Rapid Computation of thermal stress in crystals with facets and allowing for material anisotropy

Canada-China Workshop on Industrial Mathematics

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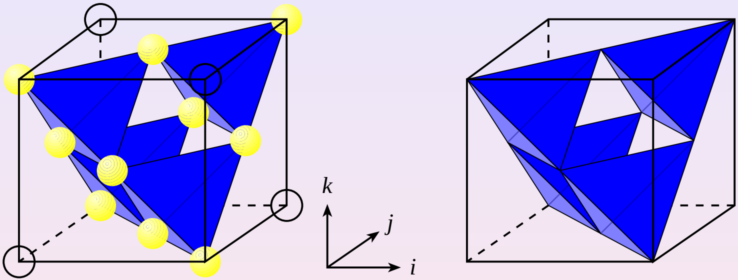
BIRS: August 6, 2007

Outline

Coordination Polyhedra

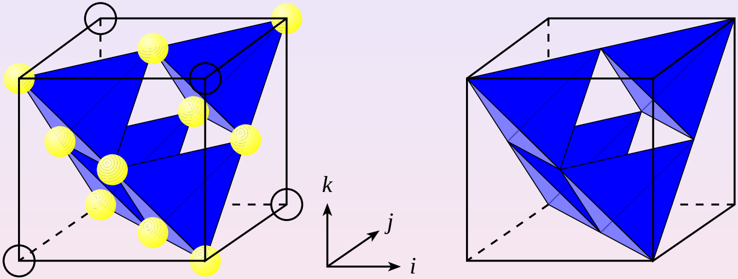
- The growth rate is based on a coordinate polyhedron model
- This is capable of naturally explaining the different growth rates between the positive and negative directions in a polar crystal such as the III-V semiconductors
- If AB is the III-V semiconductor under consideration, then its anion-coordination polyhedra are AB_4^{6-} tetrahedra

Coordination Polyhedra



Shown are the four tetrahedra of an AB unit cell. To the left only the B atoms in the unit cell are shown. B atoms in the unit cell but not included in the four growth units are represented with hollow circles. At the centre of each tetrahedral growth unit is a A atom accounting for all the atoms in the AB unit cell. On the right only the tetrahedra are shown.

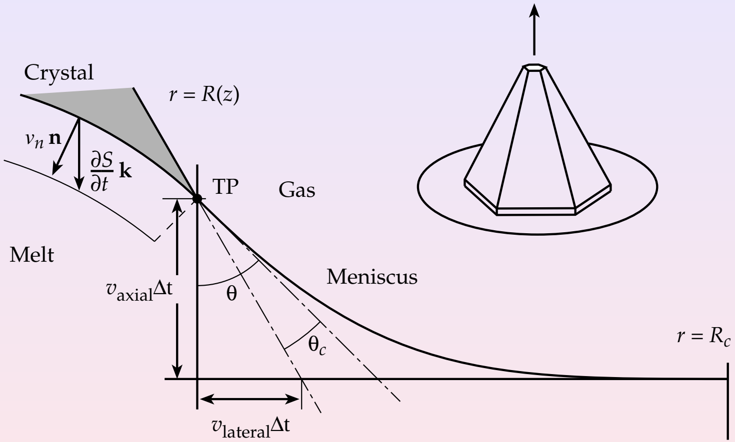
Coordination Polyhedra



For a crystal pulled in the [001] direction,

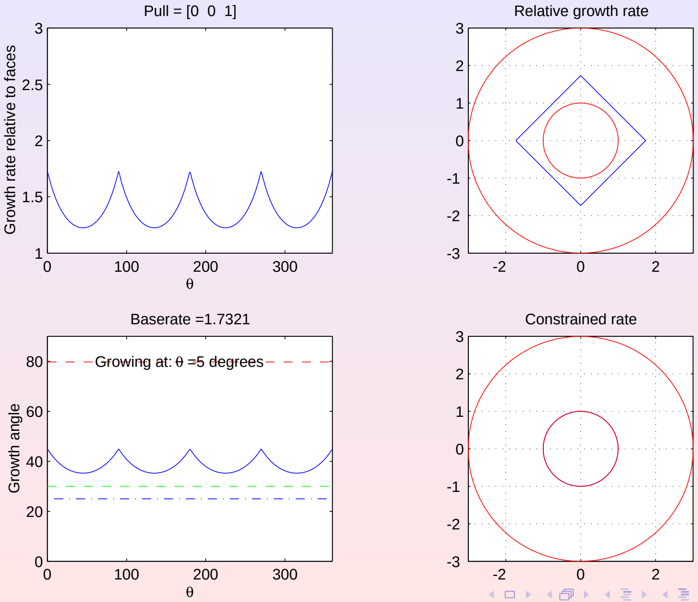
- $[00\bar{1}]$ is into the melt gives $v_{\text{axial}} = 1.7321$
- v_{lateral} has four-fold symmetry

Constrained Growth

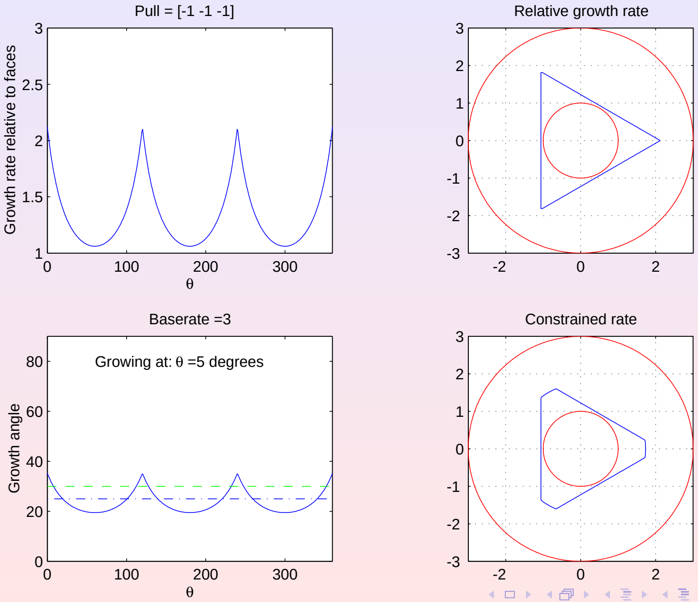


- If not constrained by the meniscus then $\tan(\theta - \theta_c) = \frac{v_{\text{lateral}}}{v_{\text{axial}}}$
- For growing a cone $\theta - \theta_c$ is $1/2$ the opening angle of the cone

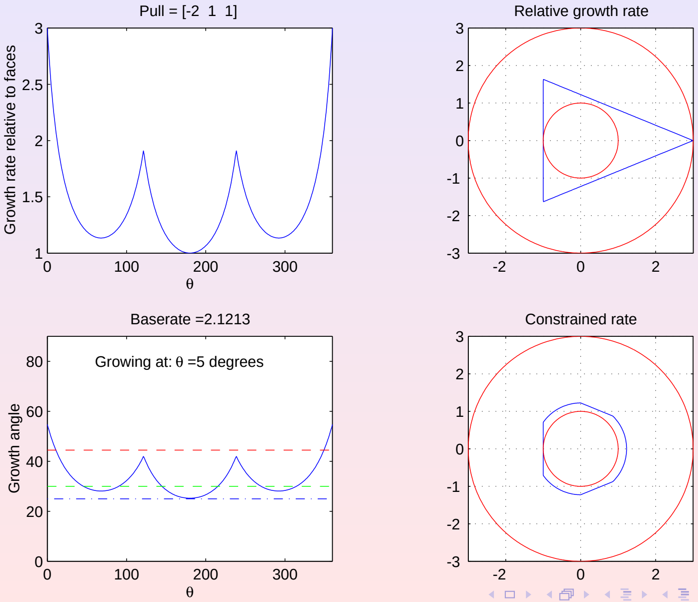
Pulling in the [001] direction



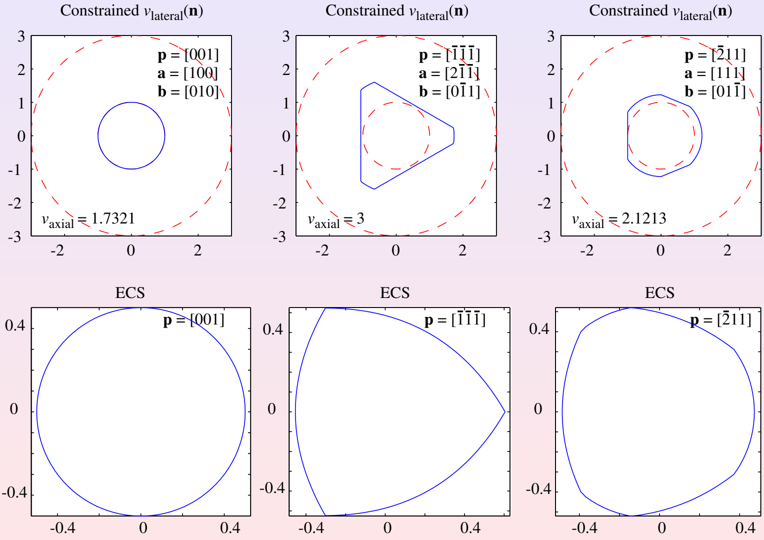
Pulling in the $[\bar{1}\bar{1}\bar{1}]$ direction



Pulling in the $[\bar{2}11]$ direction



Equilibrium Crystal Shapes



Equilibrium Crystal Shapes

For the purpose of computing thermal stress, we assume the following expression in the case of weak anisotropy (α small)

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

where m, $n_1 < n_2 < \cdots < n_m$ are positive integers and $\sum_{k=1}^{m} \beta_k^2 = 1$.

- α is the (small) geometric anisotropy factor
- 4-fold symmetry ($m = 1, n_1 = 4$)
- 6-fold symmetry ($m = 1, n_1 = 6$)
- We assume that the lateral shape of the crystal is in equilibrium

Basic Equations

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

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

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

$$-\kappa_s \frac{\partial T}{\partial \mathbf{n}} = h_{\mathrm{gs}}(T - T_g) + h_F(T^4 - T_b^4), \qquad \mathbf{x} \in \Gamma_g,$$
$$\kappa_s \frac{\partial T}{\partial z} = h_{\mathrm{ch}}(T - T_{\mathrm{ch}}), \qquad z = 0,$$

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

Basic Equations

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

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

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

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

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

Rescaled Equations

Identify the Biot number

$$\epsilon = \frac{\bar{h}_{\mathrm{gs}}\tilde{R}}{\kappa_s} \tag{1}$$

as a small parameter (small lateral heat flux). Rescaling,

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

with,

$$-\Theta_r + \frac{1}{R^2}R_\phi\Theta_\phi + \epsilon R_z\Theta_z = \epsilon F(\Theta)\left(1 + \frac{R_\phi^2}{R^2} + \epsilon R_z^2\right)^{1/2}, \quad \mathbf{x} \in \Gamma_g,$$

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

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

$$\Theta_z - \frac{1}{\epsilon}S_r\Theta_r - \frac{1}{\epsilon r^2}S_\phi\Theta_\phi = \gamma + S_t, \quad \gamma = \frac{q_l\tilde{R}}{\epsilon^{1/2}\kappa_s\Delta T}.$$

Rescaled Equations

$\beta(z) = h_{\mathrm{gs}}/\bar{h}_{\mathrm{gs}}$, and $\delta = \epsilon^{1/2} h_{\mathrm{ch}}/\bar{h}_{\mathrm{gs}}$ and γ (q_l) is the non-dimensional (dimensional) heat flux in the liquid across the crystal/melt interface in the axial direction. Also,

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

Perturbation Solution

The Biot number for the lateral heat flux is small ($\epsilon \sim 0.03$) and the geometric anisotropy is weak ($\alpha \ll 1$).
Expansion:

$$\Theta \sim \Theta_0(z,t) + \epsilon\Theta_1(r,\phi,z,t) + \epsilon^2\Theta_2(r,\phi,z,t) + \cdots,$$
$$S \sim S_0(t) + \epsilon S_1(r,\phi,t) + \epsilon^2 S_2(r,\phi,t) + \cdots.$$

Zeroth order model (Fast to compute):

$$\frac{1}{\mathrm{St}}\Theta_{0,t} - \Theta_{0,zz} = \frac{2}{\bar{R}}\left(\bar{R}'\Theta_{0,z} - F(\Theta_0)\right), \quad 0 < z < S_0(t), \quad t > 0,$$
$$\Theta_{0,z}(0,t) = \delta(\Theta_0(0,t) - \Theta_{\mathrm{ch}}), \quad t \geq 0,$$
$$\Theta_0(S_0(t),t) = 1, \quad t \geq 0,$$
$$S_0'(t) = \Theta_{0,z}(S_0(t),t) - \gamma, \quad S_0(0) = Z_0, \quad t > 0.$$

Perturbation Solution

First order model:

$$\Theta_1(r,\phi,z,t) = \Theta_1^a(z,t) + r^2\Theta_1^b(z,t) + \alpha\Theta_1^c(r,\phi,z,t) + O(\alpha^2)$$

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

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

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

These last two terms are completely determined by Θ_0 and $\bar{R}$. Θ_1^a does not play a role in the stress.

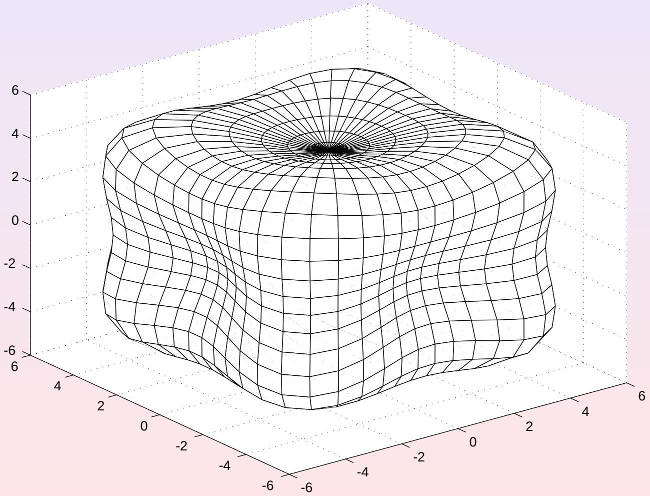
Basic Relations

For a crystal with cubic symmetry the stresses
$\underline{\sigma} = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy})^{\mathrm{T}}$ and strains
$\underline{e} = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{xz}, 2e_{xy})^{\mathrm{T}}$ are related through

$$\underline{\sigma} = C_{\mathrm{rect}}\underline{e}, \qquad C_{\mathrm{rect}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{pmatrix}.$$

For an anisotropic material the quantity $H = 2C_{44} - C_{11} + C_{12} \neq 0$.
We assume that the z-component of the displacement is zero because of the free surface at the melt.

Directional Dependence of the Young's modulus for an InSb Crystal



Operator Splitting

Split C_{rect} into a diagonal anisotropic part and an isotropic part $C_{\mathrm{rect}} = C_0 - C_{a,\mathrm{rect}}$, $C_{a,\mathrm{rect}} = H/4 \times \mathrm{diag}(2,2,2,-1,-1,-1)$, and

$$C_0 = \begin{pmatrix} C_{11}^0 & C_{12}^0 & C_{12}^0 & & & \\ C_{12}^0 & C_{11}^0 & C_{12}^0 & & & \\ C_{12}^0 & C_{12}^0 & C_{11}^0 & & & \\ & & & C_{44}^0 & & \\ & & & & C_{44}^0 & \\ & & & & & C_{44}^0 \end{pmatrix}$$

is isotropic. $C_{a,\mathrm{rect}}$ is chosen to minimize $\rho(C_0^{-1} C_{a,\mathrm{rect}})$.
E and ν in term of C_{ij} are given by

$$E = \frac{(C_{11} + 2C_{12} + H/2)(C_{11} - C_{12} + H/2)}{C_{11} + C_{12} + H/2},$$

$$\nu = \frac{C_{12}}{C_{11} + C_{12} + H/2}.$$

Operator Splitting

Denote the displacement vector as $\mathbf{w}$, the strain by $\mathbf{e} = \mathbf{S}(\mathbf{w})$ and the stress by $\sigma = C\mathbf{S}(\mathbf{w})$ with $C = C_0 - C_a$.
The thermoelastic problem becomes

$$\begin{aligned} \nabla \cdot C\mathbf{S} &= (C_{11} + 2C_{12})\nabla\Theta, && \mathbf{x} \in \Omega, \quad t > 0, \\ C\mathbf{S} \cdot \mathbf{n} &= (C_{11} + 2C_{12})\Theta\mathbf{n}, && r = R(\phi, z) \end{aligned}$$

or by rescaling

$$\begin{aligned} \nabla \cdot C\mathbf{S} &= \left(\frac{1-\nu}{1-2\nu} - \frac{H}{2}\right)\nabla\Theta, && \mathbf{x} \in \Omega, \quad t > 0, \\ C\mathbf{S} \cdot \mathbf{n} &= \left(\frac{1-\nu}{1-2\nu} - \frac{H}{2}\right)\Theta\mathbf{n}, && r = R(\phi, z) \end{aligned}$$

with $\mathbf{n}$ denoting the outward normal of the surface $r = R(\phi, z)$.

Operator Splitting

Using the form of C,

$$\nabla \cdot C\mathbf{S} = \nabla \cdot C_0\mathbf{S} - \nabla \cdot C_a\mathbf{S} = \mathcal{L}_0 - \mathcal{L}_a,$$
$$C\mathbf{S}\cdot\mathbf{n} = C_0\mathbf{S}\cdot\mathbf{n} - C_a\mathbf{S}\cdot\mathbf{n} = \mathcal{B}_0 - \mathcal{B}_a,$$

to solve for $\mathbf{w}(\mathbf{x})$ one starts with $\mathbf{w}_0$ given by

$$\mathcal{L}_0(\mathbf{w}_0) = \left(\frac{1-\nu}{1-2\nu} - \frac{H}{2}\right)\nabla\Theta, \qquad \mathbf{x}\in\Omega,\ t>0,$$
$$\mathcal{B}_0(\mathbf{w}_0) = \left(\frac{1-\nu}{1-2\nu} - \frac{H}{2}\right)\Theta\mathbf{n}, \qquad r = R(\phi, z).$$

$\mathbf{w}_0$ is the isotropic displacement found previously [Bohun et al.], multiplied by a factor of $1 - \frac{H}{2}\frac{1-2\nu}{1-\nu}$.

Operator Splitting

We know $\mathbf{w}_0$ explicitly for a given crystal shape $R(\phi, z)$.

Having defined $\mathbf{w}_0$, we denote by $\mathbf{w}_{k+1} = \mathcal{N}\mathbf{w}_k$, with $k \geq 0$, the solution to

$$
\begin{aligned}
\mathcal{L}_0(\mathbf{w}_{k+1}) &= \mathcal{L}_a(\mathbf{w}_k), && \mathbf{x} \in \Omega,\ \ t > 0,\\
\mathcal{B}_0(\mathbf{w}_{k+1}) &= \mathcal{B}_a(\mathbf{w}_k), && r = R(\phi, z).
\end{aligned}
$$

Perturbation Series

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

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

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 replaced by a finite sum. For typical cubic anisotropic materials $\omega \sim 1/3$.

	C_{11}	C_{12}	C_{44}	ω
GaAs	12.16×10^4	5.43×10^4	6.18×10^4	0.295
InP	10.76×10^4	6.08×10^4	4.233×10^4	0.288
InSb	6.70×10^4	3.65×10^4	3.02×10^4	0.329

Perturbation Series

- For a given pulling direction C_0 is invariant however, the explicit form of C_a depends on the crystal orientation
- Consequently $\mathcal{L}_a$ and $\mathcal{B}_a$ depend on the orientation
- C_a transforms as a fourth rank tensor and includes only trigonometric factors $\cos m\phi$ and $\sin m\phi$ where m depends on the orientation of the crystal

For example, if $(c_4, s_4) = (\cos 4\phi, \sin 4\phi)$ then

$$C_{a,\mathrm{cyc}}^{[001]} = \frac{H}{4}\begin{pmatrix} 1+c_4 & 1-c_4 & 0 & 0 & 0 & -s_4 \\ 1-c_4 & 1+c_4 & 0 & 0 & 0 & s_4 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ -s_4 & s_4 & 0 & 0 & 0 & -c_4 \end{pmatrix}.$$

Plane Strain

To illustrate the procedure assume that the displacement is only in the (r, ϕ) plane.
Stress strain relation for the [001] direction becomes

$$\begin{pmatrix} \sigma_{a,rr} \\ \sigma_{a,\phi\phi} \\ \sigma_{a,r\phi} \end{pmatrix} = \frac{H}{4} \begin{pmatrix} 1+c_4 & 1-c_4 & -s_4 \\ 1-c_4 & 1+c_4 & s_4 \\ -s_4 & s_4 & -c_4 \end{pmatrix} \begin{pmatrix} e_{rr} \\ e_{\phi\phi} \\ 2e_{r\phi} \end{pmatrix}.$$

For the $[\bar{1}\bar{1}\bar{1}]$ direction

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

A Canonical Problem

To find $\mathbf{w}_0 + \mathbf{w}_1 = \mathbf{w}_0 + \mathcal{N}\mathbf{w}_0$ the thermoelastic equations

$$\mathcal{L}_0(\mathbf{w}_1) = \mathcal{L}_a(\mathbf{w}_0), \qquad \mathbf{x} \in \Omega,\ t > 0,$$
$$\mathcal{B}_0(\mathbf{w}_1) = \mathcal{B}_a(\mathbf{w}_0), \qquad r = R(\phi, z)$$

reduce to finding sequence of solutions of the form

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{r\phi}}{\partial \phi} + \frac{\sigma_{rr} - \sigma_{\phi\phi}}{r} = f_r r^{k-2}\cos(n\phi + \delta), \quad r < \bar{R}(z),$$
$$\frac{\partial \sigma_{r\phi}}{\partial r} + \frac{1}{r}\frac{\partial \sigma_{\phi\phi}}{\partial \phi} + \frac{2\sigma_{r\phi}}{r} = f_\phi r^{k-2}\sin(n\phi + \delta), \quad r < \bar{R}(z),$$

with integers $n \geq 0$, $k \geq 1$, and

$$\sigma_{rr} = g_r r^{k-1}\cos(n\phi + \delta), \qquad r = \bar{R}(z),$$
$$\sigma_{r\phi} = g_\phi r^{k-1}\sin(n\phi + \delta), \qquad r = \bar{R}(z),$$

where f_r, f_ϕ, g_r, g_ϕ depend on C_a.

A Canonical Problem

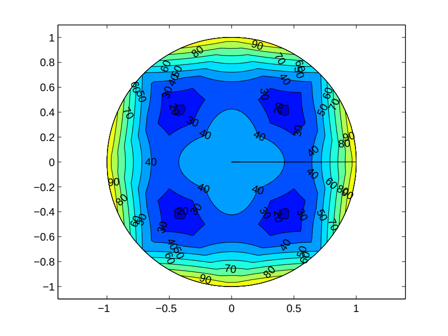
We solve this with a two stage approach.

1. Find a particular solution that does not necessarily satisfy the boundary condition
2. Find a homogeneous solution with a (perhaps) modified boundary condition

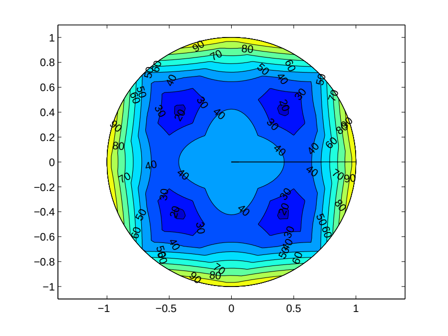
The point here is that the solution can be written out explicitly for general f_r, f_ϕ, g_r, g_ϕ so that the problem becomes a bookkeeping problem.

Fast

Results - Geometric [001]: Total Resolved Stress

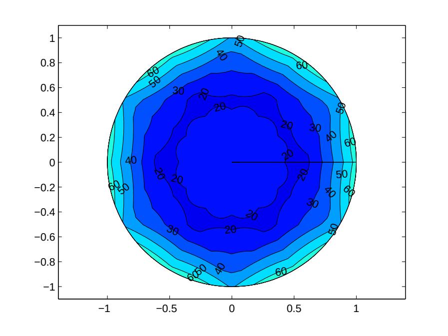


$\alpha = 0$: $\max|\sigma^{\text{tot}}_{\text{rs}}| = 9.23$

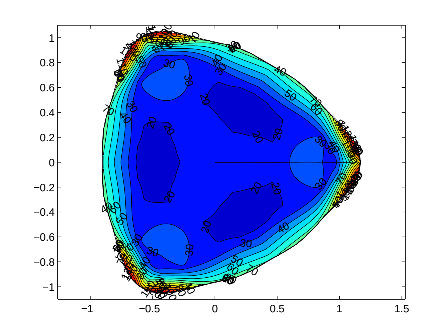


$\alpha = 0$: $\max|\sigma^{\text{tot}}_{\text{rs}}| = 9.23$

Results - Geometric $[\bar{1}\bar{1}\bar{1}]$: Total Resolved Stress

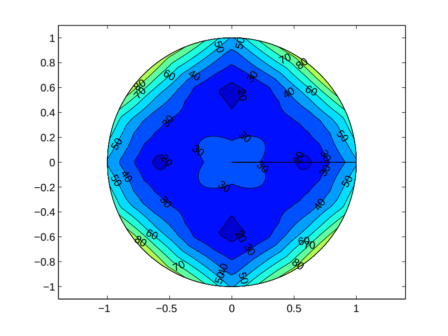


$\alpha = 0$: $\max |\sigma_{\rm rs}^{\rm tot}| = 6.07$

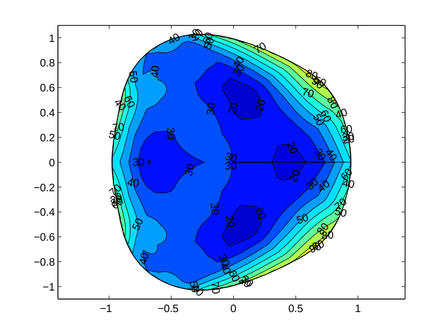


$\alpha = 0.123$: $\max |\sigma_{\rm rs}^{\rm tot}| = 13.4$

Results - Geometric $[\bar{2}11]$: Total Resolved Stress

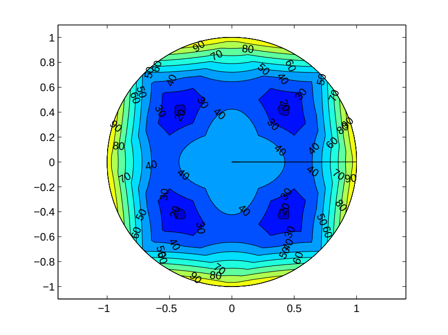


$\alpha = 0$: $\max|\sigma_{\mathrm{rs}}^{\mathrm{tot}}| = 8.19$

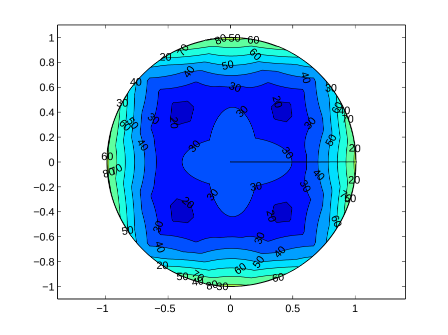


$\alpha = 0.089$: $\max|\sigma_{\mathrm{rs}}^{\mathrm{tot}}| = 8.78$

Results - Anisotropy [001]: Total Resolved Stress

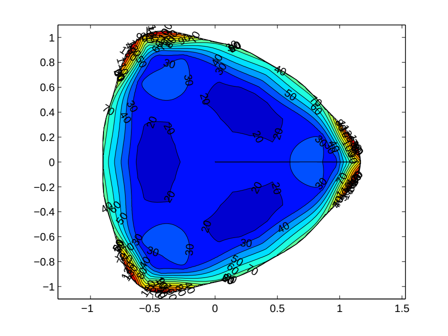


$\omega = 0$: $\max |\sigma_{\mathrm{rs}}^{\mathrm{tot}}| = 9.23$

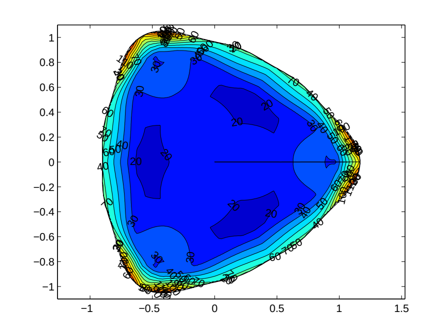


$\omega = 0.329$: $\max |\sigma_{\mathrm{rs}}^{\mathrm{tot}}| = 7.66$

Results - Anisotropy $[\bar{1}\bar{1}\bar{1}]$: Total Resolved Stress

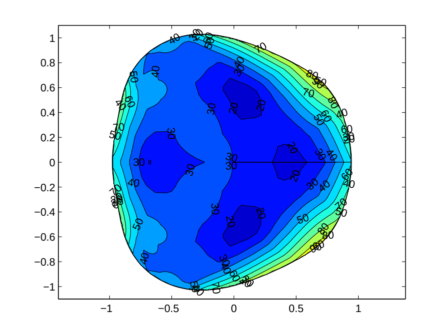


$\omega = 0$: $\max \left|\sigma_{\mathrm{rs}}^{\mathrm{tot}}\right| = 13.4$

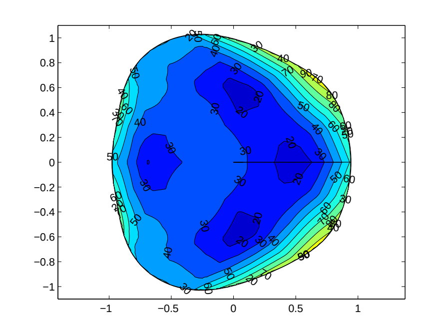


$\omega = 0.329$: $\max \left|\sigma_{\mathrm{rs}}^{\mathrm{tot}}\right| = 12.0$

Results - Anisotropy $[\bar{2}11]$: Total Resolved Stress



$\omega = 0$: $\max |\sigma_{\mathrm{rs}}^{\mathrm{tot}}| = 8.19$



$\omega = 0.329$: $\max |\sigma_{\mathrm{rs}}^{\mathrm{tot}}| = 8.78$

Conclusions

- A simple argument based on the crystal lattice structure predicts facets that depend on both the crystal orientation and growth angle
- Small opening angles tend to suppress the formation of facets
- The model naturally incorporates the polarity of III-V semiconductors
- Facet formation greatly affects the thermal stress distribution
- Anisotropy has a lesser effect when the crystal has facets
- The industry preference of the $[\bar{2}11]$ pulling direction, determined by trial and error, produces facets yet avoids the drastic increase in the stress seen in the $[\bar{1}1\bar{1}]$ orientation. Furthermore, effect of the material anisotropy is negligible in this case

Thank you