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Semi-analytic solutions for a thermoelastic problem with cubic anisotropy

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ABSTRACT

In this paper, a semi-analytic thermal stress solution is obtained for cylindrical crystals with cubic anisotropy. Based on a suitable splitting of the differential operators, a convergent series for a general elasticity problem with cubic anisotropy is derived. Each term of the series is related to an isotropic elasticity problem, which may be solved analytically. Using the analytic solution to the two-dimensional isotropic elasticity problem, a semi-analytic solution of the elasticity problem with cubic anisotropy in a disk is obtained. The novel feature of this splitting method is its ability to generate higher order terms without difficulty, unlike the perturbation solutions obtained previously where the assumption of weak anisotropy has to be made. Furthermore, for materials with cubic anisotropy the method is guaranteed to converge.

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 [1,2]. By treating the crystal as an isotropic body, Jordan et al. [2] derived an analytical formula for thermal stress inside a cylindrical body. Recently, Bohun et al. [3] derived a semi-analytical formula for thermal stress inside a non-cylindrical crystal with a non-flat crystal–melt interface, also for an isotropic body.

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 Refs. [4,5]. In this paper, we consider a linear thermoelastic mathematical model for a crystal with cubic anisotropy. Unlike the perturbation solution developed in Refs. [4,5] for weak anisotropy, our solution is valid for a wide variety of cubic anisotropic materials.

We start our discussion in a three-dimensional setting in Section 2. We introduce an anisotropic factor ω, and develop a general series for the solution to the thermoelastic problem with cubic anisotropy with each term of the series related to an isotropic elasticity problem. We prove that our solution is not restricted to weakly anisotropic materials and it is valid for all materials with cubic anisotropy. For other materials, our approach is still valid, provided we can find the "closest" isotropic elasticity problem corresponding to the anisotropic elasticity problem and regard it as the zero order expansion.

Even though the procedure developed in this paper is valid in three dimensions, most of the discussion, from Sections 3–5, is devoted to the discussion of the two-dimensional case, for simplicity and easy validation. A detailed derivation of the semi-analytic solution is given for the two-dimensional anisotropic problem on a circular disk. In this case the governing equations for a variety of pulling directions are derived based on the plane strain assumption and the differential equations in the cylindrical coordinate system [6]. In

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Section 6 we provide a proof of convergence for materials with cubic anisotropy and numerical evidence to support the indicated rate of convergence.

The analytic solution of the two-dimensional isotropic elastic problem is based on the so-called Papkovich–Neuber solution [7,8]. A method to obtain the analytic solution for a given temperature expression $\Theta_0(r) + \sum_{k=1}^{m} \Theta_k(r)\cos(n_k\theta + \delta_k)$ is given in the paper. At the zeroth order, the solution of the anisotropic thermoelastic problem is simply given by the analytic solution of an isotropic elasticity problem. Higher order corrections are given by a convergent series of solutions of problems similar to the zeroth order isotropic case.

2. The general three-dimensional elasticity problem with cubic anisotropy

Before continuing we would like to clarify notation used throughout the paper. Whenever possible, we use a normal font for matrices and tensors, bold face for vectors and script face for operators. Superscripts refer to the object under consideration and subscripts refer to the components of the object. An exception is when vectors that have operators as components, in which case we will use script face as well.

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

$$\begin{cases} \dfrac{\partial \sigma_{xx}}{\partial x} + \dfrac{\partial \sigma_{xy}}{\partial y} + \dfrac{\partial \sigma_{xz}}{\partial z} = F_1 \\ \dfrac{\partial \sigma_{xy}}{\partial x} + \dfrac{\partial \sigma_{yy}}{\partial y} + \dfrac{\partial \sigma_{yz}}{\partial z} = F_2 \quad (x,y,z) \in \Omega, \\ \dfrac{\partial \sigma_{xz}}{\partial x} + \dfrac{\partial \sigma_{yz}}{\partial y} + \dfrac{\partial \sigma_{zz}}{\partial z} = F_3 \end{cases} \tag{1}$$

where Ω is a bounded domain. Since the stress and strain tensors are symmetric, their six independent components can be represented as 6×1 vectors. With this notation, the stresses $\boldsymbol{\sigma} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy})^{\mathrm{T}}$ are related to the strains $\mathbf{e} = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{xz}, 2e_{xy})^{\mathrm{T}}$ by $\boldsymbol{\sigma} = C\mathbf{e}$ where

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

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

$$\mathscr{L}\mathbf{U} = \mathbf{F} \quad (x,y,z) \in \Omega, \tag{3}$$

where the force $\mathbf{F} = (F_1, F_2, F_3)^{\mathrm{T}}$, and $\mathscr{L}$ is an operator that acts on the displacement $\mathbf{U} = (u, v, w)^{\mathrm{T}}$ and the related strains denoted by $\mathbf{e}(\mathbf{U})$. Namely

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

The following stress conditions are imposed on the boundary:

$$\begin{cases} \sigma_{xx}n_1 + \sigma_{xy}n_2 + \sigma_{xz}n_3 = g_1 \\ \sigma_{xy}n_1 + \sigma_{yy}n_2 + \sigma_{yz}n_3 = g_2 \quad (x,y,z) \in \partial\Omega, \\ \sigma_{xz}n_1 + \sigma_{yz}n_2 + \sigma_{zz}n_3 = g_3 \end{cases} \tag{4}$$

where $\mathbf{n} = (n_1, n_2, n_3)^{\mathrm{T}}$ is the outward unit normal direction. For brevity, we also write the boundary condition (4) as

$$\mathscr{B}\mathbf{U} = \mathbf{g} \quad (x,y,z) \in \partial\Omega, \tag{5}$$

where $\mathbf{g} = (g_1, g_2, g_3)^{\mathrm{T}}$ and $\mathscr{B}$ is an appropriate operator. For the three-dimensional thermoelastic problem with cubic anisotropy as in Ref. [6], one has

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

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

For an anisotropic material the quantity $H = 2C_{44} - C_{11} + C_{12} \neq 0$. To find the stress of an anisotropic body, we split C as $C = C^0 - C^a$ where C^0 corresponds to an isotropic material, i.e., the corresponding quantity H vanishes. In Ref. [5] a splitting with $C^a = \mathrm{diag}\{0, 0, 0, -\frac{H}{2}, -\frac{H}{2}, -\frac{H}{2}\}$ was considered. Since the splitting is not unique, we wish to find a decomposition so that C^0 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 $C^a = \mathrm{diag}\{\frac{H}{2}, \frac{H}{2}, \frac{H}{2}, -\frac{H}{4}, -\frac{H}{4}, -\frac{H}{4}\}$.

To measure the degree of material anisotropy, an anisotropic factor $A = 2C_{44}/(C_{11} - C_{12})$ was introduced in Refs. [6,9]. In this paper, we introduce a different anisotropic factor

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

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.

Table 1
Anisotropic factors for a variety of cubic crystals

Crystal	C_{11}	C_{12}	C_{44}	A	ω	H
C (diamond)	107.9	12.4	57.8	1.21	0.10	0.17
W	50.1	19.8	11.5	0.76	0.14	−0.14
NaCl	4.86	1.27	1.28	0.71	0.17	−0.20
Si	16.60	6.40	7.96	1.56	0.22	0.28
Ge	12.60	4.40	6.77	1.65	0.25	0.34
GaSb	8.83	4.02	4.32	1.80	0.28	0.35
GaAs	11.90	5.34	5.96	1.82	0.29	0.36
InSb	6.70	3.65	3.02	1.98	0.33	0.37
InP	10.11	5.61	4.56	2.03	0.34	0.38
InAs	8.34	4.54	3.95	2.08	0.35	0.40
Cu	16.84	12.14	7.54	3.21	0.52	0.53
Li	1.48	1.25	1.08	9.39	0.81	0.91

The stiffness constants C_{ij} are expressed in 10^4 MPa and the H values are given by Eq. (11).

Symbolically, we can express $\mathscr{L}$ and $\mathscr{B}$ as

$$\mathscr{L} = \mathscr{L}^0 - \mathscr{L}^a, \quad \mathscr{B} = \mathscr{B}^0 - \mathscr{B}^a$$

corresponding to the decomposition of $C = C^0 - C^a$. Furthermore, we denote $\mathbf{U}_0$ as the solution to

$$\mathscr{L}^0\mathbf{U}_0 = \mathbf{F} \ \ (x,y,z) \in \Omega, \quad \mathscr{B}^0\mathbf{U}_0 = \mathbf{g} \ \ (x,y,z) \in \partial\Omega.$$

Having found $\mathbf{U}_0$, we can formally write $\mathbf{U}_{k+1} = \mathscr{N}\mathbf{U}_k$ for $k \geqslant 0$ as the solution to

$$\mathscr{L}^0\mathbf{U}_{k+1} = \mathscr{L}^a\mathbf{U}_k \quad (x,y,z) \in \Omega,$$

$$\mathscr{B}^0\mathbf{U}_{k+1} = \mathscr{B}^a\mathbf{U}_k \quad (x,y,z) \in \partial\Omega,$$

and the solution to Eqs. (3)–(4) is given by

$$\mathbf{U} = \mathbf{U}_0 + \mathscr{N}\mathbf{U}_0 + \mathscr{N}^2\mathbf{U}_0 + \cdots + \mathscr{N}^n\mathbf{U}_0 + \cdots. \tag{6}$$

Under a suitable norm $\|\cdot\|$, it can be shown that $\|\mathbf{U} - \mathbf{S}_n\| \leqslant \omega^{n+1}\|\mathbf{U}\|$, where $\mathbf{S}_n = \mathbf{U}_0 + \mathscr{N}\mathbf{U}_0 + \mathscr{N}^2\mathbf{U}_0 + \cdots + \mathscr{N}^n\mathbf{U}_0$, based on fact that $\rho((C^0)^{-1}C^a) = \omega$, or equivalently

$$\left|\sum_{i=1}^{6}\sum_{j=1}^{6} C^a_{ij}\xi_i\xi_j\right| \leqslant \omega \sum_{i=1}^{6}\sum_{j=1}^{6} C^0_{ij}\xi_i\xi_j, \quad \forall \boldsymbol{\xi} = (\xi_1,\xi_2,\xi_3,\xi_4,\xi_5,\xi_6)^{\mathrm{T}} \in \mathbb{R}^6.$$

Therefore, the series converges when $\omega < 1$, which is valid for any anisotropic cubic material. The proof of these results is given in Section 6.1.

We note that series (6) can also be applied in the finite element method to obtain a numerical approximation to the three-dimensional anisotropic elasticity problem, as shown in Ref. [5]. 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 Papkovich–Neuber solution [7,8] which makes use of the analytic solutions to Poisson equation $-\Delta u = f$. Even though the analytical solution of the three-dimensional Poisson equation can be obtained using Bessel functions, we will only consider the two-dimensional problem in most of the remainder of the paper.

3. Two-dimensional thermoelastic equation with cubic anisotropy

In this section we focus on the two-dimensional thermoelasticity problem. For simplicity, we invoke the plane strain assumption, namely the displacement is only in the plane orthogonal to the pulling direction. Following Ref. [2], 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 outward unit normal direction in polar coordinates is $\mathbf{n} = (n_1, n_2)^{\mathrm{T}} = (1,0)^{\mathrm{T}}$.

It is convenient to express the stress equations in polar coordinates

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

$$\frac{\partial\sigma_{r\theta}}{\partial r} + \frac{1}{r}\frac{\partial\sigma_{\theta\theta}}{\partial\theta} + \frac{2\sigma_{r\theta}}{r} = \frac{\alpha}{r}(C_{11} + 2C_{12})\frac{\partial\Theta}{\partial\theta}, \quad r < R, \tag{8}$$

and the related boundary conditions are

$$\sigma_{rr} = \alpha(C_{11} + 2C_{12})\Theta, \quad r = R, \tag{9}$$

$$\sigma_{r\theta} = 0, \quad r = R. \tag{10}$$

Due to the material anisotropy, the stress–strain relationship depends on the crystal orientation or the pulling direction during growth, which can obtained using the plane strain assumption, Eqs. (29) and (30)–(33) in the cylindrical (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 $c_4 = \cos 4\theta$, $s_4 = \sin 4\theta$, $c_2 = \cos 2\theta$ and $s_2 = \sin 2\theta$.

3.1. [0 0 1] *pulling direction*

From Eq. (30), we have

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

where

$$C = \begin{pmatrix} C_{11} + \frac{H}{2} & C_{12} & 0 \\ C_{12} & C_{11} + \frac{H}{2} & 0 \\ 0 & 0 & C_{44} - \frac{H}{4} \end{pmatrix} - \frac{H}{4} \begin{pmatrix} 1 + c_4 & 1 - c_4 & -s_4 \\ 1 - c_4 & 1 + c_4 & s_4 \\ -s_4 & s_4 & -c_4 \end{pmatrix} = \begin{pmatrix} C_{11} + \frac{H}{4} & C_{12} - \frac{H}{4} & 0 \\ C_{12} - \frac{H}{4} & C_{11} + \frac{H}{4} & 0 \\ 0 & 0 & C_{44} - \frac{H}{4} \end{pmatrix} - \frac{H}{4} C^{a,4}.$$

We see that for the [0 0 1] pulling direction the isotropic and anisotropic components of $C = C^0 - C^a$ are

$$C^0 = \begin{pmatrix} C_{11} + \frac{H}{4} & C_{12} - \frac{H}{4} & 0 \\ C_{12} - \frac{H}{4} & C_{11} + \frac{H}{4} & 0 \\ 0 & 0 & C_{44} - \frac{H}{4} \end{pmatrix}, \quad C^a = \frac{H}{4} C^{a,4},$$

respectively. A Young's modulus E and Poisson ratio v can be defined[1] using the isotropic coefficients in C^0. The C_{ij} and H are scaled by the factor $(1 - v)/E$ and for the [0 0 1] pulling direction the scaled value of H is

$$\tilde{H} = \frac{(1 - v)}{E} H = \frac{2\left(C_{11} + \frac{H}{4}\right) H}{(2C_{44} + C_{11} - C_{12})\left(C_{11} + 2C_{12} - \frac{H}{4}\right)}. \tag{11}$$

Dropping tildes we obtain

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

and

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

3.2. [1 1 1] *pulling direction*

Similar to the [0 0 1] direction, the stiffness matrix is given by

$$C = \begin{pmatrix} C_{11} + \frac{H}{2} & C_{12} & 0 \\ C_{12} & C_{11} + \frac{H}{2} & 0 \\ 0 & 0 & C_{44} - \frac{H}{4} \end{pmatrix} - \frac{H}{12} \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} C_{11} + \frac{H}{2} & C_{12} - \frac{H}{6} & 0 \\ C_{12} - \frac{H}{6} & C_{11} + \frac{H}{2} & 0 \\ 0 & 0 & C_{44} - \frac{H}{6} \end{pmatrix} = C^0$$

and $C^a = 0$. Using the Poisson ratio v, we have

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

and

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

[1] Note that $C^0_{11} = C_{11} + \frac{H}{4} = E(1 - v)/(1 + v)(1 - 2v)$, $C^0_{12} = C_{12} - \frac{H}{4} = Ev/(1 + v)(1 - 2v)$, $C^0_{44} = C_{44} - \frac{H}{4} = \frac{1}{2}(C^0_{11} - C^0_{12}) = E/2(1 + v)$ and $\tilde{H} = 2\omega(1 - v)H/(1 + v)|H|$.

3.3. [2 1 1] *pulling direction*

In this case,

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

Defining the Poisson ratio v using C^0, we have

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

and

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

3.4. [1 1 0] *pulling direction*

Finally, we have

$$C = \begin{pmatrix} C_{11} + \frac{7H}{16} & C_{12} - \frac{3H}{16} & 0 \\ C_{12} - \frac{3H}{16} & C_{11} + \frac{7H}{16} & 0 \\ 0 & 0 & C_{44} - \frac{3H}{16} \end{pmatrix} - \left(\frac{3H}{16} C^{a,4} - \frac{H}{8} C^{a,2} \right) = C^0 - C^a.$$

After scaling

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

and

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

Based on these matrix decompositions for C, we can systematically work out the solution series given by Eq. (6) for a variety of pulling directions. We note that C^0 is identical for the [2 1 1] and [1 1 0] pulling directions while C^a is slightly different.

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 $\mathbf{U}_0$, and the first order approximation is given by $\mathbf{U}_0 + \mathcal{N}\mathbf{U}_0$.

4.1. *Solution of the basic problem*

We consider the following problem:

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = f_r r^{k-2} \log^l r \cos(n\theta + \delta), \quad r < R, \tag{12}$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = f_\theta r^{k-2} \log^l r \sin(n\theta + \delta), \quad r < R, \tag{13}$$

with the boundary condition

$$\sigma_{rr} = g_r \cos(n\theta + \delta), \quad r = R, \tag{14}$$

$$\sigma_{r\theta} = g_\theta \sin(n\theta + \delta), \quad r = R, \tag{15}$$

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 Sections 3.1–3.4.

Generally speaking, to obtain the solution for the elasticity problem (12)–(15), first we need to find a particular solution $\mathbf{w}^p$ 4(a displacement vector) which satisfies Eqs. (12) and (13), but not necessary the boundary conditions (14) and (15).[2] Then we consider

[2] Details are given in Section 6.4.

the homogeneous version of the stress equations with the following modified boundary conditions:

$$\sigma_{rr} = g_r \cos(n\theta+\delta) - \sigma_{rr}(\mathbf{w}^p), \quad r = R,$$

$$\sigma_{r\theta} = g_\theta \sin(n\theta+\delta) - \sigma_{r\theta}(\mathbf{w}^p), \quad r = R,$$

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 $\tilde{g}_\theta$ are constants. This problem can be solved by the technique discussed in Section 6.3, and we denote the solution by $\mathbf{w}^h$. The solution to Eqs. (12) and (13) with boundary conditions (14) and (15) is a linear combination of the two, i.e., $\mathbf{w}^p + \mathbf{w}^h$.

4.2. Zero order approximation $\mathbf{U}_0$

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:

$$\frac{\partial\sigma_{rr}}{\partial r} + \frac{1}{r}\frac{\partial\sigma_{r\theta}}{\partial\theta} + \frac{\sigma_{rr}-\sigma_{\theta\theta}}{r} = \alpha(C_{11}+2C_{12})\frac{\partial\Theta}{\partial r}, \quad r<R, \tag{16}$$

$$\frac{\partial\sigma_{r\theta}}{\partial r} + \frac{1}{r}\frac{\partial\sigma_{\theta\theta}}{\partial\theta} + \frac{2\sigma_{r\theta}}{r} = \frac{\alpha}{r}(C_{11}+2C_{12})\frac{\partial\Theta}{\partial\theta}, \quad r<R, \tag{17}$$

with the boundary condition

$$\sigma_{rr} = \alpha(C_{11}+2C_{12})\Theta, \quad r = R, \tag{18}$$

$$\sigma_{r\theta} = 0, \quad r = R. \tag{19}$$

4.3. First order correction $\mathscr{N}\mathbf{U}_0$

Using $\boldsymbol{\sigma} = C^0\mathbf{e}$, we solve

$$\frac{\partial\sigma_{rr}}{\partial r} + \frac{1}{r}\frac{\partial\sigma_{r\theta}}{\partial\theta} + \frac{\sigma_{rr}-\sigma_{\theta\theta}}{r} = \mathscr{L}_r^a(\mathbf{U}_0), \quad r<R, \tag{20}$$

$$\frac{\partial\sigma_{r\theta}}{\partial r} + \frac{1}{r}\frac{\partial\sigma_{\theta\theta}}{\partial\theta} + \frac{2\sigma_{r\theta}}{r} = \mathscr{L}_\theta^a(\mathbf{U}_0), \quad r<R, \tag{21}$$

with the boundary condition

$$\sigma_{rr} = \sigma_{rr}^a(\mathbf{U}_0), \quad r = R, \tag{22}$$

$$\sigma_{r\theta} = \sigma_{r\theta}^a(\mathbf{U}_0), \quad r = R. \tag{23}$$

For a given pulling direction, we write $\mathscr{L}^a(\mathbf{V}) = (\mathscr{L}_r^a(\mathbf{V}), \mathscr{L}_\theta^a(\mathbf{V}))^{\mathrm{T}}$ and $\boldsymbol{\sigma}^a(\mathbf{V}) = (\sigma_{rr}^a(\mathbf{V}), \sigma_{r\theta}^a(\mathbf{V}))^{\mathrm{T}}$ corresponding to C^a. From the discussion in Sections 3.1–3.4, C^a can written as a linear combination of $C^{a,2}$ and $C^{a,4}$. It is easy to verify that $\mathscr{L}^{a,4}(\mathbf{V})$ and $\boldsymbol{\sigma}^{a,4}(\mathbf{V})$ have terms related to $\cos((n+4)\theta+\delta)$, $\sin((n+4)\theta+\delta)$ and $\cos((n-4)\theta+\delta)$, $\sin((n-4)\theta+\delta)$ with $\mathbf{V} = (v_r, v_\theta)^{\mathrm{T}} = (D_1 r^k \cos(n\theta+\delta), D_2 r^k \sin(n\theta+\delta))^{\mathrm{T}}$. For example, considering the [0 0 1] pulling direction where $C^a = HC^{a,4}/4$, $\mathscr{L}^a(\mathbf{V})$ and $\boldsymbol{\sigma}^a(\mathbf{V})$ are given by

$$\mathscr{L}^a(\mathbf{V}) = \frac{H}{8}r^{k-2}(D_1+D_2)(k-1-n)(k-3-n)\begin{pmatrix}\cos((n+4)\theta+\delta)\\ -\sin((n+4)\theta+\delta)\end{pmatrix} + \frac{H}{8}r^{k-2}(D_1-D_2)(k-1+n)(k-3+n)\begin{pmatrix}\cos((n-4)\theta+\delta)\\ \sin((n-4)\theta+\delta)\end{pmatrix},$$

$$\boldsymbol{\sigma}^a(\mathbf{V}) = \frac{H}{8}r^{k-1}(D_1+D_2)(k-1-n)\begin{pmatrix}\cos((n+4)\theta+\delta)\\ -\sin((n+4)\theta+\delta)\end{pmatrix} + \frac{H}{8}r^{k-1}(D_1-D_2)(k-1+n)\begin{pmatrix}\cos((n-4)\theta+\delta)\\ \sin((n-4)\theta+\delta)\end{pmatrix}.$$

The terms related to $C^{a,2}$ can be obtained similarly.

Remark 4.1. With the displacement solution in hand, we can compute stress using the stress–stain relationship (29)–(32). The thermal effect due to $-(C_{11}+2C_{12})\Theta$ will be added to yield the total stress [6]. 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 [3]

$$2(\sigma^{\mathrm{vm}})^2 = (\sigma_{rr}-\sigma_{\theta\theta})^2 + (\sigma_{rr}-\sigma_{zz})^2 + (\sigma_{\theta\theta}-\sigma_{zz})^2 + 6\sigma_{r\theta}^2. \tag{24}$$

The preferred method of dislocation generation in all III–V semiconductors is through the generation of slip defects, in particular the {1 1 1}, ⟨1 $\bar{1}$ 0⟩ slip system [3]. 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 $\mathbf{d}$ within the glide plane with normal $\mathbf{n}$ is given by

$$\sigma^{\mathrm{rs}} = \mathbf{d}^{\mathrm{T}} R_{\mathbf{p}}^{\mathrm{T}} Q^{\mathrm{T}} \boldsymbol{\sigma} Q R_{\mathbf{p}} \mathbf{n}.$$

Matrix $R_{\mathbf{p}}$ depends on the given pulling direction $\mathbf{p}$, and rotates vectors from the crystallographic frame to the solidification frame. If the stress tensor $\boldsymbol{\sigma}$ is expressed in the (r,θ,z) coordinates, Q is the coordinate transformation matrix that takes $(x,y,z) \to (r,\theta,z)$.

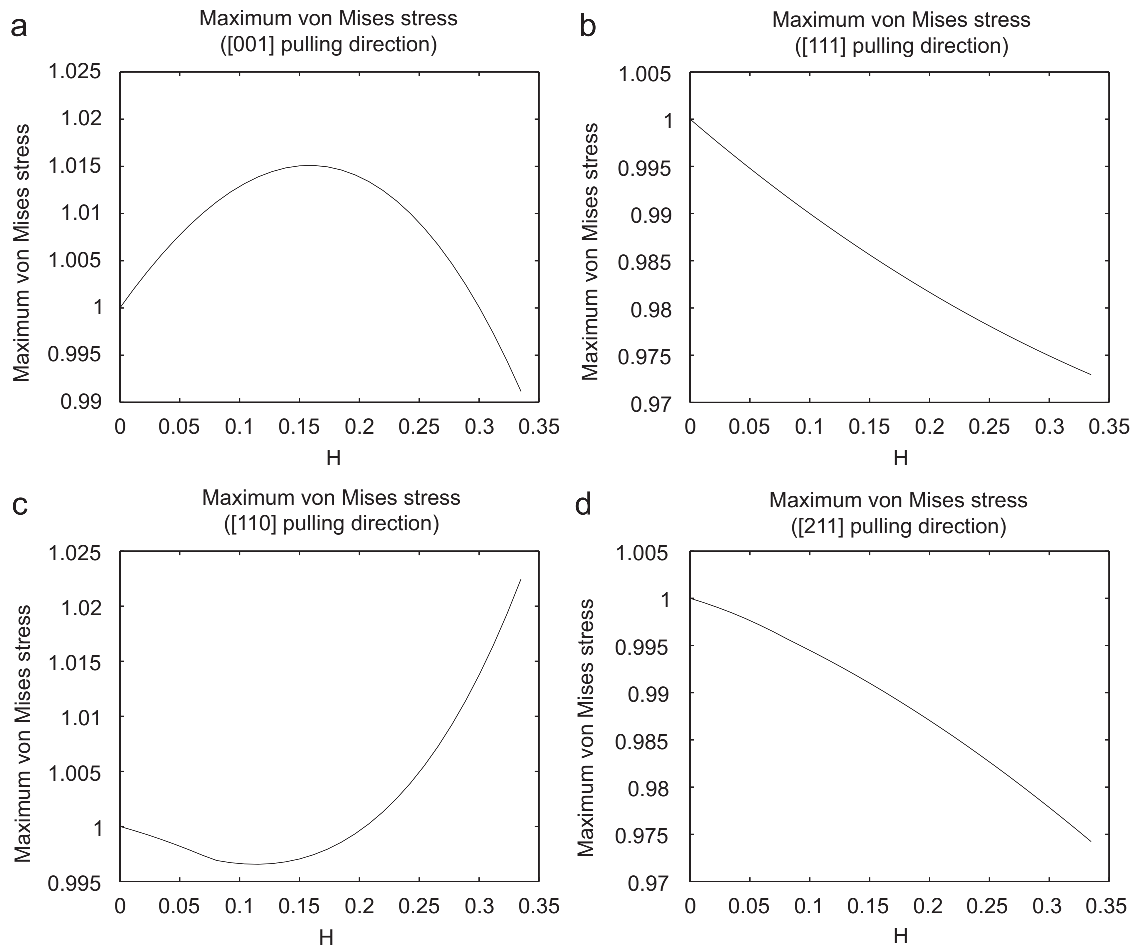

Fig. 1. Maximum von Mises stress as a function of H: (a) [0 0 1], (b) [1 1 1], (c) [1 1 0], (d) [2 1 1].

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. 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

$$\sigma^{\mathrm{rs,tot}} = \sum_{i=1}^{12} |\mathbf{d}_i^{\mathrm{T}} R_{\mathbf{p}}^{\mathrm{T}} Q^{\mathrm{T}} \boldsymbol{\sigma} Q R_{\mathbf{p}} \mathbf{n}_i|. \tag{25}$$

We assume that the temperature $\Theta = r^2$, according to Ref. [3]. In Figs. 1 and 2, the 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 scaled H, where $H \in [0, 0.34]$ (noting that the scaling is different for different pulling direction as shown in Sections 3.1–3.4). These results are obtained by high order solutions, the semi-analytic nature of the solution procedure allows us to efficiently compute the high order solutions. The figures show that the von Mises stress and resolved stress are not sensitive with respect to H, and the zero order solution (according to $H = 0$) is quite accurate in this case.

6. Details

6.1. Related lemmas on series (6)

We will prove some results on series (6). First, we define the norm

$$\|\mathbf{U}\|^2 = \sum_{i=1}^{6} \int_{\Omega} \lambda_i |e_i(\mathbf{U})|^2 \, \mathrm{d}V.$$

The weights λ_i take on the value $C_{11} - C_{12} + H/2$ for $i = 1, 2, 3$ and $C_{44} - H/4$ for $i = 4, 5, 6$ with $H = 2C_{44} - C_{11} + C_{12} \neq 0$ for an anisotropic cubic material. In Cartesian co-ordinates, $\mathbf{e}(\mathbf{U}) = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{xz}, 2e_{xy})^{\mathrm{T}}$.

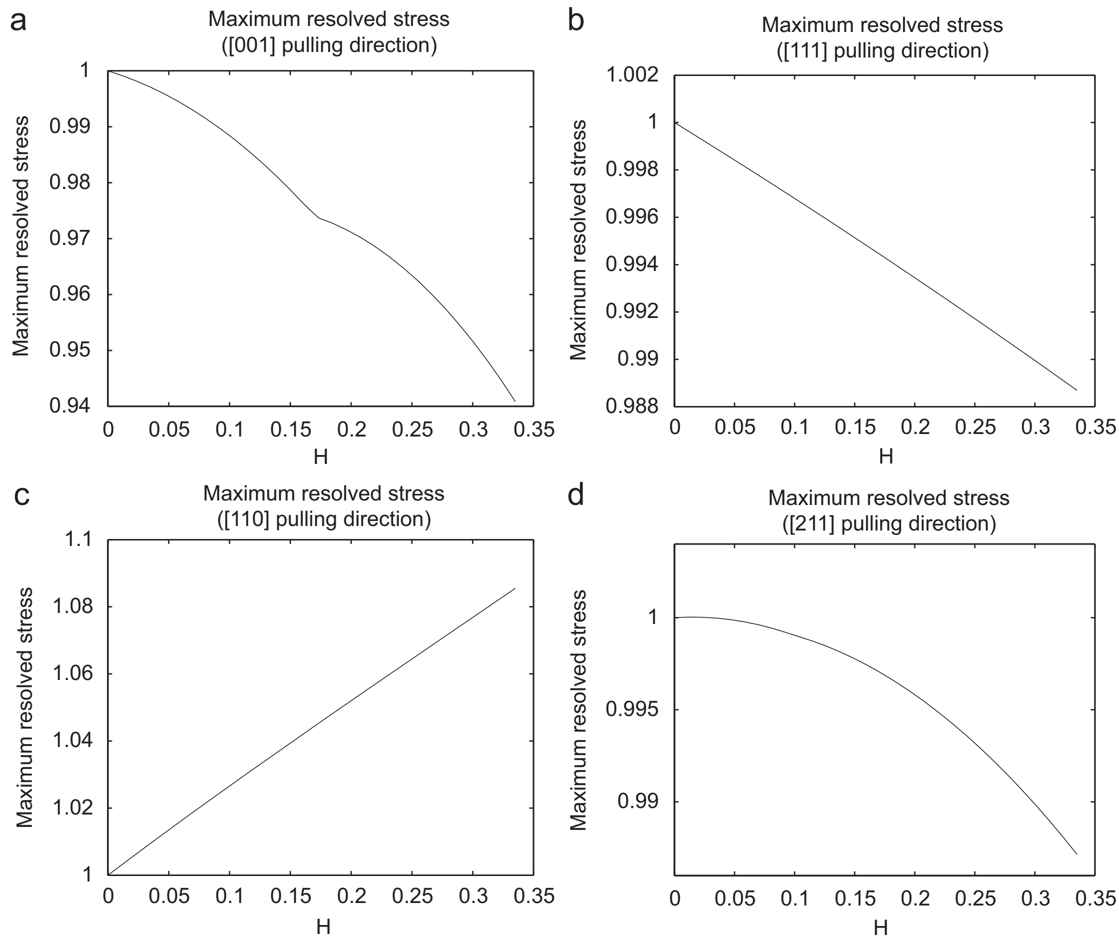

Fig. 2. Maximum resolved stress as a function of H: (a) [0 0 1], (b) [1 1 1], (c) [1 1 0], (d) [2 1 1].

Lemma 6.1. *For an anisotropic cubic material characterized by the stiffness values* $\{C_{11}, C_{12}, C_{44}\}$ *the quantity*

$$\omega = \frac{|2C_{44} - C_{11} + C_{12}|}{2C_{44} + C_{11} - C_{12}}$$

satisfies $0 < \omega < 1$.

Proof. The eigenvalues of the stiffness matrix $C_{11} + 2C_{12}$, $C_{11} - C_{12}$, and C_{44} must be positive, for otherwise the crystal would be unstable [10]. Due to the positivity constraint, we have the strict inequalities

$$-2C_{44} - C_{11} + C_{12} < 2C_{44} - C_{11} + C_{12} < 2C_{44} + C_{11} - C_{12}$$

so that $|2C_{44} - C_{11} + C_{12}| < 2C_{44} + C_{11} - C_{12}$ or $\omega < 1$. The case $\omega = 0$ corresponds to an isotropic crystal. $\square$

Lemma 6.2. *The operator* $\mathcal{N}$ *satisfies* $\|\mathcal{N}\mathbf{U}\| \leqslant \omega \|\mathbf{U}\|$, *for any given* $\mathbf{U}$.

Proof. For any given $\mathbf{U}$, let $\mathbf{W} = \mathcal{N}\mathbf{U}$. Using the boundary condition in the definition of $\mathcal{N}$, we see that $\mathbf{W}$ satisfies

$$\int_\Omega \sum_{i,j} C^0_{ij} e_i(\mathbf{W}) e_j(\mathbf{V})\, \mathrm{d}V \quad = \int_\Omega \sum_{i,j} C^a_{ij} e_i(\mathbf{U}) e_j(\mathbf{V})\, \mathrm{d}V, \quad \forall \mathbf{V}$$

and in particular for $\mathbf{V} = \mathbf{W}$,

$$\int_\Omega \sum_{i,j} C^0_{ij} e_i(\mathbf{W}) e_j(\mathbf{W})\, \mathrm{d}V \quad = \int_\Omega \sum_{i,j} C^a_{ij} e_i(\mathbf{U}) e_j(\mathbf{W})\, \mathrm{d}V. \tag{26}$$

For the left-hand side of Eq. (26), we have

$$\int_\Omega \sum_{i,j} C^0_{ij} e_i(\mathbf{W}) e_j(\mathbf{W})\, \mathrm{d}V \geqslant \int_\Omega \sum_{k=1}^{6} \lambda_k e_k^2(\mathbf{W})\, \mathrm{d}V = \|\mathbf{W}\|^2, \tag{27}$$

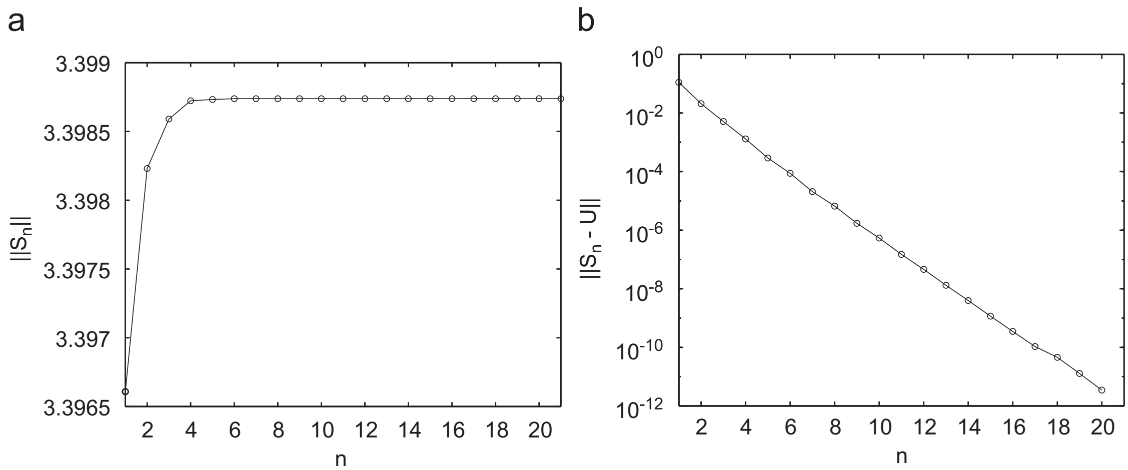

Fig. 3. The norm of (a) the approximate solution and (b) the residual as a function of the iteration n: (a) $\|\mathbf{S}_n\|$, (b) $\|\mathbf{S}_n-\mathbf{U}\|$.

while noting that C^a is itself diagonal gives

$$\int_\Omega \sum_{i,j} C^a_{ij} e_i(\mathbf{U}) e_j(\mathbf{W})\,\mathrm{d}V \quad \leqslant \int_\Omega \left(\sum_{k=1}^{3}\left|\frac{H}{2} e_k(\mathbf{U}) e_k(\mathbf{W})\right| + \sum_{k=4}^{6}\left|\frac{H}{4} e_k(\mathbf{U}) e_k(\mathbf{W})\right|\right)\mathrm{d}V. \tag{28}$$

Using the definitions of ω and H one has

$$\omega = \frac{|H/2|}{C_{11}-C_{12}+H/2} = \frac{|H/4|}{C_{44}-H/4}$$

so that estimates (27) and (28) with Eq. (26) allow us to conclude with Hölder's inequality that

$$\|\mathbf{W}\|^2 \leqslant \omega \|\mathbf{W}\|\,\|\mathbf{U}\|$$

or $\|\mathbf{W}\| \leqslant \omega\|\mathbf{U}\|$ for any given $\mathbf{U}$.

Lemma 6.3. *Let* $\mathbf{S}_n = \mathbf{U}_0 + \mathscr{N}\mathbf{U}_0 + \mathscr{N}^2\mathbf{U}_0 + \cdots + \mathscr{N}^n\mathbf{U}_0$, *with* $\mathbf{S}_0 = \mathbf{U}_0$. *Expression* (6) *converges to* $\mathbf{U}$, *and*

$$\|\mathbf{U}-\mathbf{S}_n\| \leqslant \omega^{n+1}\|\mathbf{U}\|.$$

Proof. Lemma 6.2 implies that the right-hand side of Eq. (6) converges. What remains is to show that $\mathbf{U}$ is in fact the limit. We note that

$$\mathscr{L}^0(\mathbf{U}-\mathbf{U}_0) = \mathscr{L}(\mathbf{U}) + \mathscr{L}^a(\mathbf{U}) - \mathbf{F} = \mathscr{L}^a(\mathbf{U}), \quad \mathbf{x}\in\Omega,\ t>0,$$

$$\mathscr{B}^0(\mathbf{U}-\mathbf{U}_0) = \mathscr{B}(\mathbf{U}) + \mathscr{B}^a(\mathbf{U}) - \mathbf{g} = \mathscr{B}^a(\mathbf{U}), \quad r = R(\theta, z).$$

By the definition of $\mathscr{N}$, one has $\mathbf{U}-\mathbf{U}_0 = \mathscr{N}\mathbf{U}$, $\|\mathbf{U}-\mathbf{U}_0\| = \|\mathscr{N}\mathbf{U}\| \leqslant \omega\|\mathbf{U}\|$ and $\mathbf{U}-\mathbf{S}_n = \mathscr{N}(\mathbf{U}-\mathbf{S}_{n-1})$ gives $\|\mathbf{U}-\mathbf{S}_n\| \leqslant \omega\|\mathbf{U}-\mathbf{S}_{n-1}\|$. By induction on n,

$$\|\mathbf{U}-\mathbf{S}_n\| \leqslant \omega^{n+1}\|\mathbf{U}\|, \quad \forall n\geqslant 0.$$

As an example, Fig. 3 shows both $\|\mathbf{S}_n\|$ and the residual $\|\mathbf{S}_n-\mathbf{U}\|$ as a function of iteration number n for the temperature $r^9\cos(7\theta)$, and a pulling direction of [0 0 1]. Clearly the sequence $\{\mathbf{S}_n\}$ converges in this norm and the residual approaches zero as n increases.

6.2. *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 corresponds to an isotropic material and is independent of the coordinate system. Assume

$$\boldsymbol{\sigma} = C\mathbf{e} = (C^0 - C^a)\mathbf{e}, \tag{29}$$

where

$$\boldsymbol{\sigma} = (\sigma_{rr}, \sigma_{\theta\theta}, \sigma_{zz}, \sigma_{\theta z}, \sigma_{rz}, \sigma_{r\theta})^{\mathrm{T}}, \mathbf{e} = (e_{rr}, e_{\theta\theta}, e_{zz}, 2e_{\theta z}, 2e_{rz}, 2e_{r\theta})^{\mathrm{T}}$$

are the stress and strain tensors in cylindrical coordinates (r, θ, z) expressed as a 6×1 vector.

For the [0 0 1] pulling direction, we choose the z-direction as [0 0 1], and the directions [1 0 0] and [0 1 0] corresponding to $\theta = 0$ and $\theta = \pi/2$, respectively. C^a is given by

$$\frac{1}{4}H\begin{pmatrix} 1+c_4 & 1-c_4 & 0 & 0 & 0 & -s_4 \\ 1-c_4 & 1+c_4 & 0 & 0 & 0 & s_4 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ -s_4 & s_4 & 0 & 0 & 0 & -c_4 \end{pmatrix}, \tag{30}$$

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

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

$$\frac{H}{6}\begin{pmatrix} 0 & 1 & 2 & \sqrt{2}s_3 & -\sqrt{2}c_3 & 0 \\ 1 & 0 & 2 & -\sqrt{2}s_3 & \sqrt{2}c_3 & 0 \\ 2 & 2 & -1 & 0 & 0 & 0 \\ \sqrt{2}s_3 & -\sqrt{2}s_3 & 0 & \frac{1}{2} & 0 & \sqrt{2}c_3 \\ -\sqrt{2}c_3 & \sqrt{2}c_3 & 0 & 0 & \frac{1}{2} & \sqrt{2}s_3 \\ 0 & 0 & 0 & \sqrt{2}c_3 & \sqrt{2}s_3 & -\frac{1}{2} \end{pmatrix}, \tag{31}$$

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

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

$$H\begin{pmatrix} c^2-\frac{7}{6}c^4 & \frac{1}{3}+\frac{7}{6}c^4-\frac{7}{6}c^2 & \frac{1}{6}+\frac{1}{6}c^2 & \frac{\sqrt{2}}{6}s(1-3c^2) & -\frac{\sqrt{2}}{2}cs^2 & \frac{1}{6}cs(7c^2-3) \\ \frac{1}{3}+\frac{7}{6}c^4-\frac{7}{6}c^2 & \frac{4}{3}c^2-\frac{7}{6}c^4-\frac{1}{6} & \frac{1}{3}-\frac{1}{6}c^2 & \frac{\sqrt{2}}{2}sc^2 & \frac{\sqrt{2}}{6}c(2-3c^2) & \frac{1}{6}cs(4-7c^2) \\ \frac{1}{6}+\frac{1}{6}c^2 & \frac{1}{3}-\frac{1}{6}c^2 & 0 & -\frac{\sqrt{2}}{6}s & \frac{\sqrt{2}}{6}c & -\frac{1}{6}cs \\ \frac{\sqrt{2}}{6}s(1-3c^2) & \frac{\sqrt{2}}{2}sc^2 & -\frac{\sqrt{2}}{6}s & \frac{1}{12}-\frac{1}{6}c^2 & -\frac{1}{6}cs & \frac{\sqrt{2}}{6}c(2-3c^2) \\ -\frac{\sqrt{2}}{2}cs^2 & \frac{\sqrt{2}}{6}c(2-3c^2) & \frac{\sqrt{2}}{6}c & -\frac{1}{6}cs & \frac{1}{6}c^2-\frac{1}{12} & \frac{\sqrt{2}}{6}s(1-3c^2) \\ \frac{1}{6}cs(7c^2-3) & \frac{1}{6}cs(4-7c^2) & -\frac{1}{6}cs & \frac{\sqrt{2}}{6}c(2-3c^2) & \frac{\sqrt{2}}{6}s(1-3c^2) & \frac{7}{6}c^4-\frac{7}{6}c^2+\frac{1}{12} \end{pmatrix}, \tag{32}$$

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

For the [1 1 0] pulling direction, the z-direction is [1 1 0], and [0 0 1], $[1\,\bar{1}\,0]$ correspond to $\theta = 0$ and $\theta = \pi/2$, respectively. C^a is given by

$$H\begin{pmatrix} \frac{3}{2}c^4-c^2 & \frac{3}{2}c^2s^2 & \frac{1}{2}s^2 & 0 & 0 & -\frac{3}{2}c^3s+\frac{1}{2}cs \\ \frac{3}{2}c^2s^2 & -\frac{3}{2}c^2s^2+\frac{1}{2}s^2 & \frac{1}{2}c^2 & 0 & 0 & \frac{3}{2}c^3s-cs \\ \frac{1}{2}s^2 & \frac{1}{2}c^2 & 0 & 0 & 0 & \frac{1}{2}cs \\ 0 & 0 & 0 & \frac{1}{2}c^2-\frac{1}{4} & \frac{1}{2}cs & 0 \\ 0 & 0 & 0 & \frac{1}{2}cs & -\frac{1}{2}c^2+\frac{1}{4} & 0 \\ -\frac{3}{2}c^3s+\frac{1}{2}cs & \frac{3}{2}c^3s-cs & \frac{1}{2}cs & 0 & 0 & \frac{3}{2}c^2s^2-\frac{1}{4} \end{pmatrix}. \tag{33}$$

6.3. The solution to the two-dimensional homogeneous elasticity problem

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

$$\frac{\partial\sigma_{rr}}{\partial r}+\frac{1}{r}\frac{\partial\sigma_{r\theta}}{\partial\theta}+\frac{\sigma_{rr}-\sigma_{\theta\theta}}{r}=0, \quad r<R, \tag{34}$$

$$\frac{\partial\sigma_{r\theta}}{\partial r}+\frac{1}{r}\frac{\partial\sigma_{\theta\theta}}{\partial\theta}+\frac{2\sigma_{r\theta}}{r}=0, \quad r<R, \tag{35}$$

with the boundary conditions,

$$\sigma_{rr} = g_r\cos(n\theta+\delta), \quad r=R, \tag{36}$$

$$\sigma_{r\theta} = g_\theta\sin(n\theta+\delta), \quad r=R. \tag{37}$$

When $n=0$, we have $g_\theta=0$ for the well-posedness of the elasticity problem (34)–(37). The solution $\mathbf{w}^h=(w_r^h,w_\theta^h)^{\mathrm{T}}$ is given by

$$\mathbf{w}^h=\frac{1+v}{1-v}g_r r((1-2v)\cos\delta,2(1-v)\sin\delta)^{\mathrm{T}}.$$

For $n=1$, we have $g_r=g_\theta$ for the well-posedness of Eqs. (34)–(37) and

$$\mathbf{w}^h=\frac{1+v}{1-v}\frac{g_r r^2}{2R}((1-4v)\cos(\theta+\delta),(5-4v)\sin(\theta+\delta))^{\mathrm{T}}.$$

Finally for $n\geqslant 2$, the solution $\mathbf{w}^h=(w_r^h,w_\theta^h)^{\mathrm{T}}$ is a linear combination of $r^{n+1}((2-n-4v)\cos(n\theta+\delta),(n+4-4v)\sin(n\theta+\delta))^{\mathrm{T}}$ and $r^{n-1}(\cos(n\theta+\delta),-\sin(n\theta+\delta))^{\mathrm{T}}$. More precisely, it is given by

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

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

6.4. Particular solution to the two-dimensional elasticity problem

In this subsection we detail the particular solutions to

$$\frac{\partial\sigma_{rr}}{\partial r}+\frac{1}{r}\frac{\partial\sigma_{r\theta}}{\partial\theta}+\frac{\sigma_{rr}-\sigma_{\theta\theta}}{r}=f_r r^{k-2}\cos(n\theta+\delta)\log^l r,\quad r<R, \tag{38}$$

$$\frac{\partial\sigma_{r\theta}}{\partial r}+\frac{1}{r}\frac{\partial\sigma_{\theta\theta}}{\partial\theta}+\frac{2\sigma_{r\theta}}{r}=f_\theta r^{k-2}\sin(n\theta+\delta)\log^l r,\quad r<R, \tag{39}$$

where $l\geqslant 0$ is an integer.

For $l=0$, $|k-n|=1$ the particular solution to Eqs. (38) and (39) is a linear combination of $(r^k\cos(n\theta+\delta),0)^{\mathrm{T}}$ and $r^k\log r(\zeta\cos(n\theta+\delta),\sin(n\theta+\delta))^{\mathrm{T}}$ where $\zeta=-1$ if $k=n-1$, and $\zeta=-(n-2+4v)/(n+4-4v)$ if $k=n+1$. In fact $r^k(\zeta\cos(n\theta+\delta),\sin(n\theta+\delta))^{\mathrm{T}}$ 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 $\log^l r(r^k\cos(n\theta+\delta),0)^{\mathrm{T}}$and $r^k\log^{l+1}r(\zeta\cos(n\theta+\delta),\sin(n\theta+\delta))^{\mathrm{T}}$. Because of this, we define $\mathbf{S}_{n,k,l}(f_r,f_\theta)$ for $k=n\pm1$ as

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

where

$$D_1=\begin{cases}\dfrac{1+v}{(1-v)^2}\dfrac{(2-3n-4v+4vn)f_r+(4-4v-3n+4vn)f_\theta}{8n(n-1)}, & k=n-1,\\[2ex] \dfrac{1+v}{(1-v)^2}\dfrac{(3-4v)n^2(f_r+f_\theta)+8(n+1)(1-2v)(1-v)(f_r-f_\theta)}{8n(n+1)(n+4-4v)}, & k=n+1,\end{cases} \tag{40}$$

$$D_2=\begin{cases}-\dfrac{1+v}{(1-v)^2}\dfrac{(n+2-4v)f_r+(n-4+4v)f_\theta}{8(l+1)(n-1)}, & k=n-1,\\[2ex] \dfrac{1+v}{(1-v)^2}\dfrac{(n+4-4v)(f_r+f_\theta)}{8(l+1)(n+1)}, & k=n+1,\end{cases} \tag{41}$$

$$\zeta=\begin{cases}-1, & k=n-1,\\ -\dfrac{n-2+4v}{n+4-4v}, & k=n+1.\end{cases} \tag{42}$$

In contrast, $\mathbf{S}_{n,k,l}(f_r,f_\theta)$ for $k\neq n\pm1$ is given by

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

where

$$D_1=\frac{1+v}{(1-v)^2}\frac{(k^2-2k^2v-2n^2+2n^2v+2v-1)f_r-(4nv+nk-3n)f_\theta}{((k-n)^2-1)((k+n)^2-1)}, \tag{43}$$

$$D_2=\frac{1+v}{(1-v)^2}\frac{(-4nv+nk+3n)f_r+(2k^2-2k^2v-n^2+2n^2v+2v-2)f_\theta}{((k-n)^2-1)((k+n)^2-1)}. \tag{44}$$

In compact form, we denote by $\mathbf{T}_{n,k,l}(f_r,f_\theta)$ the displacement corresponding to the particular solution to Eqs. (38) and (39) for the values of (n,k,l). When $l=0$, $\mathbf{T}_{n,k,0}(f_r,f_\theta)=\mathbf{S}_{n,k,0}(f_r,f_\theta)$. Turning to the case $l>0$, one has

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

where

$$g_{r,l} = \begin{cases} \dfrac{l(1-v)^2}{(1+v)(1-2v)}(-2kD_1 - (l+1)\zeta D_2), & k = n \pm 1, \\ \dfrac{l(1-v)}{2(1+v)(1-2v)}(-4k(1-v)D_1 - nD_2), & k \neq n \pm 1, \end{cases}$$

$$g_{\theta,l} = \begin{cases} \dfrac{l(1-v)}{2(1+v)}\left(\dfrac{n}{1-2v}D_1 - (l+1)D_2\right), & k = n \pm 1, \\ \dfrac{l(1-v)}{2(1+v)}\left(\dfrac{n}{1-2v}D_1 - 2kD_2\right), & k \neq n \pm 1, \end{cases}$$

$$h_{r,l} = -\frac{l(l-1)(1-v)^2}{(1+v)(1-2v)}D_1,$$

$$h_{\theta,l} = \begin{cases} 0, & k = n \pm 1, \\ -\dfrac{l(l-1)(1-v)}{2(1+v)}D_2, & k \neq n \pm 1, \end{cases}$$

with D_1 and D_2 given by either Eqs. (40)–(41) or Eqs. (43)–(44), 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 solutions to the isotropic body problem. The series converges for all stable crystals with cubic anisotropy since the anisotropic factor is less than one. In addition, compared to other splitting techniques which normally assume weak anisotropy, our approach is valid for all materials with other crystal symmetries as long as a suitable decomposition can be found.

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