3D modelling of the influence of the inductor on the phase boundaries in FZ crystal growth

MHD in crystal growth

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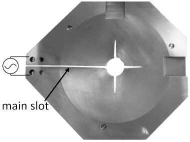
ERAF
EIROPAS REĢIONĀLĀS ATTĪSTĪBAS FONDS
EIROPAS SAVIENĪBA
IEGULDĪJUMS TAVĀ NĀKOTNĒ

Introduction

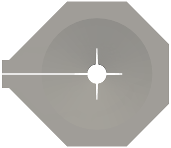
- Floating zone (FZ) silicon crystal growth – industrially important process
- Well developed mathematical modelling tools are available
- Mainly axisymmetric and simplified models
- Improvement of the existing model:
  - 3D free melt surface shape due to non-symmetric EM pressure
  - Coupling of the 3D free melt surface shape with the global heat exchange
- Numerical investigation for processes with crystal diameter of 4" and 5"

General properties of FZ silicon crystal growth

- Highest purity Si crystals
  $n_{O,C} < 10^{16}\,\mathrm{cm}^{-3}$
- HF induction coil for Si melting



Real inductor (IKZ, Berlin)



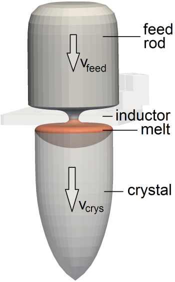
Inductor 3D model

- Large diameter (...200 mm) single crystals grown for wafer production
- Wafers used in:
  - power electronics
  - high efficiency solar cells

Experimental setup

B. Andreas et al., *Metrologia* 48, S1-S13, 2011

3D model of the process

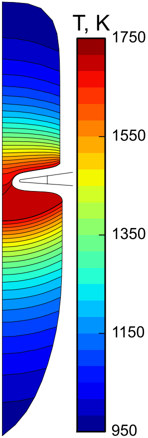


Standard Calculation Algorithm in Program FZone

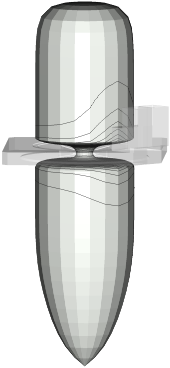
- G. Ratnieks et al.,Modelling of phase boundaries for large industrial FZ silicon crystal growth with the needle-eye technique, JCG, 255, 227-240 (2003)
- A. Muižnieks et al.,Development of numerical calculation of electromagnetic fields in FZ crystal growth process, MHD, 46, 475-486 (2010)

1. Quasi-transient approach to find quasi-stationary solution
2. 3D high frequency electromagnetic field calculations
3. Azimuthal averaging of the induced heat sources for temperature B.C. and EM pressure
4. Axisymmetric (2D) temperature calculation in silicon parts (feed rod, molten zone, crystal)
5. Iterative coupling of temperature field and radiation (view factors)
6. Axisymmetric (2D) calculation of the shape of molten zone (melt free surface, melting and crystallization interfaces)

Temperature field



Electric current lines

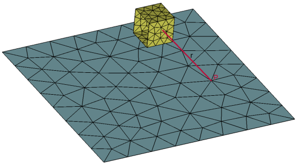


Mathematical model for 3D HF EM field

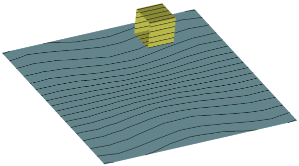
- Used for calculating heat source distribution $q_{\mathsf{EM}} = \sqrt{\frac{\pi \mu_0 f}{\sigma}} j^2$ and EM pressure $p_{\mathsf{EM}} = \frac{1}{2}\mu_0 j^2$

$\rightarrow$ $\approx 3\,\mathrm{MHz}$ frequency $\rightarrow$ distinct skin-effect $\rightarrow$ surface currents only

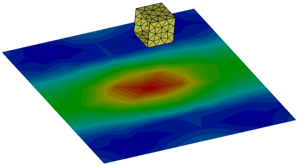
- EM field determined by surface current density $\vec{j}$: $\quad \vec{\nabla} \cdot \vec{j} = 0$
- Electric stream function $\vec{\Psi} = (0, 0, \Psi_{\mathrm{n}})$ introduced: $\quad \vec{\nabla} \times \vec{\Psi} = \vec{j}$
- BEM; Biot-Savart law for vector potential: $\quad \vec{A}(P) \approx \sum_{k=1}^{N} \frac{\vec{j}_k}{r_{P,k}} S_{\Delta,k}$



Boundary element mesh



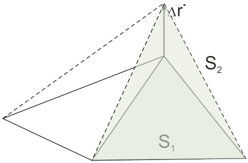
Ψ_{n} isolines



Heat source distribution

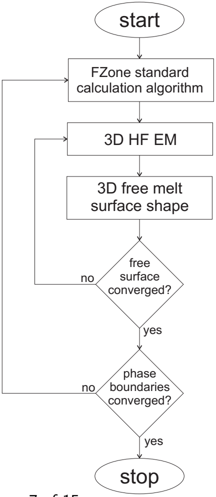
Mathematical model for 3D free melt surface

- Hydrostatic approach to find the equilibrium shape of energy minimum
- Forces acting on the free surface:
  - Surface tension $\vec{F}_\sigma = \sigma \frac{\partial S}{\partial \vec{r}}$
  - Gravity $\vec{F}_g = -\frac{\partial E_g}{\partial \vec{r}}$
  - Hydrostatic $\vec{F}_0 = p_0 \frac{\partial V}{\partial \vec{r}}$
  - **Electromagnetic** $\vec{F}_{EM} = -p_{EM} \frac{\partial V}{\partial \vec{r}}$



- Discretization with linear triangular elements
- Nodes are shifted in normal direction only
- Loop of 3D EM and free surface calculations is repeated until convergence

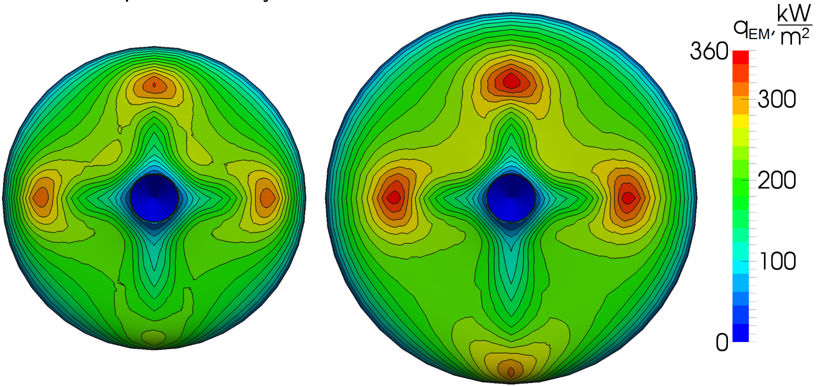
Coupling 3D EM and free surface model with 2D heat transfer model of FZone



- Initial geometry, calculation and process parameters provided for `FZone` program
- Converged solution gives new phase boundaries and inductor current
- EM pressure distribution calculated by 3D HF EM program
- 3D free melt surface shape found iteratively
- Updated phase boundaries and averaged heat sources for `FZone`
- Global coupling until stationary solution is reached

Calculation results of 3D HF EM field

Induced EM power density on the free melt surface



4" crystal 5" crystal

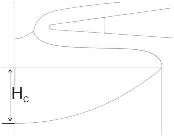
Pronounced power maxima below the edges of the additional slots
Considerably higher power maximum below main slot in 5" case

Calculation results

Inductor current and deflection of the crystallization interface for 4" and 5" processes obtained by both models.

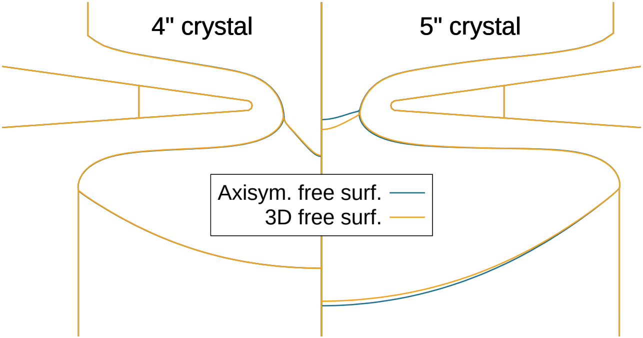
Crystal diameter	Free surface model	Inductor current I, A	Deflection H_C, mm
4"	Axisymmetric	898	16.2
	3D	896	16.3
5"	Axisymmetric	1074	24.6
	3D	1071	23.6

Definition of deflection of crystallization interface:



Calculation results

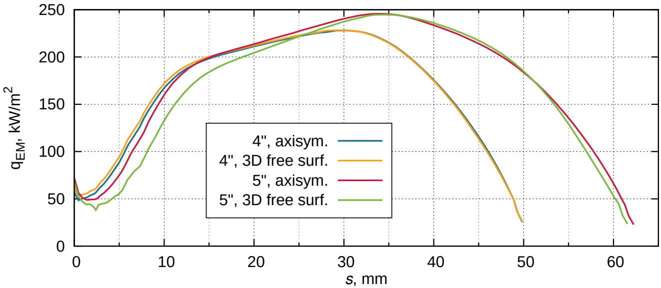
Shapes of the axisymmetric phase boundaries

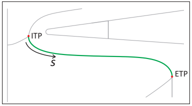


- Practically identical results in 4" case
- Decreased deflection of crystallization interface in 5" case

Calculation results

Azimuthally averaged induced heat sources on the free melt surface

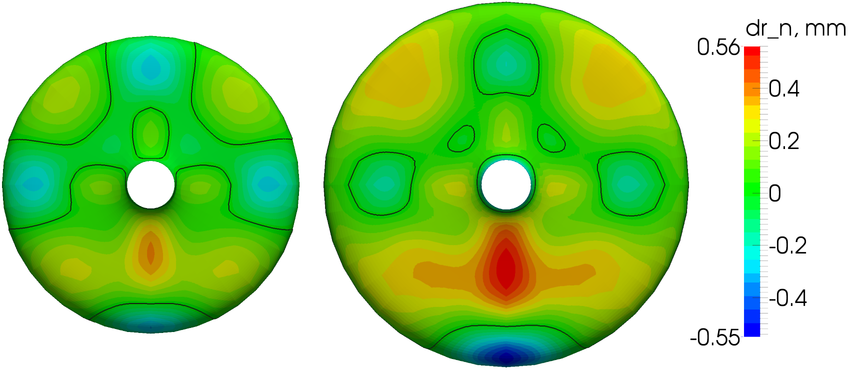




Considerably less induced power for 5" 3D free surface near ITP

Calculation results of 3D free melt surface shape

Deviation from the axisymmetric profile in the normal direction,
Black isoline corresponds to zero deviation

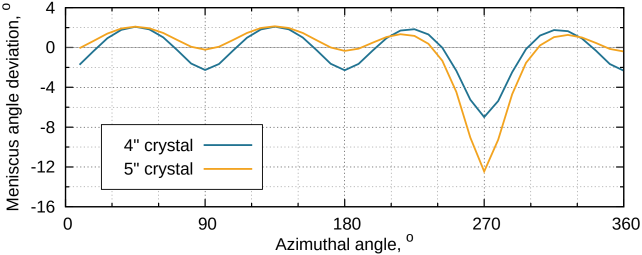


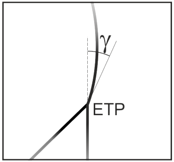
4" crystal

5" crystal

Calculation results

Azimuthal distribution of the meniscus angle deviation from the growth angle of silicon (11°)





- More pronounced non-symmetric behaviour for larger crystal diameter due to the main slot
- Crystals are rotated to avoid the non-symmetric growth

Conclusions

1. Mathematical model of coupled 3D free melt surface shape and global heat transfer has been developed
2. Influence of the 3D free melt surface shape on the whole system:
   - Negligible for 4" crystal
   - Observable for 5" crystal
   - Corresponds to the increase of non-symmetry of induced heat sources
3. The introduced coupling should be used for large diameter crystals
4. Inductor main slot has a strong influence on the meniscus angle

Thank you for your attention!