3D simulation of feed rod and fluid film in floating zone silicon crystal growth

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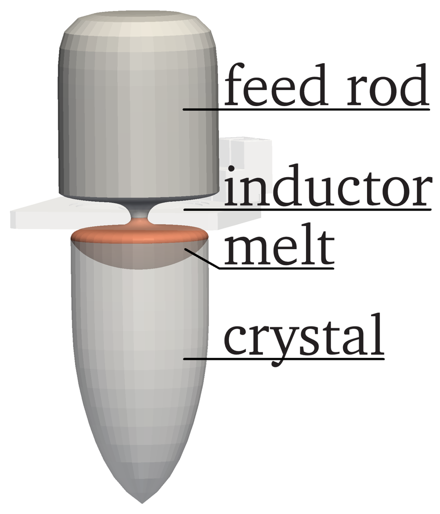
Introduction

The industrial floating zone process (FZ) of silicon crystal growth is characterized by a variety of coupled physical phenomena. Advanced global mathematical models exist for FZ process simulation, e.g., [1, 2], but they are limited to the cylindrical symmetry of the heat transfer and phase boundaries.
However, the induced electromagnetic (EM) heat sources are strongly non-axisymmetric due to the single-turn needle-eye high-frequency (HF) inductor and require three-dimensional (3D) EM field modelling. A feed rod shape too is expected to be non-axisymmetric.
Therefore a 3D transient model for the feed rod shape has been developed and implemented in the program `FZone`. An overview of the model and calculation results for a typical 4" FZ system from IKZ, Berlin, [3], are presented below.



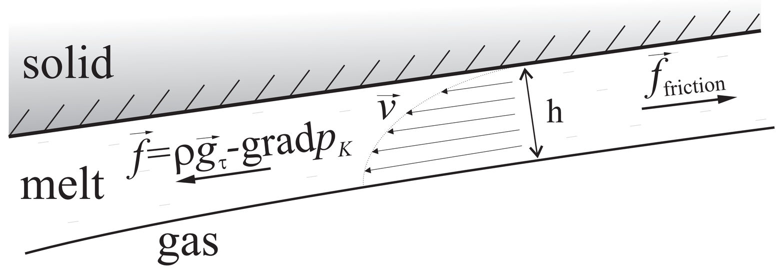
Mathematical model

Temperature in the feed rod. The 3D transient heat conduction equation is solved in the feed rod domain:

$$\rho c_{\mathrm{p}} \frac{\partial T}{\partial t} = \vec{\nabla} \cdot \left(\lambda(T) \vec{\nabla} T \right)$$

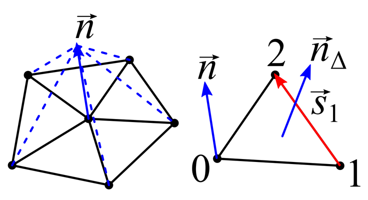
A fixed temperature boundary condition ($T_0 = 1687\,\mathrm{K}$) is applied to the inner and open fronts. A radiation boundary condition in the form $\lambda(T)\frac{\partial T}{\partial n} = \epsilon(T)\left(q_{\mathrm{inc}} - \sigma_{\mathrm{SB}} T^4\right) + q_{\mathrm{EM}}$ is imposed on the side surface. The equation is solved with a modified `OpenFOAM` solver *laplacianFoam*. Material properties are taken from [4].

Fluid field model. A quasi-steady state flow model is used for the thin molten silicon layer on the open front. The flow rate $\vec{q}$ is obtained from a parabolic velocity profile, determined by balance between the viscous drag and gravity and surface tension forces:



The surface tension pressure is given by:

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

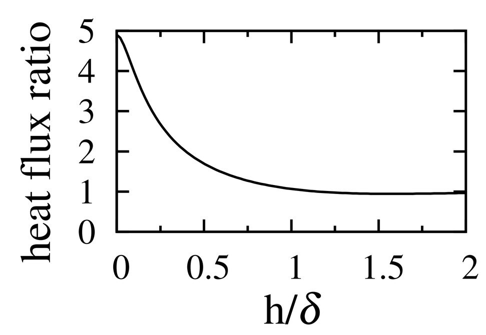


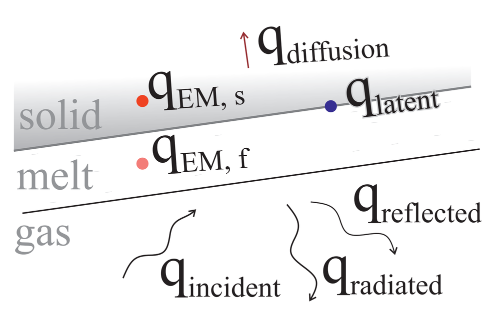
where K is the curvature of the fluid film surface. The finite volume method is used to formulate a transient equation for the fluid film thickness h:

$$\frac{\partial h}{\partial t} = \frac{1}{S} \Sigma \Delta l_i q_i + v_{\mathrm{m}} \frac{\rho_{\mathrm{c}}}{\rho_{\mathrm{m}}}$$

HF electromagnetic field. A 3D boundary element method is used to obtain the distribution of heat source density, see [5].

Open front melting. The melting rate is calculated from the heat flux balance on the open front. Thermal radiation is taken into account and a correction for the induced EM heat power density is employed depending on the fluid film thickness h.

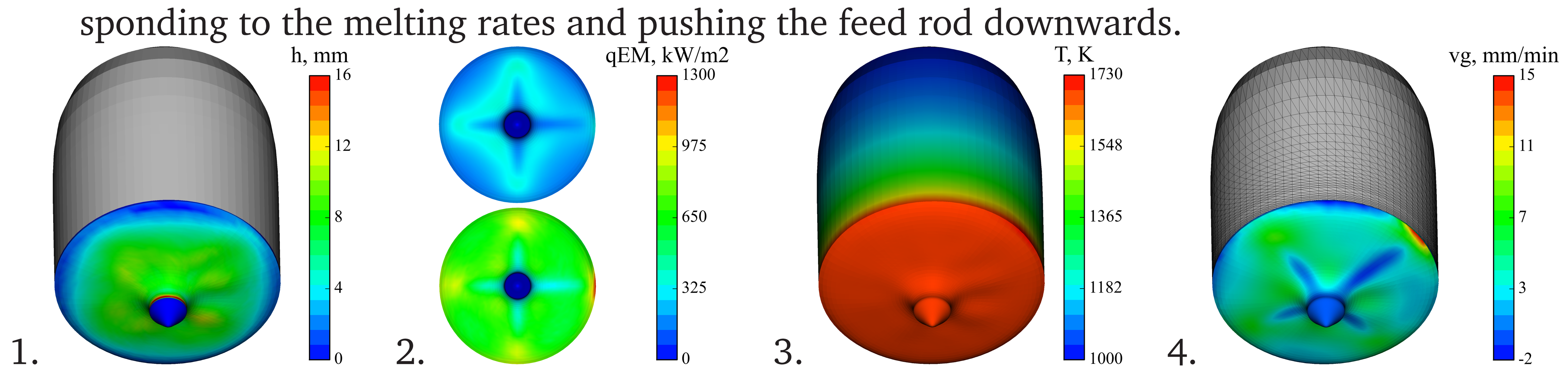




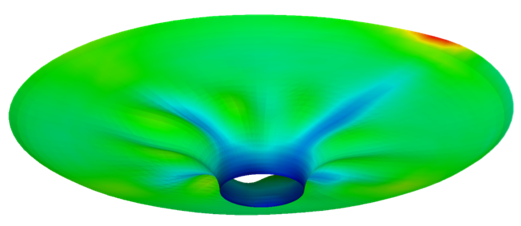
General calculation algorithm

The transient changes of the 3D feed rod shape are calculated in five stages in each times step:

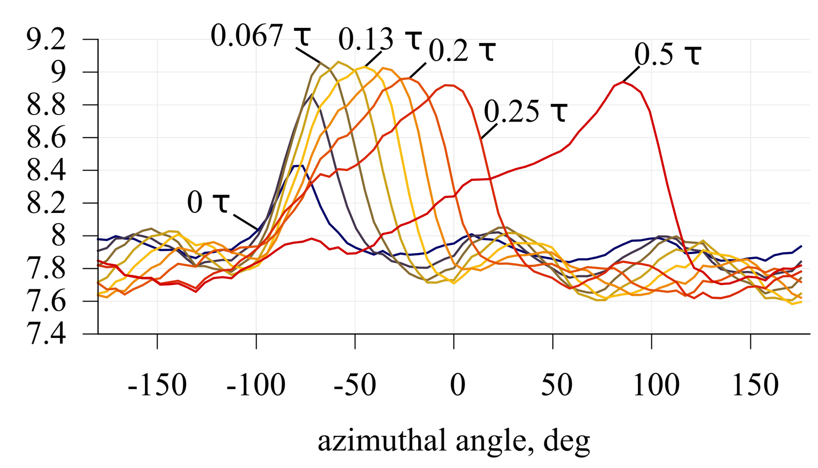
0. Rotating the inductor by an angle corresponding to the time step $\mathrm{d}t$ and rotation rate ω;
1. Obtaining the fluid film thickness h;
2. Calculating the 3D EM field and EM power distribution taking film thickness h into account;
3. Solving the transient temperature equation for the feed rod;
4. Calculating the melting rate at the open front surface. Transforming the feed rod mesh corresponding to the melting rates and pushing the feed rod downwards.



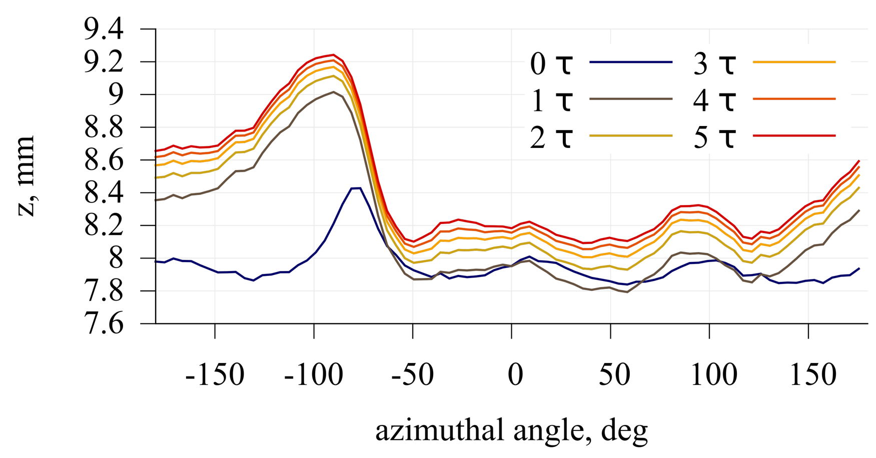
Calculation results



A process with a crystal pull rate of 3.4 mm/min and feed rod rotation rate of 1 rpm is used as a reference case. The surface tension coefficient is set to 0.2 N/m to ensure numerical stability.

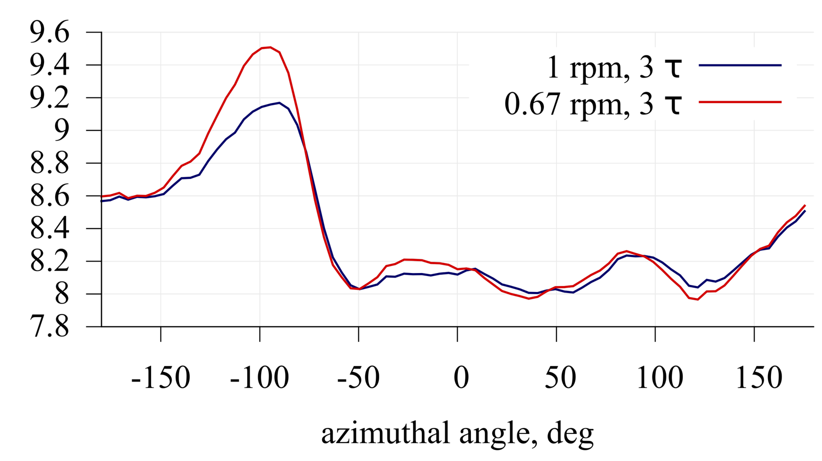


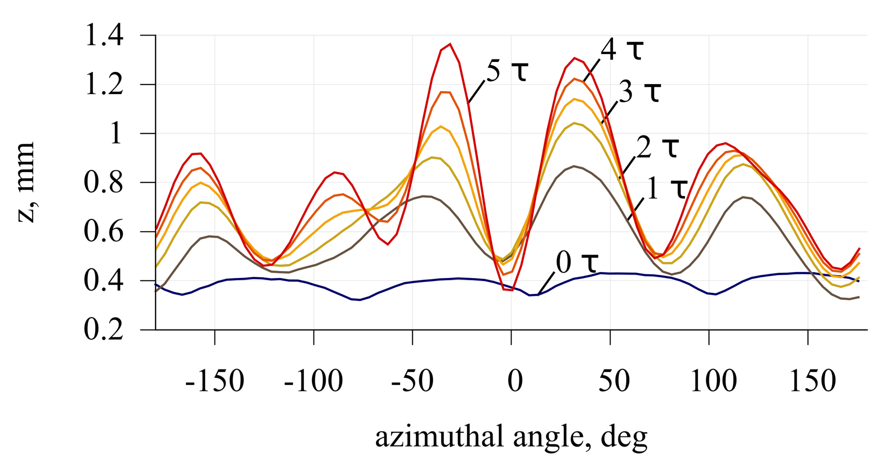
The evolution of the vertical position of the feed rod rim (right) shows a pronounced melting above the main slot due to the induced power maxima (τ is the period of a full revolution).



The molten peak above the inductor reaches its maximum value of 1 mm in roughly 1 s after the start of the simulations. Shortly after reaching saturation the molten area becomes asymmetric with respect to the azimuthal angle. The shape of the feed rod rim converges after a sufficient number of revolutions (left). More than five revolutions are necessary for a fully-periodic solution.

The height of the feed rod rim is also influenced by the side slits with a maximal height difference of 0.3 mm.
The influence of a lower feed rotation rate (0.67 rpm) on the azimuthal distribution of the feed rim height can be seen on the right. After about 1.2 revolutions the molten peak for the lower rotation is 0.4 mm higher, due to longer feed rod exposure to the EM power maximum.





Azimuthal distribution of the surface height at a middle radial position (left) shows a surface instability that is believed to occur due to interplay between gravity and EM field. Molten silicon flows downwards from the hollows, where higher EM power density is generated due to reduced thickness of the fluid film. Higher surface tension is expected to have a stabilizing effect on this instability.

References

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Acknowledgements

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