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

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with

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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 Czochalski 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* to anisotropic ones.
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Weak geometric anisotropy

Axisymmetric shape:

\[ S(t) \]

\[ C = 2\pi R \]

\[ A = \pi R^2 \]

\[ R(z) \]

\[ \Omega \]

\[ \Gamma_g \]

\[ \Gamma_S \]

\[ z=0 \]

\[ h_{gs}(z) \]
Weak geometric anisotropy: $R$ depending on the angle $\phi$. Assume

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

where $\alpha$ 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: $m=1$, $\beta_1 = 1$, $n_1 = 6$. 

Jinbiao Wu  
Semi-Analytical Model for CZ Growth with 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: \( 2C_{44} - C_{11} - C_{12} = 0. (C_{12} = \lambda, C_{44} = \mu, \text{ Lamé constants}) \)
- cubic anisotropy: \( H = 2C_{44} - C_{11} - C_{12} \geq 0. \)
elastic constant anisotropy

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- cubic anisotropy: \( H = 2C_{44} - C_{11} - C_{12} > 0. \)
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 \( \rho_s, c_s \) and \( k_s \) are the density, specific heat and thermal conductivity of the crystal. The boundary conditions are below,

\[ -\kappa_s \frac{\partial T}{\partial n} = h_{gs}(T - T_g) + h_F(T^4 - T_b^4), \quad X \in \Gamma_g \]
\[ \kappa_s \frac{\partial T}{\partial z} = h_{ch}(T - T_{ch}), \quad z = 0, \]

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 $\Gamma_S$ and is where $T = T_m$, the melting temperature. Explicitly we denote the melting isotherm by

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

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

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

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 $n$. 
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 \( h_{gs} \).

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

with boundary conditions

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

\[ \Theta = 1, \quad z = S(r, \Phi, t), \]

\[ \Theta_z = \delta(\Theta - \Theta_{ch}), \quad z = 0. \]
The right hand side of last equality is

\[ F(\Theta) = \frac{h_F}{h_{gs}} \frac{T_g^4 - T_b^4}{\Delta T} + \Theta(\beta(z) + \frac{4h_F}{h_{gs}} T_g^3) \]

\[ + \frac{h_F}{h_{gs}} \Delta T \Theta^2 (6 T_g^2 + 4 T_g \Delta T \Theta + \Delta T^2 \Theta^2) \]
Perturbation Solution

- Basic assumption: the Biot number $\epsilon(\approx 0.03)$ for the lateral heat flux is small and the geometric anisotropy is weak.

\[
\begin{align*}
\Theta & \sim \Theta_0(z, t) + \epsilon \Theta_1(r, \phi, z, t) + \cdots \\
S & \sim S_0(t) + \epsilon S_1(r, \phi, t) + \cdots
\end{align*}
\]

- Zeroth order equation

\[
\begin{align*}
\frac{1}{St} \Theta_{0,t} &= \Theta_{0,zz} - \frac{\mathcal{L}}{S} F(\Theta_0) + \frac{\Theta_{0,z} S_z}{S}, \\
\Theta_{0,z} &= \delta(\Theta_0 - \Theta_{ch}), \\
\Theta_0 &= 1, \\
\gamma + S_{0,t} &= \Theta_{0,z} \big|_{z=S_0(t)}, \\
S_0(0) &= Z_{seed}
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\frac{1}{S_t} \Theta_{0,t} = \Theta_{0,zz} - \frac{L}{S} F(\Theta_0) + \frac{\Theta_{0,z} S_z}{S}, \quad 0 < z < S_0(t),
\]
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\Theta_{0,z} = \delta(\Theta_0 - \Theta_{ch}), \quad z = 0,
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\Theta_0 = 1, \quad z = S_0(t)
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$$\Theta_0 = 1, \quad z = S_0(t)$$

$$\gamma + S_{0,t} = \Theta_{0,z} \bigg|_{z=S_0(t)}, \quad S_0(0) = Z_{seed},$$
\[ \Theta_1(r, \phi, z, t) \approx \Theta_0^0(z, t) + \frac{r^2}{4} \left( -\frac{L}{S} F(\Theta_0) + \frac{\Theta_{0,z} S_z}{S} \right) + \alpha \sum_{k=1}^{m} \beta_k r^{n_k} \frac{F(\Theta_0)}{n_k A^{n_k} - 1(z)} \cos(n_k \phi + \delta_k). \]
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- How to decide the equations with cubic anistropy?
- how to find the (Semi-)Analytic Solution?
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- How to decide the equations with cubic anistropy?
- How to find the (Semi-)Analytic Solution?
For brevity, we write the thermoelastic equation as

\[ LU = F, \quad (x, y, z) \in \Omega \]

with the boundary condition

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

where \( \mathbf{n} = (n_1, n_2, n_3)' \) is the unit outer normal direction. For the 3-D thermoelastic problem with cubic anisotropic, then

\[ F = (C_{11} + 2C_{12}) \nabla \Theta, \quad g = (C_{11} + 2C_{12}) \Theta \mathbf{n}. \]
Define $H = 2C_{44} - C_{11} + C_{12}$, split $C = C_0 - C_a$, where the isotropic part $C_0 =$

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

$C_{44} - \frac{H}{4}$

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Corresponding to the splitting, we have

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

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

$L_0 V = L_a G$,

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

$C_{00} = C_{44} - \frac{H}{4}, \quad C_{44} - \frac{H}{4}, \quad C_{44} - \frac{H}{4}$.

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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 $\|N\| \leq \omega$ with some norm $\| \cdot \|$ and the following expansion

$$U = U_0 + N U_0 + N^2 U_0 + \cdots + N^n U_0 + \cdots.$$
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$$U = U_0 + N U_0 + N^2 U_0 + \cdots + N^n U_0 + \cdots.$$
Set \( S_n = \sum_{i=0}^{n} \mathcal{N}_i U_0 \),

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

<table>
<thead>
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<th></th>
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</tr>
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The splitting in \((r, \phi, z)\) 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 \((r, \phi)\) 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 $U \approx U_0 + N U_0$, we need to know the analytic solution to

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

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

with the boundary condition

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

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

Then consider the homogeneous equations with modified boundary conditions.
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Then consider the homogeneous equations with modified boundary conditions.
Resolved stress for [0,0,1] pulling direction
Thermal stress with cubic anisotropy: $[0,0,1]$, $R(z, \phi) = A(z)(1 - 0.05 \cos(4\phi))$
Resolved stress for \([1,1,1]\) pulling direction

Thermal stress with cubic anisotropy: \([1,1,1]\), \(R(z) = A(z)\)
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Thermal stress with cubic anisotropic: \([1,1,1]\), \(R(z, \phi) = A(z)(1 + 0.05 \cos(6\phi))\)
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 \( \omega \) evaluates the anisotropic effect from elastic constants.

Future work:

- Use the asymptotic sharp.
- The effect the other coefficients in the model.
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Thank You!