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Transient modelling of Czochralski silicon crystal growth process

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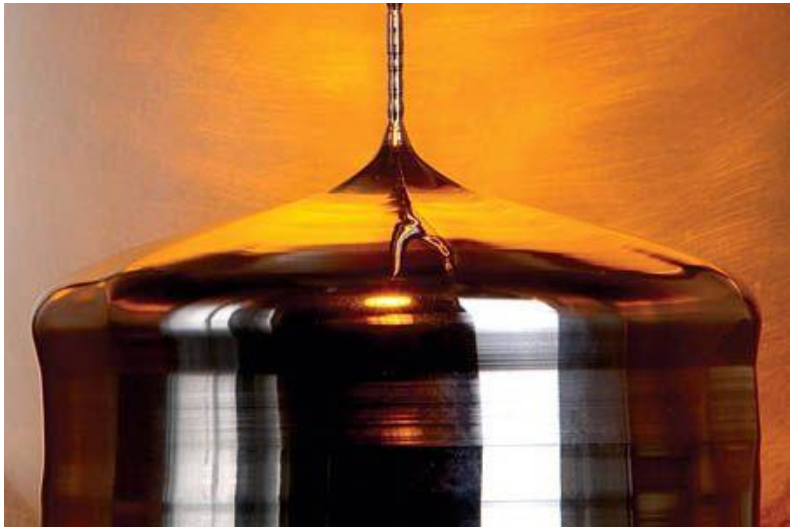


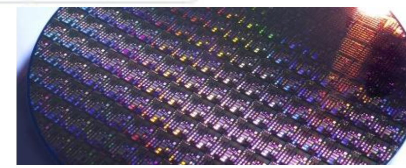
http://www.solarnovus.com/uploads/j/stories/Features/Lattice_Cz_Growth_450x300.jpg

Introduction

- Czochralski process is used to obtain single mono-crystal, which then is usually used in electronics industry

- Creating mathematical model for CZ process allows to study model parameters during crystal growth

http://huali-europe.com/en/images/sy/djgb.jpg



http://www.siliconmaterials.com/wp-content/uploads/2011/11/iStock_000011002999Medium-930x355.jpg

Mathematical model

- Heat transfer by conduction:

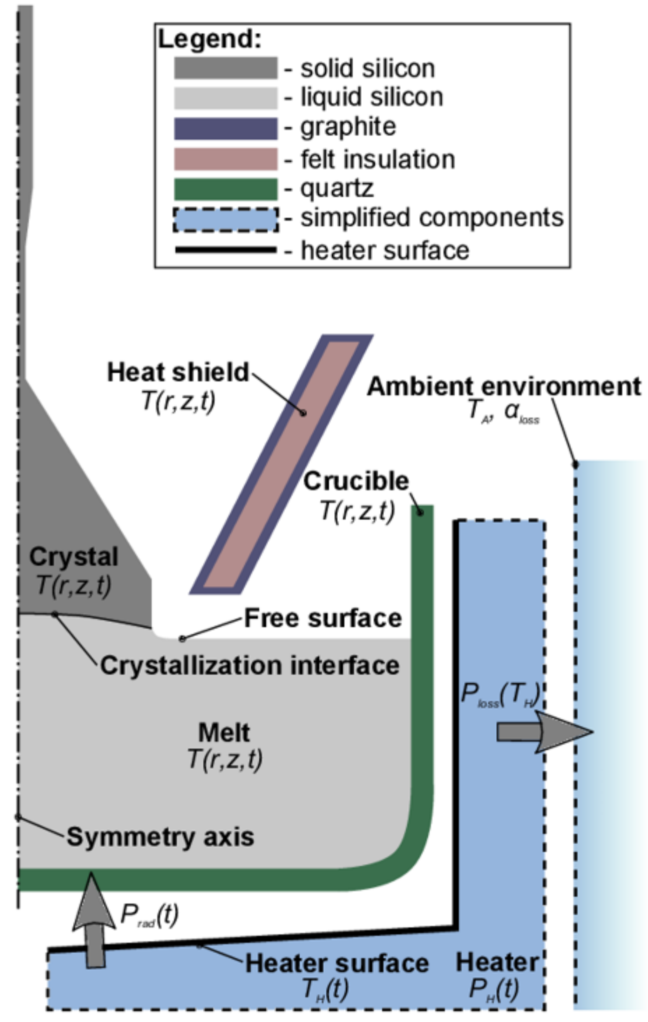
$$\rho c_p \frac{\partial T}{\partial t} = \nabla[\lambda(T)\nabla T]$$

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\lambda(T)\frac{\partial T}{\partial r}\right] + \frac{\partial}{\partial z}\left[\lambda(T)\frac{\partial T}{\partial z}\right]$$

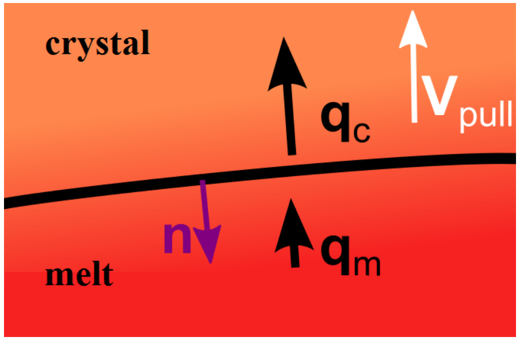
- Heat transfer by thermal radiation
  - radiation is dispersed
  - ambient temperature

$$q^{rad}(dS) = \varepsilon(dS)\sigma_{SB}T^4 - q^{amb}(dS)$$

- Boundary conditions:
  - $T = T_0$ on crystallization interface
  - $\frac{\partial T}{\partial r} = 0$ on symmetry axis($r = 0$)
  - $\lambda(T)\frac{\partial T}{\partial n} = -q^{rad}$ on radiating surfaces



Mathematical model



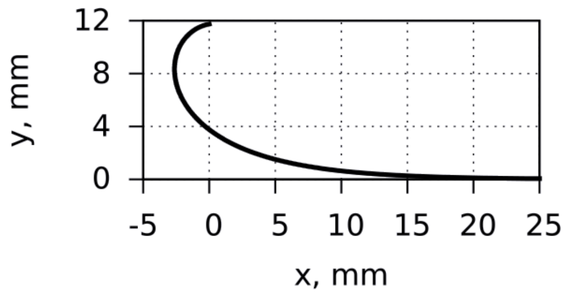
heat balance: $q_c = q_m + \rho_c q_0 V_n$

$$v_n = V_n - \vec{V}_{pull} \cdot \vec{n} = \frac{q_c - q_m}{\rho_c q_0} - \vec{V}_{pull} \cdot \vec{n}$$

interface translation: $\Delta\vec{x} = \vec{n} \cdot v_n \Delta t$

q_0 - crystallization heat
V_n - crystallization speed in $\vec{n}$ direction relative to crystal reference frame
v_n - crystallization speed in $\vec{n}$ direction relative to laboratory reference frame

Free surface shape

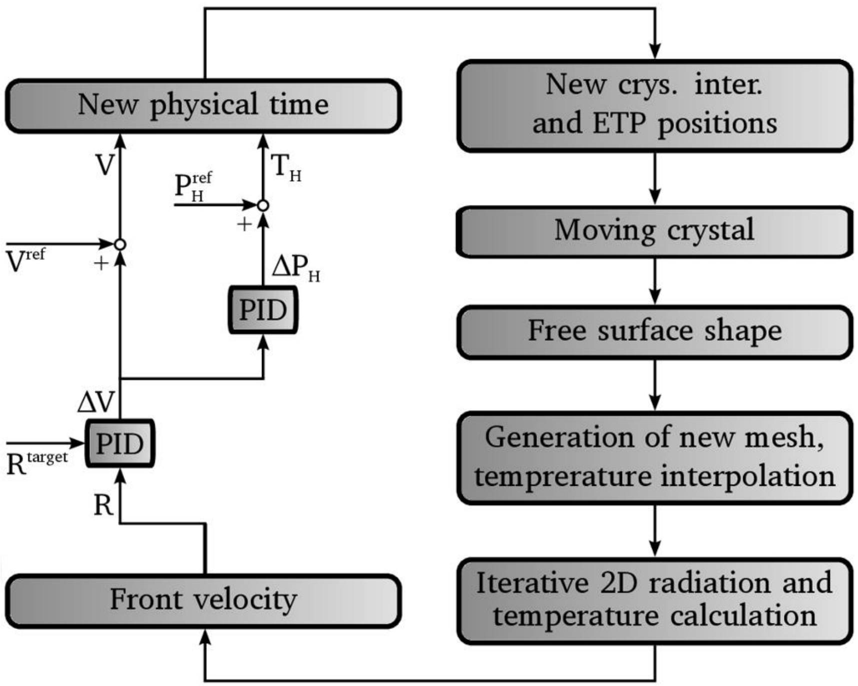


$$\gamma \frac{y''}{(1 + y'^2)^{3/2}} = \rho g y$$

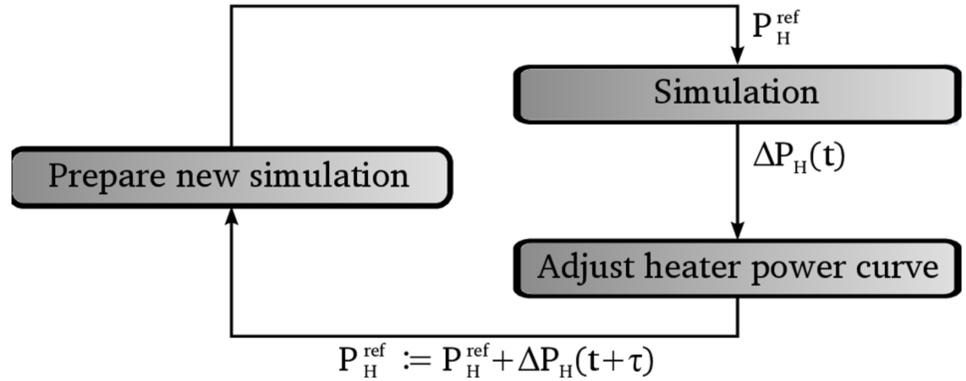
$$x = -l_c \operatorname{acosh} \frac{2 l_c}{y} + l_c \sqrt{4 - \frac{y^2}{l_c^2}} + x_0$$

γ – surface tension
$l_c = \sqrt{\frac{\gamma}{\rho g}}$ - capillarity
$h = l_c \sqrt{2 - 2 \sin \alpha}$ - meniscus height
α – angle between free surface and vertical direction
x_0 - is found from $y(x = 0) = h$

Mathematical model



calculation algorithm



algorithm for obtaining power curve

- after each simulation, necessary power curve computed by a PID controller is added to power curve
- $\tau = 40\ min$ is used

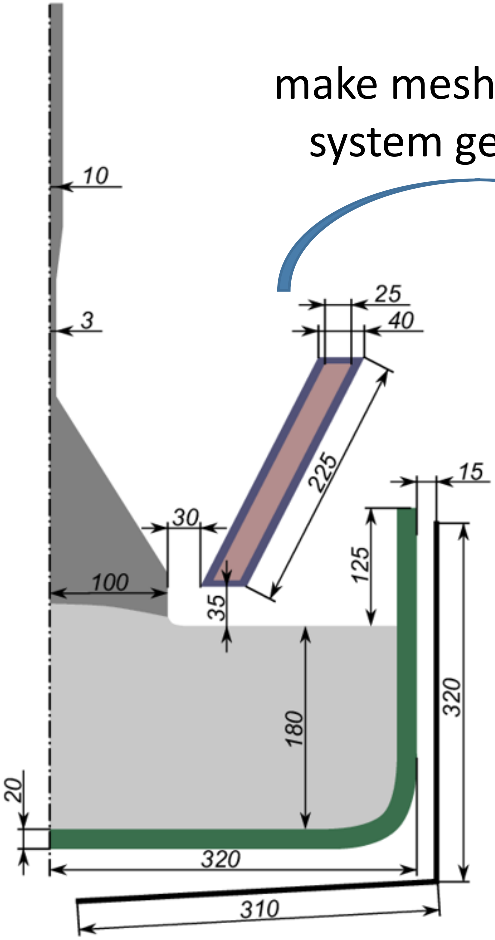
PID controller:

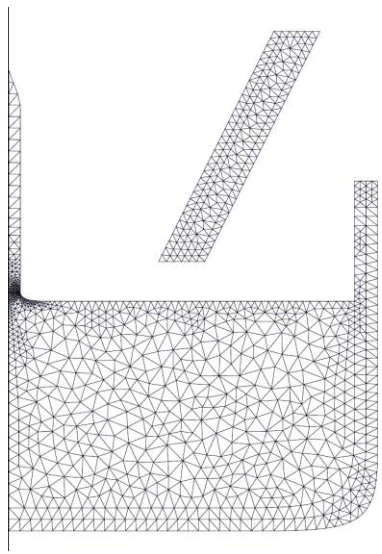
$$\Delta u(t) = K_p\left(e(t) + T_d\frac{d}{dt}e(t) + \frac{1}{T_i}\int_0^t e(\tau)d\tau\right)$$
$$e(t) = f_0(t) - f(t)$$
$$u(t) := u(t) + \Delta u(t)$$

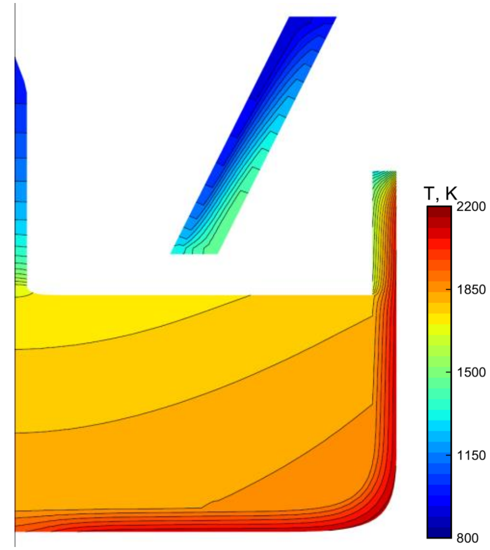
Mathematical model

make mesh for given system geometry

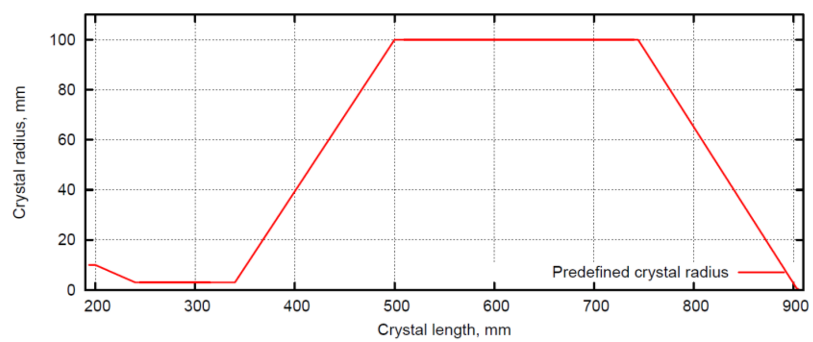
get initial state condition



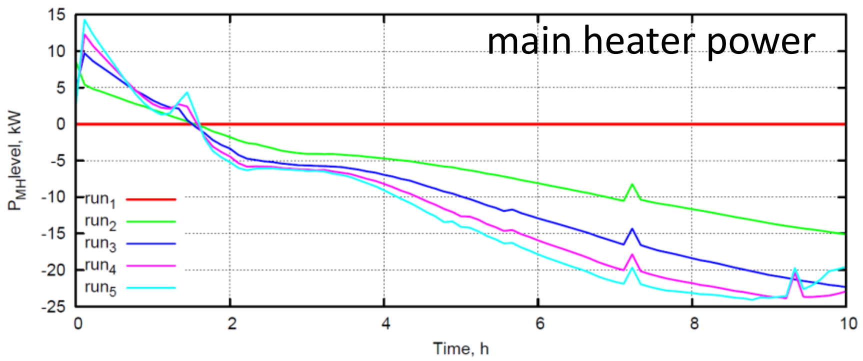


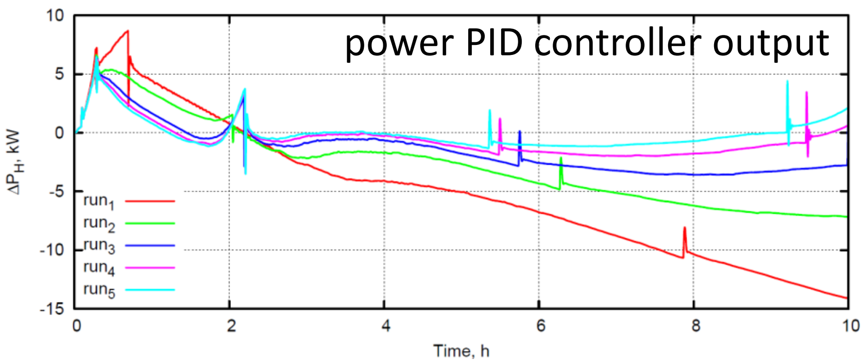


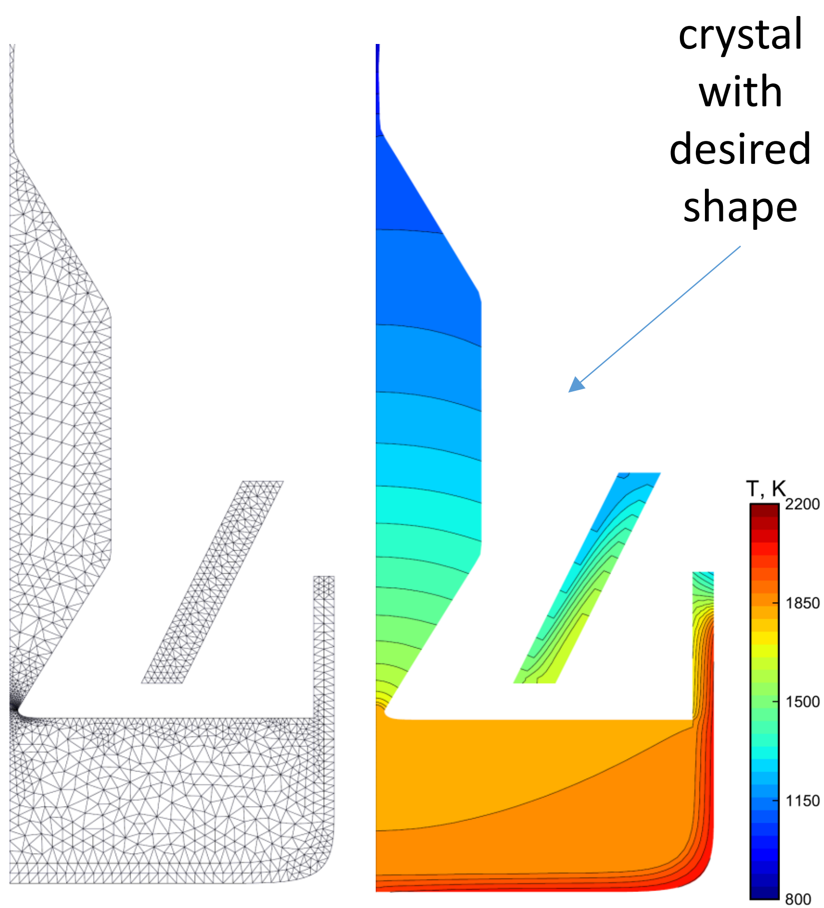
choose needed crystal shape

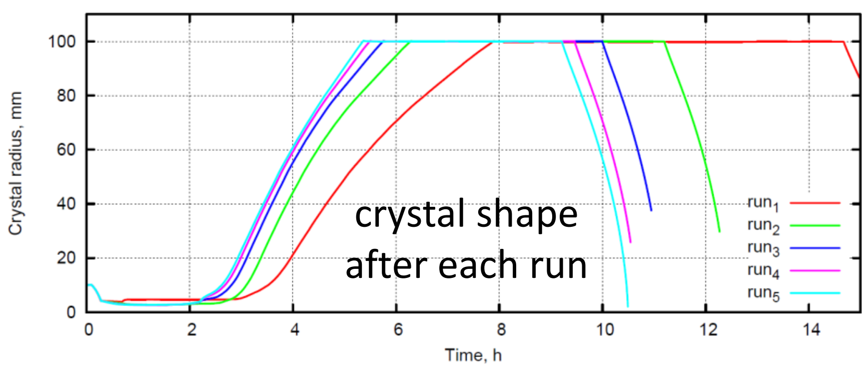


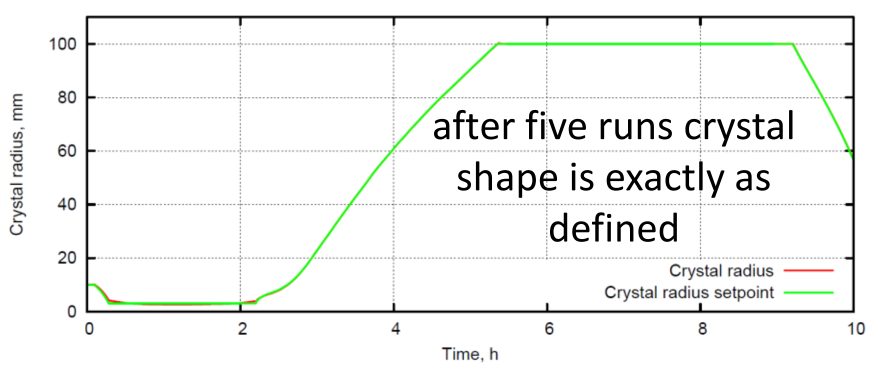
Simulation results



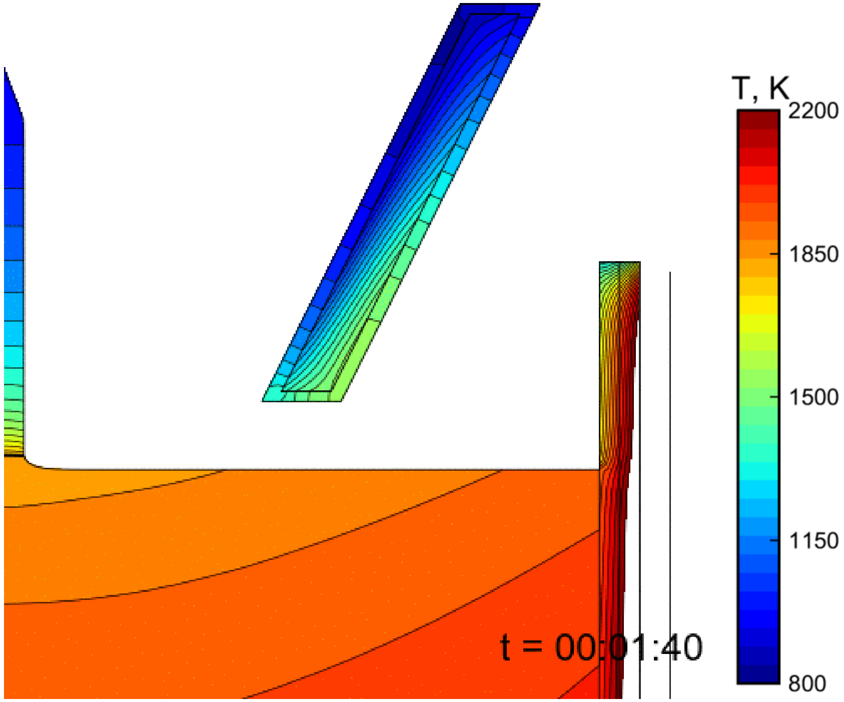








Simulation results



Thermal stresses

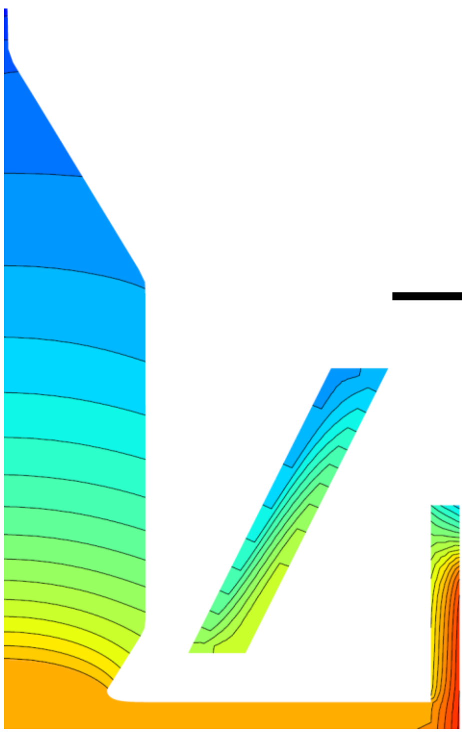
stress tensor matrix

stress vector: $\vec{T} = \lim_{\Delta S \to 0} \frac{\Delta \vec{F}}{\Delta S}$

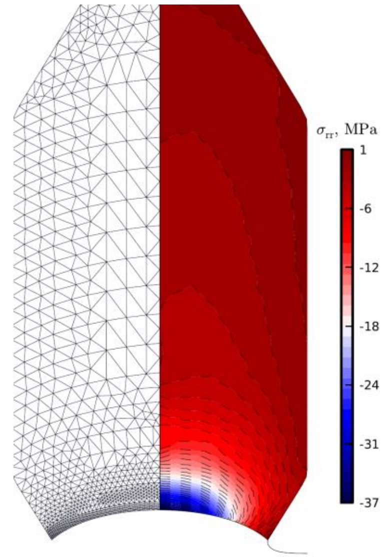
stress on surface with normal $\vec{n}$: $\vec{T} = \sigma \vec{n}$

$$\sigma_{CYL}(r,z) = \begin{pmatrix} \sigma_{rr} & 0 & \sigma_{rz} \\ 0 & \sigma_{\phi\phi} & 0 \\ \sigma_{rz} & 0 & \sigma_{zz} \end{pmatrix} \qquad c = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

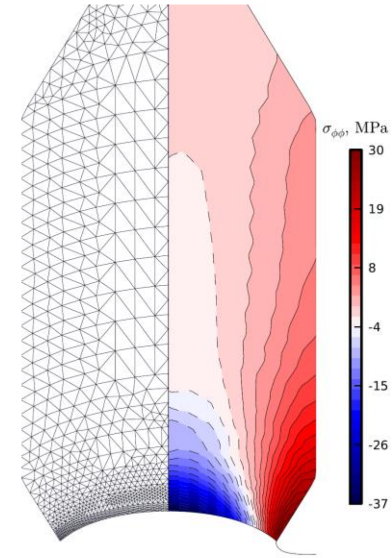
$$\sigma_{CART}(r,\phi,z) = C\sigma_{CYL}(r,z)C^{-1}$$



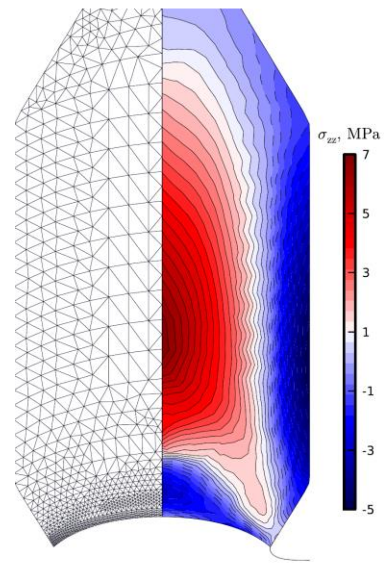
obtained temperature field is used to find thermal stresses in crystal



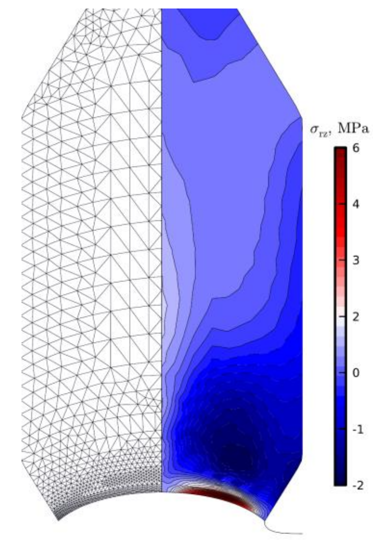
σ_{rr}



$\sigma_{\phi\phi}$



σ_{zz}

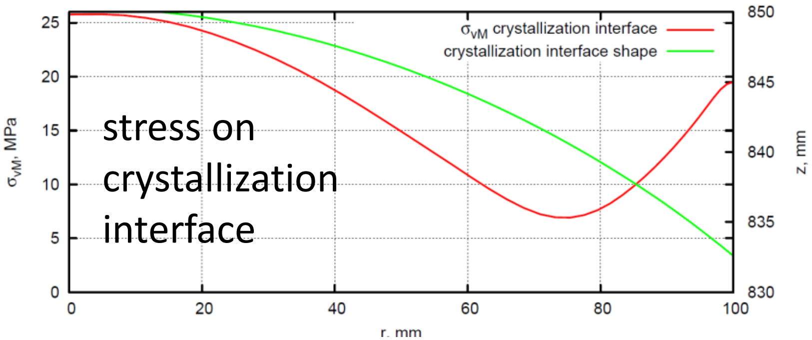


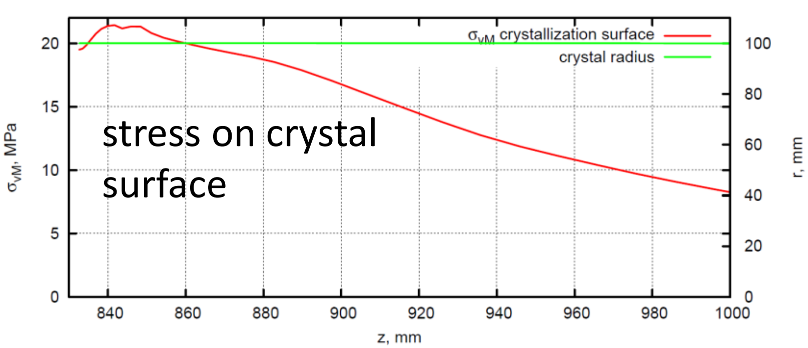
σ_{rz}

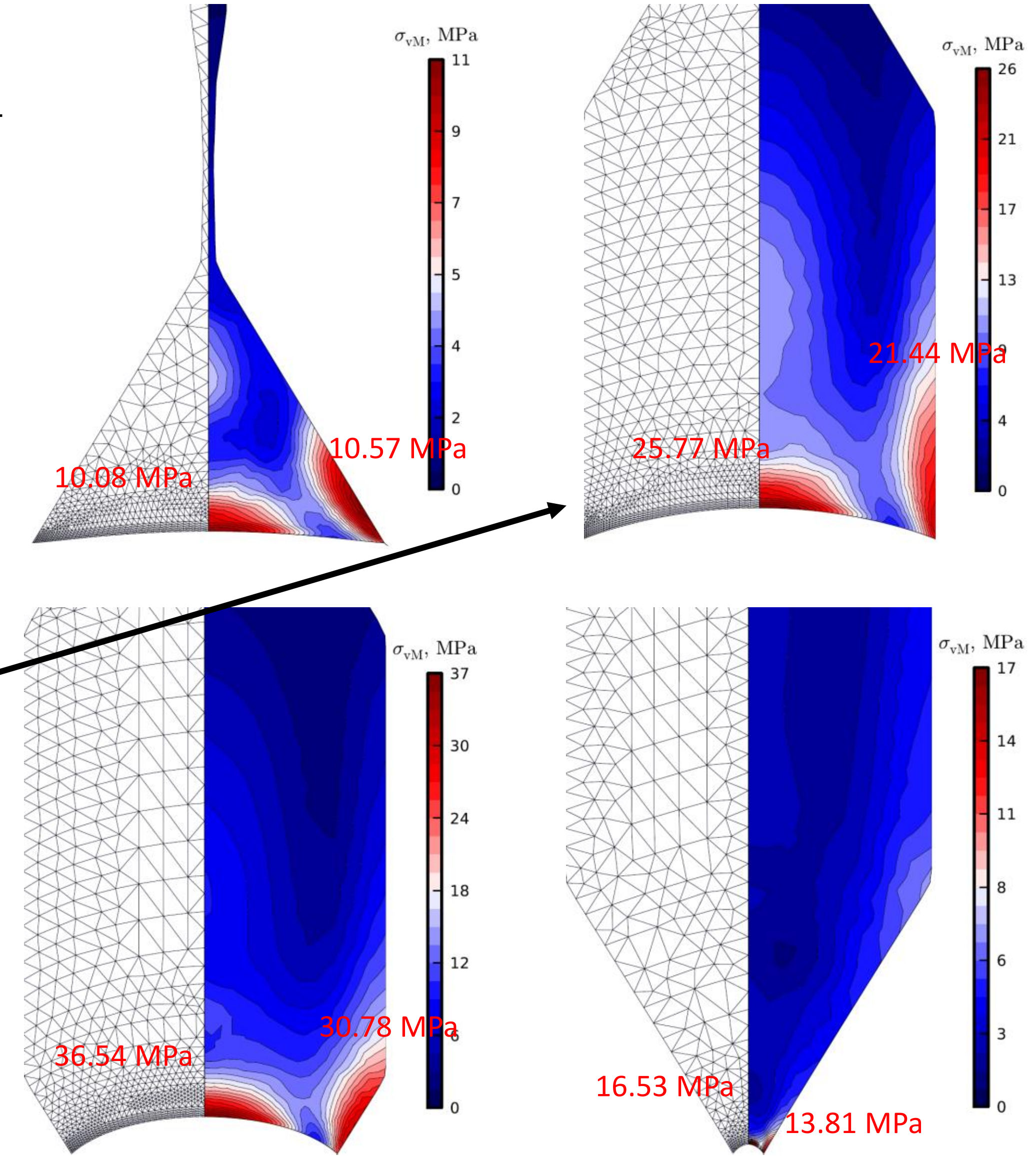
Thermal stresses

von Mises stress:

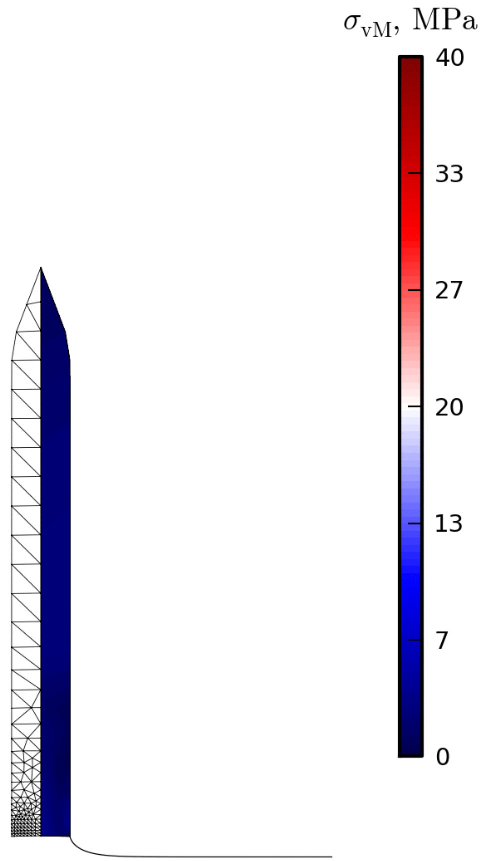
$$\sigma_{vM} = \sqrt{\frac{1}{2}\left[\begin{array}{c}(\sigma_{rr} - \sigma_{\varphi\varphi})^2 + \\ (\sigma_{\varphi\varphi} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{rr})^2 + 6(\sigma_{rz})^2\end{array}\right]}$$







Thermal stresses



Conclusions

- Transient model of CZ process has been used to simulate crystal growth
- To get optimal values for PID controller and time-shift τ parameter study is required
- Using obtained crystal thermal field, thermal stresses in crystal were found
- Obtained thermal stress field could be used for further study of point defects in crystal