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A THERMAL ELASTIC MODEL FOR DIRECTIONAL CRYSTAL GROWTH WITH WEAK ANISOTROPY*

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Abstract. In this paper we present a semi-analytical thermal stress solution for directional growth of type III–V compounds with small lateral heat flux and weak anisotropy. Both geometric and material anisotropy are considered, and our solution can be applied to crystals grown by various growth techniques such as the Czochralski (Cz) method. The semi-analytical nature of the solution allows us to compute thermal stress in crystals with weak anisotropic effects much more efficiently, compared to a full 3D simulation. Examples are given for crystals pulled in a variety of seed orientations. Our results show that the geometric effect is the dominant one while the effect of material anisotropy on thermal stress is secondary.

Key words. crystal growth, asymptotic expansion, anisotropy, facet formation, thermal stress, Czochralski technique

AMS subject classifications. 74A10, 74E10, 74F05, 74H10, 80A22, 82D25, 82D37

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1. Introduction. Directional growth techniques such as the Czochralski (Cz) method are frequently used to produce high quality single crystals. By dipping a small seed crystal into a pool of molten material in the crucible and carefully controlling the heat balance inside the grower, a large crystal can be grown by pulling the crystal away from the melt in a slow and steady fashion. The pulling rod and the crucible are normally rotated in opposite directions during the growth period. For a more detailed account of the Cz and other techniques, we refer the readers to the extremely informative handbooks by Hurle [5]. Almost perfectly cylindrical crystals are grown for silicon and other semiconductor materials despite their internal structure and material anisotropy. For these crystals, the effect of material anisotropy on thermal stress has been investigated by assuming an axisymmetric cylindrical shape [3, 9, 11, 12]. On the other hand, anisotropic effects such as facets are often visible on the surface of binary compound semiconductor crystals grown by these methods [8]. The effect of a noncylindrical shape on the thermal stress is therefore of practical interest.

In a previous paper, we developed a thermal stress model for directional growth of crystals with facets [13]. For constrained growth such as that of the Cz method, a lateral growth model consistent with the lattice structure of type III–V crystals was proposed. This model is capable of predicting facet formation on the lateral surface, which qualitatively resembles experimental observations [8] of indium antimonide (InSb) crystals. Furthermore, under the assumptions of weak lateral heat flux, we have derived perturbation solutions for temperature and related thermal stress for faceted crystals by neglecting material anisotropy.

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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 [11, 12]. It is, however, not clear whether the conclusions in [11, 12] hold for InSb crystals grown in a noncylindrical shape, especially those with facets forming on the lateral surface. The purpose of this paper is to investigate the combined effect of the geometric and material anisotropy on thermal stress inside the conic crystals considered in [13]. We start with the description of the mathematical model and the thermal problem in section 2. Since the growth model and temperature solution are identical to those in [13], they are presented without detailed derivation.

The main results of this paper are given in section 3, where the detailed derivation of the thermal stress with anisotropic elastic constants is presented. We show that the thermal stress can be expanded into an asymptotic series with respect to ω, a measure of the material anisotropy, and in Appendix A we prove that the series converges. As a result, a systematic approach can be devised to compute thermal stress to arbitrary order with the zeroth order solution corresponding to the case of isotropic material constants. In section 4, we present computational results for crystals pulled in a variety of seeding orientations. The results show that the effect of material anisotropy could be significant when the geometric effect is absent. The geometric effect, when it is present, usually dominates.

2. Model. The basic assumptions of our model are that the lateral heat flux is small and the material and geometric anisotropic effects are weak, following [1, 13]. To simplify the discussion, we assume that lateral heat transfer from the crystal to the background is known. We also assume that the heat flux from the melt is fixed while the pull rate can be adjusted in order to grow a crystal with a desirable lateral profile, e.g., a conic crystal. In principle, we could incorporate the effect of the melt flow by coupling the heat transfer process in the crystal with that in the melt. However, to focus on the thermal stress in the crystal, we neglect the effect of the melt flow and assume that the axial heat flux from the melt at the crystal/melt interface does not vary in the cross-sectional (radial and circumferential) directions.

2.1. Thermal problem. Within the crystal Ω, the temperature $T(\mathbf{x},t)$ satisfies the heat equation,

$$\rho_s c_s \frac{\partial T}{\partial t} = \nabla \cdot (\kappa_s \nabla T), \qquad \mathbf{x} \in \Omega,\ t > 0, \tag{2.1a}$$

where ρ_s, c_s, and κ_s are the density, specific heat, and thermal conductivity of the crystal, respectively. The boundary conditions on the crystal/gas interface Γ_g, and the chuck (holding the seed), are,

$$-\kappa_s \frac{\partial T}{\partial \mathbf{n}} = h_{\text{gs}}(T - T_g) + h_F(T^4 - T_b^4), \qquad \mathbf{x} \in \Gamma_g, \tag{2.1b}$$

$$\kappa_s \frac{\partial T}{\partial z} = h_{\text{ch}}(T - T_{\text{ch}}), \qquad z = 0, \tag{2.1c}$$

where h_{gs} and h_{ch} represent the heat transfer coefficients of the crystal/gas and crystal/chuck interfaces; h_F is the radiation heat transfer coefficient; and T_g, T_{ch}, and T_b denote the ambient gas temperature, the chuck temperature, and background temperature, respectively.

The crystal/melt interface is denoted Γ_S and is where $T = T_m$, which is the melting temperature. Explicitly we denote the melting isotherm by

$$z - S(\mathbf{x}, t) = 0, \qquad \mathbf{x} \in \Gamma_S, \tag{2.1d}$$

with S denoting the crystal/melt interface. The motion of the interface of the phase transition is governed by the Stefan condition,

$$\rho_s L|\mathbf{v}_n| = \kappa_s \left.\frac{\partial T}{\partial \mathbf{n}}\right|_{z\to S^-} - q_{l,n}, \qquad |\mathbf{v}_n| = v_n = \frac{\partial S}{\partial t}\mathbf{k}\cdot\mathbf{n}, \tag{2.1e}$$

where L is the latent heat, $|\mathbf{v}_n|$ is the speed of the interface in the direction of its outward normal $\mathbf{n}$, $q_{l,n}$ is the heat flux from the melt normal to the interface, and $\partial S/\partial t$ is the speed of the interface S in the $\mathbf{k}$ direction.

2.2. Crystal shape. For the purpose of computing thermal stress, we assume that the shape of the crystal is self-similar in that the crystal radius $R(\phi, z)$ scales with its angular average $\bar{R}(z)$. Such crystals are indeed seen experimentally [8], and representing the angular dependence with a truncated Fourier series gives

$$R(\phi, z) = \bar{R}(z)\left(1 + \epsilon \sum_{k=1}^{m} \beta_k \cos(n_k\phi + \delta_k)\right) = \bar{R}(z)\left(1 + \epsilon\lambda(\phi)\right). \tag{2.2a}$$

In this expression $2\pi\bar{R}(z) = \int_{-\pi}^{\pi} R(\phi, z)\, d\phi$, m, $n_1 < n_2 < \cdots < n_m$ are positive integers ($m = 1$, $n_1 = 4$ for fourfold symmetry); the $\delta_k \in [0, 2\pi)$ are chosen to ensure that $\beta_k > 0$. Note that only those n_k corresponding to $\beta_k > 0$ are represented in the series. The parameter $\epsilon \geq 0$ is a measure of the anisotropy, and choosing the β_k so that $\sum_{k=1}^{m} \beta_k^2 = 1$ yields the expression

$$\epsilon^2 = \frac{1}{\pi\bar{R}(z)^2}\int_{-\pi}^{\pi}\left(R(\phi, z) - \bar{R}(z)\right)^2 d\phi. \tag{2.2b}$$

We will assume that $\epsilon < 1$, which will certainly[1] be the case if $\max_\phi R(\phi, z) < \frac{3}{2}\bar{R}(z)$. The β_k, δ_k, and ϵ values for the cross sections used in section 4 can be found in [13].

Of particular interest are the angular integrals

$$I_{i,j}(\epsilon) = \int_0^{2\pi} (1+\epsilon\lambda)^i \left((1+\epsilon\lambda)^2 + (\epsilon\lambda')^2\right)^{j/2} \mathrm{d}\phi \tag{2.2c}$$

$$= 2\pi + \frac{\pi}{2}\left[(i+j)(i+j-1) + j\sum_{k=1}^{m} n_k^2\beta_k^2\right]\epsilon^2 + O(\epsilon^3), \tag{2.2d}$$

where $i, j \in \mathbb{Z}$ and $\lambda' = d\lambda/d\phi$. Both the enclosed area (A) and circumference (s) of R will be utilized in what follows. For any fixed z it is an easy exercise to verify $A(z) = \bar{R}^2 I_{2,0}/2$ and $s(z) = \bar{R} I_{0,1}$.

2.3. Nondimensionalization. For simplicity, we assume that the gas temperature T_g is constant. Defining the Biot number by

$$\mathrm{Bi} = \frac{\bar{h}_{\mathrm{gs}}\tilde{R}}{\kappa_s}, \tag{2.3}$$

where $\tilde{R}$ is a characteristic radius of the crystal and $\bar{h}_{\mathrm{gs}}$ is the mean value of h_{gs}, we adopt the following scalings:

$$r = \tilde{R}\hat{r}, \quad R(\phi, z) = \tilde{R}\hat{R}(\hat{\phi}, \hat{z}), \quad \mathrm{Bi}^{1/2} z = \tilde{R}\hat{z}, \quad \mathrm{Bi}^{1/2} S(r, \phi, t) = \tilde{R}\hat{S}(\hat{r}, \hat{\phi}, \hat{t}),$$

$$\mathrm{St} = \frac{L}{c_s \Delta T}, \quad \Delta T = T_m - T_g, \quad T = T_g + \Delta T\Theta, \quad t = \frac{\mathrm{St}\,\tilde{R}^2\rho_s c_s}{\kappa_s\,\mathrm{Bi}}\hat{t},$$

[1]This is simply a consequence of the positivity of R and the mean value theorem applied to (2.2b).

with $\phi = \hat{\phi}$. Here variables with hats ($\hat{}$) are the nondimensional ones. In terms of these variables, the heat equation (2.1a) becomes (after dropping hats)

$$\frac{\mathrm{Bi}}{\mathrm{St}}\Theta_t = \frac{1}{r}(r\Theta_r)_r + \frac{1}{r^2}\Theta_{\phi\phi} + \mathrm{Bi}\,\Theta_{zz}, \qquad \mathbf{x} \in \Omega,\ t > 0, \tag{2.4a}$$

and boundary conditions (2.1b)–(2.1d) under the nondimensional scaling become

$$-\Theta_r + \frac{1}{R^2}R_\phi\Theta_\phi + \mathrm{Bi}\,R_z\Theta_z = \mathrm{Bi}\,F(\Theta)\left(1 + \frac{R_\phi^2}{R^2} + \mathrm{Bi}\,R_z^2\right)^{1/2}, \qquad \mathbf{x} \in \Gamma_g, \tag{2.4b}$$

$$\Theta_z(0,\phi,t) = \delta\left(\Theta(0,\phi,t) - \Theta_{\mathrm{ch}}\right), \tag{2.4c}$$

$$\Theta = 1, \qquad \mathbf{x} \in \Gamma_S, \tag{2.4d}$$

where $\Theta_{\mathrm{ch}} = (T_{\mathrm{ch}} - T_g)/\Delta T$ and

$$F(\Theta) = \frac{h_F(T_g^4 - T_b^4)}{\bar{h}_{\mathrm{gs}}\Delta T} + \left(\beta(z) + \frac{4h_F}{\bar{h}_{\mathrm{gs}}}T_g^3\right)\Theta + \frac{h_F}{\bar{h}_{\mathrm{gs}}}\Delta T(6T_g^2 + 4T_g\Delta T\Theta + \Delta T^2\Theta^2)\Theta^2,$$

$\beta(z) = h_{\mathrm{gs}}/\bar{h}_{\mathrm{gs}}$, and $\delta = \mathrm{Bi}^{1/2}\,h_{\mathrm{ch}}/\bar{h}_{\mathrm{gs}}$. The crystal/melt interface advances according to the Stefan condition (2.1e), which in nondimensional coordinates becomes

$$\Theta_z - \frac{1}{\mathrm{Bi}}S_r\Theta_r - \frac{1}{\mathrm{Bi}\,r^2}S_\phi\Theta_\phi = \gamma + S_t, \qquad \gamma = \frac{q_l\tilde{R}}{\mathrm{Bi}^{1/2}\,\kappa_s\Delta T}, \tag{2.4e}$$

where γ (q_l) is the nondimensional (resp., dimensional) heat flux in the liquid across the crystal/melt interface in the axial direction.

2.4. Temperature solution. Equations (2.4a) and (2.4b) strongly suggest that the temperature Θ is independent of r and ϕ to leading order. If true, then the crystal/melt interface S is also independent of r and ϕ to leading order. These observations motivate the following approximates:

$$\begin{aligned}\Theta &\sim \Theta_0(z,t) + \mathrm{Bi}\,\Theta_1(r,\phi,z,t) + \mathrm{Bi}^2\,\Theta_2(r,\phi,z,t) + \cdots, \\ S &\sim S_0(t) + \mathrm{Bi}\,S_1(r,\phi,t) + \mathrm{Bi}^2\,S_2(r,\phi,t) + \cdots.\end{aligned} \tag{2.5}$$

We substitute them into the scaled model, expand in powers of Bi, and simplify and collect terms of the same orders.

The zeroth order problem is given by[2]

$$\frac{1}{\mathrm{St}}\Theta_{0,t} - \Theta_{0,zz} = \frac{2}{\bar{R}}\left(\bar{R}'\Theta_{0,z} - \frac{I_{0,1}}{I_{2,0}}F(\Theta_0)\right), \qquad 0 < z < S_0(t),\ t > 0, \tag{2.6a}$$

$$\Theta_{0,z}(0,t) = \delta(\Theta_0(0,t) - \Theta_{\mathrm{ch}}), \qquad t \geq 0, \tag{2.6b}$$

$$\Theta_0(S_0(t),t) = 1, \qquad t \geq 0, \tag{2.6c}$$

$$S_0'(t) = \Theta_{0,z}(S_0(t),t) - \gamma, \qquad S_0(0) = Z_0,\ t > 0. \tag{2.6d}$$

The first order solution is given by

$$\Theta_1(r,\phi,z,t) = \Theta_1^a(z,t) + r^2\Theta_1^b(z,t) + \epsilon\Theta_1^c(r,\phi,z,t) + O(\epsilon^2), \tag{2.7a}$$

[2] For weak anisotropy, $I_{0,1}/I_{2,0} = 1 + O(\epsilon^2)$.

where, keeping only those terms to $O(\epsilon)$,

$$\Theta_1^b(z,t) = \frac{1}{2\bar{R}}\left(\bar{R}'\Theta_{0,z} - F(\Theta_0)\right), \tag{2.7b}$$

$$\Theta_1^c(r,\phi,z,t) = \bar{R}F(\Theta_0)\sum_{k=1}^{m}\frac{\beta_k}{n_k}\left(\frac{r}{\bar{R}}\right)^{n_k}\cos(n_k\phi+\delta_k). \tag{2.7c}$$

These last two terms are completely determined by Θ_0 and $\bar{R}$. The first term $\Theta_1^a(z,t)$ can be found in [13] and is not repeated here since it is not relevant to the stress computation.

3. Thermal stress. We now turn our attention to thermal stress. In the following, the general case in 3D space is discussed first, followed by a more detailed discussion using the plane-strain assumption.

3.1. Thermoelasticity equations for solids with cubic anisotropy. We consider a 3D elasticity problem for a crystal with cubic symmetry as in [6]. In this case the stresses $\boldsymbol{\sigma} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy})^{\mathrm{T}}$ and strains $\mathbf{e} = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{xz}, 2e_{xy})^{\mathrm{T}}$ are related through

$$\boldsymbol{\sigma} = C\mathbf{e}, \qquad C = \begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{pmatrix}. \tag{3.1}$$

We denote the displacement vector by $\mathbf{w}$ and the related strain by $\mathbf{e} = \mathbf{S}(\mathbf{w})$ so that the related stress tensor is given by $\boldsymbol{\sigma} = \mathcal{D}\mathbf{S}(\mathbf{w})$. For an anisotropic material, the quantity $H = 2C_{44} - C_{11} + C_{12} \neq 0$. By defining $C = C^0 - C^a$, where $C^a = H/4 \times \mathrm{diag}(2,2,2,-1,-1,-1)$, the matrix

$$C^0 = \begin{pmatrix} C_{11}^0 & C_{12}^0 & C_{12}^0 & & & \\ C_{12}^0 & C_{11}^0 & C_{12}^0 & & & \\ C_{12}^0 & C_{12}^0 & C_{11}^0 & & & \\ & & & C_{44}^0 & & \\ & & & & C_{44}^0 & \\ & & & & & C_{44}^0 \end{pmatrix} \tag{3.2a}$$

is isotropic and the quantities E and ν in terms of C_{ij}^0 are given by [10]

$$E = \frac{(C_{11}^0 + 2C_{12}^0)(C_{11}^0 - C_{12}^0)}{C_{11}^0 + C_{12}^0}, \qquad \nu = \frac{C_{12}^0}{C_{11}^0 + C_{12}^0}. \tag{3.2b}$$

By adopting the scaling in section 2.3 for r and T in addition to (α is the thermal expansion coefficient)

$$\mathbf{w} = \tilde{R}\alpha\Delta T\hat{\mathbf{w}}, \quad \sigma_{ij} = \frac{\alpha\Delta TE}{1-\nu}\hat{\sigma}_{\hat{i}\hat{j}}, \quad e_{ij} = \alpha\Delta T\hat{e}_{\hat{i}\hat{j}},$$

we set

$$C_{ij} = \frac{E}{1-\nu}\hat{C}_{\hat{i}\hat{j}}, \qquad H = \frac{E}{1-\nu}\hat{H}$$

and obtain (after dropping hats)

$$C_{11}^0 = \frac{(1-\nu)^2}{(1+\nu)(1-2\nu)}, \quad C_{12}^0 = \frac{\nu(1-\nu)}{(1+\nu)(1-2\nu)}, \quad C_{44}^0 = \frac{1}{2}(C_{11}^0 - C_{12}^0), \tag{3.2c}$$

$$C_{11} + 2C_{12} = \frac{1-\nu}{1-2\nu} - \frac{H}{2}. \tag{3.2d}$$

According to $C = C^0 - C^a$, we have the splitting of the operator $\mathcal{D}$, $\mathcal{D} = \mathcal{D}^0 - \mathcal{D}^a$. With this notation, the linear operators $\nabla \cdot \sigma$ and $\sigma \cdot \mathbf{n}$ take the form

$$\mathcal{L} := \nabla \cdot (\mathcal{D}\mathbf{S}) = \nabla \cdot (\mathcal{D}^0\mathbf{S}) - \nabla \cdot (\mathcal{D}^a\mathbf{S}) = \mathcal{L}^0 - \mathcal{L}^a,$$
$$\mathcal{B} := (\mathcal{D}\mathbf{S}) \cdot \mathbf{n} = (\mathcal{D}^0\mathbf{S}) \cdot \mathbf{n} - (\mathcal{D}^a\mathbf{S}) \cdot \mathbf{n} = \mathcal{B}^0 - \mathcal{B}^a,$$

and the thermoelastic boundary value problem can be stated in the form

$$\mathcal{L}(\mathbf{w}) = \mathbf{F}, \qquad \mathbf{x} \in \Omega,\ t > 0, \tag{3.3a}$$
$$\mathcal{B}(\mathbf{w}) = \mathbf{g}, \qquad r = R(\phi, z), \tag{3.3b}$$

where

$$\mathbf{F} = (C_{11} + 2C_{12})\nabla\Theta = \left(\frac{1-\nu}{1-2\nu} - \frac{H}{2}\right)\nabla\Theta, \qquad \mathbf{g} = \left(\frac{1-\nu}{1-2\nu} - \frac{H}{2}\right)\Theta\mathbf{n},$$

with $\mathbf{n}$ denoting the outward normal of the surface $r = R(\phi, z)$. The total stress contains an extra diagonal term related to the scaling with respect to the isotropic quantities E and ν so that

$$\sigma_{ij}^{\text{tot,aniso}} = \sigma_{ij} - \left(\frac{1-\nu}{1-2\nu} - \frac{H}{2}\right)\Theta\delta_{ij}. \tag{3.4}$$

We assume that the displacement $\mathbf{w}$ can be written as $\sum_{k=0}^n \mathbf{w}_k$. The following procedure defines the $\mathbf{w}_k$ under the assumption that $\mathbf{w}_{k+1} = \mathcal{N}\mathbf{w}_k$ for some linear operator $\mathcal{N}$. To solve for $\mathbf{w}(\mathbf{x})$ in (3.1) we begin by finding the displacement $\mathbf{w}_0$ given by

$$\mathcal{L}^0(\mathbf{w}_0) = \mathbf{F}, \qquad \mathbf{x} \in \Omega,\ t > 0, \tag{3.5a}$$
$$\mathcal{B}^0(\mathbf{w}_0) = \mathbf{g}, \qquad r = R(\phi, z), \tag{3.5b}$$

which is the displacement found in [13], multiplied by a factor of $\mu = 1 - \frac{H}{2}\frac{1-2\nu}{1-\nu}$. Having defined $\mathbf{w}_0$, we denote by $\mathbf{w}_{k+1} = \mathcal{N}\mathbf{w}_k$, with $k \geq 0$, the solution to

$$\mathcal{L}^0(\mathbf{w}_{k+1}) = \mathcal{L}^a(\mathbf{w}_k), \qquad \mathbf{x} \in \Omega,\ t > 0, \tag{3.6a}$$
$$\mathcal{B}^0(\mathbf{w}_{k+1}) = \mathcal{B}^a(\mathbf{w}_k), \qquad r = R(\phi, z). \tag{3.6b}$$

Continuing this process, we have for $\mathbf{w}(\mathbf{x})$ in (3.1)

$$\mathbf{w} = \mathbf{w}_0 + \mathcal{N}\mathbf{w}_0 + \mathcal{N}^2\mathbf{w}_0 + \cdots + \mathcal{N}^n\mathbf{w}_0 + \cdots. \tag{3.7}$$

Since $\|\mathcal{N}\| \leq \omega$ in a suitable norm, where $\omega = \frac{|H|/2}{C_{11}-C_{12}+H/2} = \frac{|2C_{44}-C_{11}+C_{12}|}{2C_{44}+C_{11}-C_{12}} < 1$ is an anisotropic factor, the series converges and an error can be estimated when (3.7) is replaced by a finite sum; cf. Appendix A. For typical cubic anisotropic materials, $\omega \approx 1/3$ [2].

Vigdergauz and Givoli [11, 12] have discussed the fourfold symmetry case (corresponding to the [001] pulling direction in our case) for a given symmetric temperature field. However, their splitting is not optimal and is valid only for crystals with weak cubic anisotropy. Our procedure can be applied to elastic stress computations with cubic anisotropy under a relatively general setting for a wide variety of materials.

Converting the stress-strain relationship to polar coordinates, we note that C^0 will not change, so we will concern ourselves only with C^a. Corresponding to (3.1) we let $\boldsymbol{\sigma}_{\text{cyc}} = (\sigma_{rr}, \sigma_{\phi\phi}, \sigma_{zz}, \sigma_{\phi z}, \sigma_{rz}, \sigma_{r\phi})^{\mathrm{T}}$, $\mathbf{e}_{\text{cyc}} = (e_{rr}, e_{\phi\phi}, e_{zz}, 2e_{\phi z}, 2e_{rz}, 2e_{r\phi})^{\mathrm{T}}$. The components of C_{cyc} are given by

$$\begin{aligned} C_{\text{cyc},ijkl} = \frac{H}{2}(a_{i1}a_{j1}a_{k1}a_{l1} + a_{i2}a_{j2}a_{k2}a_{l2} + a_{i3}a_{j3}a_{k3}a_{l3}) - \frac{H}{4}(a_{i2}a_{j3}a_{k2}a_{l3} \\ + a_{i2}a_{j3}a_{k3}a_{l2} + a_{i3}a_{j2}a_{k2}a_{l3} + a_{i3}a_{j2}a_{k3}a_{l2} + a_{i1}a_{j3}a_{k1}a_{l3} + a_{i1}a_{j3}a_{k3}a_{l1} \\ + a_{i3}a_{j1}a_{k1}a_{l3} + a_{i3}a_{j1}a_{k3}a_{l1} + a_{i1}a_{j2}a_{k1}a_{l2} + a_{i1}a_{j2}a_{k2}a_{l1} + a_{i2}a_{j1}a_{k1}a_{l2} \\ + a_{i2}a_{j1}a_{k2}a_{l1}) \end{aligned}$$

with a_{ij} the cosine of the angle between x'_i (new axes) and x_j (old axes) [10]. Furthermore, the first two and last two suffixes are abbreviated into a single suffix according to the scheme $11 \to 1$; $22 \to 2$; $33 \to 3$; $23, 32 \to 4$; $13, 31 \to 5$; $12, 21 \to 6$. For example, $C_{\text{cyc},1111} \equiv C_{\text{cyc},11}$ and $C_{\text{cyc},1231} \equiv C_{\text{cyc},65}$.

For the [001] pulling direction, we choose the z-direction as [001], and the directions [100] and [010] correspond to $\phi = 0$ and $\phi = \pi/2$, respectively, so that

$$a_{ij}^{[001]} = \begin{pmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

For the $[\bar{1}\bar{1}\bar{1}]$ pulling direction, the z-direction is $[\bar{1}\bar{1}\bar{1}]$ and we choose $\phi = 0$ and $\phi = \pi/2$ to correspond to $[2\bar{1}\bar{1}]$ and $[0\bar{1}1]$, respectively. In this case,

$$a_{ij}^{[\bar{1}\bar{1}\bar{1}]} = \begin{pmatrix} \frac{2}{\sqrt{6}}\cos\phi & -\frac{1}{\sqrt{6}}\cos\phi - \frac{1}{\sqrt{2}}\sin\phi & -\frac{1}{\sqrt{6}}\cos\phi + \frac{1}{\sqrt{2}}\sin\phi \\ -\frac{2}{\sqrt{6}}\sin\phi & \frac{1}{\sqrt{6}}\sin\phi - \frac{1}{\sqrt{2}}\cos\phi & \frac{1}{\sqrt{6}}\sin\phi + \frac{1}{\sqrt{2}}\cos\phi \\ -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \end{pmatrix}.$$

Finally, for the $[\bar{2}11]$ pulling direction, the z-direction is $[\bar{2}11]$, $\phi = 0$ corresponds to [111], and $\phi = \pi/2$ corresponds to $[01\bar{1}]$ yielding

$$a_{ij}^{[\bar{2}11]} = \begin{pmatrix} \frac{1}{\sqrt{3}}\cos\phi & \frac{1}{\sqrt{3}}\cos\phi + \frac{1}{\sqrt{2}}\sin\phi & \frac{1}{\sqrt{3}}\cos\phi - \frac{1}{\sqrt{2}}\sin\phi \\ -\frac{1}{\sqrt{3}}\sin\phi & -\frac{1}{\sqrt{3}}\sin\phi + \frac{1}{\sqrt{2}}\cos\phi & -\frac{1}{\sqrt{3}}\sin\phi - \frac{1}{\sqrt{2}}\cos\phi \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix}.$$

Each of these transformations changes the form of C_{cyc}, and in general we have the form $C_{\text{cyc}} = \sum_k C_{\text{cyc,k}}$, where each matrix with subscript k consists of only elements $c_k = \cos(k\phi)$, $s_k = \sin(k\phi)$ and zero. The detailed expressions are given in Appendix B. Since the anisotropic part of the constitutive relation C_{cyc}^a can be decomposed into components $C_{\text{cyc},k}^a$ consisting of only s_k and c_k, we can systematically construct higher order approximations. This is accomplished by first determining the solution for a generic $C_{\text{cyc},k}^a$, and then computing an appropriate linear combination of all the solutions for a particular pulling direction. To illustrate the procedure, we now discuss a simpler problem, where we use the plane-strain assumption.

3.2. Plane-strain thermal stress for solids with cubic anisotropy. As in [13], we assume that the displacement is only in the (r,ϕ) plane so that $\mathbf{e}_{\rm cyc} = (e_{rr}, e_{\phi\phi}, 0, 0, 0, 2e_{r\phi})^{\rm T}$. We will also reintroduce the notation $(\mathcal{C}_k, \mathcal{S}_k) = (\cos(n_k\phi + \delta_k),\ \sin(n_k\phi+\delta_k))$ and its generalizations $(\mathcal{C},\mathcal{S})$ and $(\tilde{\mathcal{C}}_k, \tilde{\mathcal{S}}_k)$ with the k suffix suppressed, and $\tilde{n}_k$ replacing n_k, respectively.

Starting with the isotropic case, where $\mathbf{w}_0$ is the solution of (3.5), when ϵ is small it is shown in [13] that $\mathbf{w}_0$ can be approximated by

$$\mathbf{w}_0 \sim \begin{pmatrix} rD_r^{(1)} + r^3 D_r^{(3)} \\ 0 \end{pmatrix} + r^{n_k-1}\begin{pmatrix} D_r^- \mathcal{C}_k \\ D_\phi^- \mathcal{S}_k \end{pmatrix} + r^{n_k+1}\begin{pmatrix} D_r^+ \mathcal{C}_k \\ D_\phi^+ \mathcal{S}_k \end{pmatrix}, \tag{3.8}$$

where

$$D_r^{(1)} = \mu\left(\frac{1+\nu}{1-\nu}\right)C_1(1-2\nu), \qquad D_r^{(3)} = \mu\left(\frac{1+\nu}{1-\nu}\right)\frac{C_1}{\bar{R}^2}, \tag{3.9a}$$

$$D_r^- = \mu\left(\frac{1+\nu}{1-\nu}\right)\frac{C_1\epsilon\beta_k}{\bar{R}^{n_k-2}}n_k, \qquad D_\phi^- = -\mu\left(\frac{1+\nu}{1-\nu}\right)\frac{C_1\epsilon\beta_k}{\bar{R}^{n_k-2}}n_k, \tag{3.9b}$$

$$D_r^+ = \mu\left(\frac{1+\nu}{1-\nu}\right)\frac{C_1\epsilon\beta_k}{\bar{R}^{n_k}}(2-4\nu-n_k) + \frac{4\mu(1+\nu)}{n_k(n_k+1)}\frac{C_2\epsilon\beta_k}{\bar{R}^{n_k}}, \tag{3.9c}$$

$$D_\phi^+ = \mu\left(\frac{1+\nu}{1-\nu}\right)\frac{C_1\epsilon\beta_k}{\bar{R}^{n_k}}(4-4\nu+n_k) + \frac{4\mu(1+\nu)}{n_k(n_k+1)}\frac{C_2\epsilon\beta_k}{\bar{R}^{n_k}}, \tag{3.9d}$$

where $\mu = 1 - \frac{H}{2}\frac{1-2\nu}{1-\nu}$ (see section 3.1).

Having determined $\mathbf{w}_0$, $\mathbf{w}$ is given by the expansion (3.7). Each of the terms in the expansion is a solution of the boundary value problem (3.6). To illustrate the procedure, in the following we construct $\mathbf{w}_1 = \mathcal{N}\mathbf{w}_0$.

Due to the linearity of the equilibrium equation, we can pick a representative $\mathbf{v} = (D_r r^k\cos(n\phi+\delta),\ D_\phi r^k \sin(n\phi+\delta))^{\rm T}$ with $n \geq 0$, $k \geq 1$. From this $\mathbf{v}$, the strain

$$\mathbf{S}(\mathbf{v}) = \begin{pmatrix} e_{rr} \\ e_{\phi\phi} \\ 2e_{r\phi} \end{pmatrix} = \begin{pmatrix} kD_r r^{k-1}\mathcal{C} \\ (D_r + nD_\phi)r^{k-1}\mathcal{C} \\ (kD_\phi - D_\phi - nD_r)r^{k-1}\mathcal{S} \end{pmatrix},$$

and the stress due to the anisotropy in the material parameters is given by $C^a_{\rm cyc}\mathbf{S}(\mathbf{v})$, where the exact form of $C^a_{\rm cyc}$ depends on the orientation of the crystal. Expressions (B.1)–(B.3) show that $C^a_{\rm cyc}$ is a sum of terms, $C^a_{{\rm cyc},m}$, characterized by $\cos m\phi$ and $\sin m\phi$. Therefore, $C^a_{{\rm cyc},m}\mathbf{S}(\mathbf{v})$ can be expressed as a sum with terms of the form $r^{k-1}(\cos(\tilde{n}\phi+\delta),\ \cos(\tilde{n}\phi+\delta),\ \sin(\tilde{n}\phi+\delta))^{\rm T}$, $\tilde{n} = n \pm m$. So, we need only consider the problem

$$\frac{\partial\sigma_{rr}}{\partial r} + \frac{1}{r}\frac{\partial\sigma_{r\phi}}{\partial\phi} + \frac{\sigma_{rr}-\sigma_{\phi\phi}}{r} = f_r r^{k-2}\tilde{\mathcal{C}}, \qquad r < \bar{R}(z), \tag{3.10a}$$

$$\frac{\partial\sigma_{r\phi}}{\partial r} + \frac{1}{r}\frac{\partial\sigma_{\phi\phi}}{\partial\phi} + \frac{2\sigma_{r\phi}}{r} = f_\phi r^{k-2}\tilde{\mathcal{S}}, \qquad r < \bar{R}(z), \tag{3.10b}$$

with integers $\tilde{n} \geq 0$, $k \geq 1$, and

$$\sigma_{rr} = g_r r^{k-1}\tilde{\mathcal{C}}, \qquad r = \bar{R}(z), \tag{3.11a}$$

$$\sigma_{r\phi} = g_\phi r^{k-1}\tilde{\mathcal{S}}, \qquad r = \bar{R}(z), \tag{3.11b}$$

corresponding to (3.6) with the higher order terms omitted.

To determine the solution to (3.10)–(3.11) we take a two-step approach. We begin by finding a particular solution $\mathbf{w}_p$ which satisfies (3.10) but not necessarily (3.11). Next, we find $\mathbf{w}_h$ which solves the homogeneous version of (3.10) and the modified boundary condition

$$\sigma_{rr}^h = g_r r^{k-1}\tilde{\mathcal{C}} - \sigma_{rr}^p := \tilde{g}_r r^{k-1}\tilde{\mathcal{C}}, \qquad r = \bar{R}(z), \tag{3.12a}$$

$$\sigma_{r\phi}^h = g_\phi r^{k-1}\tilde{\mathcal{S}} - \sigma_{r\phi}^p := \tilde{g}_\phi r^{k-1}\tilde{\mathcal{S}}, \qquad r = \bar{R}(z), \tag{3.12b}$$

where σ_{rr}^p and $\sigma_{r\phi}^p$ are stress components corresponding to $\mathbf{w}_p$. Accordingly, we find

$$\mathbf{w}_p = \begin{cases} \frac{1+\nu}{(1-\nu)^2}\begin{pmatrix} a_r r^k \tilde{\mathcal{C}} \\ a_\phi r^k \tilde{\mathcal{S}} \end{pmatrix}, & (k \pm \tilde{n})^2 \neq 1, \\ \frac{1+\nu}{(1-\nu)^2}\begin{pmatrix} (b_r + b_\phi \zeta \ln r) r^k \tilde{\mathcal{C}} \\ (b_\phi r^k \ln r \tilde{\mathcal{S}}) \end{pmatrix}, & (k \pm \tilde{n})^2 = 1, \end{cases} \tag{3.13a}$$

where

$$a_r = \frac{((1-2\nu)(k^2-1) - 2\tilde{n}^2(1-\nu))f_r + \tilde{n}(3-4\nu-k)f_\phi}{((k-\tilde{n})^2-1)((k+\tilde{n})^2-1)}, \tag{3.13b}$$

$$a_\phi = \frac{\tilde{n}(3-4\nu+k)f_r + (2(1-\nu)(k^2-1) - (1-2\nu)\tilde{n}^2)f_\phi}{((k-\tilde{n})^2-1)((k+\tilde{n})^2-1)}, \tag{3.13c}$$

$$b_r = \begin{cases} -\frac{(3-4\nu)(\tilde{n}-1)(f_r+f_\phi)+(f_r-f_\phi)}{8\tilde{n}(\tilde{n}-1)}, & k = \tilde{n}-1, \\ \frac{(3-4\nu)\tilde{n}^2(f_r+f_\phi)+8(1-\nu)(1-2\nu)(\tilde{n}+1)(f_r-f_\phi)}{8\tilde{n}(\tilde{n}+1)(\tilde{n}+4-4\nu)}, & k = \tilde{n}+1, \end{cases} \tag{3.13d}$$

$$b_\phi = \begin{cases} -\frac{(\tilde{n}-1)(f_r+f_\phi)+(3-4\nu)(f_r-f_\phi)}{8(\tilde{n}-1)}, & k = \tilde{n}-1, \\ \frac{(\tilde{n}+4-4\nu)(f_r+f_\phi)}{8(\tilde{n}+1)}, & k = \tilde{n}+1, \end{cases} \tag{3.13e}$$

$$\zeta = \begin{cases} -1, & k = \tilde{n}-1, \\ -\frac{\tilde{n}-2+4\nu}{\tilde{n}+4-4\nu}, & k = \tilde{n}+1. \end{cases} \tag{3.13f}$$

The special case when $\tilde{n} = 0$ and $k = 1$ takes the form $\mathbf{w}_p = \frac{1+\nu}{2(1-\nu)^2} r \ln r \times ((1-2\nu)f_r \cos\delta,\, 2(1-\nu)f_\phi \sin\delta)^{\mathrm{T}}$. Corresponding to $\mathbf{w}_p$ are the stress components

$$\begin{pmatrix} \sigma_{rr}^p \\ \sigma_{\phi\phi}^p \\ \sigma_{r\phi}^p \end{pmatrix} = \begin{pmatrix} \frac{1-\nu}{(1+\nu)(1-2\nu)}((k-k\nu+\nu)a_r + \nu\tilde{n}a_\phi) r^{k-1}\tilde{\mathcal{C}} \\ \frac{1-\nu}{(1+\nu)(1-2\nu)}((1-\nu+k\nu)a_r + (1-\nu)\tilde{n}a_\phi) r^{k-1}\tilde{\mathcal{C}} \\ \frac{1-\nu}{2(1+\nu)}(-\tilde{n}a_r + (k-1)a_\phi) r^{k-1}\tilde{\mathcal{S}} \end{pmatrix} \tag{3.14a}$$

for $(k \pm \tilde{n})^2 \neq 1$ and

$$\begin{pmatrix} \sigma_{rr}^p \\ \sigma_{\phi\phi}^p \\ \sigma_{r\phi}^p \end{pmatrix} = \begin{pmatrix} \frac{1}{(1-\nu)(1-2\nu)} c_{rr} r^{k-1}\tilde{\mathcal{C}} \\ \frac{1}{(1-\nu)(1-2\nu)} c_{\phi\phi} r^{k-1}\tilde{\mathcal{C}} \\ \frac{1}{2(1-\nu)} c_{r\phi} r^{k-1}\tilde{\mathcal{S}} \end{pmatrix} \tag{3.14b}$$

for $(k \pm \tilde{n})^2 = 1$, where

$$c_{rr} = (k - k\nu + \nu)(b_r + b_\phi \zeta \ln r) + b_\phi((1-\nu)\zeta + \nu \tilde{n} \ln(r)), \tag{3.14c}$$

$$c_{\phi\phi} = (1 - \nu + k\nu)(b_r + b_\phi \zeta \ln r) + b_\phi(\nu\zeta + (1-\nu)\tilde{n} \ln(r)), \tag{3.14d}$$

$$c_{r\phi} = -\tilde{n}(b_r + b_\phi \zeta \ln r) + b_\phi(1 + (k-1)\ln r). \tag{3.14e}$$

For the special case when $\tilde{n} = 0$ and $k = 1$, we have

$$(\sigma^p_{rr}, \sigma^p_{\phi\phi}, \sigma^p_{r\phi})^{\mathrm{T}} = \frac{1}{2(1-\nu)}(f_r(\ln r + 1 - \nu)\cos\delta, f_r(\ln r + \nu)\cos\delta, f_\phi(1-\nu)\sin\delta)^{\mathrm{T}}.$$

Using the technique described in [13], we can find $\mathbf{w}_h$ which solves the homogeneous version of (3.10) and the boundary condition (3.12),

$$\mathbf{w}_h = \frac{1+\nu}{2(1-\nu)} \begin{pmatrix} \left(\frac{(2-\tilde{n}-4\nu)(\tilde{g}_r+\tilde{g}_\phi)r^{\tilde{n}+1}}{(\tilde{n}+1)\bar{R}^{\tilde{n}}} + \frac{(\tilde{n}\tilde{g}_r+(\tilde{n}-2)\tilde{g}_\phi)r^{\tilde{n}-1}}{(\tilde{n}-1)\bar{R}^{\tilde{n}-2}}\right)\tilde{\mathcal{C}} \\ \left(\frac{(4+\tilde{n}-4\nu)(\tilde{g}_r+\tilde{g}_\phi)r^{\tilde{n}+1}}{(\tilde{n}+1)\bar{R}^{\tilde{n}}} - \frac{(\tilde{n}\tilde{g}_r+(\tilde{n}-2)\tilde{g}_\phi)r^{\tilde{n}-1}}{(\tilde{n}-1)\bar{R}^{\tilde{n}-2}}\right)\tilde{\mathcal{S}} \end{pmatrix}. \tag{3.15}$$

The corresponding stress components are given by

$$\begin{pmatrix} \sigma^h_{rr} \\ \sigma^h_{\phi\phi} \\ \sigma^h_{r\phi} \end{pmatrix} = \begin{pmatrix} \left(\frac{(2-\tilde{n})(\tilde{g}_r+\tilde{g}_\phi)r^{\tilde{n}}}{2\bar{R}^{\tilde{n}}} + \frac{(\tilde{n}\tilde{g}_r+(\tilde{n}-2)\tilde{g}_\phi)r^{\tilde{n}-2}}{2\bar{R}^{\tilde{n}-2}}\right)\tilde{\mathcal{C}} \\ \left(\frac{(2+\tilde{n})(\tilde{g}_r+\tilde{g}_\phi)r^{\tilde{n}}}{2\bar{R}^{\tilde{n}}} - \frac{(\tilde{n}\tilde{g}_r+(\tilde{n}-2)\tilde{g}_\phi)r^{\tilde{n}-2}}{2\bar{R}^{\tilde{n}-2}}\right)\tilde{\mathcal{C}} \\ \left(\frac{\tilde{n}(\tilde{g}_r+\tilde{g}_\phi)r^{\tilde{n}}}{2\bar{R}^{\tilde{n}}} - \frac{(\tilde{n}\tilde{g}_r+(\tilde{n}-2)\tilde{g}_\phi)r^{\tilde{n}-2}}{2\bar{R}^{\tilde{n}-2}}\right)\tilde{\mathcal{S}} \end{pmatrix}. \tag{3.16}$$

In the special case when $\tilde{n} = 0$ (or $\tilde{n} = 1$), we require $\tilde{g}_\phi = 0$ (or $\tilde{g}_r = \tilde{g}_\phi$) for the homogeneous elasticity problem to be well-posed. The solution and the corresponding stress components are given by (3.15) and (3.16) without the term related to $r^{\tilde{n}-1}$ and $r^{\tilde{n}-2}$, respectively.

In the following we find the explicit form of the expression $\mathbf{w}_1 = \mathcal{N}\mathbf{w}_0$ for the $[\bar{1}\bar{1}\bar{1}]$ pulling direction. This expression generates the first order corrections to the stress of an anisotropic cubic crystal. The outline of the procedure is also given for the [001] and $[\bar{2}11]$ seeding orientations.

3.2.1. $[\bar{1}\bar{1}\bar{1}]$ pulling direction. To treat this case systematically we decompose $\mathbf{w}_0$ into five separate quantities given by

$$\mathbf{w}_{0,A} = \begin{pmatrix} D_r^{(1)} r \\ 0 \end{pmatrix}, \quad \mathbf{w}_{0,B} = \begin{pmatrix} D_r^{(3)} r^3 \\ 0 \end{pmatrix}, \quad \mathbf{w}_{0,C} = D_r^- r^k \begin{pmatrix} \mathcal{C}_k \\ -\mathcal{S}_k \end{pmatrix},$$
$$\mathbf{w}_{0,D} = \frac{D_r^+ + D_\phi^+}{2} r^k \begin{pmatrix} \mathcal{C}_k \\ \mathcal{S}_k \end{pmatrix}, \quad \mathbf{w}_{0,E} = \frac{D_r^+ - D_\phi^+}{2} r^k \begin{pmatrix} \mathcal{C}_k \\ -\mathcal{S}_k \end{pmatrix}.$$

For $\mathbf{w}_{0,C}$, $k = n_k - 1$, while for both $\mathbf{w}_{0,D}$ and $\mathbf{w}_{0,E}$, $k = n_k + 1$. What characterizes the $[\bar{1}\bar{1}\bar{1}]$ direction is the anisotropic stiffness given by C^a. From (B.1), we have in the case of plane-strain $C^a = C^a_0$, where

$$C^{a,[\bar{1}\bar{1}\bar{1}]} = \frac{H}{12}\begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and as a result $\tilde{n} = n$ for the $[\bar{1}\bar{1}\bar{1}]$ direction.

For the first component, $\mathbf{w}_{0,A}$, we find from (3.6a) and (3.10) that

$$\mathcal{L}^a(\mathbf{w}_{0,A}) = \nabla \cdot C^{a,[\bar{1}\bar{1}\bar{1}]}\mathbf{S}(\mathbf{w}_{0,A}) = \begin{pmatrix} 0 \\ 0 \end{pmatrix} = r^{k-2}\begin{pmatrix} f_r\mathcal{C} \\ f_\phi\mathcal{S} \end{pmatrix}, \tag{3.17a}$$

and for the boundary condition, (3.6b) and (3.11) give

$$\mathcal{B}^a(\mathbf{w}_{0,A}) = C^{a,[\bar{1}\bar{1}\bar{1}]}\mathbf{S}(\mathbf{w}_{0,A}) \cdot \mathbf{n} = \frac{H}{6}\begin{pmatrix} D_r^{(1)} \\ 0 \end{pmatrix} = \bar{R}^{k-1}\begin{pmatrix} g_r\mathcal{C} \\ g_\phi\mathcal{S} \end{pmatrix}, \tag{3.17b}$$

where $k = 1$, $\delta = 0$, and $n = \tilde{n} = n_k = 0$. Setting $\Lambda_A = \frac{H}{6}D_r^{(1)}$ we identify $f_r = f_\phi = 0$, $g_r = \Lambda_A$, and $g_\phi = 0$. The quantities f_r and f_ϕ applied to (3.13)–(3.14) give the particular solution for the stress as $\sigma^p_{ij,A} = 0$, which through (3.12) indicates that $\tilde{g}_r = \Lambda_A$ and $\tilde{g}_\phi = 0$. For the homogeneous solution, we solve $\mathcal{L}^0(\mathbf{w}_{1,A}) = \mathcal{L}^a(\mathbf{w}_{0,A})$ with the boundary condition $\mathcal{B}^0(\mathbf{w}_{1,A}) = \mathcal{B}^a(\mathbf{w}_{0,A})$ and by using (3.16) to determine the stress, which gives

$$\begin{pmatrix} \sigma^h_{rr,A} \\ \sigma^h_{\phi\phi,A} \\ \sigma^h_{r\phi,A} \end{pmatrix} = \Lambda_A \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}. \tag{3.17c}$$

For $\mathbf{w}_{0,B}$, we have $k = 3$, $\delta = 0$, and $n = \tilde{n} = n_k = 0$, and continuing in an analogous fashion we find that

$$\mathcal{L}^a(\mathbf{w}_{0,B}) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \qquad \mathcal{B}^a(\mathbf{w}_{0,B}) = \bar{R}^2\begin{pmatrix} g_r \\ g_\phi \end{pmatrix} = \frac{H}{6}\bar{R}^2\begin{pmatrix} D_r^{(3)} \\ 0 \end{pmatrix}. \tag{3.18a}$$

As with the previous case, we find $\sigma^p_{ij,B} = 0$, and defining $\Lambda_B = \frac{H}{6}D_r^{(3)}$ we identify $\tilde{g}_r = g_r = \Lambda_B$, and $\tilde{g}_\phi = g_\phi = f_r = f_\phi = 0$. From (3.16) we have

$$\begin{pmatrix} \sigma^h_{rr,B} \\ \sigma^h_{\phi\phi,B} \\ \sigma^h_{r\phi,B} \end{pmatrix} = \Lambda_B\bar{R}^2 \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}. \tag{3.18b}$$

For $\mathbf{w}_{0,C}$, $k = n_k - 1$, $n = \tilde{n} = n_k$, and defining $\Lambda_C = \frac{H}{6}(1 - n_k)D_r^-$ we determine

$$\mathcal{L}^a(\mathbf{w}_{0,C}) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \qquad \mathcal{B}^a(\mathbf{w}_{0,C}) = \Lambda_C\bar{R}^{n_k-2}\begin{pmatrix} \mathcal{C}_k \\ -\mathcal{S}_k \end{pmatrix}$$

so that $f_r = f_\phi = 0$, $\sigma^p_{ij,C} = 0$, $g_r = \tilde{g}_r = \Lambda_C$, and $g_\phi = \tilde{g}_\phi = -\Lambda_C$. Applying (3.16) we obtain

$$\begin{pmatrix} \sigma^h_{rr,C} \\ \sigma^h_{\phi\phi,C} \\ \sigma^h_{r\phi,C} \end{pmatrix} = \Lambda_C r^{n_k-2} \begin{pmatrix} \mathcal{C}_k \\ -\mathcal{C}_k \\ -\mathcal{S}_k \end{pmatrix}. \tag{3.19}$$

The fourth component is $\mathbf{w}_{0,D}$ and $k = n_k + 1$, $n = \tilde{n} = n_k$. By defining $\Lambda_D = \frac{H}{12}(n_k+1)(D_r^+ + D_\phi^+)$ one has

$$\mathcal{L}^a(\mathbf{w}_{0,D}) = n_k \Lambda_D r^{n_k-1} \begin{pmatrix} \mathcal{C}_k \\ -\mathcal{S}_k \end{pmatrix}, \qquad \mathcal{B}^a(\mathbf{w}_{0,D}) = \Lambda_D \bar{R}^{n_k} \begin{pmatrix} \mathcal{C}_k \\ 0 \end{pmatrix}$$

so that $f_r = -f_\phi = n_k\Lambda_D$, $g_r = \Lambda_D$, and $g_\phi = 0$. In this case the particular solution for the stress is

$$\begin{pmatrix} \sigma^p_{rr,D} \\ \sigma^p_{\phi\phi,D} \\ \sigma^p_{r\phi,D} \end{pmatrix} = \frac{\Lambda_D r^{n_k}}{n_k+4-4\nu} \begin{pmatrix} 2(n_k+1-\nu n_k)\mathcal{C}_k \\ 2(1+\nu n_k)\mathcal{C}_k \\ -n_k(1-2\nu)\mathcal{S}_k \end{pmatrix} \tag{3.20a}$$

so that

$$\begin{pmatrix} \tilde{g}_r \\ \tilde{g}_\phi \end{pmatrix} = \frac{(1-2\nu)\Lambda_D}{n_k+4-4\nu} \begin{pmatrix} 2-n_k \\ n_k \end{pmatrix},$$

and from (3.16)

$$\begin{pmatrix} \sigma^h_{rr,D} \\ \sigma^h_{\phi\phi,D} \\ \sigma^h_{r\phi,D} \end{pmatrix} = \frac{(1-2\nu)\Lambda_D r^{n_k}}{n_k+4-4\nu} \begin{pmatrix} (2-n_k)\mathcal{C}_k \\ (n_k+2)\mathcal{C}_k \\ n_k\mathcal{S}_k \end{pmatrix}. \tag{3.20b}$$

The last component, $\mathbf{w}_{0,E}$, has $k = n_k + 1$ and $n = \tilde{n} = n_k$. For this case we choose $\Lambda_E = \frac{H}{12}(D_\phi^+ - D_r^+)$ and find

$$\mathcal{L}^a(\mathbf{w}_{0,E}) = n_k \Lambda_E r^{n_k-1} \begin{pmatrix} \mathcal{C}_k \\ -\mathcal{S}_k \end{pmatrix}, \qquad \mathcal{B}^a(\mathbf{w}_{0,E}) = \Lambda_E \bar{R}^{n_k} \begin{pmatrix} (n_k-1)\mathcal{C}_k \\ -n_k\mathcal{S}_k \end{pmatrix}$$

so that $f_r = -f_\phi = n_k\Lambda_E$, $g_r = (n_k-1)\Lambda_E$, and $g_\phi = -n_k\Lambda_E$. Continuing,

$$\begin{pmatrix} \sigma^p_{rr,E} \\ \sigma^p_{\phi\phi,E} \\ \sigma^p_{r\phi,E} \end{pmatrix} = \frac{\Lambda_E r^{n_k}}{n_k+4-4\nu} \begin{pmatrix} 2(n_k+1-\nu n_k)\mathcal{C}_k \\ 2(1+\nu n_k)\mathcal{C}_k \\ -n_k(1-2\nu)\mathcal{S}_k \end{pmatrix}, \tag{3.21a}$$

yielding

$$\begin{pmatrix} \tilde{g}_r \\ \tilde{g}_\phi \end{pmatrix} = \frac{(n_k+3-2\nu)\Lambda_E}{n_k+4-4\nu} \begin{pmatrix} n_k-2 \\ -n_k \end{pmatrix}$$

and

$$\begin{pmatrix} \sigma^h_{rr,E} \\ \sigma^h_{\phi\phi,E} \\ \sigma^h_{r\phi,E} \end{pmatrix} = -\frac{(n_k+3-2\nu)\Lambda_E r^{n_k}}{n_k+4-4\nu} \begin{pmatrix} (2-n_k)\mathcal{C}_k \\ (n_k+2)\mathcal{C}_k \\ n_k\mathcal{S}_k \end{pmatrix}. \tag{3.21b}$$

Combining (3.17)–(3.21) and using both (3.9) and (3.4), we find the first order correction to the total stress in the $[\bar{1}\bar{1}\bar{1}]$ direction accounting for cubic anisotropy as

$$\begin{pmatrix}\sigma_{rr}^{\text{tot}}\\ \sigma_{\phi\phi}^{\text{tot}}\\ \sigma_{zz}^{\text{tot}}\\ \sigma_{r\phi}^{\text{tot}}\end{pmatrix}_{[\bar{1}\bar{1}\bar{1}]} = \frac{2(1-\nu)\omega C_1}{3}\begin{pmatrix}1\\1\\2\nu\\0\end{pmatrix} - \frac{4(1-\nu)^2\omega C_1 r^2}{(1+\nu)(1-2\nu)\bar{R}^2}\begin{pmatrix}1\\1\\1+\nu\\0\end{pmatrix}$$

$$- \frac{4(1-\nu)\epsilon\omega C_2}{3(1-2\nu)}\frac{\beta_k}{n_k}\left(\frac{r}{\bar{\bar{R}}}\right)^{n_k}\mathcal{C}_k\begin{pmatrix}2\frac{1-\nu+\nu^2}{1+\nu}\\ 2\frac{1-\nu+\nu^2}{1+\nu}\\ 3-5\nu+4\nu^2\\ 0\end{pmatrix} \tag{3.22}$$

$$+ \frac{\epsilon\omega C_1}{3}\beta_k(n_k+1)\left(\frac{r}{\bar{\bar{R}}}\right)^{n_k}\begin{pmatrix}(n_k+2-4\nu)\mathcal{C}_k\\ (2-n_k-4\nu)\mathcal{C}_k\\ 4\nu(1-2\nu)\mathcal{C}_k\\ -n_k\mathcal{S}_k\end{pmatrix}$$

$$- \frac{\epsilon\omega C_1}{3}\beta_k n_k(n_k-1)\left(\frac{r}{\bar{\bar{R}}}\right)^{n_k-2}\begin{pmatrix}\mathcal{C}_k\\ -\mathcal{C}_k\\ 0\\ -\mathcal{S}_k\end{pmatrix}$$

with $\omega = \frac{1+\nu}{1-\nu}\frac{|H|}{2}$ using the scaled version of H.

This procedure can of course be followed for any pulling direction provided the form of C^a is known. It can also be applied to finding higher order corrections provided that the solution (3.13) to (3.10) is generalized to allow a multiplicative factor of $(\ln r)^l$ for some integer $l \geq 1$. In the following we simply state $\mathcal{L}^a$ and $\mathcal{B}^a$ for the [001] and $[\bar{2}11]$ seeding orientations for each of the five components of the displacement (3.8).

3.2.2. [001] pulling direction. From (B.2) we have $C^a = C_0^a + C_4^a$ with

$$C_0^a = \frac{H}{4}\begin{pmatrix}1&1&0\\1&1&0\\0&0&0\end{pmatrix}, \qquad C_4^a = \frac{H}{4}\begin{pmatrix}c_4&-c_4&-s_4\\-c_4&c_4&s_4\\-s_4&s_4&-c_4\end{pmatrix}.$$

Accordingly one finds that

$$\mathcal{L}^a(\mathbf{w}_{0,A}) = \begin{pmatrix}0\\0\end{pmatrix}, \qquad \mathcal{B}^a(\mathbf{w}_{0,A}) = 3\Lambda_A\begin{pmatrix}1\\0\end{pmatrix},$$

$$\mathcal{L}^a(\mathbf{w}_{0,B}) = 12\Lambda_B r\begin{pmatrix}1\\0\end{pmatrix}, \qquad \mathcal{B}^a(\mathbf{w}_{0,B}), = 3\Lambda_B\bar{R}^2\begin{pmatrix}2+c_4\\-s_4\end{pmatrix}.$$

The composite form of $\mathcal{B}^a(\mathbf{w}_{0,B})$ shows that the condition (3.11) can generate more than one term of a particular solution for a fixed version of (3.10). For the rest of the terms we extend the notation $\{\mathcal{C}_k, \mathcal{S}_k\}$ to $\{\mathcal{C}_{k,m}, \mathcal{S}_{k,m}\}$, where $\mathcal{C}_{k,m} = \cos((n_k - m)\phi + \delta_k)$, and $\mathcal{S}_{k,m}$ is updated similarly. In this notation, one has

$$\mathcal{L}^a(\mathbf{w}_{0,C}) = 6(2-n_k)\Lambda_C r^{n_k-3}\begin{pmatrix}\mathcal{C}_{k,4}\\ \mathcal{S}_{k,4}\end{pmatrix}, \quad \mathcal{B}^a(\mathbf{w}_{0,C}) = -3\Lambda_C \bar{R}^{n_k-2}\begin{pmatrix}\mathcal{C}_{k,4}\\ \mathcal{S}_{k,4}\end{pmatrix},$$

$$\mathcal{L}^a(\mathbf{w}_{0,D}) = 3n_k\Lambda_D r^{n_k-1}\begin{pmatrix}\mathcal{C}_{k}\\ -\mathcal{S}_{k}\end{pmatrix}, \quad \mathcal{B}^a(\mathbf{w}_{0,D}) = 3\Lambda_D \bar{R}^{n_k}\begin{pmatrix}\mathcal{C}_{k}\\ 0\end{pmatrix},$$

$$\mathcal{L}^a(\mathbf{w}_{0,E}) = 3n_k\Lambda_E r^{n_k-1}\begin{pmatrix}2(1-n_k)\mathcal{C}_{k,4} - \mathcal{C}_k\\ 2(1-n_k)\mathcal{S}_{k,4} + \mathcal{S}_k\end{pmatrix},$$
$$\mathcal{B}^a(\mathbf{w}_{0,E}) = -3\Lambda_E \bar{R}^{n_k}\begin{pmatrix}n_k\mathcal{C}_{k,4} + \mathcal{C}_k\\ n_k\mathcal{S}_{k,4}\end{pmatrix}.$$

3.2.3. [$\bar{2}$11] pulling direction. From (B.3),

$$C^{a,[\bar{2}11]} = \frac{H}{48}\begin{pmatrix}3-4c_2-7c_4 & 9+7c_4 & 2s_2+7s_4\\ 9+7c_4 & 3+4c_2-7c_4 & 2s_2-7s_4\\ 2s_2+7s_4 & 2s_2-7s_4 & -3+7c_4\end{pmatrix}.$$

In the case for [$\bar{2}$11], C^a is decoupled into C_0^a, C_2^a, C_4^a, which is analogous to the [001] case. Repeating the calculation we find

$$\mathcal{L}^a(\mathbf{w}_{0,A}) = \begin{pmatrix}0\\ 0\end{pmatrix},$$
$$\mathcal{B}^a(\mathbf{w}_{0,A}) = \frac{1}{2}\Lambda_A\begin{pmatrix}3-c_2\\ s_2\end{pmatrix},$$
$$\mathcal{L}^a(\mathbf{w}_{0,B}) = 3\Lambda_B r\begin{pmatrix}1-c_2\\ s_2\end{pmatrix},$$
$$\mathcal{B}^a(\mathbf{w}_{0,B}) = \frac{1}{4}\Lambda_B\bar{R}^2\begin{pmatrix}-7c_4-6c_2+9\\ 7s_4+4s_2\end{pmatrix},$$
$$\mathcal{L}^a(\mathbf{w}_{0,C}) = \frac{1}{2}(n_k-2)\Lambda_C r^{n_k-3}\begin{pmatrix}7\mathcal{C}_{k,4}+\mathcal{C}_{k,2}\\ 7\mathcal{S}_{k,4}-\mathcal{S}_{k,2}\end{pmatrix},$$
$$\mathcal{B}^a(\mathbf{w}_{0,C}) = \frac{1}{4}\Lambda_C\bar{R}^{n_k-2}\begin{pmatrix}7\mathcal{C}_{k,4}+2\mathcal{C}_{k,2}+3\mathcal{C}_k\\ 7\mathcal{S}_{k,4}-3\mathcal{S}_k\end{pmatrix},$$
$$\mathcal{L}^a(\mathbf{w}_{0,D}) = \frac{1}{2}n_k\Lambda_D r^{n_k-1}\begin{pmatrix}-\mathcal{C}_{k,2}+3\mathcal{C}_k\\ -\mathcal{S}_{k,2}-3\mathcal{S}_k\end{pmatrix},$$
$$\mathcal{B}^a(\mathbf{w}_{0,D}) = \frac{1}{4}\Lambda_D\bar{R}^{n_k}\begin{pmatrix}-\mathcal{C}_{k,2}-\mathcal{C}_{k,-2}+6\mathcal{C}_k\\ -\mathcal{S}_{k,2}+\mathcal{S}_{k,-2}\end{pmatrix},$$
$$\mathcal{L}^a(\mathbf{w}_{0,E}) = \frac{1}{2}n_k\Lambda_E r^{n_k-1}\begin{pmatrix}7(n_k-1)\mathcal{C}_{k,4}+(n_k+1)\mathcal{C}_{k,2}\\ 7(n_k-1)\mathcal{S}_{k,4}+(3-n_k)\mathcal{S}_{k,2}\end{pmatrix},$$
$$\mathcal{B}^a(\mathbf{w}_{0,E}) = \frac{1}{4}\Lambda_E\bar{R}^{n_k}\begin{pmatrix}7n_k\mathcal{C}_{k,4}+(2n_k+1)\mathcal{C}_{k,2}+\mathcal{C}_{k,-2}+3(n_k-2)\mathcal{C}_k\\ 7n_k\mathcal{S}_{k,4}+\mathcal{S}_{k,2}-\mathcal{S}_{k,-2}-3n_k\mathcal{S}_k\end{pmatrix}.$$

In summary, the total stress is the sum of the stress components due to anisotropy in the elastic constants obtained above, plus the sum for isotropic solids given in [13] multiplied by $\mu = 1 - \frac{H}{2}\frac{1-2\nu}{1-\nu}$, which is reproduced as follows for completeness:

$$\begin{pmatrix} \sigma_{rr}^{\mathrm{tot,iso}} \\ \sigma_{\phi\phi}^{\mathrm{tot,iso}} \\ \sigma_{r\phi}^{\mathrm{tot,iso}} \end{pmatrix} = \mu C_1 \begin{pmatrix} 1-\left(\frac{r}{\bar{R}}\right)^2 \\ 1-3\left(\frac{r}{\bar{R}}\right)^2 \\ 0 \end{pmatrix} + \mu\epsilon C_1 \beta_k n_k (n_k-1)\left(\frac{r}{\bar{R}}\right)^{n_k-2} \begin{pmatrix} \mathcal{C}_k \\ -\mathcal{C}_k \\ -\mathcal{S}_k \end{pmatrix} + \mu\epsilon C_1 \beta_k (n_k+1)\left(\frac{r}{\bar{R}}\right)^{n_k} \begin{pmatrix} (2-n_k)\mathcal{C}_k \\ (n_k+2)\mathcal{C}_k \\ n_k\mathcal{S}_k \end{pmatrix} \tag{3.23a}$$

and

$$\sigma_{zz}^{\mathrm{tot,iso}} = 2\mu C_1\left(1-2\left(\frac{r}{\bar{R}}\right)^2\right) + 4\mu\epsilon\beta_k\left(\nu(n_k+1)C_1 - \frac{1-\nu}{n_k}C_2\right)\left(\frac{r}{\bar{R}}\right)^{n_k}\mathcal{C}_k. \tag{3.23b}$$

3.3. The von Mises and total resolved stresses. A characteristic amount of stress can be assigned to each point with the von Mises stress, which satisfies

$$2\sigma_{\mathrm{vm}}^2 = (\sigma_{rr}-\sigma_{\phi\phi})^2 + (\sigma_{rr}-\sigma_{zz})^2 + (\sigma_{\phi\phi}-\sigma_{zz})^2 + 6\sigma_{r\phi}^2 \tag{3.24}$$

for a cubic material, where the σ_{ij} are given by (3.23) and the corrections due to material anisotropy, such as that given by (3.22).

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], which consists 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

$$\sigma_{\mathrm{rs}} = \mathbf{d}^{\mathrm{T}} U_{\mathbf{p}}^{\mathrm{T}} Q^{\mathrm{T}} \sigma^{\mathrm{tot}} Q U_{\mathbf{p}} \mathbf{n}.$$

The matrix $U_{\mathbf{p}}$ rotates vectors from the crystallographic frame to the solidification frame. If the stress tensor σ^{tot} is expressed in the (r,ϕ,z) coordinates, Q is the coordinate transformation matrix that takes $(x,y,z) \to (r,\phi,z)$.

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

$$|\sigma_{\mathrm{rs}}^{\mathrm{tot}}| = \sum_{i=1}^{12}\left|\mathbf{d}_i^T U_{\mathbf{p}}^T Q^T \sigma^{\mathrm{tot}} Q U_{\mathbf{p}} \mathbf{n}_i\right|. \tag{3.25}$$

4. Numerical results. The physical parameters used for the simulations correspond to InSb grown with the Cz method can be found in [1]. Numerical results are obtained for a conic crystal with a half opening angle of $\varphi_{\mathrm{cone}} = 5^\circ$ so that in nondimensional coordinates $\bar{R}(z) = \bar{R}(Z_0) + \hat{\theta}_{\mathrm{cone}} z$. The initial seed length is $Z_0 = 0.054$ and the radius is $\bar{R}(Z_0) = 1/6$, corresponding to an initial dimensional radius and length of 0.005 m and 0.01 m, respectively. Here we have taken $h_{\mathrm{gs}} = \bar{h}_{\mathrm{gs}} = 4$ so that by using the characteristic radius $\tilde{R} = 0.03$ m and thermal conductivity of

TABLE 1
The maximum von Mises and resolved stress values for the three seed orientations using j correction terms.

j	Maximum von Mises stress $\mathbf{p}=[001]$	$\mathbf{p}=[\bar{1}\bar{1}\bar{1}]$	$\mathbf{p}=[\bar{2}11]$
0	3.32×10^{-3}	7.23×10^{-3}	3.83×10^{-3}
1	2.75×10^{-3}	6.80×10^{-3}	3.89×10^{-3}
12	2.85×10^{-3}	6.89×10^{-3}	4.04×10^{-3}

j	Maximum resolved stress $\mathbf{p}=[001]$	$\mathbf{p}=[\bar{1}\bar{1}\bar{1}]$	$\mathbf{p}=[\bar{2}11]$
0	9.23×10^{-3}	1.34×10^{-2}	8.78×10^{-3}
1	7.66×10^{-3}	1.20×10^{-2}	8.78×10^{-3}
12	8.15×10^{-3}	1.21×10^{-2}	8.84×10^{-3}

4.57 $\mathrm{W\,m^{-1}K^{-1}}$ we find $\mathrm{Bi} = 0.026$. The final radius and length (not including the seed) are 0.03 m and 0.286 m or 1 and 1.537, respectively, in scaled units. This gives a value of $\hat{\theta}_{\mathrm{cone}} = 0.542$.

Θ_0 is the solution of (2.6) in the pseudosteady case ($1/\mathrm{St} = 0$) with $\delta = \gamma = 0$ and $I_{0,1}/I_{2,0} = 1$. Θ_1 is given by (2.7) with $h_F = 0$ so that $F(\Theta) = \beta\Theta = \Theta$. Since 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, one has $H = 2C_{44} - C_{11} + C_{12} = 2.99 \times 10^4$ MPa and $\omega = 0.329$. In addition, the values of E and ν used in the calculation are represented by (3.2b),

$$E = \frac{(C_{11} + 2C_{12} + H/2)(C_{11} - C_{12} + H/2)}{C_{11} + C_{12} + H/2} = 5.95 \times 10^4 \text{ MPa}, \tag{4.1a}$$

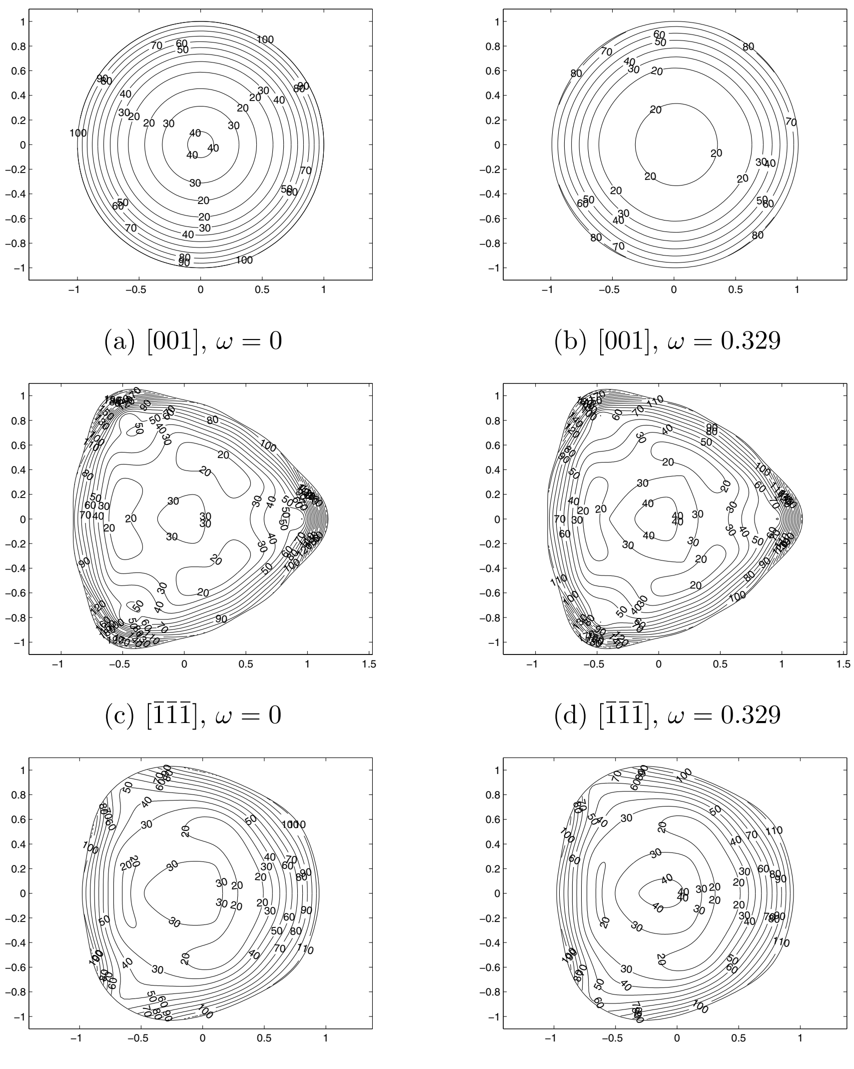
$$\nu = \frac{C_{12}}{C_{11} + C_{12} + H/2} = 0.308. \tag{4.1b}$$

When combined with the parameters above, the dimensional constant for the stress calculations is $\alpha\Delta TE/(1-\nu) \sim 93.8$ MPa, where $\alpha = 5.5 \times 10^{-6}\mathrm{K}^{-1}$ and $\Delta T = 198.4$ K [1].

We start with the expression for the displacement (3.8), which defines $D^{(1)}$, $D^{(3)}$, $D^{\pm}$, k, and n for the $\mathcal{L}^a(\mathbf{w}_0)$ and $\mathcal{B}^a(\mathbf{w}_0)$ expressions found in sections 3.2.1, 3.2.2, and 3.2.3. The $\mathcal{L}^a(\mathbf{w}_0)$ defines f_r, f_ϕ, k, and $\tilde{n}$ in (3.10), which gives σ^p_{ij}, and $\mathcal{B}^a(\mathbf{w}_0)$ defines g_r, g_ϕ, k, and $\tilde{n}$ in (3.11), which gives σ^h_{ij} with $\tilde{g}_r$ and $\tilde{g}_\phi$ given by g_r, g_ϕ, and σ^p_{ij}.

Figure 1 shows the von Mises stress for the three seeding orientation: [001], $[\bar{1}\bar{1}\bar{1}]$ and $[\bar{2}11]$. To the left of each pair is the isotropic case corresponding to the material in [13], and to the right is the anisotropic case corresponding to one correction term, namely, $\mathbf{w} \sim \mathbf{w}_0 + \mathbf{w}_1$. Reported stress values are given in percentages with 100% corresponding to the outer edge of a cylindrical crystal ($\alpha = 0$) grown in the [001] direction or $|\sigma_{\mathrm{vm}}| = 3.32 \times 10^{-3}$. In the [001] pulling direction the von Mises stress retains its axial symmetry even when anisotropic stiffness coefficients are included. For the $[\bar{1}\bar{1}\bar{1}]$ and $[\bar{2}11]$ seeding orientations the geometric effect dominates the amount of stress. Table 1 lists the maximum value of the von Mises stress for the three orientations using zero (isotropic, $\omega = 0$), one, and twelve correction terms for the total stress. It can be seen that the von Mises stress can either decrease or increase when material anisotropy is considered, depending on seed orientation.

Figure 2 shows the corresponding resolved stress $\sigma^{\mathrm{tot}}_{\mathrm{rs}}$ as given by (3.25), which is relevant to dislocation generation. The computed peak values for the total resolved stress are listed in Table 1 and once again we conclude that the effect of the material



(a) [001], $\omega = 0$ (b) [001], $\omega = 0.329$

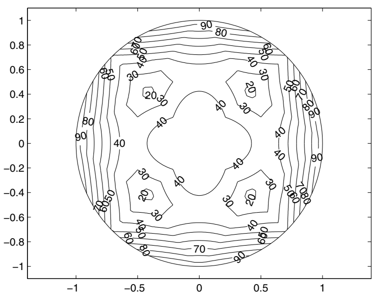
(c) $[\bar{1}\bar{1}\bar{1}]$, $\omega = 0$ (d) $[\bar{1}\bar{1}\bar{1}]$, $\omega = 0.329$

(e) $[\bar{2}11]$, $\omega = 0$ (f) $[\bar{2}11]$, $\omega = 0.329$

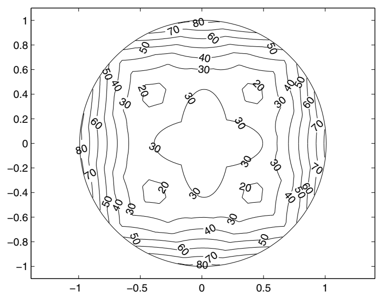
FIG. 1. *The von Mises stress computed using* (3.24) *at the indicated orientation, just inside the crystal/melt interface at the end of the growth. All reported stress values are expressed in percentages with* 100% *occurring at the outer edge of a crystal grown in the* [001] *direction, which corresponds to a value of* $|\sigma_{vm}| = 3.32 \times 10^{-3}$(0.311 MPa). *The* $\omega = 0.329$ *case utilizes one correction term.*

anisotropy is more significant for the [001] orientation since there is no geometric effect in that case. For the other two directions, the geometric effect dominates and the material anisotropy has a limited effect.

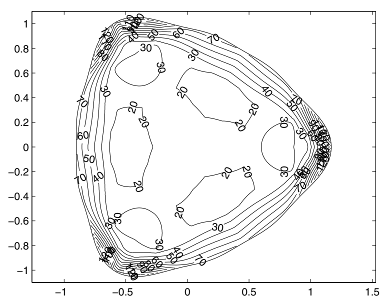
5. Conclusion. In this paper we have discussed the effect of material anisotropy on the thermal stress and compared it with that of geometric anisotropy due to facet formation. We have presented a systematic procedure which computes the stress iteratively, using an asymptotic series. We have also shown that the series converges for any anisotropic cubic material. Numerical results are obtained for InSb crystals



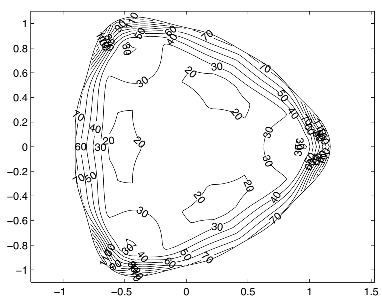
(a) [001], $\omega = 0$



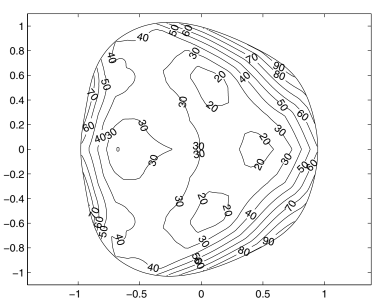
(b) [001], $\omega = 0.329$



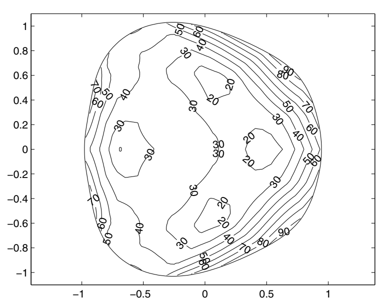
(c) $[\bar{1}\bar{1}\bar{1}]$, $\omega = 0$



(d) $[\bar{1}\bar{1}\bar{1}]$, $\omega = 0.329$



(e) $[\bar{2}11]$, $\omega = 0$



(f) $[\bar{2}11]$, $\omega = 0.329$

FIG. 2. *The total resolved stress computed using* (3.25) *at the indicated orientation, just inside the crystal/melt interface at the end of the growth. All reported stress values are expressed in percentages with* 100% *occurring at the outer edge of a crystal grown in the* [001] *direction, which corresponds to a value of* $|\sigma_{vm}^{tot}| = 9.23\times10^{-3}(0.866\,\mathrm{MPa})$. *The* $\omega = 0.329$ *case utilizes one correction term.*

grown by the Cz method in three pulling directions. When the seed orientation is in the [001] direction, since no facet forms and no geometric anisotropy is present, the material anisotropy has a visible effect on both the von Mises and the total resolved stresses. For the $[\bar{1}\bar{1}\bar{1}]$ and $[\bar{2}11]$ seeding orientations, however, the material anisotropy has only a limited effect, while the geometric (facet formation) has a much stronger effect. Our results suggest that for faceted crystals, it is much more important to take the geometric effect into account, while neglecting the material anisotropy is justified. Finally, the methodology used in this paper is not limited to the case of Cz crystals.

It can be applied to other elastic problems, such as the ones investigated in [7, 14], by including the effect of an anisotropic material property.

Appendix A. Proof of (3.7). We begin by introducing the weighted direct sum Hilbert space

$$\overset{\circ}{\mathcal{H}} = \left\{ \mathbf{w} \in \left(H^1(\Omega)\right)^3 : \int_\Omega \mathbf{w}\ \mathrm{d}V = \mathbf{0}, \int_\Omega \mathrm{rot}(\mathbf{w})\ \mathrm{d}V = \mathbf{0}, \|\mathbf{w}\|^2_{\overset{\circ}{\mathcal{H}}} = \sum_{i=1}^{6} \lambda_i \|e_i(\mathbf{w})\|_0^2 \right\}$$

on the bounded domain Ω. $\|\cdot\|_0$ denotes the standard L^2 norm, and the quantity $\mathbf{e}(\mathbf{w})$ consists of elements of the strain tensor associated with the displacement $\mathbf{w}$. 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 coordinates, $\mathbf{e}(\mathbf{w}) = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{xz}, 2e_{xy})^{\mathrm{T}}$, where $e_{ij} = (w_{i,j} + w_{j,i})/2$, the comma denoting partial differentiation.

For the uniqueness of (3.3), (3.5), and (3.6), we assume that the displacement solutions to these equations belong to $\overset{\circ}{\mathcal{H}}$.

LEMMA A.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. □

The space $\overset{\circ}{\mathcal{H}}$ is the natural choice for an anisotropic cubic crystal. The next lemma states that convergence in $\overset{\circ}{\mathcal{H}}$ is equivalent to convergence in $(H^1)^3$.

LEMMA A.2. $\|\cdot\|_{\overset{\circ}{\mathcal{H}}}$ *is equivalent to* $\|\cdot\|_1$ *(the* $(H^1)^3$ *norm) in* $\overset{\circ}{\mathcal{H}}$.

Proof. This is a direct consequence of the Korn inequality [4],

$$\|\mathbf{w}\|_1^2 \le C(\Omega) \left(\sum_{i=1}^{6} \|e_i(\mathbf{w})\|_0^2 \right) \quad \forall \mathbf{w} \in \overset{\circ}{\mathcal{H}},$$

where $C(\Omega)$ is a constant depending only on the domain Ω. □

Next we illustrate that the operator $\mathcal{N}$ is a contraction mapping on $\overset{\circ}{\mathcal{H}}$.

LEMMA A.3. *The operator* $\mathcal{N}$ *in* (3.7) *satisfies* $\|\mathcal{N}\|_{\overset{\circ}{\mathcal{H}} \mapsto \overset{\circ}{\mathcal{H}}} \le \omega < 1$.

Proof. For any given $\mathbf{u} \in \overset{\circ}{\mathcal{H}}$, let $\mathbf{w} = \mathcal{N}\mathbf{u}$. Using the boundary condition in the definition of $\mathcal{N}$, we see that $\mathbf{w}$ satisfies

$$\int_\Omega C^0_{ij} e_i(\mathbf{w}) e_j(\mathbf{v})\,\mathrm{d}V = \int_\Omega C^a_{ij} e_i(\mathbf{u}) e_j(\mathbf{v})\,\mathrm{d}V \quad \forall \mathbf{v} \in \overset{\circ}{\mathcal{H}},$$

and in particular for $\mathbf{v} = \mathbf{w}$,

$$\int_\Omega C^0_{ij} e_i(\mathbf{w}) e_j(\mathbf{w})\, \mathrm{d}V = \int_\Omega C^a_{ij} e_i(\mathbf{u}) e_j(\mathbf{w})\, \mathrm{d}V. \tag{A.1}$$

Taking only the diagonal terms of the left-hand side of (A.1) yields

$$\int_\Omega C^0_{ij} e_i(\mathbf{w}) e_j(\mathbf{w})\, \mathrm{d}V \geq \int_\Omega \sum_{k=1}^{6} \lambda_k e_k^2(\mathbf{w})\, \mathrm{d}V = \|\mathbf{w}\|^2_{\overset{\circ}{\mathcal{H}}}, \tag{A.2}$$

while noting that C^a is itself diagonal gives

$$\int_\Omega C^a_{ij} e_i(\mathbf{u}) e_j(\mathbf{w})\, \mathrm{d}V \leq \int_\Omega \left(\sum_{k=1}^{3} \left| \frac{H}{2} e_k(\mathbf{u}) e_k(\mathbf{w}) \right| + \sum_{k=4}^{6} \left| \frac{H}{4} e_k(\mathbf{u}) e_k(\mathbf{w}) \right| \right) \mathrm{d}V. \tag{A.3}$$

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 (A.2) and (A.3) with (A.1) allow us to conclude, with Hölder's inequality, that

$$\|\mathbf{w}\|^2_{\overset{\circ}{\mathcal{H}}} \leq \omega \|\mathbf{w}\|_{\overset{\circ}{\mathcal{H}}} \|\mathbf{u}\|_{\overset{\circ}{\mathcal{H}}}$$

or $\|\mathbf{w}\|_{\overset{\circ}{\mathcal{H}}} \leq \omega \|\mathbf{u}\|_{\overset{\circ}{\mathcal{H}}}$ for any given $\mathbf{u} \in \overset{\circ}{\mathcal{H}}$. Using Lemma A.1, $\|\mathcal{N}\|_{\overset{\circ}{\mathcal{H}} \mapsto \overset{\circ}{\mathcal{H}}} \leq \omega < 1$. ◻

Proposition A.4. *Let* $\mathbf{s}_n = \mathbf{w}_0 + \mathcal{N}\mathbf{w}_0 + \mathcal{N}^2\mathbf{w}_0 + \cdots + \mathcal{N}^n\mathbf{w}_0$, *with* $\mathbf{s}_0 = \mathbf{w}_0$. *Expression* (3.7) *converges to* $\mathbf{w}$ *in* $\overset{\circ}{\mathcal{H}}$, *and*

$$\|\mathbf{w} - \mathbf{s}_n\|_{\overset{\circ}{\mathcal{H}}} \leq \omega^{n+1} \|\mathbf{w}\|_{\overset{\circ}{\mathcal{H}}}.$$

Proof. Lemma A.3 implies that the right-hand side of (3.7) converges. What remains is to show that $\mathbf{w}$ is in fact the limit. We note that

$$\begin{aligned} \mathcal{L}^0(\mathbf{w} - \mathbf{w}_0) &= \mathcal{L}(\mathbf{w}) + \mathcal{L}^a(\mathbf{w}) - \mathbf{F} = \mathcal{L}^a(\mathbf{w}), && \mathbf{x} \in \Omega, \quad t > 0, \\ \mathcal{B}^0(\mathbf{w} - \mathbf{w}_0) &= \mathcal{B}(\mathbf{w}) + \mathcal{B}^a(\mathbf{w}) - \mathbf{g} = \mathcal{B}^a(\mathbf{w}), && r = R(\phi, z). \end{aligned}$$

By the definition of $\mathcal{N}$, one has $\mathbf{w} - \mathbf{w}_0 = \mathcal{N}\mathbf{w}$ and $\|\mathbf{w} - \mathbf{w}_0\| = \|\mathcal{N}\mathbf{w}\| \leq \omega \|\mathbf{w}\|$. $\mathbf{w} - \mathbf{s}_n = \mathcal{N}(\mathbf{w} - \mathbf{s}_{n-1})$ gives $\|\mathbf{w} - \mathbf{s}_n\| \leq \omega \|\mathbf{w} - \mathbf{s}_{n-1}\|$ with all norms taken in $\overset{\circ}{\mathcal{H}}$. By induction on n

$$\|\mathbf{w} - \mathbf{s}_n\|_{\overset{\circ}{\mathcal{H}}} \leq \omega^{n+1} \|\mathbf{w}\|_{\overset{\circ}{\mathcal{H}}} \quad \forall n \geq 0$$

so that letting $n \to \infty$ and using Lemma A.3 gives the result. ◻

Appendix B. Detailed form of C_{cyc}. For the $[\bar{1}\bar{1}\bar{1}]$ pulling direction we obtain $C_{\mathrm{cyc}}^{a,[\bar{1}\bar{1}\bar{1}]} = C_{\mathrm{cyc},0}^{a,[\bar{1}\bar{1}\bar{1}]} + C_{\mathrm{cyc},3}^{a,[\bar{1}\bar{1}\bar{1}]}$, where

$$C_{\mathrm{cyc},0}^{a,[\bar{1}\bar{1}\bar{1}]} = \frac{H}{12}\begin{pmatrix} 0 & 2 & 4 & 0 & 0 & 0 \\ 2 & 0 & 4 & 0 & 0 & 0 \\ 4 & 4 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \tag{B.1a}$$

$$C_{\mathrm{cyc},3}^{a,[\bar{1}\bar{1}\bar{1}]} = \frac{\sqrt{2}H}{6}\begin{pmatrix} 0 & 0 & 0 & s_3 & -c_3 & 0 \\ 0 & 0 & 0 & -s_3 & c_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ s_3 & -s_3 & 0 & 0 & 0 & c_3 \\ -c_3 & c_3 & 0 & 0 & 0 & s_3 \\ 0 & 0 & 0 & c_3 & s_3 & 0 \end{pmatrix}. \tag{B.1b}$$

For the [001] pulling direction, $C_{\mathrm{cyc}}^{a,[001]} = C_{\mathrm{cyc},0}^{a,[001]} + C_{\mathrm{cyc},4}^{a,[001]}$, where

$$C_{\mathrm{cyc},0}^{a,[001]} = \frac{H}{4}\begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{B.2a}$$

$$C_{\mathrm{cyc},4}^{a,[001]} = \frac{H}{4}\begin{pmatrix} c_4 & -c_4 & 0 & 0 & 0 & -s_4 \\ -c_4 & c_4 & 0 & 0 & 0 & s_4 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -s_4 & s_4 & 0 & 0 & 0 & -c_4 \end{pmatrix}. \tag{B.2b}$$

Finally, for the $[\bar{2}11]$ pulling direction, $C_{\mathrm{cyc}}^{a,[\bar{2}11]} = C_{\mathrm{cyc},0}^{a,[\bar{2}11]} + C_{\mathrm{cyc},1}^{a,[\bar{2}11]} + C_{\mathrm{cyc},2}^{a,[\bar{2}11]} + C_{\mathrm{cyc},3}^{a,[\bar{2}11]} + C_{\mathrm{cyc},4}^{a,[\bar{2}11]}$, where

$$C_{\mathrm{cyc},0}^{a,[\bar{2}11]} = \frac{H}{16}\begin{pmatrix} 1 & 3 & 4 & 0 & 0 & 0 \\ 3 & 1 & 4 & 0 & 0 & 0 \\ 4 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \tag{B.3a}$$

$$C_{\mathrm{cyc},1}^{a,[\bar{2}11]} = \frac{\sqrt{2}H}{24}\begin{pmatrix} 0 & 0 & 0 & -s_1 & 3c_1 & 0 \\ 0 & 0 & 0 & -3s_1 & c_1 & 0 \\ 0 & 0 & 0 & 4s_1 & -4c_1 & 0 \\ -s_1 & -3s_1 & 4s_1 & 0 & 0 & c_1 \\ 3c_1 & c_1 & -4c_1 & 0 & 0 & -s_1 \\ 0 & 0 & 0 & c_1 & -s_1 & 0 \end{pmatrix}, \tag{B.3b}$$

$$C^{a,[\bar{2}11]}_{\mathrm{cyc},2} = \frac{H}{24}\begin{pmatrix} -2c_2 & 0 & 2c_2 & 0 & 0 & s_2 \\ 0 & 2c_2 & -2c_2 & 0 & 0 & s_2 \\ 2c_2 & -2c_2 & 0 & 0 & 0 & -2s_2 \\ 0 & 0 & 0 & -2c_2 & -2s_2 & 0 \\ 0 & 0 & 0 & -2s_2 & 2c_2 & 0 \\ s_2 & s_2 & -2s_2 & 0 & 0 & 0 \end{pmatrix}, \tag{B.3c}$$

$$C^{a,[\bar{2}11]}_{\mathrm{cyc},3} = \frac{\sqrt{2}H}{8}\begin{pmatrix} 0 & 0 & 0 & s_3 & -c_3 & 0 \\ 0 & 0 & 0 & -s_3 & c_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ s_3 & -s_3 & 0 & 0 & 0 & c_3 \\ -c_3 & c_3 & 0 & 0 & 0 & s_3 \\ 0 & 0 & 0 & c_3 & s_3 & 0 \end{pmatrix}, \tag{B.3d}$$

$$C^{a,[\bar{2}11]}_{\mathrm{cyc},4} = \frac{7H}{48}\begin{pmatrix} -c_4 & c_4 & 0 & 0 & 0 & s_4 \\ c_4 & -c_4 & 0 & 0 & 0 & -s_4 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ s_4 & -s_4 & 0 & 0 & 0 & c_4 \end{pmatrix}. \tag{B.3e}$$

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