

THE EFFECT OF INTERFACE SHAPE
ON DISLOCATION GENERATION
DURING CRYSTAL GROWTH

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ABSTRACT

We adopt the quasi-steady-state thermoelastic analysis with the effect of interface shape to predict the dislocation density pattern in Czochralski-pulled single crystal. The results show that the dislocation density deduced from the analysis with effect of curved interface is quite different from that with effect of the planar interface. Quantitatively, this difference of the dislocation density on sections near the interface between the two cases (planar and curved interfaces) may exceed more than 20%, under normal operation condition.

1. INTRODUCTION

The dislocations generated during the growth from the melt of semiconductor crystals by the Czochralski method can greatly degrade the electronic properties of the grown material [1]. Although dislocation-free Si is routinely grown, the control of dislocations is more severe in III-V compounds such as GaAs and InP, which have low yield stress near their melting point, unless the lattice is properly hardened [2-5]. The generation of

dislocations has been attributed to excessive thermal stresses by Penning for the growth of Ge [6], and by Jordan et al. for the growth of GaAs and InP [7].

Following the seminal work of Jordan et al. on GaAs [7], several thermal stress calculations have been published. Analytical solutions for the stresses have been presented by Iwaki and Kobayashi [8-10] and by Szabo [11]. Numerical solutions have been presented by Duseaux [12] who examined some limited aspects of the effect of neck geometry, by Motakef and Witt [13] who examined the effect of the encapsulant, and by Lambropoulos [14] 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 [15,16].

A common conclusion of these works [7-17] is that all significant stress variation, including maximum values, occurs within one or two radii from the solid-liquid interface.

All the thermal stress calculations mentioned above assumed that the solid-liquid interface is planar. But in reality, experimental evidence showed that the interface is curved during the growth of GaAs by the liquid encapsulated Czochralski method [18]. Wilcox and Duty [19] solved the steady state problem under the consideration of a heat balance on the melt-solid interface. They showed that the interface is concave into the crystal. For large Biot number and that the shape of the interface is approximately like parabolic. This conclusion was adopted by Lambropoulos et al. [20], who modeled the interface as parabolic and implemented finite element techniques to quantify the effect of the deviation from planarity of the solid-liquid interface on thermal stresses during Czochralski growth. Lambropoulos et al. 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 [19] and of Lambropoulos et al. [20] have neglected the transient term in the governing conduction equation.

In this work, we intend to analyze the quasi-steady-state equation under the consideration of a uniform heat flux through the bottom of the melt-solid interface [21]. While doing this, we expect not only that the transient temperature profiles will be determined, but also that the shape of the interface will simultaneously be determined by imposing a constant melting temperature on it. These results will be shown later on in figures and

we'll see that the shape of the interface is also deduced to be parabolic-like. The radial, tangential, and axial thermal stress components for a growing cylinder in a close form are determined right after the quasi-steady-state temperature profiler are solved. These stresses are then employed in evaluating the 12 resolved shear stress components of the $\{111\}, \langle 1\bar{1}0 \rangle$ slip system causing glide. Following Penning's hypothesis [6], the dislocation density is taken to be proportional to the same of these shear stresses, the total excess shear stress. For this reason, it is convenient for us to only look on the distributions of the total excess shear stress.

2. THEORY

We assume that a uniform heat flux q_0 transfers from the bottom of the crystal and that the constant temperature at the curved interface is the melting point, T_f . The other assumptions are followed after Jordan et al. [7].

Fig.1 sketches the coordinate system relevant to our Czochralski growth model. In the interest of clarity, the vertical axes (Z and s) have been displaced from the crystal axes. If a transform $s = Z + pt$ and dimensionless variables $\Theta = \frac{T - T_s}{T_f - T_s}$, $p_1 = \frac{pr_0}{k}$, $h_1 = r_0 h$, $h_p = \frac{p_1}{2} + h_1$, $\rho = \frac{r}{r_0}$, $\psi = \frac{s}{r_0}$, $\psi_t = \frac{p_1 t}{r_0}$, $Q = \frac{q_0 r_0}{k_s(T_f - T_s)}$ are introduced, the heat conduction equation and all the corresponding boundary conditions will take the forms.

$$\left(\frac{\partial^2 \Theta}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \Theta}{\partial \rho} + \frac{\partial^2 \Theta}{\partial \psi^2} \right) = p_1 \frac{\partial \Theta}{\partial \psi_t}, \quad (1)$$

$$\frac{\partial \Theta}{\partial \rho} + h_1 \Theta|_{\rho=1} = 0, \quad (2a)$$

$$\frac{\partial \Theta}{\partial \psi} + h_1 \Theta|_{\psi=\psi_t} = 0, \quad (2b)$$

$$\frac{\partial \Theta}{\partial \psi}|_{\psi=0} = -Q. \quad (2c)$$

The dimensionless temperature is then sloved as

$$\Theta = e^{\frac{p_1 \psi}{2}} \sum_{n=1}^{\infty} J_0(\rho \alpha_n) \times [A_n \sinh \beta_n(\psi_t - \psi) + B_n \cosh \beta_n(\psi_t - \psi)], \quad (3)$$

where

$$\beta_n^2 = \alpha_n^2 + \left(\frac{p_1}{2}\right)^2. \quad (4)$$

$$A_n = -2h_1 h_p Q \sum_{n=1}^{\infty} \frac{1}{J_0(\alpha_n) X_n} \times \frac{1}{Y_n}, \quad (5)$$

$$B_n = -2h_1 Q \sum_{n=1}^{\infty} \frac{\beta_n}{J_0(\alpha_n) X_n} \times \frac{1}{Y_n}, \quad (6)$$

with

$$X_n = h_1^2 + \alpha_n^2, \quad (7)$$

$$Y_n = \left[\frac{p_1 h_p}{2} - \beta_n^2 \right] \sinh \beta_n \psi_t - \left[\frac{p_1 \beta_n}{2} - h_p \beta_n \right] \cosh \beta_n \psi_t, \quad (8)$$

$$Q = -\frac{1}{2h_1} \frac{1}{\sum_{n=1}^{\infty} \frac{1}{X_n} \times \frac{W_n}{Y_n}}, \quad (9)$$

$$W_n = h_p \sinh \beta_n \psi_t + \beta_n \cosh \beta_n \psi_t, \quad (10)$$

$$V_n = h_p \sinh \beta_n (\psi_t - \psi) + \beta_n \cosh \beta_n (\psi_t - \psi). \quad (11)$$

Furthermore, since the temperature on the curved interface is assume to be T_f , we substitute $\Theta = 1$ into equation (3) and have the equation of the interface expressed as

$$1 = e^{\frac{p_1 \psi}{2}} \frac{\sum_{n=1}^{\infty} J_0(\rho \alpha_n) V_n}{J_0(\alpha_n) X_n} \frac{1}{Y_n} \times \frac{1}{\sum_{n=1}^{\infty} \frac{1}{X_n} \frac{W_n}{Y_n}}. \quad (12)$$

Here we see that equation (12) determines the shape of the interface to be parabolic-like.

Then, assuming that the induced thermal stresses are in the "plane strain" case, the dimensionless axial stress σ_{ψ^*} , the dimensionless radial stress σ_{ρ^*} and the dimensionless tangential stress σ_{θ^*} are [7]:

$$\sigma_{\rho^*} = \frac{\sigma_r(1-\nu)}{aE(T_f - T_a)} = \int_0^1 \Theta \rho d\rho - \frac{1}{\rho^2} \int_0^1 \Theta \rho d\rho \quad (13a)$$

$$\sigma_{\theta^*} = \frac{\sigma_{\theta}(1-\nu)}{aE(T_f - T_a)} = \int_0^1 \Theta \rho d\rho + \frac{1}{\rho^2} \int_0^1 \Theta \rho d\rho - \Theta \quad (13b)$$

$$\sigma_{\psi^*} = \frac{\sigma_z(1-\nu)}{aE(T_f - T_a)} = 2\left(\int_0^1 \Theta \rho d\rho - \Theta\right) \quad (13c)$$

where E , ν , a , are Young's modulus, Poisson's ratio, and the linear thermal expansion coefficient, respectively.

All the integrals in equation (13) can be readily performed by applying equation (3). Hence, the stress components become

$$\sigma_{\rho^*} = e^{\frac{\rho^*}{2}} \sum_{n=1}^{\infty} \frac{1}{J_0(\alpha_n) X_n} \frac{V_n}{Y_n} \times \frac{1}{\sum_{n=1}^{\infty} \frac{1}{X_n} \frac{W_n}{Y_n}} \left[\frac{J_1(\alpha_n)}{\alpha_n} - \frac{J_1(\alpha_n \rho)}{\alpha_n \rho} \right], \quad (14a)$$

$$\sigma_{\theta^*} = e^{\frac{\rho^*}{2}} \sum_{n=1}^{\infty} \frac{1}{J_0(\alpha_n) X_n} \frac{V_n}{Y_n} \times \frac{1}{\sum_{n=1}^{\infty} \frac{1}{X_n} \frac{W_n}{Y_n}} \left[\frac{J_1(\alpha_n)}{\alpha_n} + \frac{J_1(\alpha_n \rho)}{\alpha_n \rho} - J_0(\alpha_n \rho) \right], \quad (14b)$$

$$\sigma_{\psi^*} = e^{\frac{\rho^*}{2}} \sum_{n=1}^{\infty} \frac{1}{J_0(\alpha_n) X_n} \frac{V_n}{Y_n} \times \frac{1}{\sum_{n=1}^{\infty} \frac{1}{X_n} \frac{W_n}{Y_n}} \left[\frac{2J_1(\alpha_n)}{\alpha_n} - J_0(\alpha_n \rho) \right]. \quad (14c)$$

3. RESOLVED SHEAR STRESS

According to Schmid's Law [22], glide occurs when the resolved shear stress (σ_{RS}) exceeds a certain critical value, the so-called critical resolved shear stress. Since the dislocation density d_L is proportional to the glide strain, we may also take it to be proportional to the σ_{RS} within an additive constant.

Slips in GaAs and other semi-conductors crystallizing in the diamond or Zinc blende structure are associated with the $\{111\}, <1\bar{1}0>$ slip system [23]. The $\{111\}, <1\bar{1}0>$ slip system represents 12 permissible glide operations, that is, four $\{111\}$ slip planes, each containing three possible $<1\bar{1}0>$ slip directions.

According to the work of Jordan et al. [7], setting an appropriate coordinates system to perform the stress transformation, we have the proportionality

$$d_L \propto \sigma_{tot^*} \equiv 4|\sigma_{I^*}| + 2[|\sigma_{II^*}| + |\sigma_{III^*}| + |\sigma_{IV^*}| + |\sigma_{V^*}|], \quad (15)$$

where

$$\sigma_{I^*} = \frac{-\sqrt{6}}{6} (\sigma_{\rho^*} - \sigma_{\theta^*}) \cos 2\theta,$$

$$\begin{aligned}
\sigma_{II} &= \frac{\sqrt{6}}{6} [(\sigma_{\psi} - \sigma_{\theta}) - (\sigma_{\rho} - \sigma_{\theta}) \frac{2}{\sqrt{2}} \sin \theta \sin(\theta + \pi/4)], \\
\sigma_{III} &= \frac{\sqrt{6}}{6} [(\sigma_{\psi} - \sigma_{\theta}) - (\sigma_{\rho} - \sigma_{\theta}) \frac{2}{\sqrt{2}} \sin \theta \sin(\theta - \pi/4)], \\
\sigma_{IV} &= \frac{-\sqrt{6}}{6} [(\sigma_{\psi} - \sigma_{\theta}) - (\sigma_{\rho} - \sigma_{\theta}) \frac{2}{\sqrt{2}} \cos \theta \sin(\theta + \pi/4)], \\
\sigma_V &= \frac{-\sqrt{6}}{6} [(\sigma_{\psi} - \sigma_{\theta}) + (\sigma_{\rho} - \sigma_{\theta}) \frac{2}{\sqrt{2}} \cos \theta \sin(\theta - \pi/4)].
\end{aligned}$$

4. RESULTS AND DISCUSSION

Inspecting on equations (3), (14), and (15), we realize that the results of this work are qualitatively like to that Jordan et al. [7] obtained. This means that all the parameters influencing the temperature, the induced thermal stresses, and the dislocation density have the qualitatively same effects. However, results of the present study are quantitatively different from that of Jordan et al. [7]. Fig. 2 ~ Fig. 4 are sketched by computer to compare both the results of this study and the work of Jordan et al.

Fig. 2 show the dimensionless temperature distributions at $t=3600$ sec with isothermal lines under conditions of planar melt-solid interface and curved interface, respectively. The isothermal lines under the conditions of curved interface are denser than those in the planar interface case, both in ψ - and ρ - directions. This means that the temperature gradients in the case of curve interface, both in ψ - and ρ - directions, are larger than those in the case of planar interface. For this reason, 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. Fig. 3 compares the three components of thermal stress, at time $t=3600$ sec and height $\psi = 0.5$, in both the cases. It is obvious that there are apparent differences of the stresses between the two cases. Also at time $t=3600$, the distributions of dislocation density on the section at the height $\psi = 0.5$ is shown in the Fig. 4. There are two diagrams in Fig. 4: the distribution of dislocation density of the planar interface case is on the left and the other is on the right. It can be seen that although both the two diagram possess the same qualitative characteristics, there is obviously quantitative difference between them. The dislocation distribution under the curved interface condition is higher than that in the planar interface case at every point on the section. Comparing both the dislocation density around the peripheries in the $\langle 100 \rangle$ direction, we see that the difference between the dislocation maximums may exceed more than 20%.

5. CONCLUSION

Here we apply the condition of constant heat flux through the plane at $\psi = 0$ to investigate the QSS system with the effect of curved interface. The absolute values of the induced thermal stresses in this case are seen to be larger than those deduced from the assumption of planar interface. The results show that the maximum dislocation density is evaluated to exceed more than 20%, when compared to the result of Jorden et al. [7].

6. NOMENCLATURE

α	linear thermal expansion coefficient,	p	pulling rate, cm/s
$d_{\perp}$	dislocation density,	p_1	dimensionless pulling rate,
E	Young's modulus,	q_0	heat flux, W/cm^2
h	heat transfer coefficient, cm^{-1}	Q_0	dimensionless heat flux,
h_a	heat convection coefficient, $W/cm \cdot K$	r	radial position, cm
h_1	dimensionless heat convection coefficient,	r_0	crystal radius, cm
$h_p = p_1/2 + h_1$		t	time, sec
J_0	bessel function of the first kind with order zero,	T_a	ambient temperature, K
J_1	bessel function of the first kind with order one,	T_f	melting of solid, K
k	thermal diffusivity, cm^2/s	s	height of crystal, cm
k_s	heat conduction coefficient, $W/cm \cdot K$	Z	axial position, cm

Greek symbols

α_n	eigenvalues,	ψ	dimensionless height = s/r_0 ,
ν	Poisson's ratio,	ψ_t	dimensionless height = pt/r_0 ,
σ_r	radial stress,	σ_{ρ}	dimensionless radial stress,
σ_{θ}	tangential stress,	σ_{ψ}	dimensionless axial stress,
σ_z	axial stress,	σ_{θ}	dimensionless tangential stress,
ρ	dimensionless radial,	σ_{tot}	dimensionless the sum of the absolute stress.

7. REFERENCES

- [1] A. S. Jordan, A. R. Von Neida and R. Caruso, *J. Crystal Growth* 76 (1986) 243.
- [2] A. S. Jordan, A. R. Von Neida and R. Caruso, *J. Crystal Growth* 70 (1984) 555.
- [3] A. S. Jordan, G. T. Brown, B. Cockayne, D. Brasen and W. A. Bonner, *J. Appl. Phys.* 58 (1985) 4383.
- [4] S. Guruswamy, R. S. Tsai, K. T. Faber and J. P. Hirth, *J. Appl. Phys.* 62 (1987) 4130.
- [5] A. R. Von Neida and A. S. Jordan, *J. Metals* 38 (1986) 35.
- [6] P. Penning, *Philips Res. Rept.* 13 (1985) 79.
- [7] A. S. Jordan, A. R. Von Neida and R. Caruso, *Bell System Tech. J.* 59 (1980) 593.
- [8] T. Iwaki and N. Kobayashi, *J. Appl. Mech.* 48 (1981) 866.
- [9] T. Iwaki and N. Kobayashi, *J. Crystal Growth* 73 (1985) 96.
- [10] T. Iwaki and N. Kobayashi, *Intern. J. Solids Structures* 22 (1986) 307.
- [11] G. Szabo, *J. Crystal Growth* 73 (1985) 131.
- [12] M. Duseaux, *J. Crystal Growth* 61 (1983) 576.
- [13] S. Motakef and A. F. Witt, *J. Crystal Growth* 80 (1987) 576.
- [14] J. C. Lambropoulos, *J. Crystal Growth* 80 (1987) 245.
- [15] J. C. Lambropoulos, *J. Crystal Growth* 80 (1987) 349.
- [16] J. C. Lambropoulos, *J. Crystal Growth* 80 (1988) 531.
- [17] C. E. Schvezov, I. V. Samarasekera and F. Weinberg, *J. Crystal Growth* 85 (1987) 142.
- [18] S. Ozawa and T. Fukuda, *J. Crystal Growth* 76 (1986) 323.
- [19] W. R. Wilcox and R. L. Duty, *J. Heat Transfer, Trans. ASME*, 88, 45 1966.
- [20] J. C. Lambropoulos and C. N. Delametter, *J. Crystal Growth* 92 (1988) 390.
- [21] W. R. Wilcox, *Preparation and Properties of Solid-State Materials*, vol. 6, 176.
- [22] E. Schmid and W. Boas, *Plasticity of Crystals*, London: Chapman and Hall, 1968.
- [23] D. Laister and G. M. Jenkins, *J. Mater. Sci.*, 8 (1973) 1218.

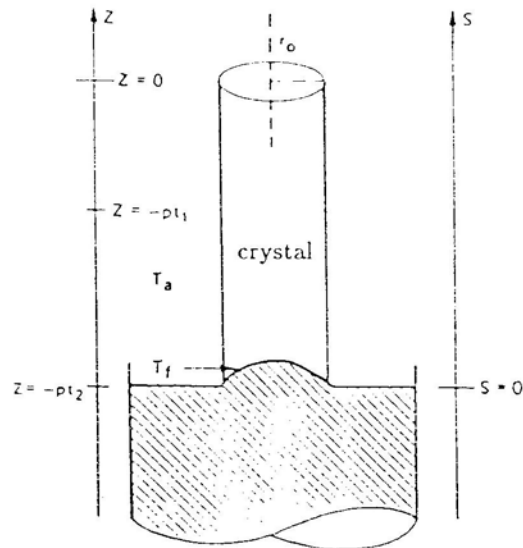


Fig. 1 -Stationary (z) and moving (s) coordinate systems for Czochoalski growth. The stationary and moving systems are anchored at the top-end and solid-liquid interface, respectively. Above the interface, the temperature of the surroundings is uniformly T_a .

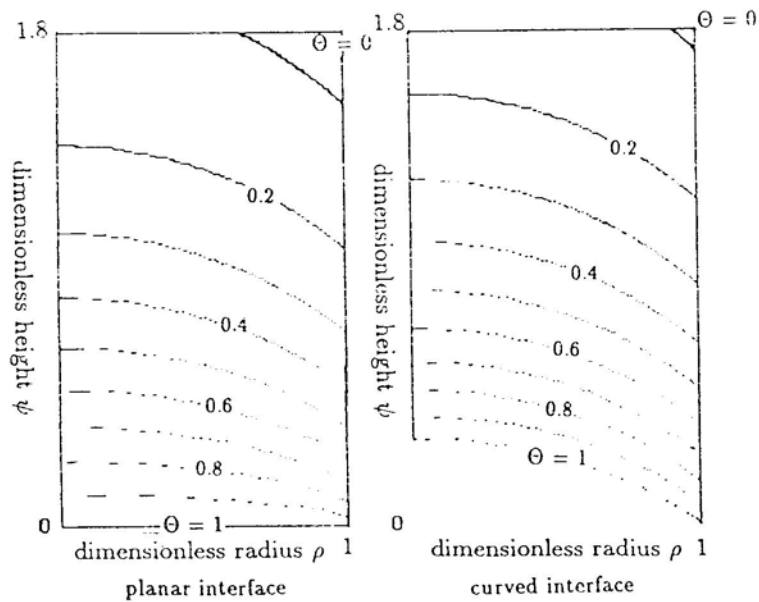


Fig. 2 -Constant dimensionless temperature contour lines in the ψ - ρ plane for GaAs. The relevant parameters are $t = 3600s$, $p = 0.001cm/s$, $r_0 = 2cm$, $k = 0.04cm^2/s$, $h = 0.6cm^{-1}$.

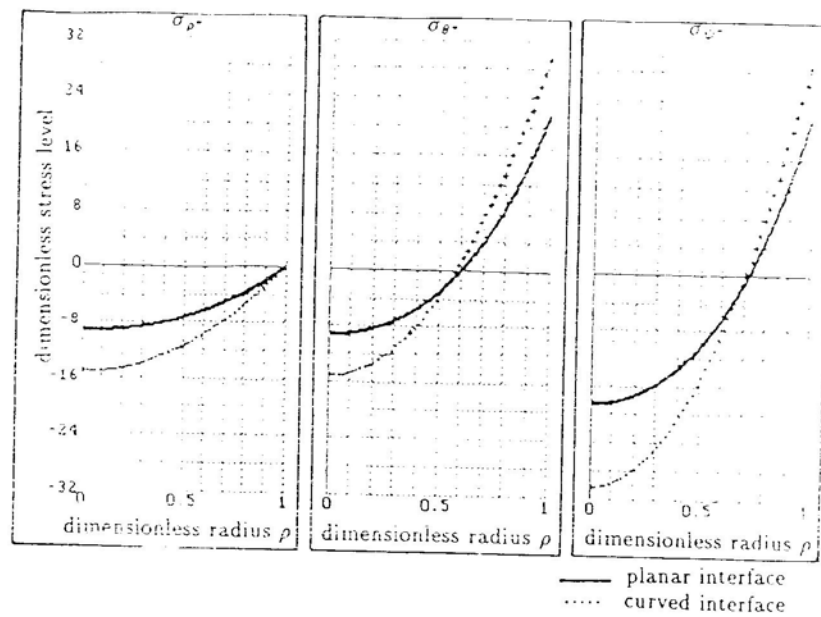


Fig. 3 -Dimensionless radial (σ_{ρ}), tangential (σ_{θ}) and axial (σ_{ψ}) stress levels versus dimensionless radius (ρ) for GaAs at $\psi = 0.5$. The relevant parameters are same as in Fig. 2.

