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Simulation of the influence of gas flow on melt convection and phase boundaries in FZ silicon single crystal growth

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ERAF
EIROPAS REĢIONĀLĀS ATTĪSTĪBAS FONDS
EIROPAS SAVIENĪBA
IEGULDĪJUMS TAVĀ NĀKOTNĒ

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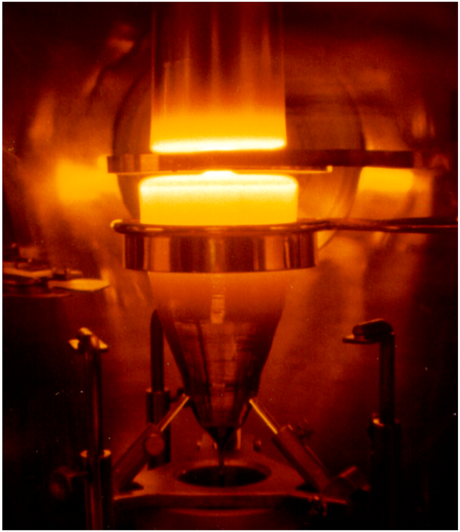
2. 2D axisymmetric mathematical model for turbulent argon flow in FZ puller using `OpenFOAM`

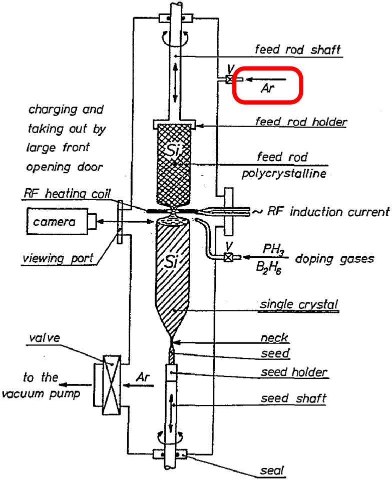
3. Calculation example of ICG (Berlin, Dr. H. Riemann) floating zone system with crystal diameter 4 inches

4. Conclusions

Si single crystal growth with FZ technique

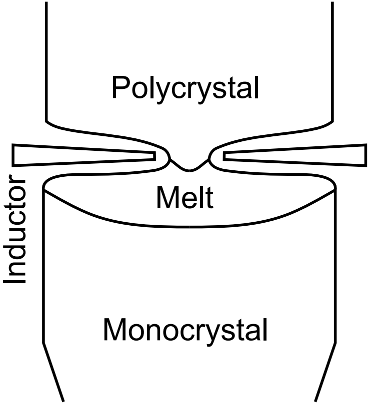


Courtesy of Dr. H. Riemann (ICG, Berlin)



W. Zulehner. Mater. Sci. Eng. B, 73(1):7-15, 2000

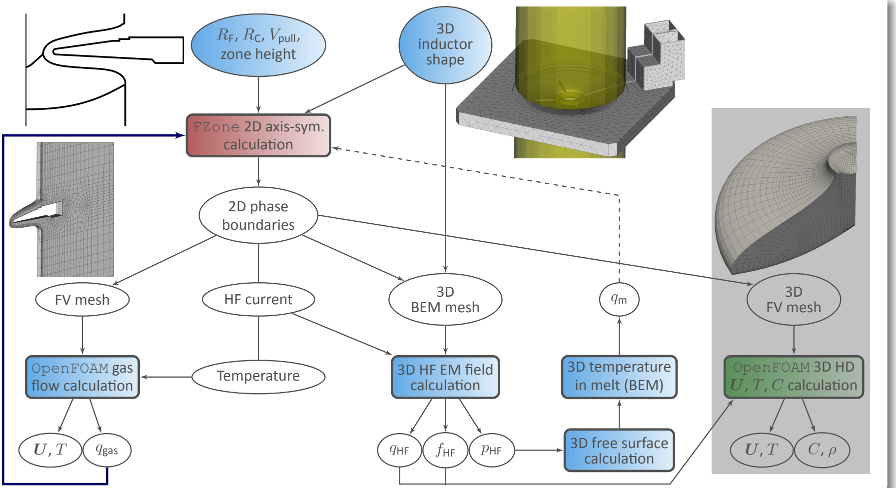
Axisymmetric quasi-stationary FZ model



- High-frequency electromagnetic field (BEM), 2D or 3D
- Thermal radiation, including reflector (view factor model)
- Heat transfer in crystals, melt and reflector (FEM)
- Free melt surface shape (iterative approach)
- Solid-liquid interface positions
- Open melting front model

- Model implemented in the program `FZone` (Ratnieks, 2003)
- Further development of the model is still ongoing

Actual mathematical model



R_F, R_C, V_pull, zone height

3D inductor shape

`FZone` 2D axis-sym. calculation

2D phase boundaries

FV mesh

HF current

3D BEM mesh

q_m

3D FV mesh

`OpenFOAM` gas flow calculation

Temperature

3D HF EM field calculation

3D temperature in melt (BEM)

`OpenFOAM` 3D HD U, T, C calculation

U, T

q_gas

q_HF

f_HF

p_HF

3D free surface calculation

U, T

C, ρ

Gas flow: Introduction

Density: Ideal gas law

- Large temperature and density variations

$$\rho = p\frac{M}{RT}$$

ρ density
p pressure
M molar mass
R universal gas constant
T absolute temperature

Viscosity: Sutherland's law

$$\mu(T) = \frac{A_S\sqrt{T}}{1 + T_S/T}$$

Parameter values

	Argon	Helium	
M	39.948	4.0026	$\mathrm{g\ mol^{-1}}$
c_p	520	5193	$\mathrm{J\ kg^{-1}\ K^{-1}}$
A_S	2.130	1.811	$\mu\mathrm{Pa\ s\ K^{-1/2}}$
T_S	199.2	205.3	K
Pr	0.67	0.67	-

- Thermal conductivity and kinematic viscosity of helium is 8 times higher than of argon

Turbulence

- SST k-omega turbulence model

Gas flow: Basic equations (steady-state)

Continuity equation

$$\nabla \left(\rho \boldsymbol{U} \right) = 0$$

Pressure

$$p_{\mathsf{rgh}} = p - \rho \, \boldsymbol{g} \, \boldsymbol{x}$$

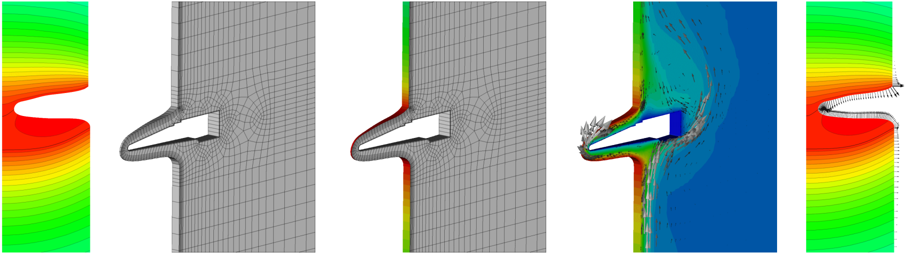
Navier-Stokes equations

$$\nabla \left(\rho \boldsymbol{U} \otimes \boldsymbol{U} \right) = -\nabla \left(p_{\mathsf{rgh}} + \frac{2}{3} \mu_{\mathsf{eff}} \nabla \boldsymbol{U} \right) - \boldsymbol{g} \, \boldsymbol{x} \, \nabla \rho + \\ + \nabla \left[\mu_{\mathsf{eff}} \left(\nabla \boldsymbol{U} + \nabla \boldsymbol{U}^{T} \right) \right], \quad \mu_{\mathsf{eff}} = \mu + \mu_{t}$$

Enthalpy equation

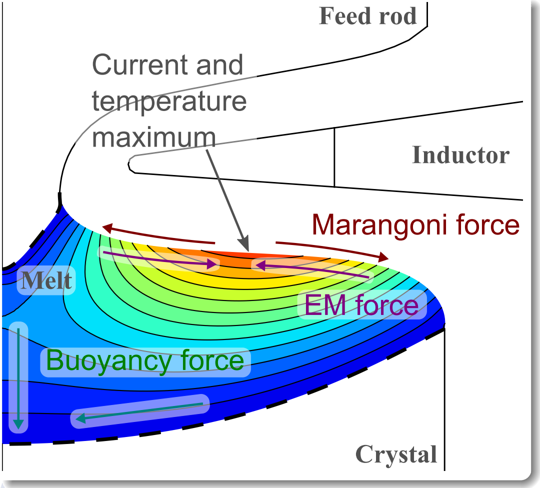
$$\rho \boldsymbol{U} \nabla \left(h + \frac{U^2}{2} \right) = \nabla \left(\alpha_{\mathsf{eff}} \nabla h \right), \quad \alpha_{\mathsf{eff}} = \alpha + \alpha_{t}$$

`FZone` and `OpenFOAM` iteration algorithm



1. Calculation of the quasi-stationary shape of **phase boundaries** and **temperature** field in silicon using `FZone`
2. Creation of the **geometry** for argon flow calculations and automatic **mesh** generation
3. **Interpolation** of the temperature field on the silicon surfaces of the generated finite volume mesh
4. Calculation of the axisymmetric steady state **argon flow** using `OpenFOAM` standard solver `buoyantSimpleFoam`
5. Calculation of the quasi-stationary shape of **phase boundaries** with **argon cooling** taken into account using `FZone`

Melt flow



$$\nabla \boldsymbol{u} = 0$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\nabla)\boldsymbol{u} = -\frac{\nabla p}{\rho_0} + \nu\nabla^2\boldsymbol{u} + \boldsymbol{g}\beta(T - T_0)$$

$$\frac{\partial T}{\partial t} + (\boldsymbol{u}\nabla)T = \frac{\lambda}{\rho c_p}\nabla^2 T$$

Free surface: EM and Marangoni surface forces

$$\boldsymbol{f}_{\mathrm{EM}} = \frac{\mu_0\delta}{4}\frac{\partial(i^2)}{\partial\tau}$$

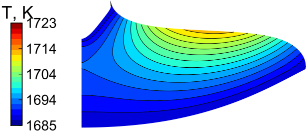
$$\boldsymbol{f}_{\mathrm{Ma}} = \frac{\partial\gamma}{\partial T}\frac{\partial T}{\partial\tau} = M\frac{\partial T}{\partial\tau}$$

Influence of Marangoni coefficient

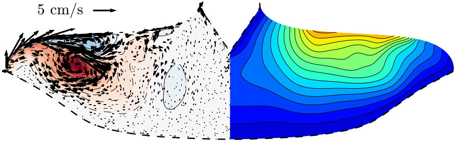
Marangoni coefficient $M = \frac{\partial \gamma}{\partial T}$, γ – surface tension

M is not exactly known, therefore several coefficients were used

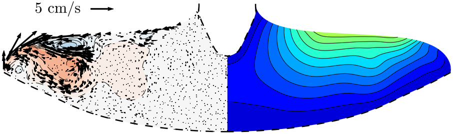
No HD



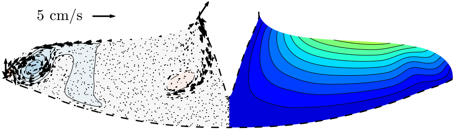
$M = -1.3 \cdot 10^{-4}\,\mathrm{N/(m \cdot K)}$



$\boldsymbol{M = -1.6 \cdot 10^{-4}}\,\mathrm{N/(m \cdot K)}$

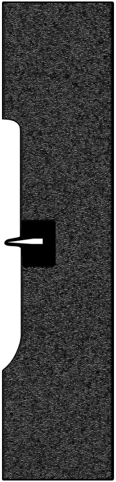


$M = -2.5 \cdot 10^{-4}\,\mathrm{N/(m \cdot K)}$



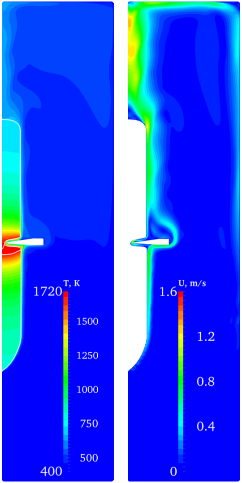
4” FZ process: Global view

Mesh

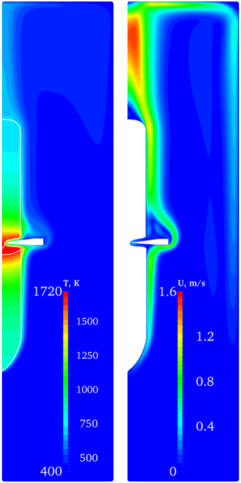


1.3 m × 0.3 m, ca. 73 000 cells

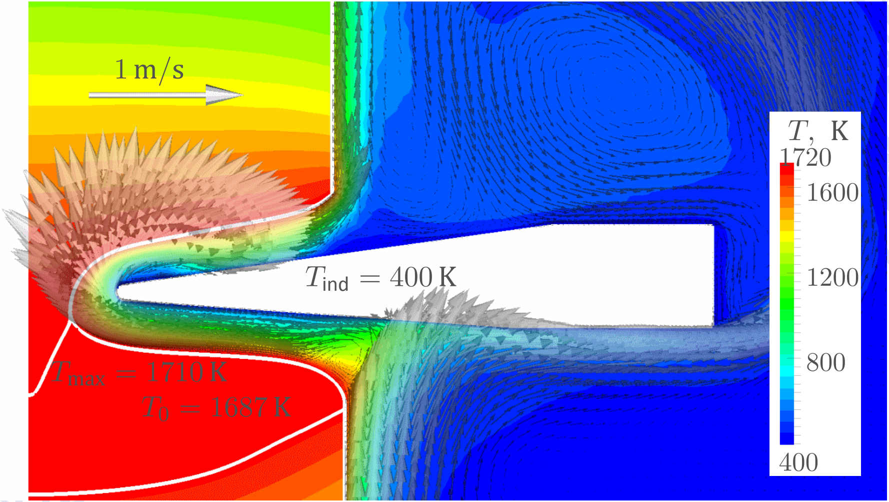
Argon flow



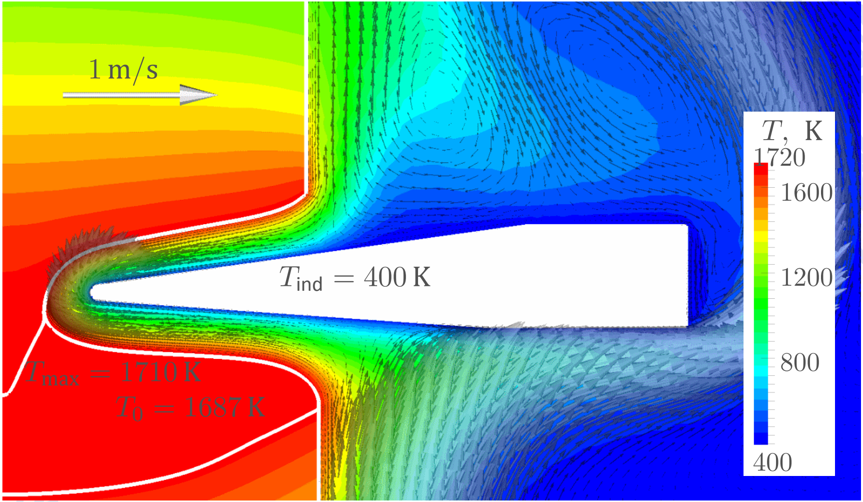
Helium flow



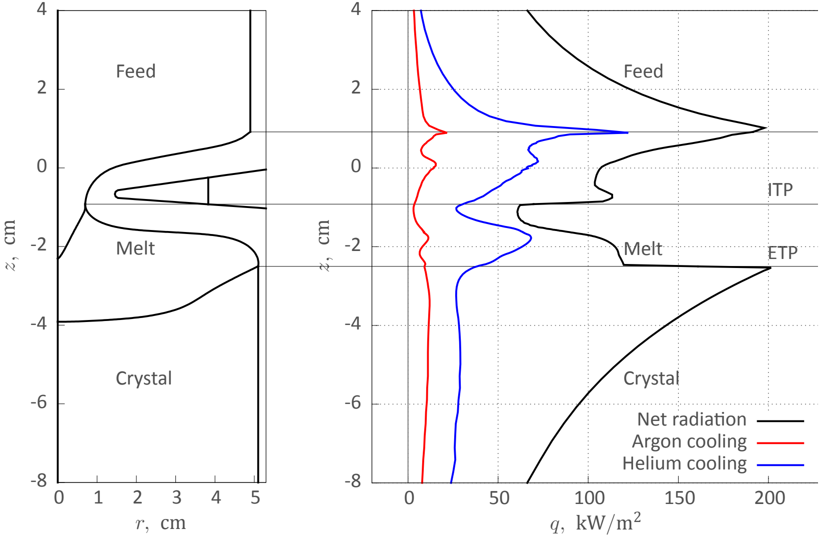
T and U fields near the inductor: Argon



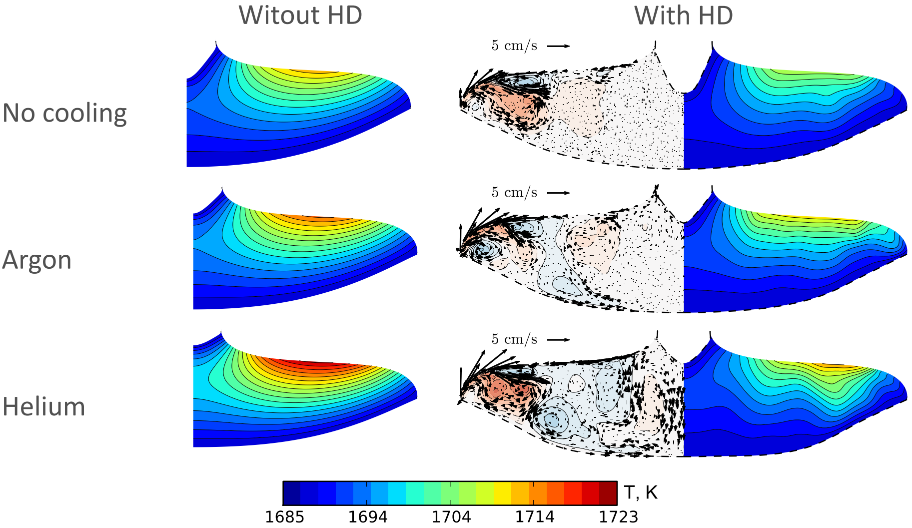
T and U fields near the inductor: Helium



Cooling by argon and helium

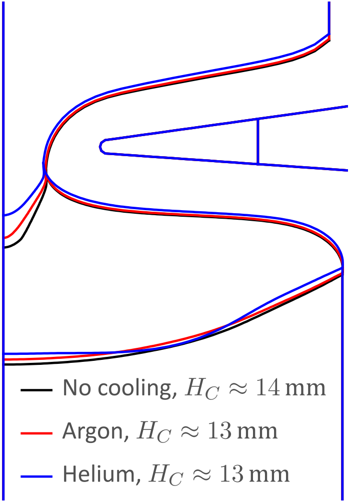


Influence of gas cooling

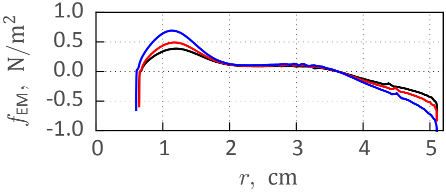


Influence of gas cooling

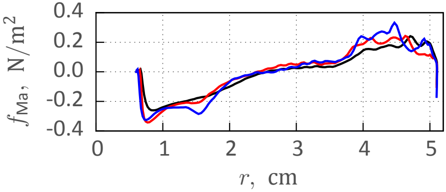
Phase boundaries



EM force



Marangoni force



Conclusions

1. Axisymmetric calculations of argon and helium flow in FZ system have been carried out using `OpenFOAM`
2. Argon cooling power density can be as large as 10% of net radiation heat flux density, for helium it can reach about 50%
3. Argon flow only slightly changes f_{EM} and f_{Ma}, while strong helium cooling requires significantly larger inductor current, noticeably increasing EM force
4. Shear stress of gas flow is by at least an order of magnitude smaller than f_{EM} and f_{Ma} ($0.02\,\mathrm{N/m^2}$ for argon and $0.008\,\mathrm{N/m^2}$ for helium) and therefore has a weak influence