

Semi-analytic solution for thermoelastic problem with cubic anisotropy

Jinbiao Wu^a, C. Sean Bohun^b, Huaxiong Huang^c

^a*School of Mathematical Sciences, Peking University, Beijing, China 100871.*

^b*Faculty of Science, University of Ontario Institute of Technology, Oshawa, Ontario,
Canada L1H 7K4.*

^c*Department of Mathematics and Statistics, York University, Toronto, Ontario, Canada
M3J 1P3.*

Abstract

In this paper, a semi-analytic thermal stress computation for single crystals with cubic anisotropy is developed, by introducing a new anisotropic factor. Based on a suitable splitting of the differential operators, a convergence series for general elasticity problem with cubic anisotropy is derived. Each term of the series is related to an isotropic elasticity problem. Using the analytic solution to two-dimensional isotropic elasticity problem, semi-analytic solution of elasticity problem cubic anisotropy in a disk is obtained. This procedure can be applied to elastic stress computation with cubic anisotropy under a general setting.

Key words: Crystals, Cubic anisotropy, Thermoelasticity, Stress

PACS: 61.50.A

1 Introduction

Directional growth techniques such as the Czochralski (Cz) method are frequently used to produce high quality single crystals. The thermal stress experienced by the crystal during growth could lead to the generation of structural defects in the crystal (3; 8). By treating the crystal as an isotropic body, Jordan et al. (8) derived analytical formula for thermal stress inside a cylindrical body. Bohun et al. (1) derived semi-analytical formula for thermal stress inside a non-cylindrical crystal with a curved moving interface, also for an isotropic body.

Email addresses: jwu@math.pku.edu.cn (Jinbiao Wu),
Sean.Bohun@uoit.ca (C. Sean Bohun), hhuang@yorku.ca (Huaxiong Huang).

The effect of material anisotropy on thermal stress, on the other hand, could be significant for cylindrical crystals with an underlying cubic lattice structure, as shown in (16; 15). In this paper, we consider a mathematical model for a linear thermoelasticity crystal with cubic anisotropy. Unlike the perturbation solution developed in (16; 15) for weak anisotropy, our solution is valid for all cubic anisotropic materials.

We introduce an anisotropic factor ω , and develop a general series for the solution to the thermoelastic problem with cubic anisotropy, each term of the series is related to an isotropic elasticity problem. Our solution is not restricted to weak anisotropic material, provided that we can find the “closest” isotropic elasticity problem for the anisotropic elasticity problem and regard it as the zero order expansion.

Even though the procedure used in this paper is valid in three-dimensions, the rest part of the paper is devoted to a semi-analytic solution for two-dimensional anisotropic problem on a circular disk. for simplicity and easy validation. The two-dimensional governing equations for different pulling direction are derived based on the plane strain assumption and the differential equations in the cylindrical coordinate system (9).

The analytic solution of the two-dimensional isotropic elastic problem is based on the so-called Papkovitch-Neuber solution (2; 11). A method to obtain analytic solution for a given temperature expression $\Theta_0(r) + \sum_{k=1}^m \Theta_k(r) \cos(n_k \theta + \delta_k)$ is developed in the paper. At the zeroth order, the solution of the anisotropic thermoelastic problem is simply given by the analytic solution of isotropic elastic problem. Higher order corrections are given by a convergence series of solutions of problems similar to the zeroth order isotropic case.

2 General 3-D elasticity problem with cubic anisotropy

In this section we consider the three-dimensional elasticity problem with cubic anisotropy,

$$\nabla \cdot \sigma_{xyz} = F, \quad (x, y, z) \in \Omega, \quad (1)$$

where Ω is a bounded domain, and

$$\sigma_{xyz} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix}.$$

Here the stresses $\sigma = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy})^T$ are related to the strains $e = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{xz}, 2e_{xy})^T$ by $\sigma = Ce$ where

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{pmatrix}. \quad (2)$$

For brevity, we also write the elasticity problem (1) as

$$LU = F, \quad (x, y, z) \in \Omega \quad (3)$$

where the displacement $U = (u, v, w)^T$, the related strains is denoted by $e(U)$. Namely

$$\begin{aligned} e_{xx} &= \frac{\partial u}{\partial x}, & e_{yy} &= \frac{\partial v}{\partial y}, & e_{zz} &= \frac{\partial w}{\partial z}, \\ e_{xy} &= \frac{1}{2} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), & e_{xz} &= \frac{1}{2} \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right), & e_{yz} &= \frac{1}{2} \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right). \end{aligned}$$

The following stress conditions are imposed on the boundary

$$\sigma_{xyz} \mathbf{n} = g, \quad (x, y, z) \in \partial\Omega \quad (4)$$

where $\mathbf{n} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)^T$ is the unit outer normal direction. For the three-dimensional thermoelastic problem with cubic anisotropy as in (9), one has

$$F = \alpha_0(C_{11} + 2C_{12})\nabla\Theta, \quad g = \alpha_0(C_{11} + 2C_{12})\Theta\mathbf{n}$$

where Θ is the temperature field, and α_0 is the thermal expansion coefficient.

For an anisotropic material the quantity $H = 2C_{44} - C_{11} + C_{12} \neq 0$. To find stress of anisotropic body, we split C as $C = C_0 - C_a$ where C_0 is corresponding to an isotropic material, i.e., the corresponding quantity H vanishes. In (16), a splitting with $C_a = \text{diag}\{0, 0, 0, -\frac{H}{2}, -\frac{H}{2}, -\frac{H}{2}\}$ was considered. Since the splitting is not unique, we wish to find a decomposition so that C_0 which is ‘‘close’’ to C . Using the spectral radius of $C_0^{-1}C_a$ ($\rho(C_0^{-1}C_a)$) as a measure of the closeness between C_0 and C , the closest splitting is found to be given by $C_a = \text{diag}\{\frac{H}{2}, \frac{H}{2}, \frac{H}{2}, -\frac{H}{4}, -\frac{H}{4}, -\frac{H}{4}\}$.

To measure the degree of material anisotropy, an anisotropic factor $A = 2C_{44}/(C_{11} -$

Table 1

Anisotropic factors for a variety of cubic crystals. The stiffness constants C_{ij} are expressed in 10^4 MPa

Crystal	C_{11}	C_{12}	C_{44}	A	ω
NaCl	4.86	1.27	1.28	0.71	-0.17
W	50.1	19.8	11.5	0.76	-0.14
C (diamond)	107.9	12.4	57.8	1.21	0.10
Si	16.60	6.40	7.96	1.56	0.22
Ge	12.60	4.40	6.77	1.65	0.25
GaSb	8.83	4.02	4.32	1.80	0.28
GaAs	11.90	5.34	5.96	1.82	0.29
InSb	6.67	3.65	3.02	2.00	0.33
InP	10.11	5.61	4.56	2.03	0.34
InAs	8.34	4.54	3.95	2.08	0.35
Cu	16.48	12.14	7.54	3.21	0.52
Li	1.48	1.25	1.08	9.39	0.81

C_{12}) was introduced in (7; 9). In this paper, we introduce a different anisotropic factor

$$\omega = \frac{H/2}{C_{11} - C_{12} + H/2} = \frac{2C_{44} - C_{11} + C_{12}}{2C_{44} + C_{11} - C_{12}},$$

and it is straightforward to verify that $\omega = (A - 1)/(A + 1)$. Table 1 lists the elasticity constants, A and ω for a variety of cubic crystals.

Symbolically, we can express L and σ_{xyz} as

$$L = L_0 - L_a, \quad \sigma_{xyz} = \sigma_{0,xyz} - \sigma_{a,xyz},$$

corresponding to the decomposition of $C = C_0 - C_a$. Furthermore, we denote U_0 as the solution to

$$L_0 U_0 = F, \quad (x, y, z) \in \Omega; \quad \sigma_{0,xyz} \mathbf{n} = g, \quad (x, y, z) \in \partial\Omega.$$

Having found U_0 , we can formally write $U_{k+1} = \mathcal{N}U_k$ for $k \geq 0$, as the solution to

$$L_0 U_{k+1} = L_a U_k, \quad (x, y, z) \in \Omega; \quad \sigma_{0,xyz}(U_{k+1}) \mathbf{n} = \sigma_{a,xyz}(U_k) \mathbf{n}, \quad (x, y, z) \in \partial\Omega.$$

And the solution to (3-4) is given by,

$$U = U_0 + \mathcal{N}U_0 + \mathcal{N}^2 U_0 + \cdots + \mathcal{N}^n U_0 + \cdots. \quad (5)$$

Under a suitable norm $\|\cdot\|$, it can be shown that $\|U - S_n\| \leq \omega^{n+1}$, where $S_n =$

$U_0 + \mathcal{N}U_0 + \mathcal{N}^2U_0 + \dots + \mathcal{N}^nU_0$, based on factor that $\rho(C_0^{-1}C_a) = \omega$, or

$$\left| \sum_{i=1}^3 \sum_{j=1}^3 C_{a,ij} \xi_i \xi_j \right| \leq \omega \sum_{i=1}^3 \sum_{j=1}^3 C_{0,ij} \xi_i \xi_j, \quad \forall \xi = (\xi_1, \xi_2, \xi_3).$$

Therefore, the series converges when $\omega < 1$.

We note that the series (5) can also be applied in the finite element method to obtain a numerical approximation to the three-dimensional anisotropic elasticity problem, as shown in (16). In this paper, we show that this procedure can be used to obtain an analytic solution to the anisotropic elastic problem. Our solution technique is based on the so-called Papkovitch-Neuber solution (2; 11) which makes use of the analytic solutions to Poisson equation $-\Delta u = f$. Since the analytic solution of the three-dimensional Poisson equation is related to Bessel functions, which loses its superiority in a finite element approach, we will only consider the two dimensional problem in the rest of the paper.

3 2-D thermoelastic equation with cubic anisotropy

In this section we focus on the two dimensional thermoelasticity problem. For simplicity, we evoke the plane strain assumption, namely the displacement is only on plane orthogonal to the pulling direction.

Following (8), we assume that the temperature is given by a general form $\Theta = \Theta_0(r) + \sum_{k=1}^m \Theta_k(r) \cos(n_k \theta + \delta_k)$. The domain is $\Omega = \{r < R\}$, with boundary $\partial\Omega = \{r = R\}$ and the outer normal direction in polar coordinate is $\mathbf{n} = (n_1, n_2)^T = (1, 0)^T$.

It is convenient to express the stress equations in polar coordinates

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = \alpha_0 (C_{11} + 2C_{12}) \frac{\partial \Theta}{\partial r}, \quad r < R \quad (6)$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = \frac{\alpha_0}{r} (C_{11} + 2C_{12}) \frac{\partial \Theta}{\partial \theta}, \quad r < R, \quad (7)$$

and the related boundary conditions are

$$\sigma_{rr} = \alpha_0 (C_{11} + 2C_{12}) \Theta, \quad r = R, \quad (8)$$

$$\sigma_{r\theta} = 0, \quad r = R. \quad (9)$$

Due to material anisotropy, the stress-strain relationship depends on the crystal orientation or the pulling direction during growth, which can be obtained using the plane strain assumption and (24) and (25-28) in the r, θ, z coordinate system. For

brevity, we introduce the following notation before discussing the details

$$C_{a,4} = \begin{pmatrix} c_4 & -c_4 & -s_4 \\ -c_4 & c_4 & s_4 \\ -s_4 & s_4 & -c_4 \end{pmatrix}, \quad C_{a,2} = \begin{pmatrix} -2c_2 & 0 & s_2 \\ 0 & 2c_2 & s_2 \\ s_2 & s_2 & 0 \end{pmatrix}$$

where $c_4 = \cos 4\theta$ and $s_4 = \sin 4\theta$; $c_2 = \cos 2\theta$ and $s_2 = \sin 2\theta$.

3.1 [001] pulling direction

From (25), we have

$$(\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{r\theta})^T = C_{r\theta}(e_{rr}, e_{\theta\theta}, 2e_{r\theta})^T,$$

where

$$\begin{aligned} C_{r\theta} &= \begin{pmatrix} C_{11} + \frac{H}{2} & C_{12} & 0 \\ C_{12} & C_{11} + \frac{H}{2} & 0 \\ 0 & 0 & C_{44} - \frac{H}{4} \end{pmatrix} - \frac{H}{4} \begin{pmatrix} 1 + c_4 & 1 - c_4 & -s_4 \\ 1 - c_4 & 1 + c_4 & s_4 \\ -s_4 & s_4 & -c_4 \end{pmatrix} \\ &= \begin{pmatrix} C_{11} + \frac{H}{4} & C_{12} - \frac{H}{4} & 0 \\ C_{12} - \frac{H}{4} & C_{11} + \frac{H}{4} & 0 \\ 0 & 0 & C_{44} - \frac{H}{4} \end{pmatrix} - \frac{H}{4} C_{a,4} \\ &= C_0 - C_a. \end{aligned}$$

A Poisson ratio ν can be defined according the isotropic coefficients in C_0 . After scaling, we obtain

$$C_{11} = \frac{(1 - \nu)^2}{(1 + \nu)(1 - 2\nu)} - \frac{H}{4}, \quad C_{12} = \frac{\nu(1 - \nu)}{(1 + \nu)(1 - 2\nu)} + \frac{H}{4},$$

and

$$C_{11} + 2C_{12} = \frac{1 - \nu}{1 - 2\nu} + \frac{H}{4}.$$

3.2 [111] pulling direction

Similar to the [001] direction, the stiffness matrix is given by

$$\begin{aligned}
C_{r\theta} &= \begin{pmatrix} C_{11} + \frac{H}{2} & C_{12} & 0 \\ C_{12} & C_{11} + \frac{H}{2} & 0 \\ 0 & 0 & C_{44} - \frac{H}{4} \end{pmatrix} - \frac{H}{12} \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
&= \begin{pmatrix} C_{11} + \frac{H}{2} & C_{12} - \frac{H}{6} & 0 \\ C_{12} - \frac{H}{6} & C_{11} + \frac{H}{2} & 0 \\ 0 & 0 & C_{44} - \frac{H}{6} \end{pmatrix} \\
&= C_0 - C_a.
\end{aligned}$$

Using the Poisson ratio ν , we have

$$C_{11} = \frac{(1-\nu)^2}{(1+\nu)(1-2\nu)} - \frac{H}{2}, \quad C_{12} = \frac{\nu(1-\nu)}{(1+\nu)(1-2\nu)} + \frac{H}{6}$$

and

$$C_{11} + 2C_{12} = \frac{1-\nu}{1-2\nu} - \frac{H}{6}.$$

3.3 [211] pulling direction

In this case,

$$\begin{aligned}
C_{r\theta} &= \begin{pmatrix} C_{11} + \frac{7H}{16} & C_{12} - \frac{3H}{16} & 0 \\ C_{12} - \frac{3H}{16} & C_{11} + \frac{7H}{16} & 0 \\ 0 & 0 & C_{44} - \frac{3H}{16} \end{pmatrix} - \left(-\frac{7H}{48}C_{a,4} + \frac{H}{24}C_{a,2} \right) \\
&= C_0 - C_a.
\end{aligned}$$

Defining the Poisson ratio ν using C_0 , we have

$$C_{11} = \frac{(1-\nu)^2}{(1+\nu)(1-2\nu)} - \frac{7H}{16}, \quad C_{12} = \frac{\nu(1-\nu)}{(1+\nu)(1-2\nu)} + \frac{3H}{16}$$

and

$$C_{11} + 2C_{12} = \frac{1-\nu}{1-2\nu} - \frac{H}{16}.$$

3.4 [110] pulling direction

Finally, we have

$$C_{r\theta} = \begin{pmatrix} C_{11} - \frac{H}{16} & C_{12} - \frac{3H}{16} & 0 \\ C_{12} - \frac{3H}{16} & C_{11} - \frac{H}{16} & 0 \\ 0 & 0 & C_{44} - \frac{H}{16} \end{pmatrix} - \left(\frac{3H}{16}C_{a,4} - \frac{H}{8}C_{a,2} \right)$$

$$= C_0 - C_a.$$

and

$$C_{11} = \frac{(1-\nu)^2}{(1+\nu)(1-2\nu)} + \frac{H}{16}, \quad C_{12} = \frac{\nu(1-\nu)}{(1+\nu)(1-2\nu)} + \frac{3H}{16}$$

and

$$C_{11} + 2C_{12} = \frac{1-\nu}{1-2\nu} + \frac{7H}{16}.$$

Based on these matrix decompositions for $C_{r\theta}$, we can work out the solution series as (5) systematically for a variety of pulling directions.

4 Approximate solution

As an illustration of the method, in this section we derive the solutions up to the first order. The zeroth order approximation is given by U_0 , and the first order approximation is given by $U_0 + \mathcal{N}U_0$.

4.1 Solution of a basic problem

We consider the following problem,

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = f_r r^{k-2} \log^l r \cos(n\theta + \delta), \quad r < R, \quad (10)$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = f_\theta r^{k-2} \log^l r \sin(n\theta + \delta), \quad r < R, \quad (11)$$

with the boundary condition

$$\sigma_{rr} = g_r \cos(n\theta + \delta), \quad r = R, \quad (12)$$

$$\sigma_{r\theta} = g_\theta \sin(n\theta + \delta), \quad r = R, \quad (13)$$

where $f_r, f_\theta, g_r, g_\theta$ and δ are given constants, $k-2, l, n$ are non-negative integers. Here the stress-strain relationship corresponds to isotropic part C_0 in subsection 3.1-3.4.

General speaking, to obtain the solution for the elasticity problem (10-13), first we need to find a particular solution \mathbf{w}_p which satisfies equations (10) and (11),

but not necessary the boundary conditions (12) and (13).¹ Then we consider the homogeneous version of the stress equations with the following modified boundary conditions,

$$\begin{aligned}\sigma_{rr} &= g_r \cos(n\theta + \delta) - \sigma_{rr}(\mathbf{w}_p), & r = R, \\ \sigma_{r\theta} &= g_\theta \sin(n\theta + \delta) - \sigma_{r\theta}(\mathbf{w}_p), & r = R,\end{aligned}$$

where $\sigma_{rr}(\mathbf{w}_p) = \tilde{g}_r \cos(n\theta + \delta)$, $\sigma_{r\theta}(\mathbf{w}_p) = \tilde{g}_\theta \sin(n\theta + \delta)$ on $r = R$, and \tilde{g}_r and \tilde{g}_θ are constants. This problem can be solved by the technique discussed in section 6.2, and we denote the solution by \mathbf{w}_h . The solution to (10) and (11) with boundary conditions (12) and (13) is a linear combination of the two, i.e., $\mathbf{w}_p + \mathbf{w}_h$.

4.2 Zero order approximation U_0

By the procedure described in section 4.1, we can obtain the zero order solution by substituting the temperature $\Theta = \Theta_0(r) + \sum_{k=1}^m \Theta_k(r) \cos(n_k\theta + \delta_k)$ into the following equations and boundary conditions

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = \alpha_0(C_{11} + 2C_{12}) \frac{\partial \Theta}{\partial r}, \quad r < R, \quad (14)$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = \frac{\alpha_0}{r}(C_{11} + 2C_{12}) \frac{\partial \Theta}{\partial \theta}, \quad r < R, \quad (15)$$

with the boundary condition

$$\sigma_{rr} = \alpha_0(C_{11} + 2C_{12})\Theta, \quad r = R, \quad (16)$$

$$\sigma_{r\theta} = 0, \quad r = R. \quad (17)$$

4.3 First order correction $\mathcal{N}U_0$

Using $\sigma = C_0 e$, we solve

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = L_a^r(U_0), \quad r < R, \quad (18)$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = L_a^\theta(U_0), \quad r < R, \quad (19)$$

with the boundary condition

$$\sigma_{rr} = \sigma_{a,rr}(U_0), \quad r = R, \quad (20)$$

$$\sigma_{r\theta} = \sigma_{a,r\theta}(U_0), \quad r = R. \quad (21)$$

¹ Details are given in section 6.3.

For a given pulling direction, we write $L_a(V) = (L_a^r(V), L_a^\theta(V))$ and $\sigma_a(V)$. From the discussion in section 3.1-3.4, C_a can be written into a linear combination of $C_{a,2}$ and $C_{a,4}$. It is easy to verify that $L_{a,4}(V)$ and $\sigma_{a,4}(V)$ have terms related to $\cos((n+4)\theta+\delta)$, $\sin((n+4)\theta+\delta)$ and $\cos((n-4)\theta+\delta)$, $\sin((n-4)\theta+\delta)$. For example, $L_a(\mathbf{v})$ and $(\sigma_{a,rr}(V), \sigma_{a,r\theta}(V))^T$ with $V = (v^r, v^\theta) = (D_1 r^k \cos(n\theta + \delta), D_2 r^k \sin(n\theta + \delta))$ are given by

$$\begin{aligned} L_a(V) &= \frac{1}{2} r^{k-2} (D_1 + D_2) (k-1-n)(k-3-n) \begin{pmatrix} \cos((n+4)\theta + \delta) \\ -\sin((n+4)\theta + \delta) \end{pmatrix} \\ &\quad + \frac{1}{2} r^{k-2} (D_1 - D_2) (k-1+n)(k-3+n) \begin{pmatrix} \cos((n-4)\theta + \delta) \\ \sin((n-4)\theta + \delta) \end{pmatrix}, \\ \begin{pmatrix} \sigma_{a,rr}(V) \\ \sigma_{a,r\theta}(V) \end{pmatrix} &= \frac{1}{2} r^{k-1} (D_1 + D_2) (k-1-n) \begin{pmatrix} \cos((n+4)\theta + \delta) \\ -\sin((n+4)\theta + \delta) \end{pmatrix} \\ &\quad + \frac{1}{2} r^{k-1} (D_1 - D_2) (k-1+n) \begin{pmatrix} \cos((n-4)\theta + \delta) \\ \sin((n-4)\theta + \delta) \end{pmatrix}. \end{aligned}$$

Remark 4.1 *With the displacement solution in hand, we can compute stress using the stress-strain relationship (24-27). The thermal effect due to $-(C_{11} + 2C_{12})\Theta$ will be added to yield the total stresses (9). The axial stress σ_{zz} will be modified by Saint Venant's principle.*

5 Computational results and discussion

A characteristic amount of stress can be assigned to each point with the von Mises stress which satisfies

$$\begin{aligned} 2\sigma_{\text{vm}}^2 &= (\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2 \\ &= (\sigma_{rr} - \sigma_{\phi\phi})^2 + (\sigma_{rr} - \sigma_{zz})^2 + (\sigma_{\phi\phi} - \sigma_{zz})^2 + 6\sigma_{r\phi}^2 \end{aligned} \quad (22)$$

where $\sigma_1, \sigma_2, \sigma_3$ denote the eigenvalues of the total stress tensor.

The preferred method of dislocation generation in all III-V semiconductors, is through the generation of slip defects, in particular the $\{111\}$, $\langle 1\bar{1}0 \rangle$ slip system (1). Consisting of four glide planes within which atoms can slip in one of three directions, the resolved stress σ_{rs} , in a particular slip direction \vec{g} within the glide plane with normal is given by

$$\sigma_{\text{rs}} = \vec{g}^T U_{\text{p}}^T Q^T \sigma^{\text{tot}} Q U_{\text{p}} \vec{n}.$$

The matrix U_{p} rotates vectors from the crystallographic frame to the solidification frame so that for a given pulling direction, the rows of U_{p} are the vectors \mathbf{a} , \mathbf{b} and \mathbf{p} .

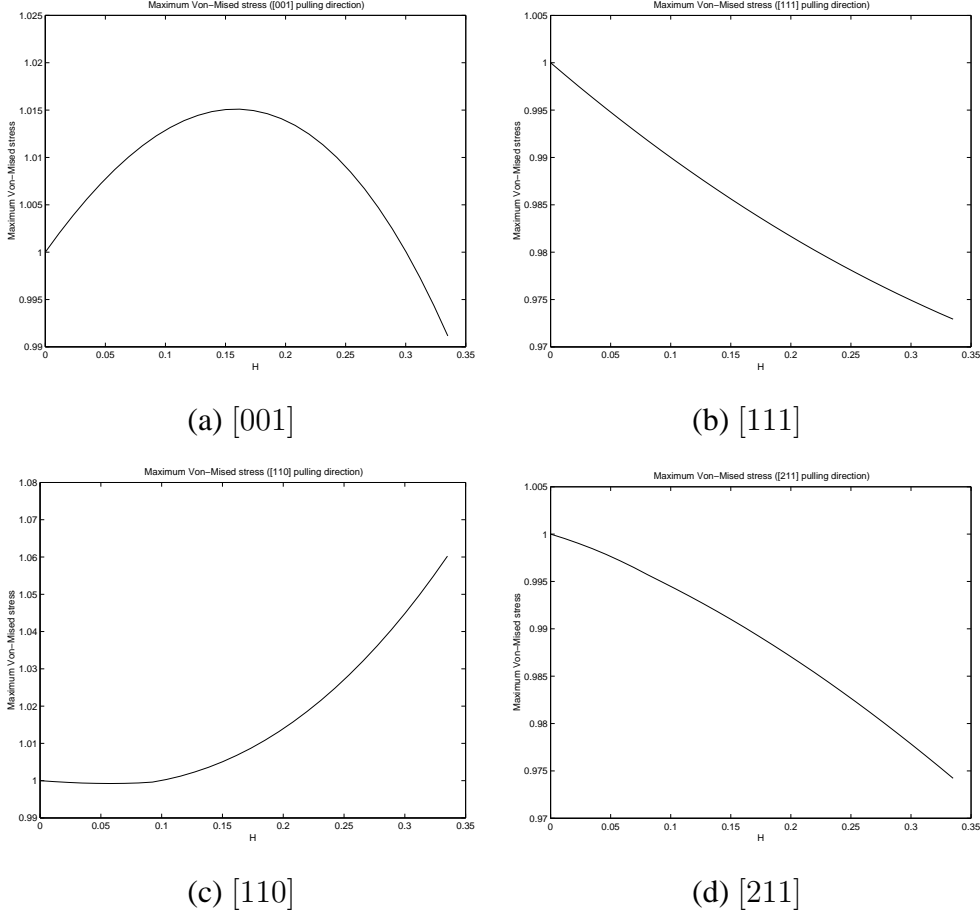


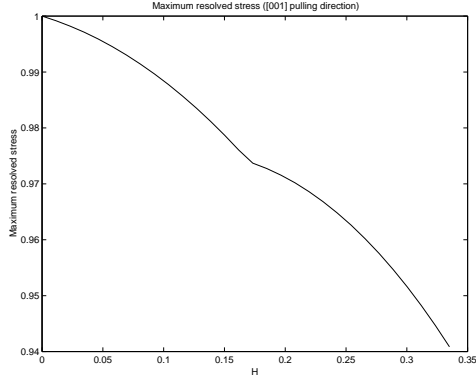
Fig. 1. Maximum Von-Mises stress as a function of H .

If the stress tensor σ^{tot} is expressed in the (r, ϕ, z) coordinates, Q is the coordinate transformation matrix that takes $(x, y, z) \rightarrow (r, \phi, z)$.

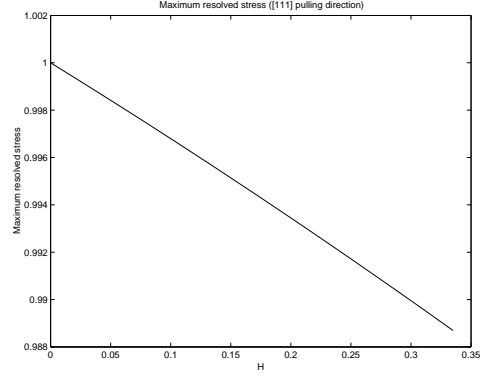
Plastic deformation of the crystal occurs if the stress in any of the 12 slip directions exceeds a maximum value known as the critical resolved shear stress, σ_{crss} . To leading order, the actual density of dislocations suffered by the crystal is proportional to the total excess stress at any given point within the crystal. In this sense, an estimation of where dislocations are likely to occur is given by the distribution of the total absolute resolved stress

$$|\sigma_{\text{rs}}^{\text{tot}}| = \sum_{i=1}^{12} \left| \vec{g}_i^T U_{\text{P}}^T Q^T \sigma^{\text{tot}} Q U_{\text{P}} \vec{n}_i \right|. \quad (23)$$

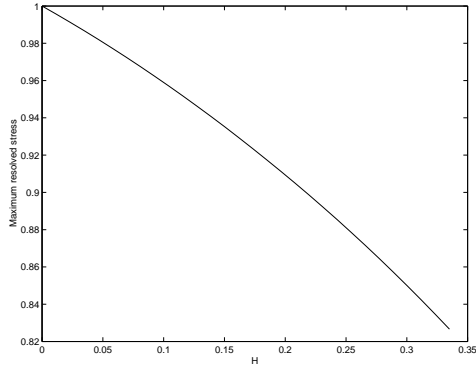
We assume that the temperature $\Theta = r^2$, according to (1). The stiffness constants for InSb are $C_{11} = 6.70 \times 10^4$, $C_{12} = 3.65 \times 10^4$, $C_{44} = 3.02 \times 10^4$ MPa. In Figs. 1 and 2, maximum Von-Mises stress and the maximum resolved stress respectively (scaling by the related maximum stress when $H = 0$) are shown as a function of H , where $H \in [0, 0.34]$.



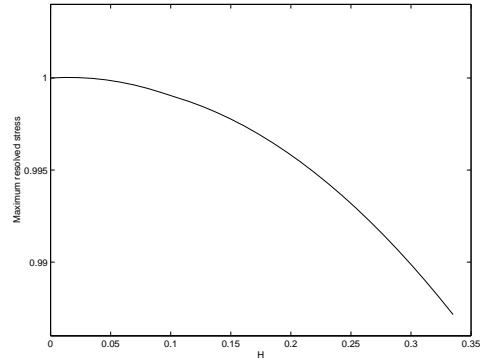
(a) [001]



(b) [111]



(c) [110]



(d) [211]

Fig. 2. Maximum resolved stress as a function of H .

6 Computational details

6.1 Stress-strain relationship in a cylindrical coordinate system

In this subsection, we give the stress-strain relationship in the cylindrical coordinate system. In particular, we derive the expression for C_a since C_0 is corresponding to an isotropic material and independent of the coordinator systems. Assume

$$\sigma_{r\theta z} = C_{r\theta z} e_{r\theta z} = (C_0 - C_{a,r\theta z}) e_{r\theta z}, \quad (24)$$

where

$$\sigma_{r\theta z} = (\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{zz}, \sigma_{\theta z}, \sigma_{rz}, \sigma_{r\theta})^T, \quad e_{r\theta z} = (e_{rr}, e_{\theta\theta}, e_{zz}, 2e_{\theta z}, 2e_{rz}, 2e_{r\theta})^T.$$

For [001] pulling direction, we choose the z -direction as [001], and the directions

[100] and [010] correspond to $\theta = 0$ and $\theta = \pi/2$, respectively. $C_{a,r\theta z}$ is given by

$$\frac{1}{4}H \begin{pmatrix} 1 + c_4 & 1 - c_4 & 0 & 0 & 0 & -s_4 \\ 1 - c_4 & 1 + c_4 & 0 & 0 & 0 & s_4 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ -s_4 & s_4 & 0 & 0 & 0 & -c_4 \end{pmatrix} \quad (25)$$

where $c_4 = \cos 4\theta$ and $s_4 = \sin 4\theta$.

For [111] pulling direction, the z -direction is [111], and $[11\bar{2}]$ and $[\bar{1}10]$ are the directions corresponded to $\theta = 0$ and $\theta = \pi/2$, respectively. In this case $C_{a,r\theta z}$ is written as

$$\frac{H}{6} \begin{pmatrix} 0 & 1 & 2 & \sqrt{2}s_3 & -\sqrt{2}c_3 & 0 \\ 1 & 0 & 2 & -\sqrt{2}s_3 & \sqrt{2}c_3 & 0 \\ 2 & 2 & -1 & 0 & 0 & 0 \\ \sqrt{2}s_3 & -\sqrt{2}s_3 & 0 & \frac{1}{2} & 0 & \sqrt{2}c_3 \\ -\sqrt{2}c_3 & \sqrt{2}c_3 & 0 & 0 & \frac{1}{2} & \sqrt{2}s_3 \\ 0 & 0 & 0 & \sqrt{2}c_3 & \sqrt{2}s_3 & -\frac{1}{2} \end{pmatrix} \quad (26)$$

where $c_3 = \cos 3\theta$ and $s_3 = \sin 3\theta$.

For [211] pulling direction, the z -direction is [211], and we choose $\theta = 0$ and $\theta = \pi/2$ to correspond to $[1\bar{1}\bar{1}]$ and $[01\bar{1}]$ respectively. $C_{a,r\theta z}$ is given by

$$H \begin{pmatrix} c^2 - \frac{7}{6}c^4 & \frac{1}{3} + \frac{7}{6}c^4 - \frac{7}{6}c^2 & \frac{1}{6} + \frac{1}{6}c^2 & \frac{\sqrt{2}}{6}s(1 - 3c^2) & -\frac{\sqrt{2}}{2}cs^2 & \frac{1}{6}cs(7c^2 - 3) \\ \frac{1}{3} + \frac{7}{6}c^4 - \frac{7}{6}c^2 & \frac{4}{3}c^2 - \frac{7}{6}c^4 - \frac{1}{6} & \frac{1}{3} - \frac{1}{6}c^2 & \frac{\sqrt{2}}{2}sc^2 & \frac{\sqrt{2}}{6}c(2 - 3c^2) & \frac{1}{6}cs(4 - 7c^2) \\ \frac{1}{6} + \frac{1}{6}c^2 & \frac{1}{3} - \frac{1}{6}c^2 & 0 & -\frac{\sqrt{2}}{6}s & \frac{\sqrt{2}}{6}c & -\frac{1}{6}cs \\ \frac{\sqrt{2}}{6}s(1 - 3c^2) & \frac{\sqrt{2}}{2}sc^2 & -\frac{\sqrt{2}}{6}s & \frac{1}{12} - \frac{1}{6}c^2 & -\frac{1}{6}cs & \frac{\sqrt{2}}{6}c(2 - 3c^2) \\ -\frac{\sqrt{2}}{2}cs^2 & \frac{\sqrt{2}}{6}c(2 - 3c^2) & \frac{\sqrt{2}}{6}c & -\frac{1}{6}cs & \frac{1}{6}c^2 - \frac{1}{12} & \frac{\sqrt{2}}{6}s(1 - 3c^2) \\ \frac{1}{6}cs(7c^2 - 3) & \frac{1}{6}cs(4 - 7c^2) & -\frac{1}{6}cs & \frac{\sqrt{2}}{6}c(2 - 3c^2) & \frac{\sqrt{2}}{6}s(1 - 3c^2) & \frac{7}{6}c^4 - \frac{7}{6}c^2 + \frac{1}{12} \end{pmatrix} \quad (27)$$

where $c = \cos \theta$ and $s = \sin \theta$.

For [110] pulling direction, the z -direction is [110], and [001] and $[1\bar{1}0]$ are the

directions corresponded to $\theta = 0$ and $\theta = \pi/2$, respectively. $C_{a,r\theta z}$ is given by

$$H \begin{pmatrix} -\frac{3}{2}c^2s^2 + \frac{1}{2}c^2 & \frac{3}{2}c^2s^2 & 1 - \frac{1}{2}c^2 & 0 & 0 & -\frac{3}{2}c^3s + \frac{1}{2}cs \\ \frac{3}{2}c^2s^2 & \frac{3}{2}c^4 - 2c^2 + \frac{1}{2} & \frac{1}{2}c^2 & 0 & 0 & \frac{3}{2}c^3s - cs \\ 1 - \frac{1}{2}c^2 & \frac{1}{2}c^2 & 0 & 0 & 0 & \frac{1}{2}cs \\ 0 & 0 & 0 & \frac{1}{2}c^2 - \frac{1}{4} & \frac{1}{2}cs & 0 \\ 0 & 0 & 0 & \frac{1}{2}cs & -\frac{1}{2}c^2 + \frac{1}{4} & 0 \\ -\frac{3}{2}c^3s + \frac{1}{2}cs & \frac{3}{2}c^3s - cs & \frac{1}{2}cs & 0 & 0 & \frac{3}{2}c^2s^2 - \frac{1}{4}. \end{pmatrix} \quad (28)$$

6.2 The solution to the 2-d homogeneous elasticity problem

In this subsection, we consider the solution to the following homogeneous equation,

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0, \quad r < R, \quad (29)$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = 0, \quad r < R, \quad (30)$$

with the boundary conditions,

$$\sigma_{rr} = g_r \cos(n\theta + \delta), \quad r = R, \quad (31)$$

$$\sigma_{r\theta} = g_\theta \sin(n\theta + \delta), \quad r = R. \quad (32)$$

When $n = 0$, we have $g_\theta = 0$ for the well-posedness of the elasticity problem (29-32). The solution is given by

$$w_h^r = g_r \frac{1 + \nu}{(1 - \nu)} (1 - 2\nu) r \cos \delta,$$

$$w_h^\theta = 2g_r (1 + \nu) r \sin \delta.$$

For $n = 1$, we have $g_r = g_\theta$ for the well-posedness of (29-32). The solution is given by

$$w_h^r = \frac{(1 + \nu)(1 - 4\nu)g_r r^2}{2(1 - \nu)R} \cos(\theta + \delta),$$

$$w_h^\theta = \frac{(1 + \nu)(5 - 4\nu)g_r r^2}{2(1 - \nu)R} \sin(\theta + \delta).$$

Finally for $n \geq 2$, the solution is a linear combination of $r^{n+1}((2 - n - \nu) \cos(n\theta + \delta), (n + 4 - 4\nu) \sin(n\theta + \delta))$ and $r^{n-1}(\cos(n\theta + \delta), -\sin(n\theta + \delta))$. More precisely,

it is given by

$$w_h^r = \frac{1+\nu}{2(1-\nu)} \left(\frac{(2-n-4\nu)(g_r+g_\theta)r^{n+1}}{(n+1)R^n} + \frac{(ng_r+(n-2)g_\theta)r^{n-1}}{(n-1)R^{n-2}} \right) \cos(n\theta+\delta),$$

$$w_h^\theta = \frac{1+\nu}{2(1-\nu)} \left(\frac{(n+4-4\nu)(g_r+g_\theta)r^{n+1}}{(n+1)R^n} - \frac{(ng_r+(n-2)g_\theta)r^{n-1}}{(n-1)R^{n-2}} \right) \sin(n\theta+\delta).$$

6.3 Particular solution to the 2-d elasticity problem

In this subsection we detail the particular solutions to

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = f_r r^{k-2} \cos(n\theta + \delta) \log^l r, \quad r < R, \quad (33)$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = f_\theta r^{k-2} \sin(n\theta + \delta) \log^l r, \quad r < R, \quad (34)$$

where $l \geq 0$ is an integer.

For $l = 0$, $|k - n| = 1$ the particular solution to (33) and (34) is a linear combination of $(r^k \cos(n\theta + \delta), 0)$ and $r^k \log r (\zeta \cos(n\theta + \delta), \sin(n\theta + \delta))$ where $\zeta = -1$ if $k = n - 1$, and $\zeta = -(n - 2 + 4\nu)/(n + 4 - 4\nu)$ if $k = n + 1$. In fact $r^k (\zeta \cos(n\theta + \delta), \sin(n\theta + \delta))$ is a solution to the homogeneous two-dimensional elasticity problem. Particular solutions for $l > 0$ are composed of these lower order solutions and a linear combination of $\log^l r (r^k \cos(n\theta + \delta), 0)$ and $r^k \log^{l+1} r (\zeta \cos(n\theta + \delta), \sin(n\theta + \delta))$. Because of this, we define $\mathcal{F}_{n,k,l}(f_r, f_\theta)$ for $k = n \pm 1$ as

$$\mathcal{F}_{n,k,l}(f_r, f_\theta) = r^k \log^l r ((D_1 + D_2 \zeta \log r) \cos(n\theta + \delta), D_2 \log r \sin(n\theta + \delta)),$$

where

$$D_1 = \begin{cases} \frac{1+\nu}{(1-\nu)^2} \frac{(2-3n-4\nu+4\nu n)f_r + (4-4\nu-3n+4\nu n)f_\theta}{8n(n-1)} & k = n - 1, \\ \frac{1+\nu}{(1-\nu)^2} \frac{(3-4\nu)n^2(f_r+f_\theta) + 8(n+1)(1-2\nu)(1-\nu)(f_r-f_\theta)}{8n(n+1)(n+4-4\nu)}, & k = n + 1, \end{cases} \quad (35)$$

$$D_2 = \begin{cases} -\frac{1+\nu}{(1-\nu)^2} \frac{(n+2-4\nu)f_r + (n-4+4\nu)f_\theta}{8(l+1)(n-1)}, & k = n - 1, \\ \frac{1+\nu}{(1-\nu)^2} \frac{(n+4-4\nu)(f_r+f_\theta)}{8(l+1)(n+1)}, & k = n + 1, \end{cases} \quad (36)$$

$$\zeta = \begin{cases} -1, & k = n - 1, \\ -\frac{n-2+4\nu}{n+4-4\nu}, & k = n + 1. \end{cases} \quad (37)$$

In contrast, $\mathcal{F}_{n,k,l}(f_r, f_\theta)$ for $k \neq n \pm 1$ is given by

$$\mathcal{F}_{n,k,l}(f_r, f_\theta) = r^k \log^l r (D_1 \cos(n\theta + \delta), D_2 \sin(n\theta + \delta)),$$

where

$$D_1 = \frac{1 + \nu}{(1 - \nu)^2} \frac{(k^2 - 2k^2\nu - 2n^2 + 2n^2\nu + 2\nu - 1)f_r - (4n\nu + nk - 3n)f_\theta}{((k - n)^2 - 1)((k + n)^2 - 1)}, \quad (38)$$

$$D_2 = \frac{1 + \nu}{(1 - \nu)^2} \frac{(-4n\nu + nk + 3n)f_r + (2k^2 - 2k^2\nu - n^2 + 2n^2\nu + 2\nu - 2)f_\theta}{((k - n)^2 - 1)((k + n)^2 - 1)}. \quad (39)$$

In compact form, we denote by $\mathcal{S}_{n,k,l}(f_r, f_\theta)$ the particular solution to (33) and (34) corresponding to the values of (n, k, l) . When $l = 0$, $\mathcal{S}_{n,k,0}(f_r, f_\theta) = \mathcal{F}_{n,k,0}(f_r, f_\theta)$. Turning to the case $l > 0$, one has

$$\mathcal{S}_{n,k,l}(f_r, f_\theta) = \mathcal{F}_{n,k,l}(f_r, f_\theta) + \mathcal{S}_{n,k,l-1}(g_{r,l}, g_{\theta,l}) + \mathcal{S}_{n,k,l-2}(h_{r,l}, h_{\theta,l}),$$

where

$$\begin{aligned} g_{r,l} &= \begin{cases} \frac{l(1-\nu)^2}{(1+\nu)(1-2\nu)} (-2kD_1 - (l+1)\zeta D_2), & k = n \pm 1, \\ \frac{l(1-\nu)}{2(1+\nu)(1-2\nu)} (-4k(1-\nu)D_1 - nD_2), & k \neq n \pm 1, \end{cases} \\ g_{\theta,l} &= \begin{cases} \frac{l(1-\nu)}{2(1+\nu)} \left(\frac{n}{1-2\nu} D_1 - (l+1)D_2 \right), & k = n \pm 1, \\ \frac{l(1-\nu)}{2(1+\nu)} \left(\frac{n}{1-2\nu} D_1 - 2kD_2 \right), & k \neq n \pm 1, \end{cases} \\ h_{r,l} &= -\frac{l(l-1)(1-\nu)^2}{(1+\nu)(1-2\nu)} D_1, \\ h_{\theta,l} &= \begin{cases} 0, & k = n \pm 1, \\ -\frac{l(l-1)(1-\nu)}{2(1+\nu)} D_2, & k \neq n \pm 1, \end{cases} \end{aligned}$$

with D_1 and D_2 given by either (35-36) or (38-39), dependent on the values of k and n .

7 Conclusion

In this paper, we have presented a procedure to compute the thermal stress inside a cylindrical body with a cubic lattice structure under a general temperature field. By choosing a suitable splitting of the anisotropic elastic coefficient matrix, the stress can be constructed using a series of the solutions to the isotropic body. The series is convergent as long as the anisotropic factor is less than one, which is the case for most materials of interest. Compared to other splitting techniques which normally assumes weak anisotropy, our approach is valid for all materials as long as a suitable decomposition can be found.

Acknowledgment

The authors would like to acknowledge the support from NSERC of Canada (HH), MITACS of Canada (JW and HH) and MCME of China (JW).

References

- [1] Bohun, C.S., Frigaard, Huang, H. & Liang S. (2006). *A Semianalytical Thermal Stress Model for the Czochralski Growth of Type III-V Compounds*. SIAM Journal of Applied Mathematics, 66(5), 1533-1562.
- [2] Boley, B.A & Weiner, J.H. (1997). *Theory of Thermal Stresses*, 3rd. ed. Dover Publications: New York.
- [3] D.E. Bornside, T.A. Kinney and R.A. Brown (1991), *Minimization of thermoelastic stress in Czochralski grown silicon: application of the integrated system model*. J. Cryst. Growth 108, 779-805.
- [4] T.-C. Chen, H.-C. Wu and C.-I. Weng (1997), *The effect of interface shape on anisotropic thermal stress of bulk single crystal during Czochralski growth*, Journal of Crystal Growth, 173, 367-379.
- [5] S. H. Davis (2001), *Theory of Solidification*, Cambridge University Press.
- [6] A. H. England (1971), *Complex Variable Methods in Elasticity*, Wiley-Interscience., London, New York.
- [7] J. Hirth and J. Lothe (1982), *Theory of Dislocations*, 2nd ed., Wiley, New York.
- [8] A.S. Jordan, R. Caruso and A.R. von Neida (1980), *A thermoelastic analysis of dislocation generation in pulled GaAs crystals*. The Bell Syst. Tech. J. 59 (4), 593-637.
- [9] J. C. Lambropoulos (1987), *The isotropic assumption during the Czochralski growth of single semiconductors crystals*, Journal of Crystal Growth, 84, 349-358.
- [10] L.D. Landau and E.M. Lifschitz (1986), *Theory of Elasticity*, Pergamon, Oxford.
- [11] R. Mindlin (1936), *Note on the Galerkin and Papkovitch stress functions*. Bulletin of the American Mathematics Society, 42, 373-376.
- [12] N. Miyazaki (2002), *Development of a thermal stress analysis system for anisotropy single crystal growth*, Journal of Crystal Growth, 236, 455-465.
- [13] J. Nitsche (1981), *On Korn's second inequality*, RAIRO Anal. Numér. 15, 237.
- [14] G. Russo and P. Smereka (2000), *A level-set method for the revolution of faceted crystals*, SIAM J. Sci. Comput., 21 (6), 2073-2095.
- [15] S. Vigdergauz and D. Givoli (1999), *Thermoelastic stresses in a cylinder or disk with cubic anisotropy*. International Journal of Solids and Structures, 36 (14), 2109-2125.

- [16] S. Vigdergauz and D. Givoli (1999), *Thermoelastic stresses in a crystal with weak anisotropy*. Journal of Crystal Growth, 198-199 (part 1), 125-128.