of the Gibbs free energy of the segment due to the presence of the interface change $\varepsilon f(\xi, \theta)\boldsymbol{n}$; $(\delta\mathcal{F})$ is the variation of total surface energy of this segment and $(\delta\mathcal{V})$ is the variation of the total volume Gibbes free energy induced by the phase transition.

It is noted that the total area of the interface (S) of the segment of the perturbed needle (V_{B}) is

$$A = \int_{(S)} \mathrm{d}A = \int_{(A)} |\boldsymbol{X}_\xi \times \boldsymbol{X}_\theta| \mathrm{d}\xi\mathrm{d}\theta$$
$$= \int_{(A)} h_\xi h_\theta \mathrm{d}\xi\mathrm{d}\theta - \varepsilon\int_{(A)} f(\xi,\theta)(\mathcal{K}_\theta + \mathcal{K}_\xi)\mathrm{d}\xi\mathrm{d}\theta + O(\varepsilon^2) \quad \text{(A-41)}$$

Hence, the variation of the surface area can be written as:

$$\left.\frac{\mathrm{d}A}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = -\int_{(A)} f(\xi,\theta)(\mathcal{K}_\theta + \mathcal{K}_\xi)\mathrm{d}\xi\mathrm{d}\theta$$
$$= \int_{(A)} f\mathcal{H}\mathrm{d}\xi\mathrm{d}\theta \quad \text{(A-42)}$$

where $\mathcal{H} = -(\mathcal{K}_\theta + \mathcal{K}_\xi)$. Accordingly, the corresponding variation of the total volume is

$$\left.\frac{\mathrm{d}V}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = \int_{(A)} f(\xi,\theta)\mathrm{d}A \quad \text{(A-43)}$$

In view of the above, one may write that

$$\delta\mathcal{F} = \left.\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}\delta\varepsilon = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\int_{(S)} \gamma(\Phi, \Theta)\mathrm{d}A\right)\delta\varepsilon$$
$$= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(\int_{(A)} \gamma(\Phi, \Theta)|\boldsymbol{X}_\xi \times \boldsymbol{X}_\theta|\mathrm{d}\xi\mathrm{d}\theta\right)\delta\varepsilon \quad \text{(A-44)}$$

and

$$\delta\mathcal{V} = \left.\frac{\mathrm{d}\mathcal{V}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}\delta\varepsilon = \left(\int_{(S)} \Lambda f(\xi,\theta)\mathrm{d}A\right)\delta\varepsilon \quad \text{(A-45)}$$

where Λ is the change of Gibbs free energy per unit volume of solid due to the phase transition.

From (A-45), it is derived that

$$\left.\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = \int_{(A)} [\gamma(\Phi^{(0)}, \Theta^{(0)})f\mathcal{H} + \gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})\Phi^{(1)}$$
$$+ \gamma_\Theta(\Phi^{(0)}, \Theta^{(0)})\Theta^{(1)}]h_\xi h_\theta \mathrm{d}\xi\mathrm{d}\theta$$
$$= \text{(I)} + \text{(II)} + \text{(III)} \quad \text{(A-46)}$$

Each of the terms on the right hand side of (A-46) are calculated as follows:

- $\text{(I)} = \int_{(A)} \mathcal{F}_{\text{(I)}} f\mathrm{d}\xi\mathrm{d}\eta$, where

$$\mathcal{F}_{\text{(I)}} = \gamma(\Phi^{(0)}, \Theta^{(0)})\mathcal{H} \quad \text{(A-47)}$$

- $\text{(II)} = \int_{(A)} \mathcal{F}_{\text{(II)}} f\mathrm{d}\xi\mathrm{d}\eta$. Note that

$$\text{(II)} = \int_{(A)} \gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})\Phi^{(1)}h_\xi h_\theta \mathrm{d}\xi\mathrm{d}\theta$$
$$= \int \gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})\left(\frac{f_\xi}{h_\xi}\right)h_\xi h_\theta \mathrm{d}\xi\mathrm{d}\theta$$
$$= -\int_{(A)} f(\xi,\theta)\frac{\partial}{\partial\xi}[\gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})h_\theta]\mathrm{d}\xi\mathrm{d}\theta \quad \text{(A-48)}$$

In the above derivation, we have applied the integral by parts and assume that $f(\xi, \theta) = 0$ at the boundary (C) of the domain (A). On the other hand, we have

$$\frac{\partial}{\partial\xi}\big[\gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})h_\theta\big]$$
$$= \gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})\frac{\partial h_\theta}{\partial\xi} + h_\theta\big[\gamma_{\Phi\Phi}(\Phi^{(0)}, \Theta^{(0)})\Phi_\xi^{(0)}$$
$$+ \gamma_{\Phi\Theta}(\Phi^{(0)}, \Theta^{(0)})\Theta_\xi^{(0)}\big]$$
$$= \gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})\frac{\partial h_\theta}{\partial\xi} + \gamma_{\Phi\Phi}(\Phi^{(0)}, \Theta^{(0)})h_\theta\Phi_\xi^{(0)} \quad \text{(A-49)}$$

Here, we have used $\Theta_\xi^{(0)} = 0$. We finally derive

$$\mathcal{F}_{\text{(II)}} = \gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})\frac{\partial h_\theta}{\partial\xi} + \gamma_{\Phi\Phi}(\Phi^{(0)}, \Theta^{(0)})h_\theta\Phi_\xi^{(0)} \quad \text{(A-50)}$$

- $\text{(III)} = \int_{(A)} \mathcal{F}_{\text{(III)}} f\mathrm{d}\xi\mathrm{d}\eta$. Note that

$$\text{(III)} = \int_A \gamma_\Theta(\Phi^{(0)}, \Theta^{(0)})\Theta^{(1)}h_\xi h_\theta \mathrm{d}\xi\mathrm{d}\theta$$
$$= \int \gamma_\Theta(\Phi^{(0)}, \Theta^{(0)})\left(-\frac{f_\theta h_\xi}{h_\theta^2}\right)h_\xi h_\theta \mathrm{d}\xi\mathrm{d}\theta$$

$$= -\int \gamma_\Theta(\Phi^{(0)}, \Theta^{(0)}) \frac{f_\theta h_\xi^2}{h_\theta} \mathrm{d}\xi \mathrm{d}\theta$$

$$= \int f(\xi,\theta) \frac{\partial}{\partial\theta}\left[\gamma_\Theta(\Phi^{(0)}, \Theta^{(0)}) \frac{h_\xi^2}{h_\theta}\right] \mathrm{d}\xi \mathrm{d}\theta \quad \text{(A-51)}$$

In the above derivation, we once again used the integral by parts and the boundary condition: $f(\xi,\theta) = 0$, at $(\xi,\theta) \in (C)$. Note that

$$\frac{\partial}{\partial\theta}\left[\gamma_\Theta(\Phi^{(0)}, \Theta^{(0)}) \frac{h_\xi^2}{h_\theta}\right] = \gamma_\Theta(\Phi^{(0)}, \Theta^{(0)}) \frac{\partial}{\partial\theta}\left(\frac{h_\xi^2}{h_\theta}\right) + \left[\gamma_{\Theta\Phi}(\Phi^{(0)}, \Theta^{(0)})\Phi_\theta^{(0)} + \gamma_{\Theta\Theta}(\Phi^{(0)}, \Theta^{(0)})\Theta_\theta^{(0)}\right]\frac{h_\xi^2}{h_\theta}$$

$$= \gamma_{\Theta\Theta}(\Phi^{(0)}, \Theta^{(0)}) \cdot \frac{h_\xi^2}{h_\theta} \cdot \Phi_\theta^{(0)} \quad \text{(A-52)}$$

Here, we have used

$$\Theta_\theta^{(0)} = 0$$

$$\frac{\partial h_\theta}{\partial\xi} = \eta_0^2, \quad \frac{\partial h_\xi}{\partial\theta} = 0, \quad \frac{\partial h_\theta}{\partial\theta} = 0, \quad \frac{\partial}{\partial\theta}\left(\frac{h_\xi^2}{h_\theta}\right) = 0 \quad \text{(A-53)}$$

So that, we derive

$$\mathcal{F}_{(\mathrm{III})} = \gamma_{\Theta\Theta}(\Phi^{(0)}, \Theta^{(0)}) \cdot \frac{h_\xi^2}{h_\theta} \cdot \Phi_\theta^{(0)} \quad \text{(A-54)}$$

Putting all the terms together, we get

$$\left.\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} = \int \left[\gamma(\Phi^{(0)}, \Theta^{(0)})\mathcal{H} - \frac{\gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})}{h_\xi h_\theta}\frac{\partial h_\theta}{\partial\xi} - \frac{\gamma_{\Phi\Phi}(\Phi^{(0)}, \Theta^{(0)})}{h_\xi h_\theta} h_\theta \Phi_\xi^{(0)} + \frac{\gamma_{\Theta\Theta}(\Phi^{(0)}, \Theta^{(0)})}{h_\xi h_\theta}\frac{h_\xi^2}{h_\theta}\Theta_\theta^{(0)}\right] f h_\xi h_\theta \mathrm{d}\xi \mathrm{d}\theta \quad \text{(A-55)}$$

we have derived

$$\Theta^{(0)} = \theta, \quad \Phi^{(0)} = \phi$$

$$\Theta_\theta^{(0)} = 1, \quad \Phi_\xi^{(0)} = -\frac{1}{1+\xi^2}$$

Combining (A-55) with (A-45) and noting that $f(\xi,\theta)$ is arbitrary function, we derive that to ensure the interface is in the local thermodynamic equilibrium state, the parameter Λ must take the following form:

$$\Lambda = \gamma(\Phi^{(0)}, \Theta^{(0)})\mathcal{H} - \frac{\gamma_\Phi(\Phi^{(0)}, \Theta^{(0)})}{h_\xi h_\theta}\frac{\partial h_\theta}{\partial\xi} - \gamma_{\Phi\Phi}(\Phi^{(0)}, \Theta^{(0)})\frac{\Phi_\xi^{(0)}}{h_\xi} + \gamma_{\Theta\Theta}(\Phi^{(0)}, \Theta^{(0)})\frac{h_\xi \Theta_\theta^{(0)}}{h_\theta^2} \quad \text{(A-56)}$$

which yields the local interface temperature.

5 Herring formula

It is known that the dimensional form of the Herring formula can be described as:

$$T_\mathrm{I} = T_\mathrm{M}\left(1 + \frac{1}{\Delta H}\Lambda\right) \quad \text{(A-57)}$$

The interfacial energy can be described as:

$$\gamma = \gamma_0(1 + \hat{\alpha}_4 Q_4) \quad \text{(A-58)}$$

where

$$Q_4(\boldsymbol{n}) = n_x^4 + n_y^4 + n_z^4 = \sin^4\phi\left(\cos^4\theta + \sin^4\theta\right) + \cos^4\phi$$

$$= \sin^4\phi\left(\frac{3}{4} + \frac{1}{4}\cos 4\theta\right) + \cos^4\phi$$

$$= \frac{\frac{3}{4}\xi^4 + 1}{(1+\xi^2)^2} + \frac{\frac{1}{4}\xi^4}{(1+\xi^2)^2}\cos 4\theta \quad \text{(A-59)}$$

One may calculate

$$\frac{\partial^2\gamma}{\partial\Theta^2} = \gamma_0\hat{\alpha}_4\frac{\partial^2 Q_4}{\partial\Theta^2} = -4\gamma_0\hat{\alpha}_4\sin^4\phi\cos 4\theta = \frac{-4\gamma_0\hat{\alpha}_4\xi^4}{(1+\xi^2)^2}\cos 4\theta$$

$$\frac{\partial\gamma}{\partial\Phi} = \gamma_0\hat{\alpha}_4\frac{\partial Q_4}{\partial\Phi} = \hat{\alpha}_4\left[4\sin^3\phi\cos\phi\left(\frac{3}{4} + \frac{1}{4}\cos 4\theta\right) - 4\cos^3\phi\sin\phi\right] = \gamma_0\hat{\alpha}_4\left[\frac{-3\xi^3 + 4\xi}{(1+\xi^2)^2} + \frac{-\xi^3}{(1+\xi^2)^2}\cos 4\theta\right]$$

$$\frac{\partial^2\gamma}{\partial\Phi^2} = \gamma_0\hat{\alpha}_4\frac{\partial^2 Q_4}{\partial\Phi^2} = \hat{\alpha}_4\left[(12\sin^2\phi\cos^2\phi - 4\sin^4\phi)\left(\frac{3}{4} + \frac{1}{4}\cos 4\theta\right) + (12\sin^2\phi\cos^2\phi - 4\cos^4\phi)\right]$$

$$= \gamma_0\hat{\alpha}_4\left[\frac{9\xi^2 - 3\xi^4 + 12\xi^2 - 4}{(1+\xi^2)^2} + \frac{3\xi^2 - \xi^4}{(1+\xi^2)^2}\cos 4\theta\right]$$

By using the formulas

$$h_\xi = \eta_0^2\sqrt{1+\xi^2}, \quad h_\theta = \eta_0^2\xi, \quad \frac{1}{h_\xi h_\theta} = \frac{1}{\eta_0^4\xi\sqrt{1+\xi^2}} \quad \text{(A-60)}$$

$$\frac{\partial h_\theta}{\partial\xi} = \eta_0^2, \quad \frac{\partial h_\xi}{\partial\theta} = 0, \quad \frac{\partial h_\theta}{\partial\theta} = 0, \quad \frac{\partial}{\partial\theta}\left(\frac{h_\xi^2}{h_\theta}\right) = 0 \quad \text{(A-61)}$$

and

$$\mathcal{K}_\theta = -\frac{1}{h_\xi}, \quad \mathcal{K}_\xi = -\frac{\eta_0^4}{h_\xi^3}$$

$$\mathcal{H} = -(\mathcal{K}_\theta + \mathcal{K}_\xi) = \frac{2+\xi^2}{\eta_0^2(1+\xi^2)^{\frac{3}{2}}} \tag{A-62}$$

we finally obtain the parameter

$$\begin{aligned}
\Lambda &= \gamma_0\left[1+\hat{\alpha}_4\left(\frac{\frac{3}{4}\xi^4+1}{(1+\xi^2)^2}+\frac{\frac{1}{4}\xi^4}{(1+\xi^2)^2}\cos 4\theta\right)\right]\frac{2+\xi^2}{\eta_0^2(1+\xi^2)^{\frac{3}{2}}} \\
&\quad -\hat{\alpha}_4\left[\frac{-3\xi^3+4\xi}{(1+\xi^2)^2}+\frac{-\xi^3}{(1+\xi^2)^2}\cos 4\theta\right]\frac{1}{\eta_0^4\xi\sqrt{1+\xi^2}}\eta_0^2 \\
&\quad -\hat{\alpha}_4\left[\frac{-3\xi^4+21\xi^2-4}{(1+\xi^2)^2}+\frac{3\xi^2-\xi^4}{(1+\xi^2)^2}\cos 4\theta\right] \\
&\quad \cdot\frac{1}{\eta_0^2\sqrt{1+\xi^2}}\frac{-1}{1+\xi^2}+\left[\frac{-4\hat{\alpha}_4\xi^4}{(1+\xi^2)^2}\cos 4\theta\right]\frac{\eta_0^2\sqrt{1+\xi^2}}{\eta_0^4\xi^2} \\
&= \frac{\gamma_0}{\eta_0^2}\left[\frac{2+\xi^2}{\sqrt{1+\xi^2}}+\hat{\alpha}_4(F_0+F_4\cos 4\theta)\right]
\end{aligned} \tag{A-63}$$

where

$$\begin{aligned}
F_0 &= \frac{\frac{3}{4}\xi^4+1}{(1+\xi^2)^2}\frac{2+\xi^2}{(1+\xi^2)^{3/2}}-\frac{-3\xi^3+4\xi}{(1+\xi^2)^2}\frac{1}{\xi\sqrt{1+\xi^2}} \\
&\quad +\frac{-3\xi^4+21\xi^2-4}{(1+\xi^2)^2}\frac{1}{\sqrt{1+\xi^2}}\frac{1}{1+\xi^2} \\
&= \frac{1}{(1+\xi^2)^{7/2}}\left[\left(\frac{3}{4}\xi^4+1\right)(2+\xi^2)\right. \\
&\quad \left.-(-3\xi^2+4)(1+\xi^2)+(-3\xi^4+21\xi^2-4)\right] \\
&= \frac{1}{(1+\xi^2)^{7/2}}\left(\frac{3}{4}\xi^6+\frac{3}{2}\xi^4+21\xi^2-6\right)
\end{aligned} \tag{A-64}$$

and

$$\begin{aligned}
F_4 &= \frac{\frac{1}{4}\xi^4}{(1+\xi^2)^2}\frac{2+\xi^2}{(1+\xi^2)^{3/2}}-\frac{-\xi^3}{(1+\xi^2)^2}\frac{1}{\xi\sqrt{1+\xi^2}} \\
&\quad +\frac{3\xi^2-\xi^4}{(1+\xi^2)^2}\frac{1}{\sqrt{1+\xi^2}}\frac{1}{1+\xi^2}-\frac{4\xi^4}{(1+\xi^2)^2}\frac{\sqrt{1+\xi^2}}{\xi^2} \\
&= \frac{1}{(1+\xi^2)^{7/2}}\left[\frac{1}{4}\xi^4(2+\xi^2)+\xi^2(1+\xi^2)\right. \\
&\quad \left.+(3\xi^2-\xi^4)-4\xi^2(1+\xi^2)^2\right] \\
&= -\frac{1}{(1+\xi^2)^{7/2}}\left(\frac{15}{4}\xi^6+\frac{15}{2}\xi^4\right)
\end{aligned} \tag{A-65}$$

$$K_0 = \frac{2+\xi^2}{(1+\xi^2)^{3/2}}, \quad F_0 = \frac{\frac{3}{4}\xi^6+\frac{3}{2}\xi^4+21\xi^2-6}{(1+\xi^2)^{7/2}}$$

$$F_4 = \frac{-\frac{15}{4}\xi^6-\frac{15}{2}\xi^4}{(1+\xi^2)^{7/2}} \tag{A-66}$$

With the length scale ℓ_{T}, we may derive the following dimensionless form of the Herring formula from (A-57):

$$T_{\mathrm{I}} = -\varepsilon^2\left[\frac{2+\xi^2}{\sqrt{1+\xi^2}}+\hat{\alpha}_4\big(F_0+F_4\cos 4\theta\big)\right]+\mathcal{O}(\varepsilon^4) \tag{A-67}$$

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