A Semi-Analytical Thermal Elastic Model for Directional Crystal Growth with Weakly Anisotropy

Jinbiao Wu

School of Mathematical Sciences
Peking University

with

Sean Bohun, Penn State University
Huaxiong Huang, York University

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Cz growth and anisotropy

The thermal model with weak anisotropy

The elasticity model with cubic anisotropy

Numerical Results

- Directional growth techniques such as Czocholski method is frequently used to produce high quality single crystals.
- anisotropic effects such as facets are often visible on the surface of the crystals grown by Cz method.
- We extend perturbation model for axisymmetric crystals developed in
  C. Sean Bojun, Ian Frigaard, Huaxiong Huang & Shuqing Liang, *A Semi-Analytical Model for the Cz growth of Type III-V Compounds*
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- Both the geometry and elastic parameters anisotropy effect are considered.

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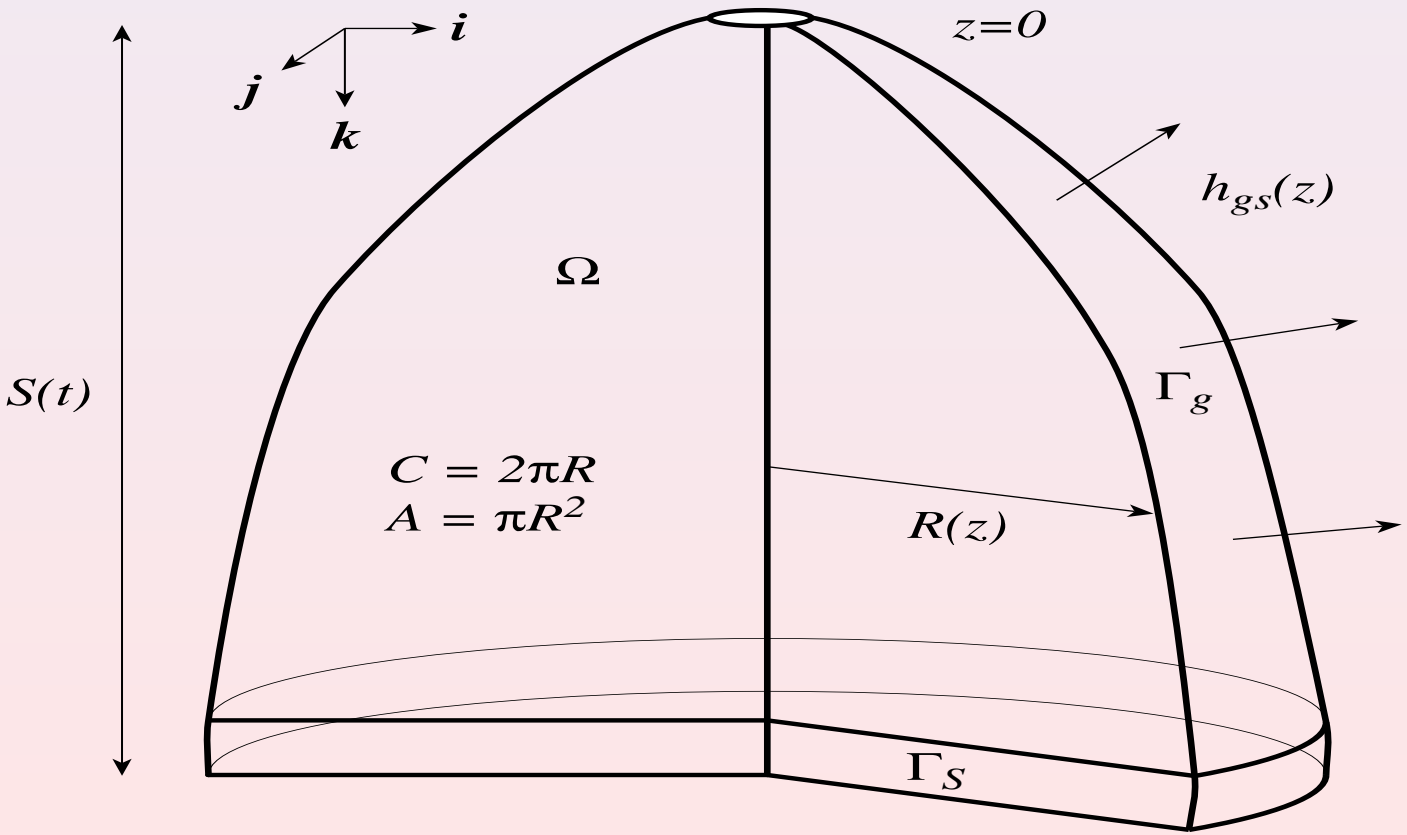
Weak geometric anisotropy

Axisymmetric shape:



Weak geometric anisotropy (cont.)

Weak geometric anisotropy: R depending on the angle ϕ. Assume

$$R(z,\phi,t) = A(z,t)(1+\alpha\sum_{k=1}^{m}\beta_k\cos(n_k(\phi+\delta_k))$$

where α is small constant (weak anisotropy), and $\sum_{k=1}^{m}\beta_k^2 = 1$.
For [1,0,0] pulling direction, 4-fold symmetric: m=1, $\beta_1 = 1$, $n_1 = 4$.
For [1,1,1] pulling direction, 6-fold symmetric: m=1, $\beta_1 = 1$, $n_1 = 6$.

elastic constant anisotropy

The effect of elasticity problem with cubic anisotropy
The stresses $\sigma = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy})'$ are related to the strains $e = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{xz}, 2e_{xy})'$ by

$$\sigma = \begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{pmatrix} e = Ce.$$

- isotropic case: $2C_{44} - C_{11} - C_{12} = 0.(C_{12} = \lambda, C_{44} = \mu$, Lamé constants)
- cubic anisotropy: $H = 2C_{44} - C_{11} - C_{12} > 0.$

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Basic Equations

$$\rho_s c_s \frac{\partial T}{\partial t} = \kappa_s \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right), \quad X = (x, y, z) \in \Omega, t > 0.$$

where ρ_s, c_s and k_s are the density, specific heat and thermal conductivity of the crystal. The boundary conditions are below,

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

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

where h_{gs} and h_{ch} represent the heat transfer coefficients; h_F the radiation heat transfer coefficients; 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 $T = T_m$, the melting temperature. Explicitly we denote the melting isotherm by

$$z - S(X, t) = 0, \qquad X \in \Gamma_S.$$

The motion of the interface of the phase transition is governed by the Stefan condition

$$\rho_s L \frac{\partial S}{\partial t} = \kappa_s \frac{\partial T}{\partial \mathbf{n}}\bigg|_{z \to S^-} - q_l,$$

where L is the latent heat and q_l is the heat flux from the melt. The speed $\frac{\partial S}{\partial t}$ above is the speed at which S moves in the direction of the outward normal $\mathbf{n}$.

Basic equations after non-dimensionlization

Define the Biot number by

$$\epsilon = \frac{\bar{h}_{gs}\bar{R}}{\kappa_s}.$$

where $\bar{h}_{gs}$ is the mean value of h_{gs}.

$$\frac{\epsilon}{\mathrm{St}}\Theta_t = \frac{1}{r}(r\Theta_r)_r + \frac{1}{r^2}\Theta_{\phi\phi} + \epsilon\Theta_{zz}, \qquad X \in \Omega, t > 0;$$

with boundary conditions

$$\frac{-\Theta_r + \epsilon R_z\Theta_z + \Theta_\phi R_\phi/R^2}{\sqrt{1+\epsilon(R_z)^2 + (R_\phi)^2/R^2}} = \epsilon F(\Theta), \qquad r = R(\phi, z),$$

$$\Theta = 1, \qquad z = S(r, \Phi, t),$$

$$\Theta_z = \delta(\Theta - \Theta_{ch}), \qquad z = 0.$$

The right hand side of last equality is

$$
\begin{aligned}
F(\Theta) &= \frac{h_F(T_g^4 - T_b^4)}{\bar{h}_{gs}\triangle T} + \Theta(\beta(z) + \frac{4h_F}{\bar{h}_{gs}} T_g^3) \\
&+ \frac{h_F}{\bar{h}_{gs}} \triangle T \Theta^2 (6T_g^2 + 4T_g \triangle T \Theta + \triangle T^2 \Theta^2)).
\end{aligned}
$$

Perturbation Solution

- Basic assumption: the Biot number $\epsilon(\approx 0.03)$ for the lateral heat flux is small and the geometric anisotropy is weak.
- $$\Theta \sim \Theta_0(z,t) + \epsilon\Theta_1(r,\phi,z,t) + \cdots$$
$$S \sim S_0(t) + \epsilon S_1(r,\phi,t) + \cdots$$
- Zeroth order equation

$$\frac{1}{\mathrm{St}}\Theta_{0,t} = \Theta_{0,zz} - \frac{\mathcal{L}}{\mathcal{S}}F(\Theta_0) + \frac{\Theta_{0,z}\mathcal{S}_z}{\mathcal{S}}, \qquad 0 < z < S_0(t),$$
$$\Theta_{0,z} = \delta(\Theta_0 - \Theta_{ch}), \qquad z = 0,$$
$$\Theta_0 = 1, \qquad z = S_0(t)$$
$$\gamma + S_{0,t} = \Theta_{0,z}\big|_{z=S_0(t)}, \qquad S_0(0) = Z_{\mathrm{seed}}\ ,$$

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$$\begin{aligned}\Theta_1(r,\phi,z,t) &\approx \Theta_1^0(z,t) + \frac{r^2}{4}\left(-\frac{\mathcal{L}}{\mathcal{S}}F(\Theta_0) + \frac{\Theta_{0,z}\mathcal{S}_z}{\mathcal{S}}\right) \\ &+ \alpha\sum_{k=1}^{m}\beta_k r^{n_k}\frac{F(\Theta_0)}{n_k A^{n_k-1}(z)}\cos(n_k\phi+\delta_k).\end{aligned}$$

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3-D General elastic problem with cubic anisotropy

- For brevity, we write the thermoelastic equation as

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

with the boundary condition

$$\sigma_{xyz}\mathbf{n} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix} \mathbf{n} = g, \qquad (x, y, z) \in \partial\Omega$$

where $\mathbf{n} = (\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3)'$ is the unit outer normal direction. For the 3-D thermoelastic problem with cubic anisotropic, then

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

- Define $H = 2C_{44} - C_{11} + C_{12}$, split $C = C_0 - C_a$, where the isotropic part $C_0 =$

$$\begin{pmatrix} C_{11} + \frac{H}{2} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} + \frac{H}{2} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} + \frac{H}{2} & & & \\ & & & C_{44} - \frac{H}{4} & & \\ & & & & C_{44} - \frac{H}{4} & \\ & & & & & C_{44} - \frac{H}{4} \end{pmatrix}$$

. Corresponding to the splitting, we have

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

- Define $V = \mathcal{N} G$ if V satisfies

$$L_0 V = L_a G,$$

with boundary condition $\sigma_{0,xyz}(V)\mathbf{n} = \sigma_{a,xyz}(G)\mathbf{n}$.

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- We assume that U_0 is the solution to

$$L_0 U_0 = F,$$

with boundary condition

$$\sigma_{0,xyz} = g$$

- Define the anisotropic factor

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

- We can get that $\|\mathcal{N}\| \leq \omega$ with some norm $\|\cdot\|$ and the following expansion

$$U = U_0 + \mathcal{N} U_0 + \mathcal{N}^2 U_0 + \cdots + \mathcal{N}^n U_0 + \cdots .$$

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- Set $S_n = \sum_{i=0}^{n} \mathcal{N}^i U_0$,

$$\|U - S_n\| \leq \omega^{n+1} \|U\|$$

-

	C_{11}	C_{12}	C_{44}	ω
GaAs	12.16e4	5.43e4	6.18e4	0.295
InP	10.76e4	6.08e4	4.233e4	0.288
InSb	6.70e4	3.65e4	3.02e4	0.329

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The splitting in (r, ϕ, z) coordinates

The stress-stain relationship:

$$C_{r\phi z} = C_0 + C_{a,r\phi z}$$

For example [0,0,1] pulling direction, we choose the z-direction is [0,0,1], [1,0,0] and [0,1,0] are the directions related to $\phi = 0$ and $\phi = \pi/2$. $C_{a,r\phi z}$ is given by

$$\frac{1}{4}H\begin{pmatrix} 1+\cos(4\phi) & 1-\cos(4\phi) & 0 & 0 & 0 & -\sin(4\phi) \\ 1-\cos(4\phi) & 1+\cos(4\phi) & 0 & 0 & 0 & \sin(4\phi) \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ -\sin(4\phi) & \sin(4\phi) & 0 & 0 & 0 & -\cos(4\phi) \end{pmatrix}$$

For [1,1,1] pulling direction, it is nature to choose the z-direction is [1,1,1], [1,1,-2] and [-1,1,0] are the directions related to $\phi = 0$ and $\phi = \pi/2$. $C_{a,r\phi z}$ is

$$H \begin{pmatrix} 0 & \frac{1}{6} & \frac{1}{3} & \frac{\sqrt{2}}{6}s & -\frac{\sqrt{2}}{6}c & 0 \\ \frac{1}{6} & 0 & \frac{1}{3} & -\frac{\sqrt{2}}{6}s & \frac{\sqrt{2}}{6}c & 0 \\ \frac{1}{3} & \frac{1}{3} & -\frac{1}{6} & 0 & 0 & 0 \\ \frac{\sqrt{2}}{6}s & -\frac{\sqrt{2}}{6}s & 0 & \frac{1}{12} & 0 & \frac{\sqrt{2}}{6}c \\ -\frac{\sqrt{2}}{6}c & \frac{\sqrt{2}}{6}c & 0 & 0 & \frac{1}{12} & \frac{\sqrt{2}}{6}s \\ 0 & 0 & 0 & \frac{\sqrt{2}}{6}c & \frac{\sqrt{2}}{6}s & -\frac{1}{12} \end{pmatrix}$$

where $c = \cos(3\phi)$ and $s = \sin(3\phi)$

Semi-analytic solution for 2-D problem

Now we assume that the displacement is only in the (r, ϕ) plane. The previous 3-D problem reduce to 2-D problem. For [0,0,1] pulling direction

$$\begin{pmatrix} \sigma_{a,rr} \\ \sigma_{a,\phi\phi} \\ \sigma_{a,r\phi} \end{pmatrix} = \frac{H}{4} \begin{pmatrix} 1+\cos(4\phi) & 1-\cos(4\phi) & -\sin(4\phi) \\ 1-\cos(4\phi) & 1+\cos(4\phi) & \sin(4\phi) \\ -\sin(4\phi) & \sin(4\phi) & -\cos(4\phi) \end{pmatrix} \begin{pmatrix} e_{rr} \\ e_{\phi\phi} \\ 2e_{r\phi} \end{pmatrix}$$

For [1,1,1] pulling direction

$$\begin{pmatrix} \sigma_{a,rr} \\ \sigma_{a,\phi\phi} \\ \sigma_{a,r\phi} \end{pmatrix} = H \begin{pmatrix} 0 & \frac{1}{6} & 0 \\ \frac{1}{6} & 0 & 0 \\ 0 & 0 & -\frac{1}{12} \end{pmatrix} \begin{pmatrix} e_{rr} \\ e_{\phi\phi} \\ 2e_{r\phi} \end{pmatrix}$$

Solution technique

If we want to know the solution $U \approx U_0 + \mathcal{N} U_0$, we need to know the analytic solution to

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{r\phi}}{\partial \phi} + \frac{\sigma_{rr} - \sigma_{\phi\phi}}{r} = d_1 r^{k-2} \cos(n\phi + \delta), \qquad r < A(z),$$

$$\frac{\partial \sigma_{r\phi}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{\phi\phi}}{\partial \phi} + \frac{2\sigma_{r\phi}}{r} = d_2 r^{k-2} \sin(n\phi + \delta), \qquad r < A(z),$$

with the boundary condition

$$\sigma_{rr} = d_3 \cos(n\phi + \delta), \qquad r = A(z),$$

$$\sigma_{r\phi} = d_4 \sin(n\phi + \delta), \qquad r = A(z).$$

- To find the solution to the equations with the boundary conditions, first we need to find a particular solution to the equations, like $W = (W^r, W^\phi) = (c_1 r^k \cos(n\phi + \delta), c_2 r^k \sin(n\phi + \delta))$ (in the case that $k = n + 1$ or $k = n - 1$, need another particular solution like $c_3 \log r((r^k \cos(n\phi + \delta), \gamma_2 r^k \sin(n\phi + \delta))$ where $((r^k \cos(n\phi + \delta), \gamma_2 r^k \sin(n\phi + \delta))$ is a solution to homogeneous elasticity equation).
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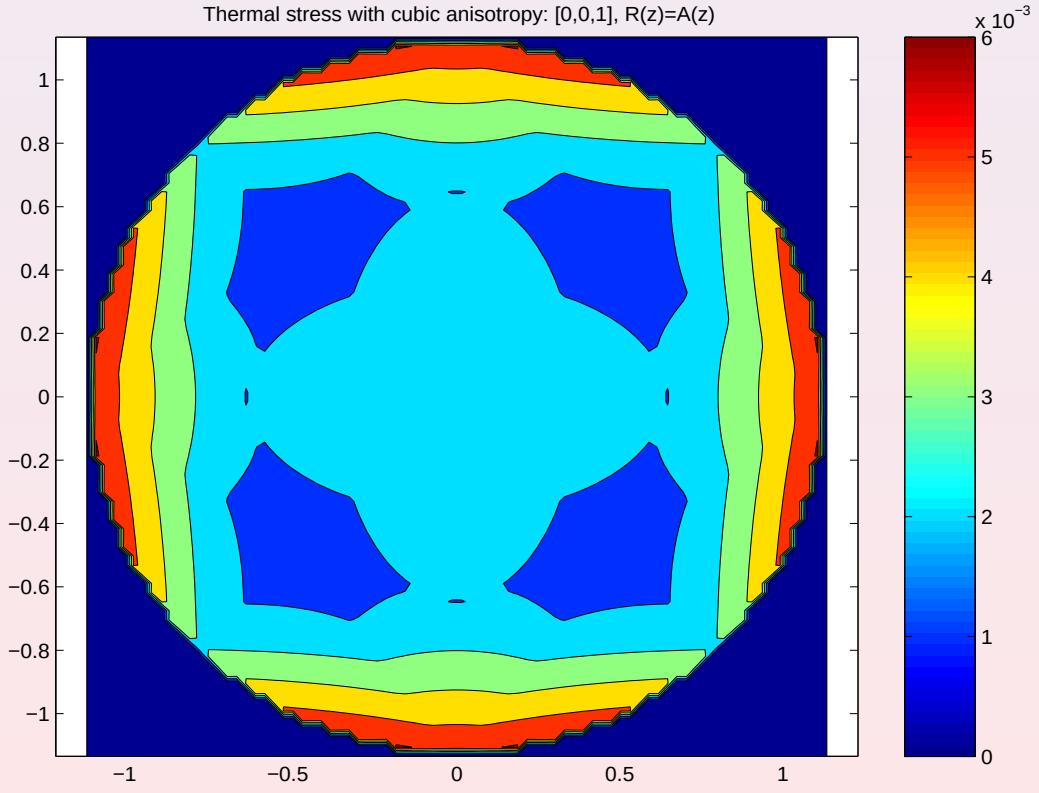
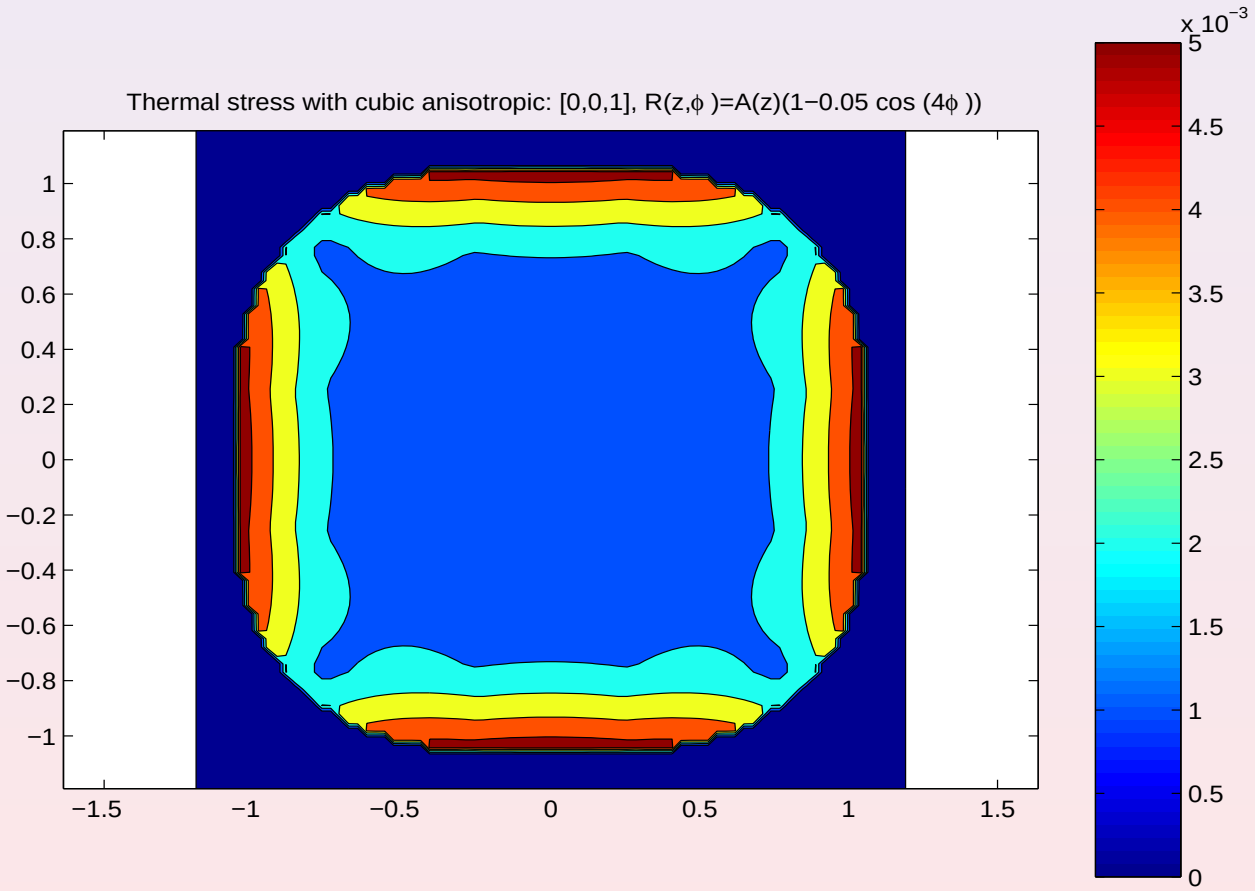
Resolved stress for [0,0,1] pulling direction




Thermal stress with cubic anisotropic: [0,0,1], R(z,ϕ)=A(z)(1−0.05 cos (4ϕ))
x 10^−3
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
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−1.5
−1
−0.5
0
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1
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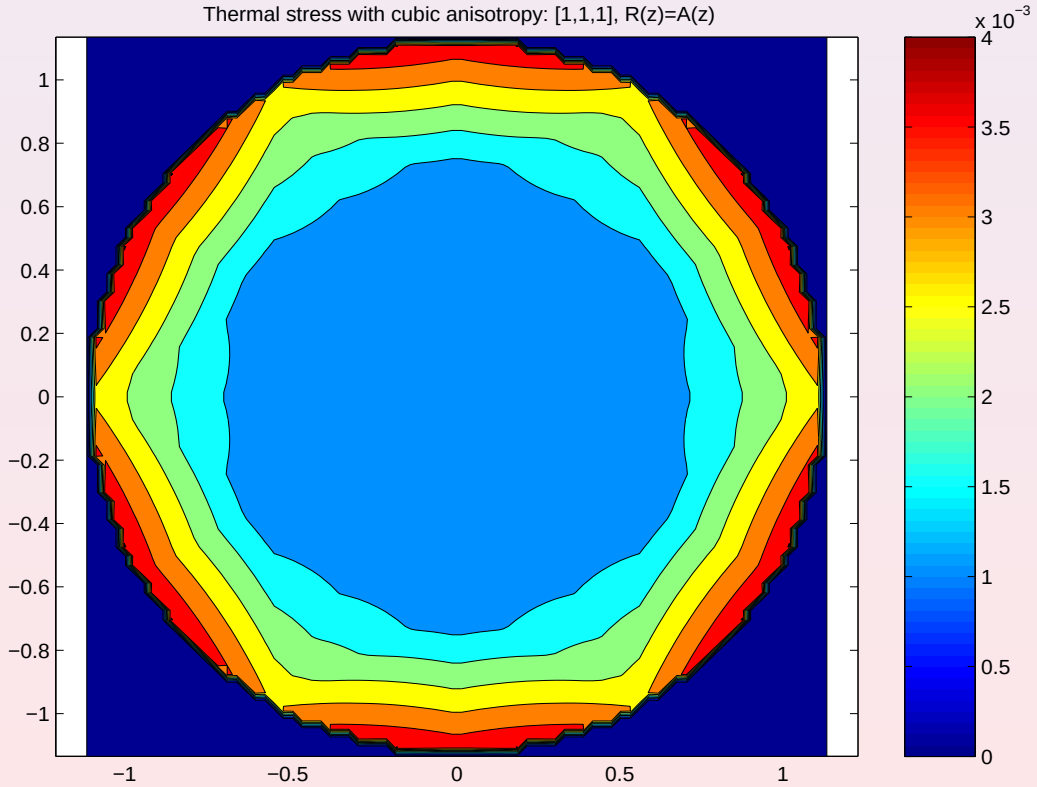
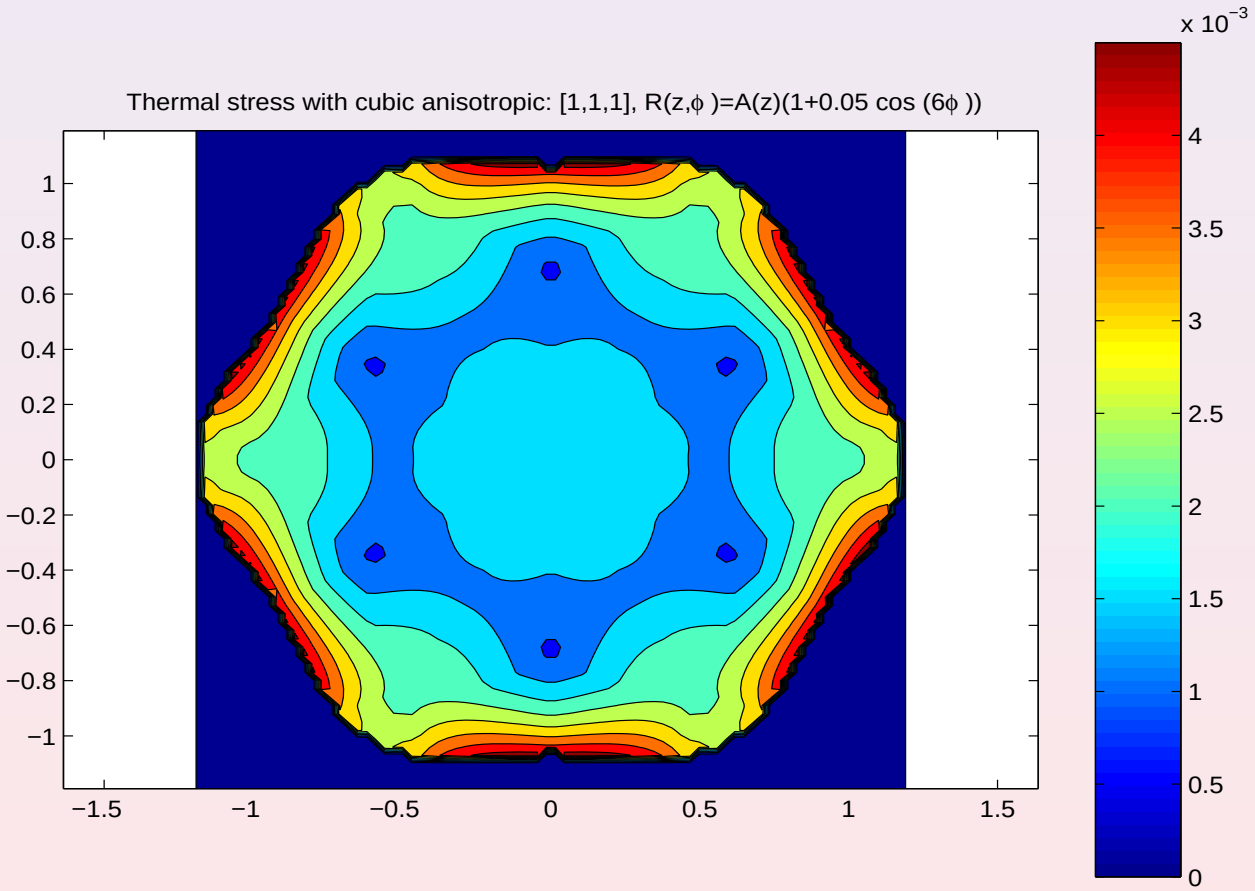
Resolved stress for [1,1,1] pulling direction

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Conclusion and future work

Conclusion:

- The anisotropy may not be ignored for accurate simulation.
- The closest isotropic part for elastic problem with cubic anisotropy is setting $\lambda = C_{12}$ and $\mu = \frac{2C_{44}+C_{11}-C_{12}}{4}$.
- The anisotropic factor ω evaluates the anisotropic effect from elastic constants.

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- The closest isotropic part for elastic problem with cubic anisotropy is setting $\lambda = C_{12}$ and $\mu = \frac{2C_{44}+C_{11}-C_{12}}{4}$.
- The anisotropic factor ω evaluates the anisotropic effect from elastic constants.

Future work:

- use the asymtopic sharp.
- The effect the other coefficients in the model.

Thank You!