

The effect of curved interface shape on thermal stress during Czochralski crystal growth

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Analytical solutions of the quasi-steady-state thermal stresses in the crystal with finite length during Czochralski growth are obtained. In the temperature analysis, both the temperature distribution and the shape of the solid–liquid interface are simultaneously solved. It is found that the shape of the interface is parabolic-like and the Biot number is the dominating parameter. In the thermal stress analysis, we found that the results of the curved interface model are qualitatively similar to, but quantitatively different from those of the planar interface model. In addition, we also find that the effect of the crystal length should not be neglected, especially when the length is small.

1. Introduction

In recent years, there has been a rapidly growing interest in research on the thermal stress produced in a single crystal by temperature variations during Czochralski growth, because the thermal stress may deform the crystal plastically and generate dislocations which then will degrade the electronic properties of the grown material [1]. Actually, both Penning, [2] who studied the growth of Ge, and Jordan et al. [3], who researched to growth of GaAs and InP, have pointed out that the generation of dislocation is attributed to excessive thermal stresses.

Following the work of Jordan et al. on GaAs [3], several thermal stress calculations have been published. Some of them are based on the plane strain assumption [1–5]. However, the plane strain assumption is not always satisfied because the axial variation of the thermal stress is not negligible during growth. Analytical solutions for the stresses have been presented by Iwaki and Kobayashi [6–8] and by Szabo [9]. Numerical solutions have been presented by Duseaux [10], who examined some limited aspects of the effects of neck geometry, by Motakef and Witt [11], who

examined the effect of the encapsulant, and by Lambropoulos [12], who examined the stresses near the solid–liquid interface and the effect of creep thereby, and the effect of crystalline anisotropy on the resulting thermal stress and dislocation density [13,14]. A common conclusion of the works mentioned above is that all significant stress variations, including maximum values, occur within one or two radii from the solid–liquid interface. Also, the calculations mentioned above have started with a knowledge of the temperature distribution within the growing crystal, and they have modeled the material as linear-elastic with the exception of the limited account of high temperature creep presented by Lambropoulos [12]. Furthermore, in these thermal stress calculations, a planar solid–liquid interface is assumed.

However, in reality, experimental and numerical evidence showed that the interface is curved during the growth of GaAs by the liquid encapsulated Czochralski method [15,16]. Wilcox and Duty [17] solved the steady state problem by using a heat balance at the solid–liquid interface. They showed that the interface is concave into the crystal for a large Biot number and that the shape of the interface is approximately parabolic.

This conclusion was adopted by Lambropoulos and Delametter [18], who modeled the interface as parabolic and implemented finite element technique to quantify the effect of the deviation from planarity of the solid-liquid interface on thermal stresses during Czochralski growth. Lambropoulos and Delametter [18] claimed that the thermal stresses increase with the maximum characteristic height of the interface curve especially near the center of the crystal. However, both the works of Wilcox and Duty [17] and of Lambropoulos and Delametter [18] have neglected the transient term in the governing heat conduction equation.

Recently, Chen et al. [19] undertook a quasi-steady-state thermoelastic analysis with the effect of interface shape to predict the dislocation density pattern in Czochralski-pulled single crystals. They considered a uniform heat flux through the bottom of the solid-liquid interface and imposed a constant melting temperature on the interface. Then the transient temperature profiles as well as the shape of the interface will be determined simultaneously. However, they have adopted the plane strain assumption in the thermal stress analysis.

In this work we intent to improve the work of Chen et al. [19] by introducing a displacement potential and a Love stress function as in Iwaki and Kobayashi [6–8], so that hence the plane strain assumption is no longer used. We discuss the effects of the Biot number and the Peclet number on the thermal stress in a crystal during Czochralski growth. In addition, we determine the effect of the crystal's length. We compare our results with those of Iwaki and Kobayashis [8], to emphasize the effect of curved interface.

2. Temperature distribution

We assume that a uniform heat flux q_0 is transferred from the bottom of the crystal and that the solid-liquid interface is maintained at the melting temperature T_m [16]. The other assumptions include [3]:

(1) Initially, at $t \leq 0$, the semi-infinite space between $z = 0$ and $-\infty$ is completely filled by a

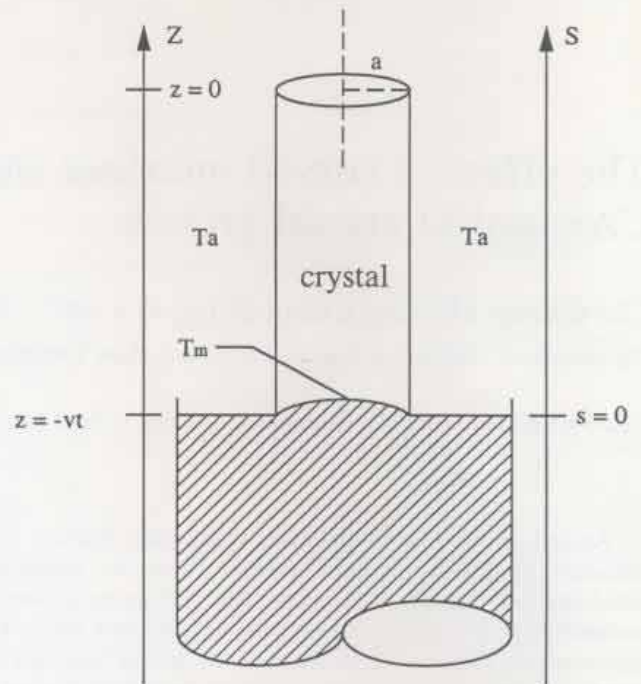


Fig. 1. Physical plane diagram of a Czochralski growth system.

stoichiometric liquid solution contained in a crucible and held at the melting point of the liquid solution, T_m .

(2) The crystal is grown by the removal of the crucible in the $-z$ direction at rate v , and its shape is cylindrical from top to bottom.

(3) The growing boule is surrounded by an ambient fluid at temperature $T_a = \text{constant} \leq T_m$, while the melt is continuously maintained at T_m .

(4) The temperature distribution is not significantly influenced by crucible or crystal rotation.

(5) At the top and on the lateral surface of the boule, the heat loss is proportional to the temperature difference between the surface and the ambient fluid.

Fig. 1 sketches the coordinate system relevant to our Czochralski growth model. In the interest of clarity, the vertical axis (z and s) have been displaced from the crystal axes. Let a , v , t , T , T_a , κ , k , and h denote the radius of crystal, the pulling rate, the pulling time, the temperature, the ambient temperature, the thermal diffusivity, the thermal conductivity, and the convective heat-transfer coefficient, respectively. Then, if the transformation $s = z + vt$ and dimensionless vari-

ables $\Theta = (T - T_a)/(T_m - T_a)$, $P = av/\kappa$, $H = ah/k$, $\rho = r/a$, $\psi = s/a$, $\psi_t = vt/a$ and $Q^* = q_0 a/k(T_m - T_a)$ are introduced, the heat conduction equation and the corresponding boundary conditions will take the forms:

$$\frac{\partial^2 \Theta}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \Theta}{\partial \rho} + \frac{\partial^2 \Theta}{\partial \psi^2} = P \frac{\partial \Theta}{\partial \psi}, \quad (2.1)$$

$$\left[\frac{\partial \Theta}{\partial \rho} + H \Theta \right]_{\rho=1} = 0, \quad (2.2a)$$

$$\left[\frac{\partial \Theta}{\partial \psi} + H \Theta \right]_{\psi=\psi_t} = 0, \quad (2.2b)$$

$$\frac{\partial \Theta}{\partial \psi} \Big|_{\psi=0} = -Q^*, \quad (2.2c)$$

$$\Theta|_{\psi=0, \rho=1} = 1. \quad (2.2d)$$

Here P and H denote the Peclet number and the Biot number, respectively. By the method of eigenfunction expansion, we assume the solution of the temperature field be

$$\Theta = \sum_{n=1}^{\infty} [A_n e^{\alpha_n(\psi-\psi_t)} + B_n e^{\beta_n(\psi-\psi_t)}] J_0(\lambda_n \rho), \quad (2.3)$$

where J_0 is a Bessel function of the first type of order zero and

$$\alpha_n = \frac{1}{2}P + \sqrt{\left(\frac{1}{2}P\right)^2 + \lambda_n^2},$$

$$\beta_n = \frac{1}{2}P - \sqrt{\left(\frac{1}{2}P\right)^2 + \lambda_n^2}.$$

Introducing (2.3) into (2.2a), we have the characteristic equation

$$-\lambda_n J_1(\lambda_n) + H J_0(\lambda_n) = 0, \quad (2.4a)$$

where J_1 is a Bessel function of the first type of order one and λ_n is the n th eigenvalue. If we substitute (2.3) into (2.2b), then we have the relation between A_n and B_n :

$$A_n = -\frac{\beta_n + H}{\alpha_n + H} B_n. \quad (2.4b)$$

From (2.2c), we will relate B_n and Q^* as

$$B_n = \frac{-2HQ^*}{(H^2 + \lambda_n^2) J_0(\lambda_n) W_n}, \quad (2.4c)$$

where

$$W_n = -\alpha_n \frac{\beta_n + H}{\alpha_n + H} e^{-\alpha_n \psi_t} + \beta_n e^{-\beta_n \psi_t}.$$

Finally, we obtain Q^* from (2.2d)

$$Q^* = \left[\sum_{n=1}^{\infty} \frac{-2H}{(H^2 + \lambda_n^2) W_n} \times \left(e^{-\beta_n \psi_t} - \frac{\beta_n + H}{\alpha_n + H} e^{-\alpha_n \psi_t} \right) \right]^{-1}. \quad (2.4d)$$

The temperature field in the crystal is completely determined by substituting (2.4) into (2.3).

Since we have imposed the interfacial temperature to be the melting point, the shape of the solid-liquid interface can be sketched by the equation

$$\sum_{n=1}^{\infty} (A_n e^{-\alpha_n(\psi-\psi_t)} + B_n e^{\beta_n(\psi-\psi_t)}) J_0(\lambda_n \rho) = 1, \quad (2.5)$$

which represents the relation between ψ and ρ if both H and P are fixed.

3. The thermal stresses

According to Iwaki and Kobayashi's work [6], to analyze the thermal stresses, we first introduce the displacement potential ϕ_0^* and the Love stress function ϕ_r^* [6] which, respectively, have to satisfy

$$\Delta^* \phi_0^* = \Theta, \quad (3.1)$$

$$\Delta^* \Delta^* \phi_r^* = 0, \quad (3.2)$$

where

$$\Delta^* = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial \psi^2}.$$

Then the thermal stresses are given by

$$\sigma_{ij}^* = \sigma_{0ij}^* + \sigma_{lij}^*, \quad (3.3)$$

where

$$\sigma_{0\rho\rho}^* = \frac{\partial^2 \phi_0^*}{\partial \rho^2} - \Delta^* \phi_0^*, \quad (3.4a)$$

$$\sigma_{0\theta\theta}^* = \frac{1}{\rho} \frac{\partial \phi_0^*}{\partial \rho} - \Delta^* \phi_0^*, \quad (3.4b)$$

$$\sigma_{0\psi\psi}^* = \frac{\partial^2 \phi_0^*}{\partial \psi^2} - \Delta^* \phi_0^*, \quad (3.4c)$$

$$\sigma_{0\rho\psi}^* = \frac{\partial^2 \phi_0^*}{\partial \rho \partial \psi}, \quad (3.4d)$$

and

$$\sigma_{l\rho\rho}^* = \frac{\partial}{\partial \psi} \left(\nu \Delta^* \phi_l^* - \frac{\partial^2 \phi_l^*}{\partial \rho^2} \right), \quad (3.5a)$$

$$\sigma_{l\theta\theta}^* = \frac{\partial}{\partial \psi} \left(\nu \Delta^* \phi_l^* - \frac{1}{\rho} \frac{\partial \phi_l^*}{\partial \rho} \right), \quad (3.5b)$$

$$\sigma_{l\psi\psi}^* = \frac{\partial}{\partial \psi} \left[(2 - \nu) \Delta^* \phi_l^* - \frac{\partial^2 \phi_l^*}{\partial \psi^2} \right], \quad (3.5c)$$

$$\sigma_{l\rho\psi}^* = \frac{\partial}{\partial \rho} \left[(1 - \nu) \Delta^* \phi_l^* - \frac{\partial^2 \phi_l^*}{\partial \psi^2} \right]. \quad (3.5d)$$

Here ν denotes the Poisson's ratio. The corresponding boundary conditions are

$$\sigma_{\rho\rho}^*|_{\rho=1} = \sigma_{\rho\psi}^*|_{\rho=1} = 0, \quad (3.6)$$

$$\phi_{\psi\psi}^*|_{\psi=\psi_l} = \sigma_{\rho\psi}^*|_{\psi=\psi_l} = 0, \quad (3.7)$$

and

$$\sigma_{ij}^* n_j = 0, \quad (i, j = \rho, \psi) \text{ at the interface,} \quad (3.8)$$

where the n_j 's are the components of the normal unit vector at the solid-liquid interface.

Since the dimensionless temperature Θ has been found in the preceding section, we will have a particular solution of eq. (3.1):

$$\phi_0^* = \sum_{n=1}^{\infty} (C_n e^{\alpha_n(\psi-\psi_l)} + D_n e^{\beta_n(\psi-\psi_l)}) J_0(\lambda_n \rho), \quad (3.9)$$

where

$$C_n = A_n / (\alpha_n^2 - \lambda_n^2), \quad (3.10a)$$

$$D_n = B_n / (\beta_n^2 - \lambda_n^2). \quad (3.10b)$$

The Love stress function is constructed in the form

$$\phi_l^* = \phi_1^* + \phi_2^*, \quad (3.11)$$

thus $\sigma_{lij}^* = \sigma_{1ij}^* + \sigma_{2ij}^*$ where the stresses σ_{1ij}^* and σ_{2ij}^* are derived from ϕ_1^* and ϕ_2^* , respectively. The function ϕ_1^* has the form

$$\begin{aligned} \phi_1^* = \sum_{n=1}^{\infty} [& E_n e^{\alpha_n(\psi-\psi_l)} J_0(\alpha_n \rho) \\ & + F_n e^{\beta_n(\psi-\psi_l)} J_0(\beta_n \rho) \\ & + G_n e^{\alpha_n(\psi-\psi_l)} \rho J_1(\alpha_n \rho) \\ & + H_n e^{\beta_n(\psi-\psi_l)} \rho J_1(\beta_n \rho)], \end{aligned} \quad (3.12)$$

where the unknowns E_n , F_n , G_n , and H_n are determined by the boundary conditions at the cylindrical surface

$$\sigma_{0\rho\rho}^* + \sigma_{1\rho\rho}^* = 0, \quad \text{at } \rho = 1, \quad (3.13a)$$

$$\sigma_{0\rho\psi}^* + \sigma_{1\rho\psi}^* = 0, \quad \text{at } \rho = 1. \quad (3.13b)$$

Consequently, we have

$$E_n = C_n \Gamma(\alpha_n), \quad (3.14a)$$

$$F_n = D_n \Gamma(\beta_n), \quad (3.14b)$$

$$G_n = C_n \Lambda(\alpha_n), \quad (3.14c)$$

$$H_n = D_n \Lambda(\beta_n), \quad (3.14d)$$

where

$$\begin{aligned} \Gamma(\alpha_n) = & \{ \lambda_n J_1(\lambda_n) [2(1-\nu) J_1(\alpha_n) \\ & - \alpha_n^2 J_1(\alpha_n) + 2(1-\nu) \alpha_n J_0(\alpha_n)] \\ & - \alpha_n^2 J_0(\lambda_n) [2(1-\nu) J_1(\alpha_n) \\ & + \alpha_n J_0(\alpha_n)] \} \\ & \times \{ [2(1-\nu) - \alpha_n^2] J_1^2(\alpha_n) \\ & - \alpha_n^2 J_0^2(\alpha_n) \}^{-1} \alpha_n^{-2}, \end{aligned} \quad (3.15a)$$

$$\begin{aligned} \Lambda(\alpha_n) = & [\alpha_n J_1(\alpha_n) J_0(\alpha_n) - \alpha_n J_0(\lambda_n) J_1(\alpha_n)] \\ & \times \{ [2(1-\nu) - \alpha_n^2] J_1^2(\alpha_n) \\ & - \alpha_n^2 J_0^2(\alpha_n) \}^{-1}. \end{aligned} \quad (3.15b)$$

To satisfy the boundary condition (3.8), we assume ϕ_2^* be of the form [20]:

$$\phi_2^* = Q e^{s\psi} J_0(s\rho) + R e^{s\psi} \rho J_1(s\rho). \quad (3.16)$$

The stresses which are derived from ϕ_2^* must satisfy the boundary conditions at the cylindrical surface:

$$\sigma_{2\rho\rho}^* = \sigma_{2\rho\psi}^* = 0, \quad \text{at } \rho = 1. \quad (3.17)$$

Thus, combining (3.5a), (3.5b), (3.16), and (3.17) leads to

$$\begin{bmatrix} \Pi_{11} & \Pi_{12} \\ \Pi_{21} & \Pi_{22} \end{bmatrix} \begin{Bmatrix} Q \\ R \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}, \quad (3.18)$$

where

$$\Pi_{11} = sJ_0(s) - J_1(s),$$

$$\Pi_{12} = (2\nu - 1)J_0(s) + sJ_1(s),$$

$$\Pi_{21} = -sJ_1(s), \quad \Pi_{22} = 2(1 - \nu)J_1(s) + sJ_0(s).$$

For the existence of a nontrivial solution of (3.18), s must be the root of the transcendental equation:

$$[s^2 - 2(1 - \nu)] J_1^2(s) + s^2 J_0^2(s) = 0, \quad (3.19)$$

This equation has infinitely many complex roots. If the n th root is defined by s_n whose real and imaginary parts are positive, $\bar{s}_n$, $-s_n$, and $-\bar{s}_n$ are also the roots of eq. (3.19). We taken s_n and $-\bar{s}_n$ as two roots and truncate as infinite number of roots at $n = N$. Naturally, large N leads to more accurate results and a theoretically exact solution requires that N is taken to be infinite. The final form of ϕ_2^* is given by

$$\begin{aligned} \phi_2^* = & \sum_{n=1}^N [L_n e^{s_n(\psi - \psi_t)} - M_n e^{-s_n(\psi - \psi_t)}] \\ & \times [Q(s_n) J_0(s_n \rho) + R(s_n) \rho J_1(s_n \rho)], \end{aligned} \quad (3.20)$$

where

$$Q(s_n) = 2(1 - \nu) J_1(s_n) + s_n J_0(s_n) \quad (3.21a)$$

$$R(s_n) = s_n J_1(s_n), \quad (3.21b)$$

and L_n and M_n are unknown complex coefficients. The unknown coefficients can be deter-

mined by the boundary conditions (3.7) and (3.8), i.e., by

$$\sigma_{2\psi\psi}^* = -\sigma_{0\psi\psi}^* - \sigma_{1\psi\psi}^*, \quad \psi = \psi_t, \quad (3.22a)$$

$$\sigma_{2\rho\psi}^* = -\sigma_{0\rho\psi}^* - \sigma_{1\rho\psi}^*, \quad \psi = \psi_t, \quad (3.22b)$$

and

$$\sigma_{2ij}^* n_j = -(\sigma_{0ij}^* + \sigma_{1ij}^*) n_j, \quad \text{at the interface.} \quad (3.23)$$

From (3.5) and (3.20)–(3.23), the exact solution is analytically expected. However, due to the constraint of the form of power series, these coefficients can only be approximately determined by numerical methods. In this work, they are determined by the method of least squares, so that the boundary conditions (3.22) and (3.23) may be satisfied at a number of midpoints (ρ_m , $m = 1, 2, \dots, M$) across the top and bottom surfaces. Thus we obtain the simultaneous equations

$$[S]_{4 \times 4} [U]_{4 \times 1} = [V]_{4 \times 1}, \quad (3.24)$$

where the elements of each matrix are shown in the appendix.

After ϕ_0^* , ϕ_1^* and ϕ_2^* have been solved, we then can combine (3.3)–(3.5) and (3.11) to obtain the thermal stresses σ_{ij} .

4. Results and discussion

In this study, the Poisson ratio is chosen as $\nu = 0.3$ for all calculations. Fig. 2 shows the di-

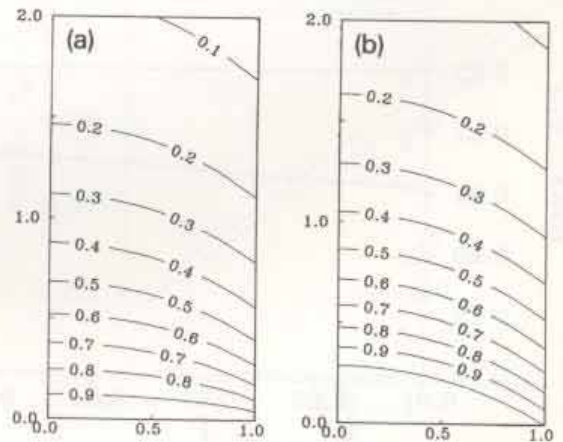


Fig. 2. Temperature distributions for $\psi_t = 2$, $H = 1$, and $P = 0.02$: (a) with planar interface; (b) with curved interface.

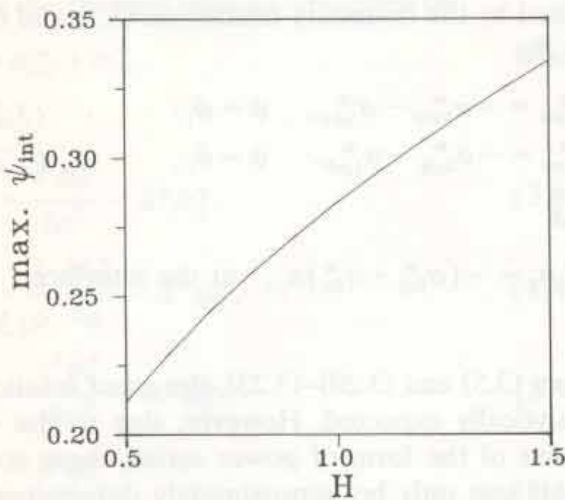


Fig. 3. Variation of the steady-state maximum height of the interface, $\max. \psi_{int}$, with the Biot number, for $P = 0.02$.

mensionless temperature distributions, with and without curved interface, when $\psi_i = 2.0$. From this figure, it is rational to believe that the induced thermal stresses in the case of curved interface will be larger than those in the planar interface case, because the isothermal lines in the former case are denser. The interfacial curve varies with time, such that, as time goes on, it will approach to the steady-state one. Fig. 3 shows that the steady-state maximum height of the interface ($\psi = \psi_{int}$ as $\rho = 0$) varies proportionally with the Biot number for $P = 0.02$. The explanation of such behavior starts with the definition of the Biot number. The Biot number H represents the rate of heat loss through the crystal's surfaces relative to conduction through the crystal. If the

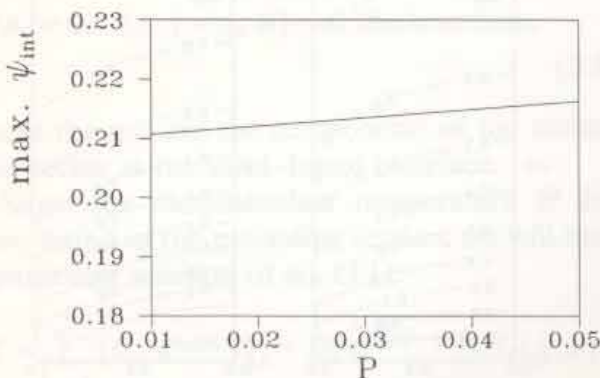


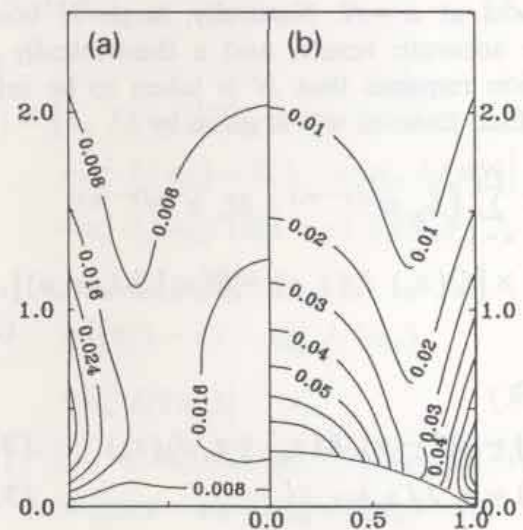
Fig. 4. Variation of the steady-state maximum height of the interface, $\max. \psi_{int}$, with the Peclet number, for $H = 1$.

heat loss through the crystal's surfaces is fixed, larger H requires shorter distances between the interface and the surfaces. So, the steady-state height of the interface will sensitively and proportionally vary with H . The effect of the Peclet number P on the steady-state maximum height of the interface, for $H = 1$, is shown in fig. 4. Since P in large part provides the transient effect, as can be seen in the heat conduction equation (2.1), it will not sensitively influence the steady-state height of the interface.

In this article, the thermal stress that is calculated is the equivalent shear stress τ_e which is defined by

$$\tau_e = \sqrt{S_{ij}S_{ij}/2}, \quad (4.1)$$

where S_{ij} is the stress deviator $S_{ij} = \sigma_{ij} - \sigma_{kk}\delta_{ij}/3$. We choose τ_e to be calculated, because it is a measure of that part of the stress tensor which causes plastic deformation by dislocation slip. Although in the thermal stress analysis, we have obtained the analytical solutions of the thermal stress tensor, only numerical results in fact calculated. In this paper, all the stresses are measured in units of $E\alpha(T_m - T_a)/(1 - \nu)$, where E denotes the modulus of elasticity and α is the coefficient of thermal expansion. In addition, a choice of $N = 20$ and $M \leq 21$ is made in order to provide better accuracy in the calculations of



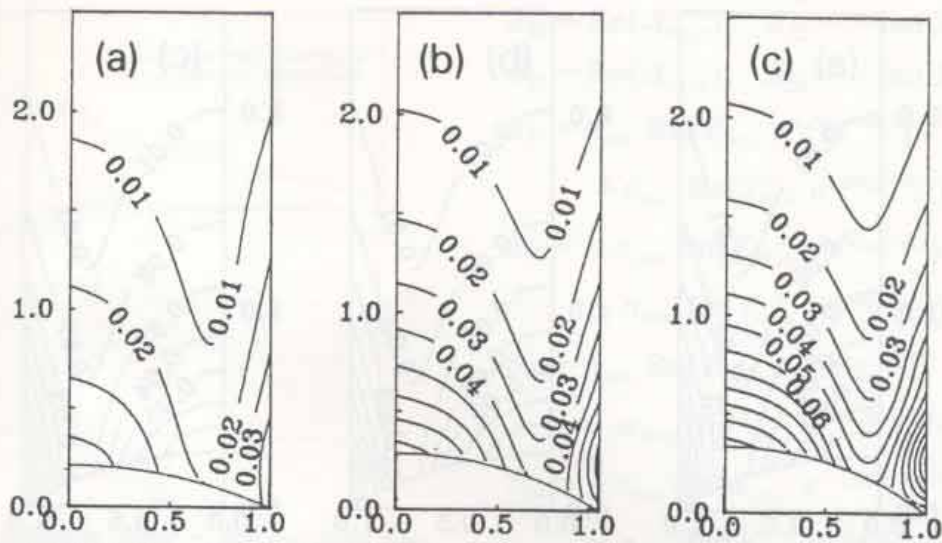


Fig. 6. Distributions of τ_e for $P = 0.02$ and $\psi_t = 6$ when: (a) $H = 0.5$; (b) $H = 1.0$; (c) $H = 1.5$.

thermal stress (cf. refs. [6] and [8]). Fig. 5 shows the stress distributions calculated from this work and Iwaki and Kobayashi's work [8], for $P = 0.02$, $\psi_t = 4$, and $H = 1$. Obviously, the thermal stresses are affected by the Biot number H , the Peclet number P , and the dimensionless height of the crystal ψ_t . Fig. 6 shows the distributions of τ_e for $P = 0.02$, $\psi_t = 6$, under $H = 0.5$, 1.0 , and 1.5 , respectively. Generally speaking, the equivalent shear stress increases with H , because, as mentioned previously, large H induces larger central height of the interface and hence, denser isothermal lines. In turn, denser isothermal lines lead to larger temperature gradient and consequently, larger thermal stresses. Fig. 7 shows the dependences of the maximum center τ_e ($\rho = 0$) and the edge τ_e ($\rho = 1$) on the Biot number H , in the cases with and without curved interface, respectively. It is seen that although the trends in both causes are qualitatively similar, the differences between them are significant.

Fig. 8 shows the distributions of τ_e for $H = 1$, $\psi_t = 4$ under $P = 0.01$, 0.02 , and 0.04 . To see the effect of P on the maximum center τ_e and on the maximum edge τ_e , we sketch fig. 9. From fig. 9, we realize that the Peclet number affects the maximum center τ_e , and the maximum edge τ_e only little. This only indicates that the case $\psi_t = 4$ is close to the steady-state case since P theoretically dominates the transient thermal behavior.

Fig. 10 shows the distributions of τ_e for $H = 1$ and $P = 0.02$ under $\psi = t = 2, 4$ and 6 . The effects of the dimensionless height of the crystal on the maximum center τ_e and the maximum edge τ_e are shown in fig. 11.

It is interesting to see that, in the case of a curved interface, the maximum edge τ_e decreases as ψ_t increases, while, in the case of planar interface, the maximum edge τ_e is almost independent of ψ_t . The decrease of the maximum edge τ_e in the case of the curved interface will slow down and the maximum edge τ_e will approach a constant as ψ_t becomes large, because

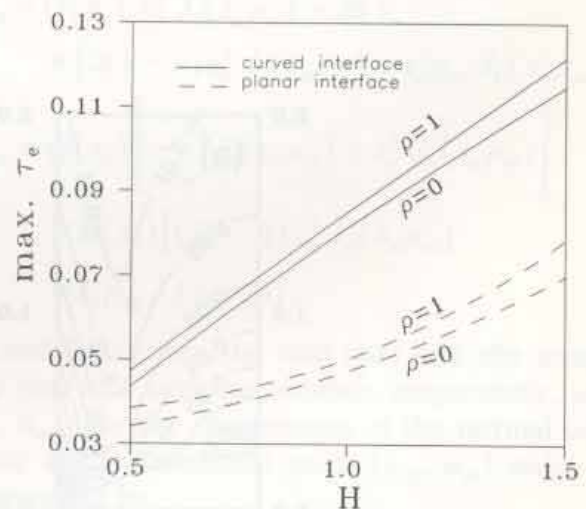


Fig. 7. Variations of maximum center τ_e and maximum edge τ_e with H ; $P = 0.02$.

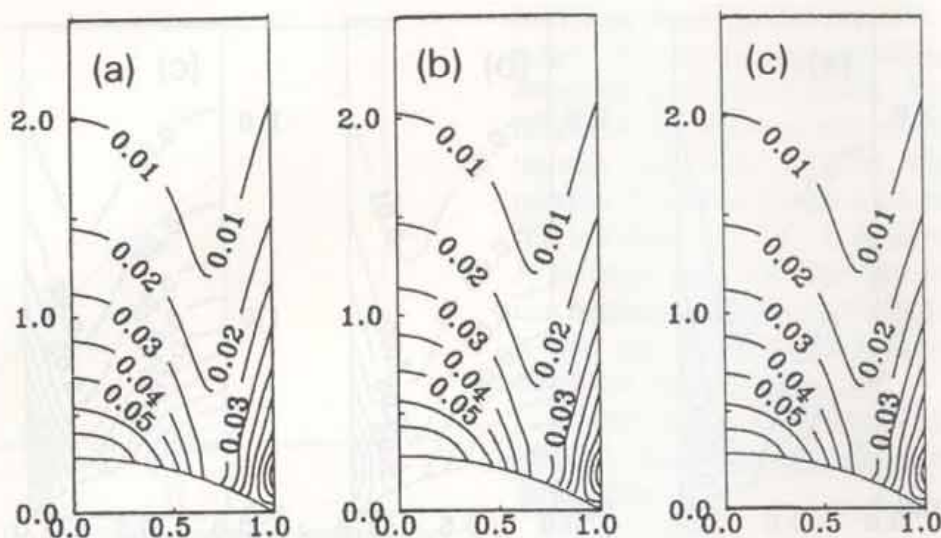


Fig. 8. Distributions of τ_e for $H = 1$ and $\psi_i = 4$ when: (a) $P = 0.01$; (b) $P = 0.02$; (c) $P = 0.04$.

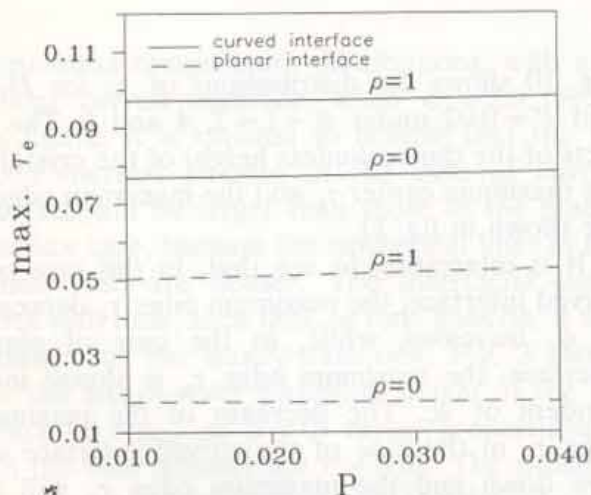


Fig. 9. Variations of maximum center τ_e and maximum edge τ_e with P ; $H = 1$.

as ψ_i increases, one moves closer to the steady-state case.

5. Conclusion

In this paper, we undertake the quasi-steady-state analysis on the thermal stresses of the Czochralski-grown crystal with finite length. Analytical solutions are obtained, although only numerical results can be finally reached. Under appropriate assumptions on the interfacial boundary condition, the shape of the solid-liquid interface is shown to be parabolic-like. The shape of the interface is greatly affected by the Biot

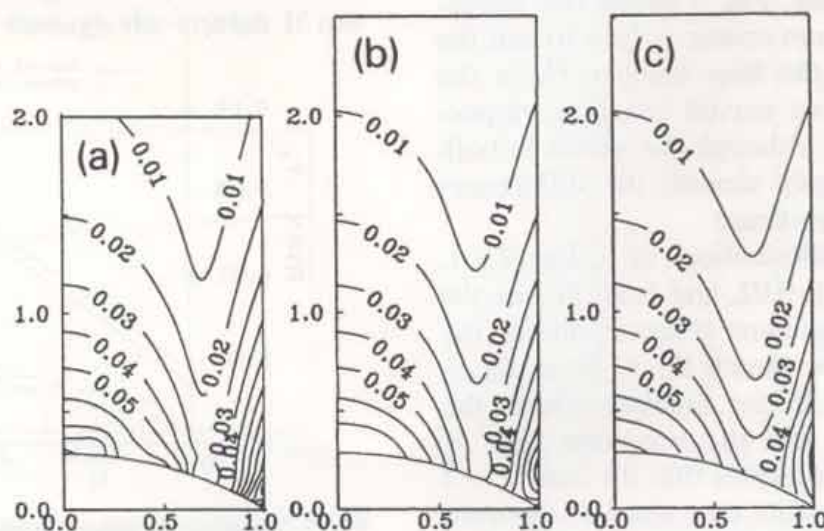


Fig. 10. Distributions of τ_e for $H = 1$ and $P = 0.02$ when: (a) $\psi_i = 2$; (b) $\psi_i = 4$; (c) $\psi_i = 6$.

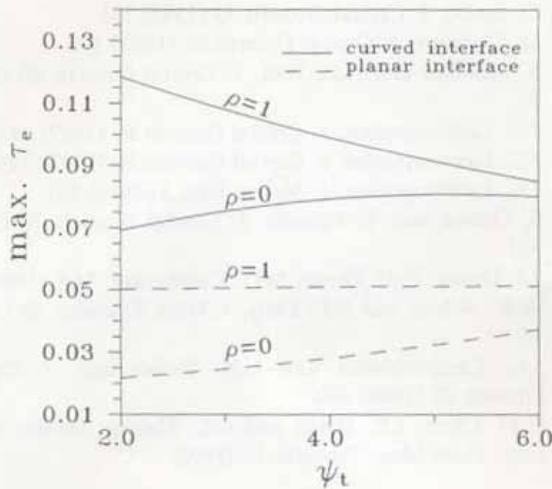


Fig. 11. Variations of maximum center τ_c and maximum edge τ_e with ψ_t ; $H = 1$, $P = 0.02$.

number. In the thermal stress analysis, comparisons between the calculations from the cases with and without curved interface reveal that the trends of variations of the maximum edge τ_e and the maximum center τ_c on H and P are qualitatively similar in both cases. However, the quantitative differences between them are significant, more than 50%. In addition, in the quasi-steady-state analysis, we find that the effect of the crystal length is also significant, especially when the length is short.

Appendix

The corresponding elements of $[S]_{4 \times 4}$, $[U]_{4 \times 1}$, and $[V]_{4 \times 1}$ in (3.24) are:

$$\begin{aligned} S_{11} &= n_{\psi m} \operatorname{Re}(X_{m,n} e^{s_n(\psi_m - \psi_t)}) \\ &\quad + n_{\rho m} \operatorname{Re}(Y_{m,n} e^{s_n(\psi_m - \psi_t)}), \\ S_{12} &= -n_{\psi m} \operatorname{Im}(X_{m,n} e^{s_n(\psi_m - \psi_t)}) \\ &\quad - n_{\rho m} \operatorname{Im}(Y_{m,n} e^{s_n(\psi_m - \psi_t)}), \\ S_{13} &= n_{\psi m} \operatorname{Re}(X_{m,n} e^{-s_n(\psi_m - \psi_t)}) \\ &\quad - n_{\rho m} \operatorname{Re}(Y_{m,n} e^{-s_n(\psi_m - \psi_t)}), \\ S_{14} &= -n_{\psi m} \operatorname{Im}(X_{m,n} e^{-s_n(\psi_m - \psi_t)}) \\ &\quad + n_{\rho m} \operatorname{Im}(Y_{m,n} e^{-s_n(\psi_m - \psi_t)}), \end{aligned}$$

$$\begin{aligned} S_{21} &= \operatorname{Re}(X_{m,n}), \quad S_{22} = -\operatorname{Im}(X_{m,n}), \\ S_{23} &= \operatorname{Re}(X_{m,n}), \quad S_{24} = -\operatorname{Im}(X_{m,n}), \\ S_{31} &= n_{\rho m} \operatorname{Re}(Z_{m,n} e^{s_n(\psi_m - \psi_t)}) \\ &\quad + n_{\psi m} \operatorname{Re}(Y_{m,n} e^{s_n(\psi_m - \psi_t)}), \\ S_{32} &= -n_{\rho m} \operatorname{Im}(Z_{m,n} e^{s_n(\psi_m - \psi_t)}) \\ &\quad - n_{\psi m} \operatorname{Im}(Y_{m,n} e^{s_n(\psi_m - \psi_t)}), \\ S_{33} &= n_{\rho m} \operatorname{Re}(Z_{m,n} e^{-s_n(\psi_m - \psi_t)}) \\ &\quad - n_{\psi m} \operatorname{Re}(Y_{m,n} e^{-s_n(\psi_m - \psi_t)}), \\ S_{34} &= -n_{\rho m} \operatorname{Im}(Z_{m,n} e^{-s_n(\psi_m - \psi_t)}) \\ &\quad + n_{\psi m} \operatorname{Im}(Y_{m,n} e^{-s_n(\psi_m - \psi_t)}), \\ S_{41} &= \operatorname{Re}(Y_{m,n}), \quad S_{42} = -\operatorname{Im}(Y_{m,n}), \\ S_{43} &= -\operatorname{Re}(Y_{m,n}), \quad S_{44} = \operatorname{Im}(Y_{m,n}), \\ U_{11} &= \operatorname{Re}(L_n), \quad U_{21} = \operatorname{Im}(L_n), \\ U_{31} &= \operatorname{Re}(L_n), \quad U_{41} = \operatorname{Im}(L_n), \\ V_{11} &= -n_{\psi m}(\sigma_{0\psi\psi}^* + \sigma_{1\psi\psi}^*) - n_{\rho m}(\sigma_{0\rho\rho}^* + \sigma_{1\rho\rho}^*), \\ V_{21} &= -\sigma_{0\psi\psi}^* - \sigma_{1\psi\psi}^*, \\ V_{31} &= -n_{\psi m}(\sigma_{0\rho\psi}^* + \sigma_{1\rho\psi}^*) - n_{\rho m}(\sigma_{0\rho\rho}^* + \sigma_{1\rho\rho}^*), \\ V_{41} &= -\sigma_{0\rho\psi}^* - \sigma_{1\rho\psi}^*, \end{aligned}$$

where

$$\begin{aligned} X_{m,n} &= -Q(s_n) s_n^3 J_0(s_n \rho_m) + R(s_n) \\ &\quad \times [2(2 - \nu) s_n^2 J_0(s_n \rho_m) - s_n^3 \rho_m J_1(s_n \rho_m)], \\ Y_{m,n} &= Q(s_n) s_n^3 J_1(s_n \rho_m) - R(s_n) \\ &\quad \times [2(1 - \nu) s_n^2 J_1(s_n \rho_m) + s_n^3 \rho_m J_0(s_n \rho_m)], \\ Z_{m,n} &= Q(s_n) \left[\frac{-s_n^2}{\rho_m} J_1(s_n \rho_m) + s_n^3 J_0(s_n \rho_m) \right] \\ &\quad \times R(s_n) [(2\nu - 1) s_n^2 J_0(s_n \rho_m) \\ &\quad + s_n^3 \rho_m J_1(s_n \rho_m)], \end{aligned}$$

Re and Im denote the real part and the imaginary part of a complex number, respectively, and $n_{\rho m}$, $n_{\psi m}$ are the components of the normal unit vector at the interfacial point (ρ_m, ψ_m) which is represented by

$$n_m^{\wedge} = n_{\rho m} e_{\rho}^{\wedge} + n_{\psi m} e_{\psi}^{\wedge}. \quad (\text{A.1})$$

References

- [1] A.S. Jordan, A.R. Von Neida and R. Caruso, *J. Crystal Growth* 76 (1986) 243.
- [2] P. Penning, *Philips Res. Rept.* 13 (1958) 79.
- [3] A.S. Jordan, A.R. Von Neida and R. Caruso, *Bell System Tech. J.* 59 (1980) 593.
- [4] A.S. Jordan, A.R. Von Neida and R. Caruso, *J. Crystal Growth* 70 (1984) 555.
- [5] A.R. Von Neida and A.S. Jordan, *J. Metals* 38 (1986) 35.
- [6] T. Iwaki and N. Kobayashi, *ASME J. Appl. Mech.* 48 (1981) 866.
- [7] N. Kobayashi and T. Iwaki, *J. Crystal Growth* 73 (1985) 96.
- [8] T. Iwaki and N. Kobayashi, *Intern. J. Solid Structures* 22 (1986) 307.
- [9] G. Szabo, *J. Crystal Growth* 73 (1985) 131.
- [10] M. Duseaux, *J. Crystal Growth* 61 (1983) 576.
- [11] S. Motakef and A.F. Witt, *J. Crystal Growth* 80 (1987) 37.
- [12] J.C. Lambropoulos, *J. Crystal Growth* 80 (1987) 245.
- [13] J.C. Lambropoulos, *J. Crystal Growth* 80 (1987) 349.
- [14] J.C. Lambropoulos, *J. Mater. Res.* 3 (1988) 531.
- [15] S. Ozawa and T. Fukuda, *J. Crystal Growth* 76 (1986) 323.
- [16] J.J. Derby, PhD Thesis, MIT, Cambridge, MA (1986).
- [17] W.R. Wilcox and R.L. Duty, *J. Heat Transfer*, 88 (1966) 45.
- [18] J.C. Lambropoulos and C.N. Delametter, *J. Crystal Growth* 92 (1988) 390.
- [19] K.M. Chen, J.Y. Hsieh and C.C. Hwang, *Intern. Commun. Heat Mass Transfer* 19 (1992) 175.