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IEGULDĪJUMS TAVĀ NĀKOTNĒ

3D simulation of feed rod melting in floating zone silicon single crystal growth

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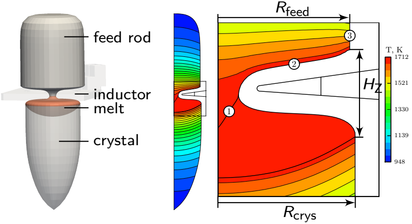
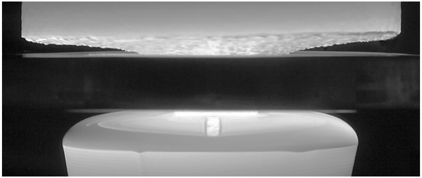
Open melting front of the feed rod

Overall view of the system



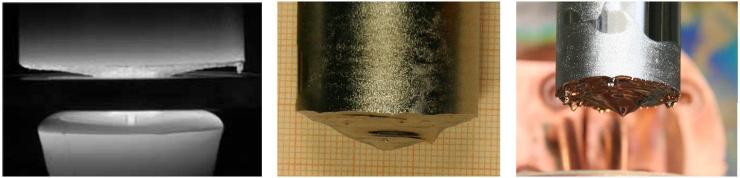
Inhomogeneous structure



Th. Duffar. *Crystal Growth Processes Based on Capillarity*, 2010

Instabilities

Formation of spikes or "noses" deteriorate the process

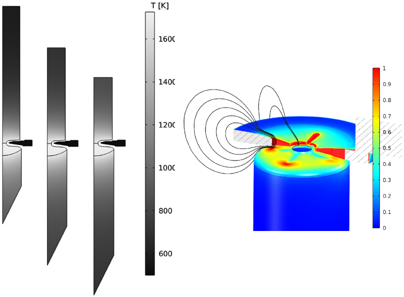


M. Wünscher. PhD Thesis, 2011

Existing models for the open melting front

- Only axisymmetric

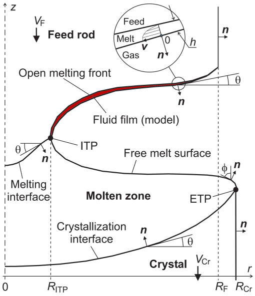
The shape is taken from experimental data



M. Wünscher et al. *JCG*, 2014

The shape is obtained numerically

Fluid film model



G. Ratnieks et al. *JCG*, 2003

Mathematical model

Aim

Time-dependent distribution of the local melting rate on the open melting front

Balance of the heat flux densities

- Heat conduction q_{diff}
- Thermal radiation q_{rad}
- Induced heat sources q_{EM}

} disbalance causes melting or crystallization

Separate models for:

Temperature field

Heat flux in the feed rod due to diffuse heat transfer

HF EM field

Induced heat sources on the open front

Liquid silicon layer

For the correction of the EM heat sources because heat sources are induced in both phases

Melting of the open front found from the heat flux balance

Temperature field

Equation

- 3D unsteady heat conduction in the feed rod:

$$\rho_s c_p \frac{\partial T}{\partial t} = \vec{\nabla} \cdot \left(\lambda(T) \vec{\nabla} T \right) \tag{1}$$

ρ_s – density

c_p – heat capacity at constant pressure

$\lambda(T)$ – temperature dependent heat conductivity

- No convective terms – reference frame linked to the feed rod

Boundary conditions

- Constant temperature on the melting fronts: $T_0 = 1687\,\mathrm{K}$
- On the side surface: $\lambda(T)\frac{\partial T}{\partial n} = \epsilon(T)\left(q_{inc} - \sigma_{SB} T^4\right) + q_{EM}$

HF EM field

Main equations

- Introduction of the linear current density $\vec{j}$: $\vec{\nabla} \cdot \vec{j} = 0$
- Electrical vector potential $\vec{\Psi} = (0, 0, \Psi_{\mathrm{n}})$: $\vec{\nabla} \times \vec{\Psi} = \vec{j}$

Induced power density

$$q_{EM} = \underbrace{\frac{j_l^2}{\delta_l \sigma_l}}_{\substack{\text{Infinite}\\\text{liquid}\\\text{layer}}} \cdot \underbrace{\frac{1 - (1-\kappa)\, e^{-2l}}{1 - 2\,(1-\kappa)\, e^{-l} \cos l + (1-\kappa)^2\, e^{-2l}}}_{\text{Correction due to finite layer thickness}} \qquad (2)$$

Parameters: $\kappa = \sqrt{\frac{\sigma_s}{\sigma_l}}$ un $l = \frac{h}{\delta_l}$, where h – thickness of the fluid film

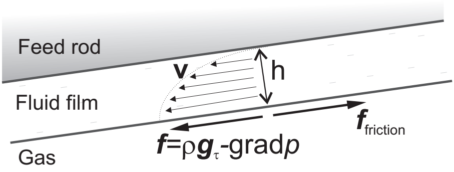
Liquid silicon layer

Equation

- Unsteady mass conservation law:

$$\iint_S \frac{\mathrm{d}h}{\mathrm{d}t}\mathrm{d}S = -\oint_{\partial S} \vec{q}\cdot \mathrm{d}\vec{l} + \iint_S v_{\mathrm{m}} \frac{\rho_{\mathrm{s}}}{\rho_{\mathrm{l}}}\mathrm{d}S \quad (3)$$

- Velocity is integrated over the film thickness: $\vec{q} = \int_0^h \vec{v}\mathrm{d}h$
- Balance of friction and tangential forces: $-\eta \frac{\mathrm{d}^2\vec{v}}{\mathrm{d}h^2} = \vec{f}$



Parabolic velocity distribution in the fluid film and force equilibrium

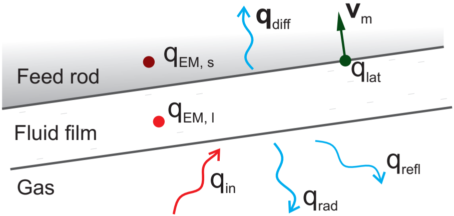
Melting of the open front

- Local melting rate:

$$v_{\mathrm{m}} = \frac{q_{\mathrm{EM}} - q_{\mathrm{diff}} - q_{\mathrm{rad}}}{L\rho_{\mathrm{s}}} \tag{4}$$

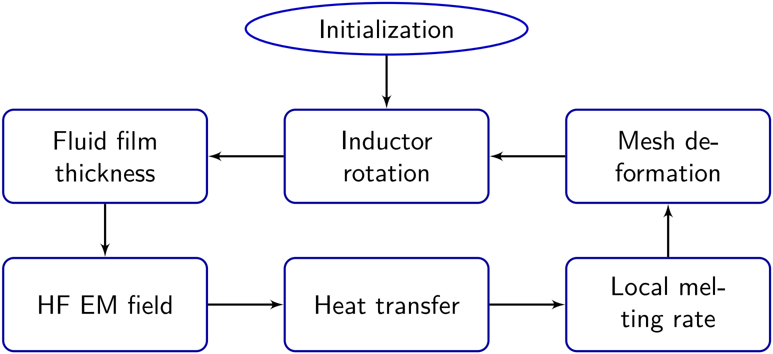
L – latent heat

- Heat flux in feed rod: $q_{\mathrm{diff}} = -\lambda_s \frac{\partial T}{\partial n}$
- Net radiation power density: $q_{\mathrm{rad}} = \epsilon_l \left(\sigma_{\mathrm{SB}} T_0^4 - q_{\mathrm{inc}}\right)$



Balance of the heat fluxes

Overall calculation scheme



Fluid film calculations

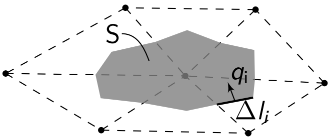
Discretization

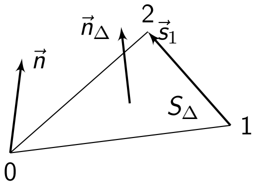
- Transient equation for the fluid film:

$$\frac{h_1 - h_0}{\Delta t_h} = \frac{1}{S}\Sigma \Delta l_\mathrm{i} q_\mathrm{i} + v_\mathrm{m}\frac{\rho_\mathrm{c}}{\rho_\mathrm{m}} \quad (5)$$

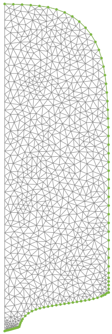
- Pressure due to surface tension:

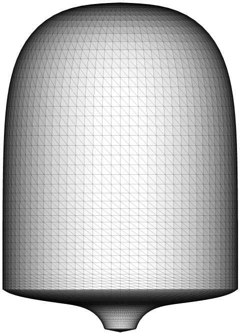
$$p_\mathrm{K} = \gamma \frac{3}{2}\frac{\sum \vec{n}_\triangle \cdot (\vec{s}_1 \times \vec{n})}{\sum \vec{S}_\triangle \cdot \vec{n}} \quad (6)$$

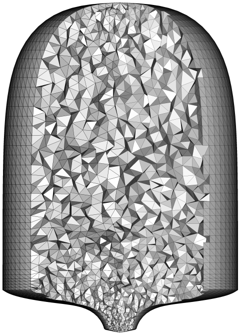




Generation of 3D element mesh







2D finite elements

Axisymmetric *FZone* calculations

3D boundary elements

HF EM field calculations

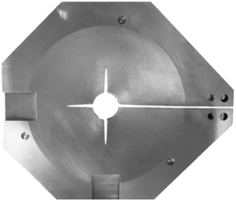
Volume elements

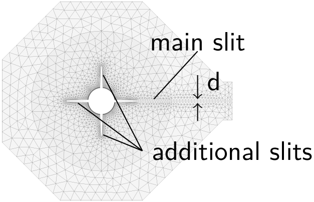
Unsteady temperature field calculations

Surface points coincide for all meshes

The considered 4" FZ system from ICG, Berlin

Inductor



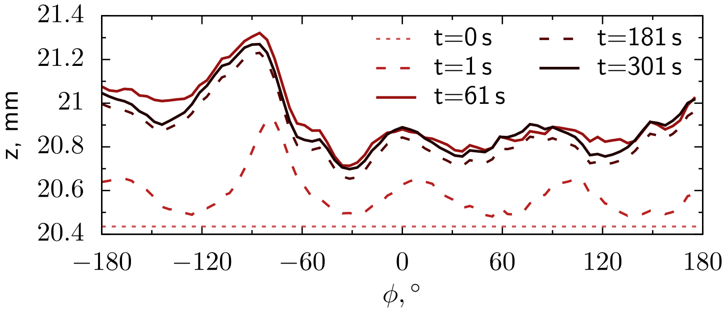


Process parameters

Parameter and designation		Value	Dimension
Target zone height	H_z	32.5	mm
Inductor current frequency	f	3	MHz
Crystal pull rate	v_c	2.55	mm/min
Feed rod push rate	v_f	2.76	mm/min
Crystal radius	R_{crys}	51	mm
Feed rod radius	R_{feed}	49	mm

Time development of the open front melting

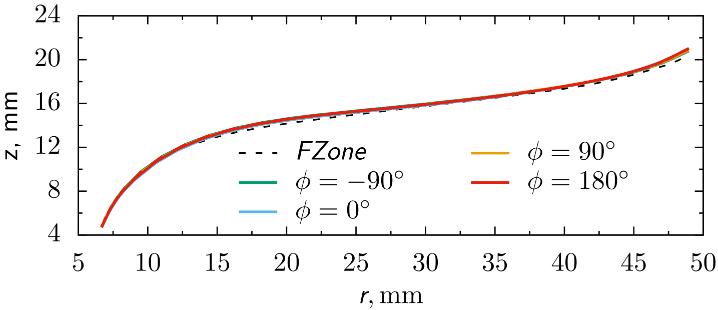
Azimuthal profile at the feed rod rim



The shape stabilizes after ≈ 5 periods

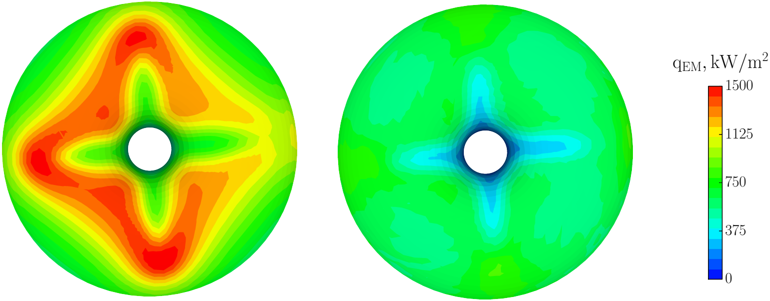
Comparison between axisymmetric and 3D results

Radial profiles of the open front



Melting of the open front

Distribution of the induced power density



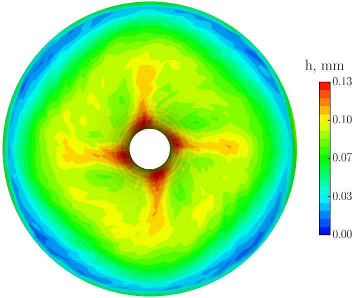
Dry feed rod surface

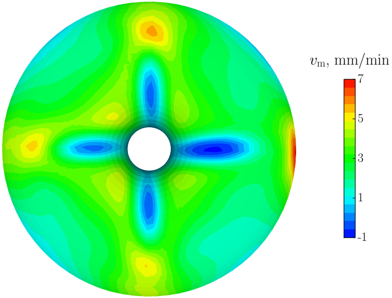
With fluid film correction

- Differences of the induced power density up to $\kappa = \sqrt{\frac{\sigma_s}{\sigma_l}} \approx 4.9$ times

Melting of the open front

Distribution of the fluid film thichness and melting velocity

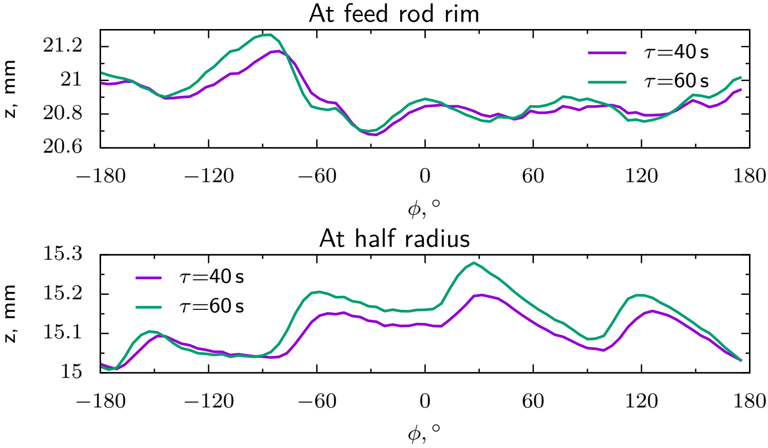




- Highest fluid film thickness around the neck
- Lowest fluid film thickness near the feed rod rim
- Melting rate corresponds to the EM heat source distribution

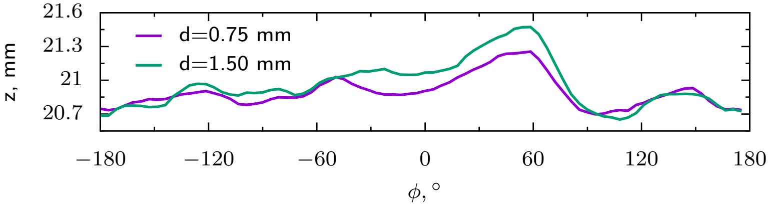
Influence of rotation period

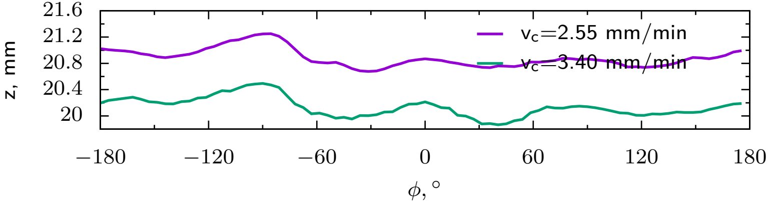
Azimuthal profiles of the open front



Influence of process parameters

Azimuthal profiles of the open front





Conclusions

- For the first time a 3D transient mathematical model for feed rod melting has been developed and implemented in a calculation program
- The shape of the open front tends to stabilize after several feed rod revolutions
- The obtained 3D shape of the open melting front remains close to the axisymmetric profile with differences of order $\sim 1\,\mathrm{mm}$
- The asymmetry increases with:
  - higher pulling velocity
  - lower feed rod rotation rate
  - narrower main slit of the inductor
- The obtained results are useful for a comparison with experimental data

Thank you for your attention!