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Effect of EM field frequency on 3D melt convection during floating zone growth of silicon

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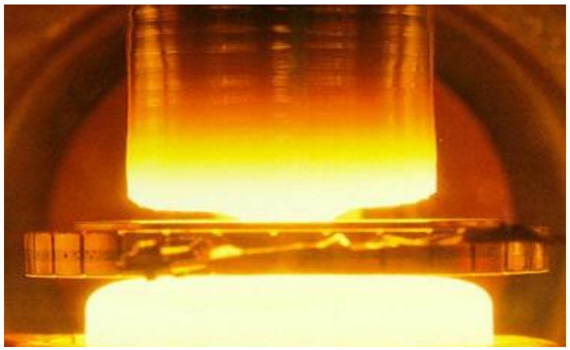
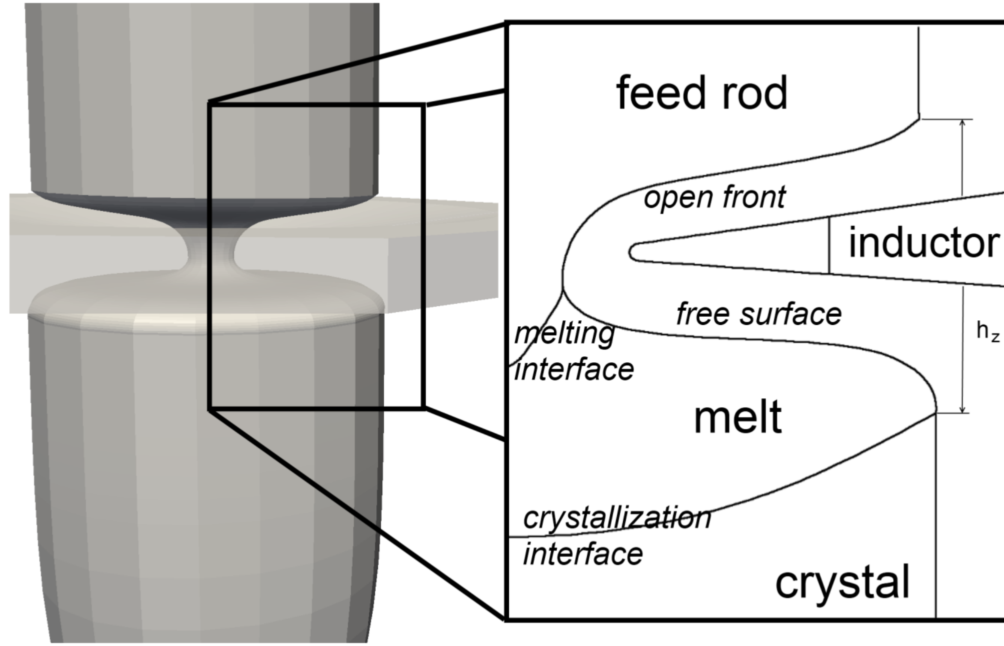
Content of the presentation

- Introduction
- Mathematical models
- Results
- Conclusions

Introduction



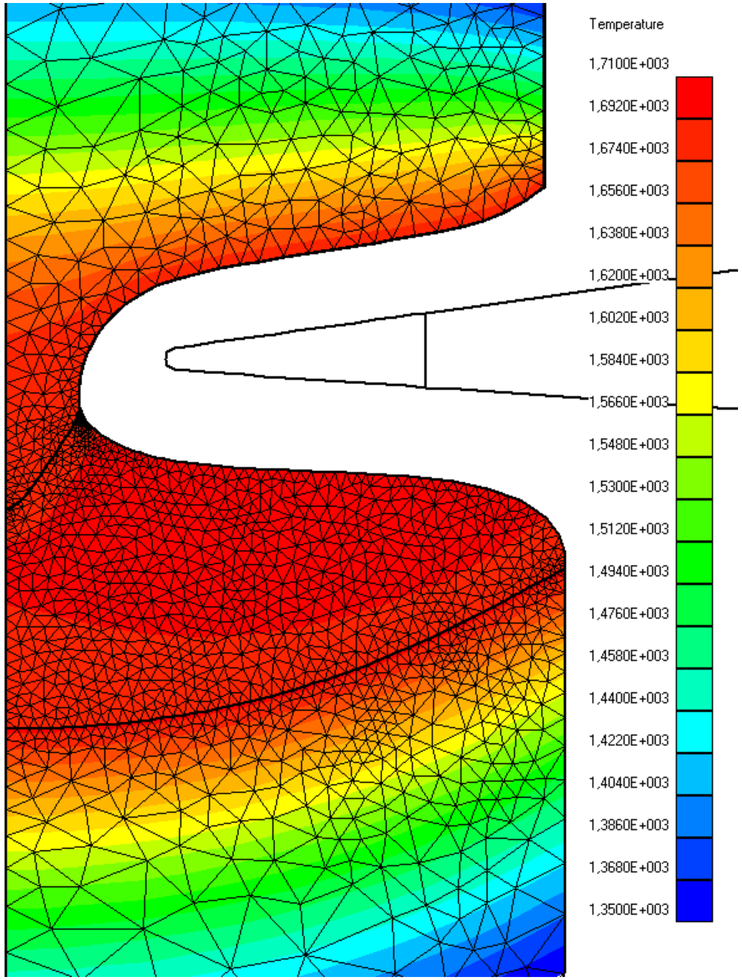


- Floating zone process of single crystal growth can be modelled using `FZone` (axially symmetrical shape of phase boundaries) and `fzsiFOAM` (3D melt flow) programs
- In this presentation, an improvements in boundary conditions of these programs are described. These improvements allows to describe electromagnetic (EM) heat sources and Lorentz force more precisely.
- To verify these programs, results were compared to experimental data for different inductor current frequencies.

Mathematical model: phase boundaries

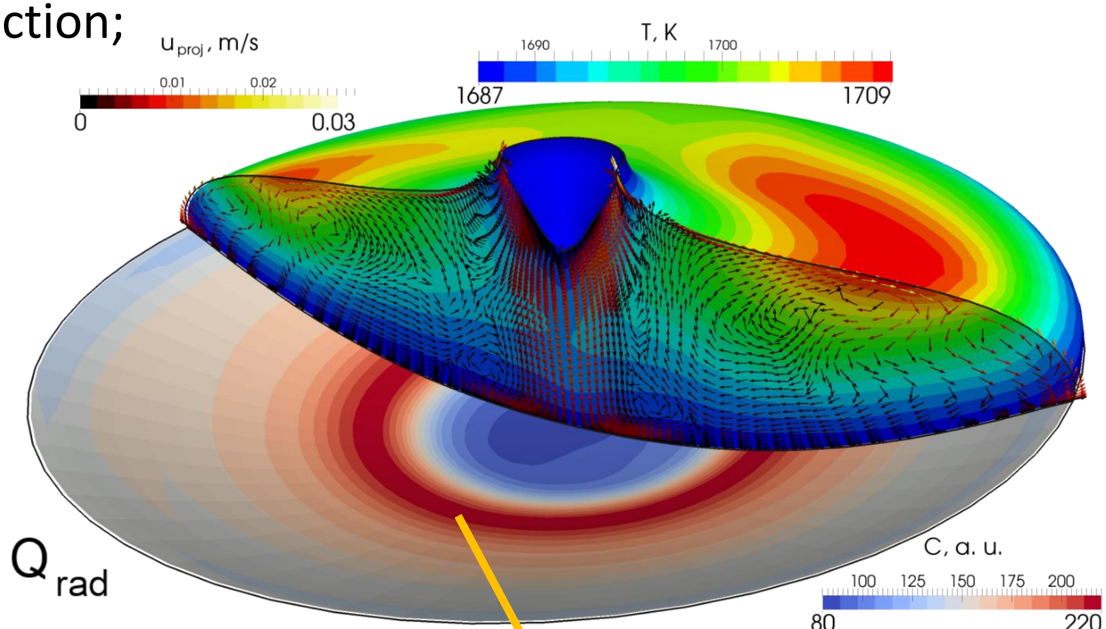
Main principles of FZone program:

- Temperature field in silicon is found using 2D finite element method.
- Thermal radiation (surfaces are optically grey) is solved using 3D view factor method for axially symmetrical shape.
- High-frequency EM field for heat sources on silicon is obtained using 3D boundary element method (distinct skin layer, 0.3 mm in melt).
- Phase boundaries between solid and liquid silicon are found considering balance of heat fluxes; for free surface – hydrostatical balance (capillarity, gravity, EM pressure).
- Quasi-stationary solution is obtained.

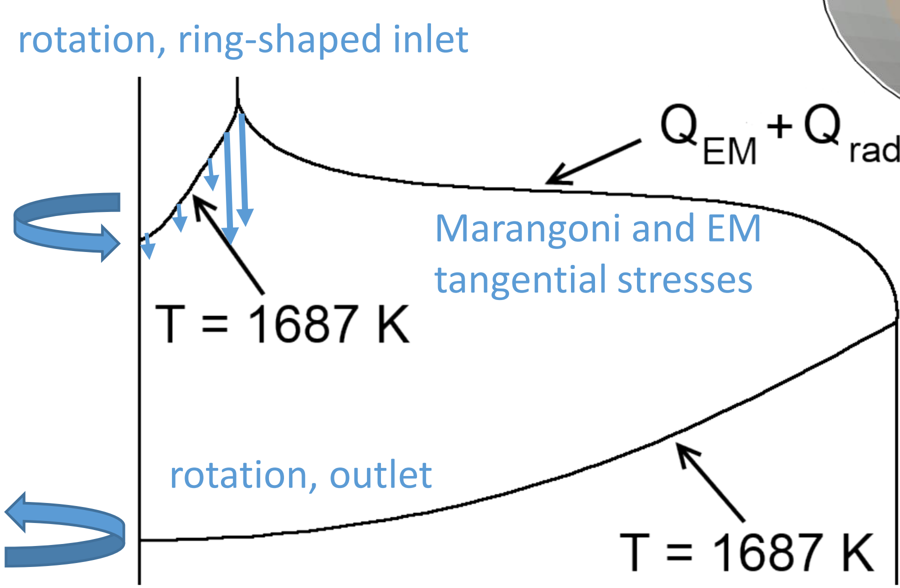


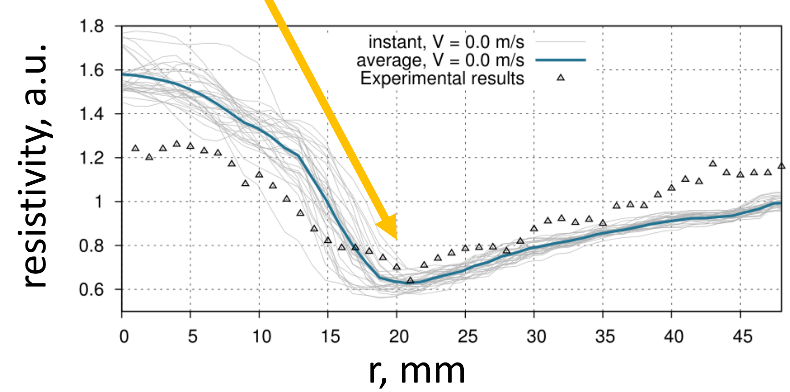
Mathematical model: melt flow

- `fzsiFOAM` program, based on `OpenFOAM` library:
  - velocity – non-stationary, incompressible, laminar, Bousinesq approach for description of convection;
  - pressure;
  - temperature;
  - concentration.



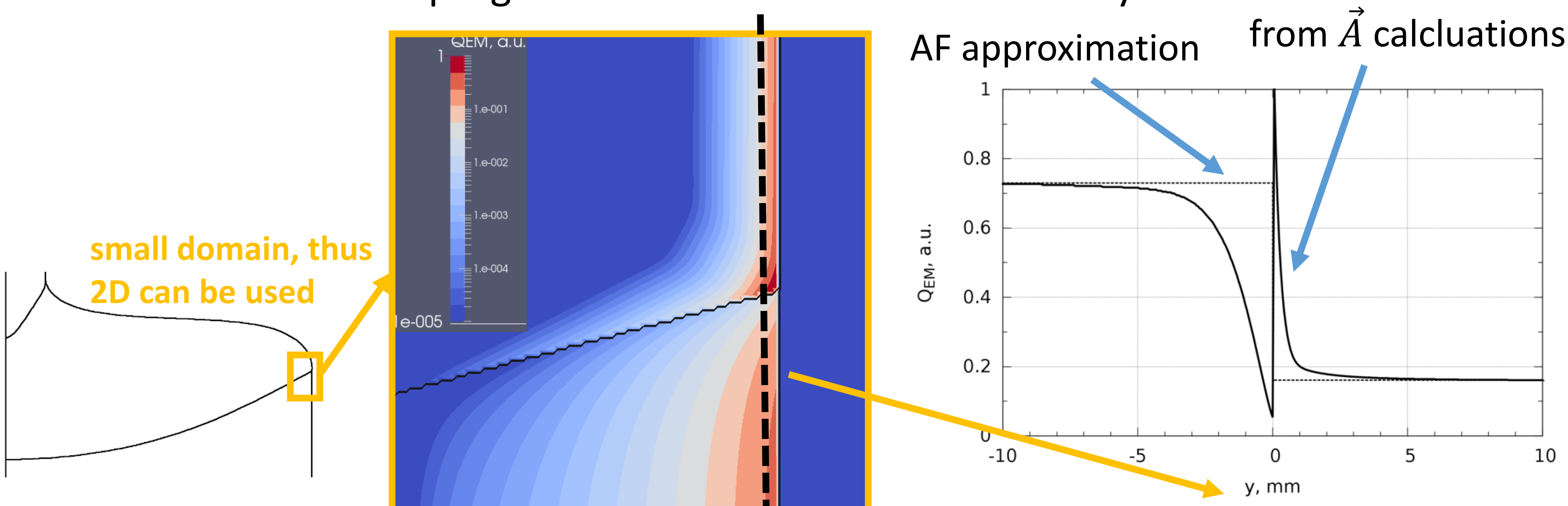
- Boundary condition:



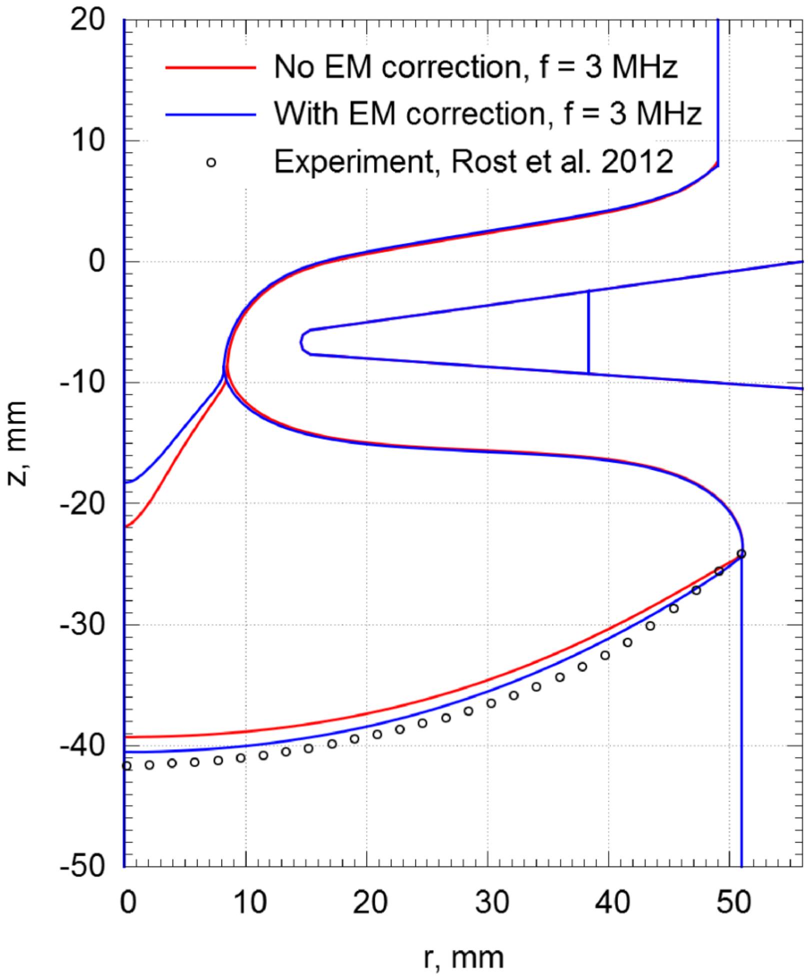


Mathematical model: EM field

- In the vicinity of external triple point (ETP) high-frequency (HF) approximation must be modified, because skin depth changes 5 times.
- Thus, EM correction algorithm was developed:
  - Vector potential $\vec{A}$ of EM field is solved in complex number formulation. Only azimuthal currents are considered ($\vec{A} = (0,0,A_z)$): $\Delta \mathrm{A_z} - i\omega\sigma\mu A_z = -\mu I$
  - Induced current and heat flow density in silicon: $\mathrm{j} = -i\,\sigma\mu A_z\,,\quad q = \frac{|j|^2}{\sigma}$ results are implemented in `FZone` and `fzsiFOAM` programs as a correction in the vicinity of ETP.



Results: phase boundaries

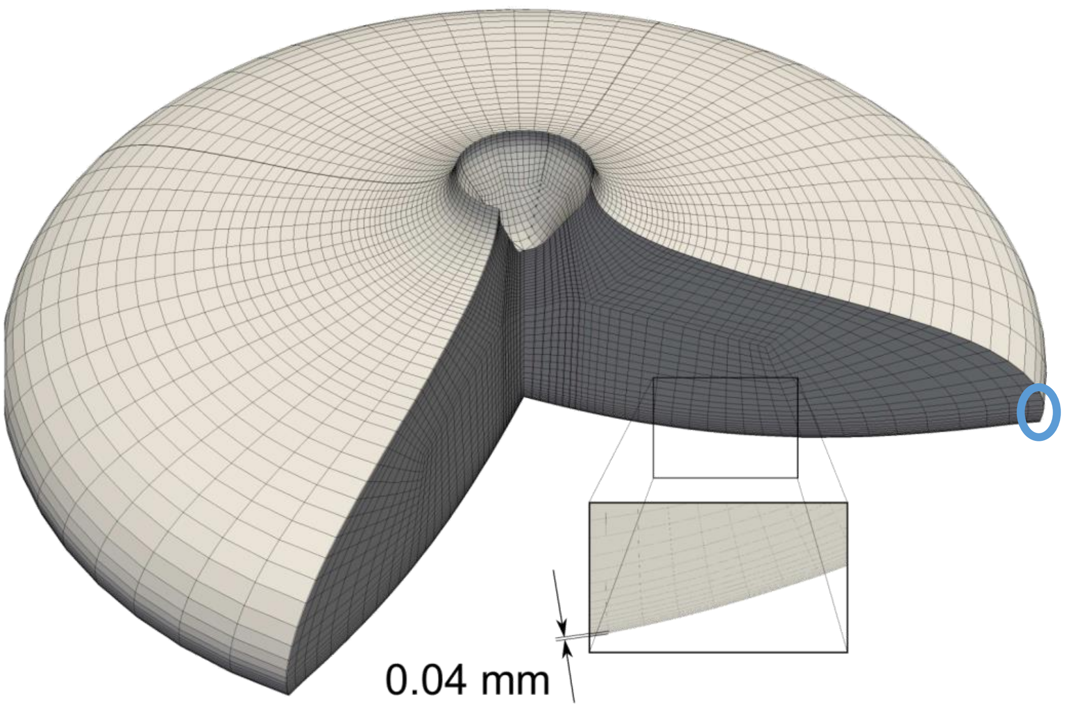


First, EM correction was used for axially symmetrical calculation of phase boundaries via FZone.

- Due to change in heat sources, inductor current increases to hold prescribed zone height (as it is required by calculation algorithm).
- Obtained shape of crystallization interface is closer to the experimental one (*ICG*, Berlin)

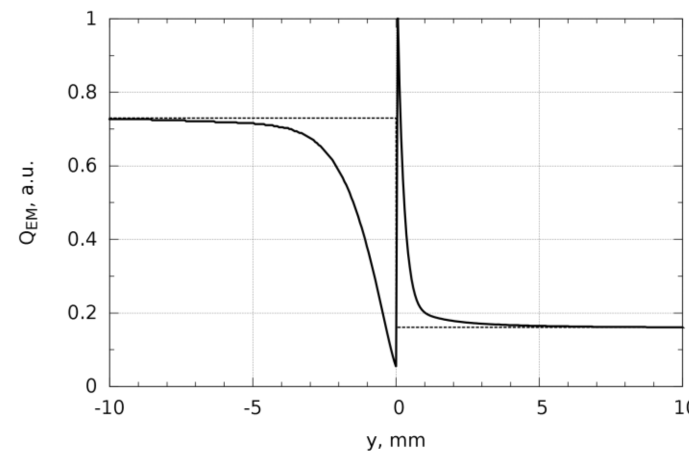
	I, A	H_C, mm
Without EM correction	870	15.0
With EM correction	884	16.2
Experiment	-	16.9

Calculations of melt flow



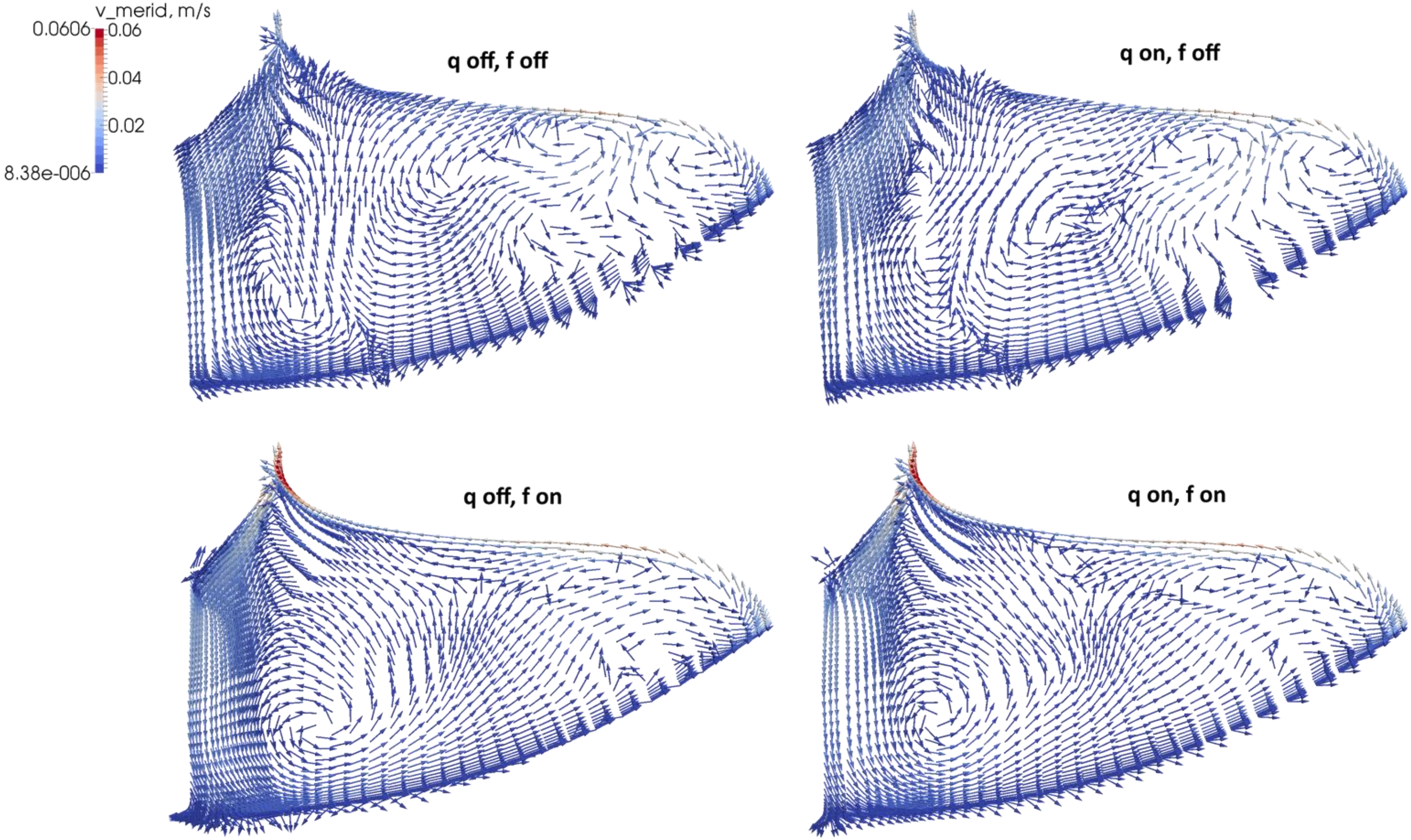
- 3D finite volume mesh, obtained by rotating profile from FZone program.
- 80 000 hexahedral elements

EM correction near the ETP ($\Delta y \leq 2$ mm)



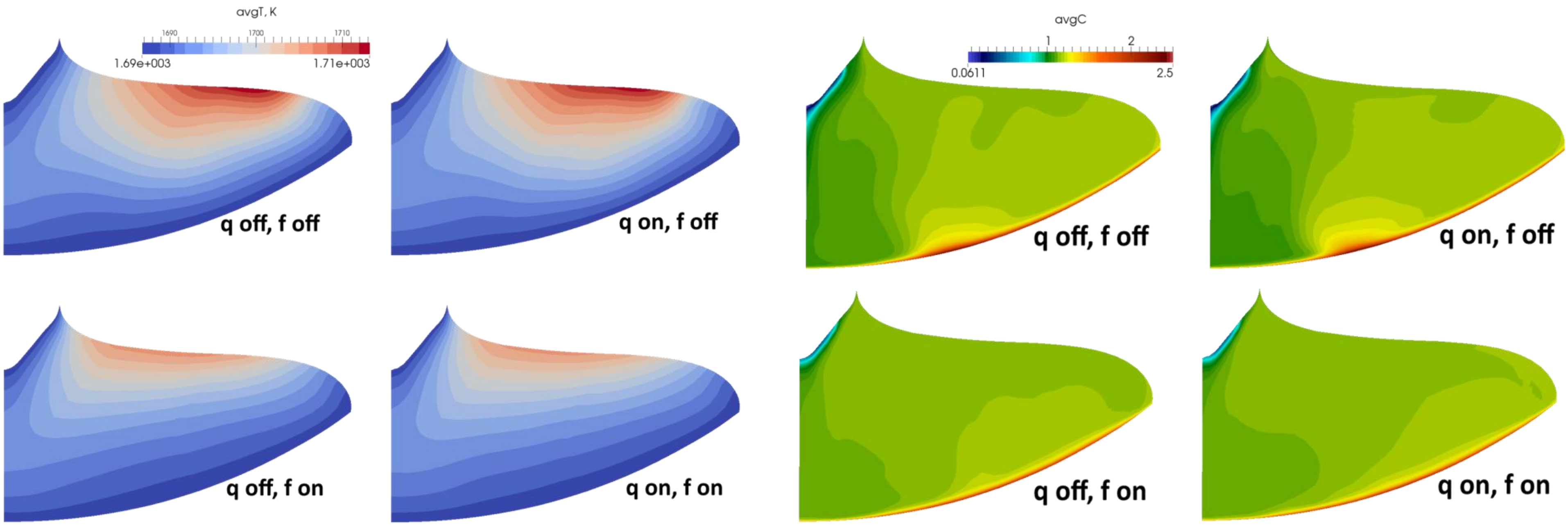
Heat source correction (denoted by *q* on/ off) and Lorentz force correction (*f* on/off) were considered separately.

Results: 3D melt flow



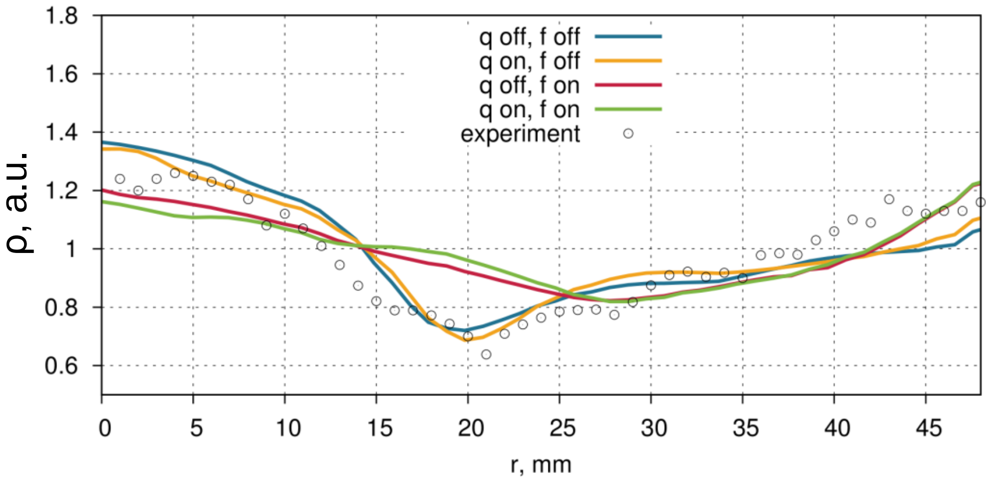
Time-averaged (5 s) meridional velocity field in the vertical slice of melt

Results: 3D melt flow



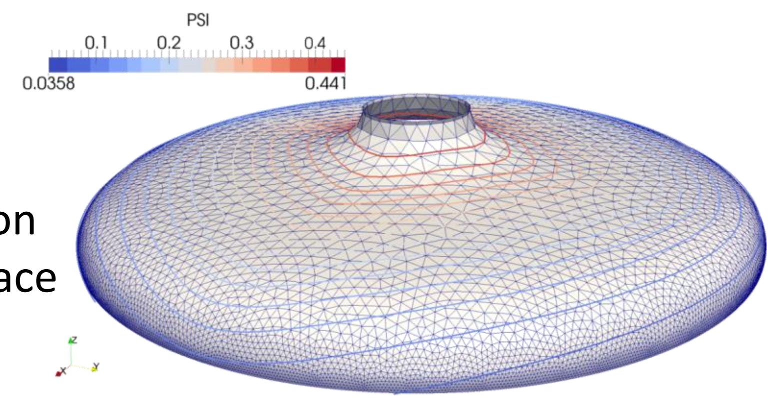
Time-averaged (5 s) temperature and dopant concentration fields

Results and analysis

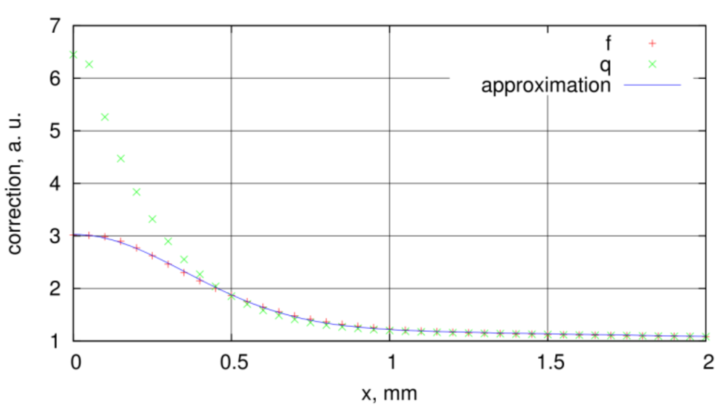


Influence of heat source correction is very small. Lorentz force correction leads to more homogeneous profile due to strong meridional convection.

Radial distribution of crystal resistivity

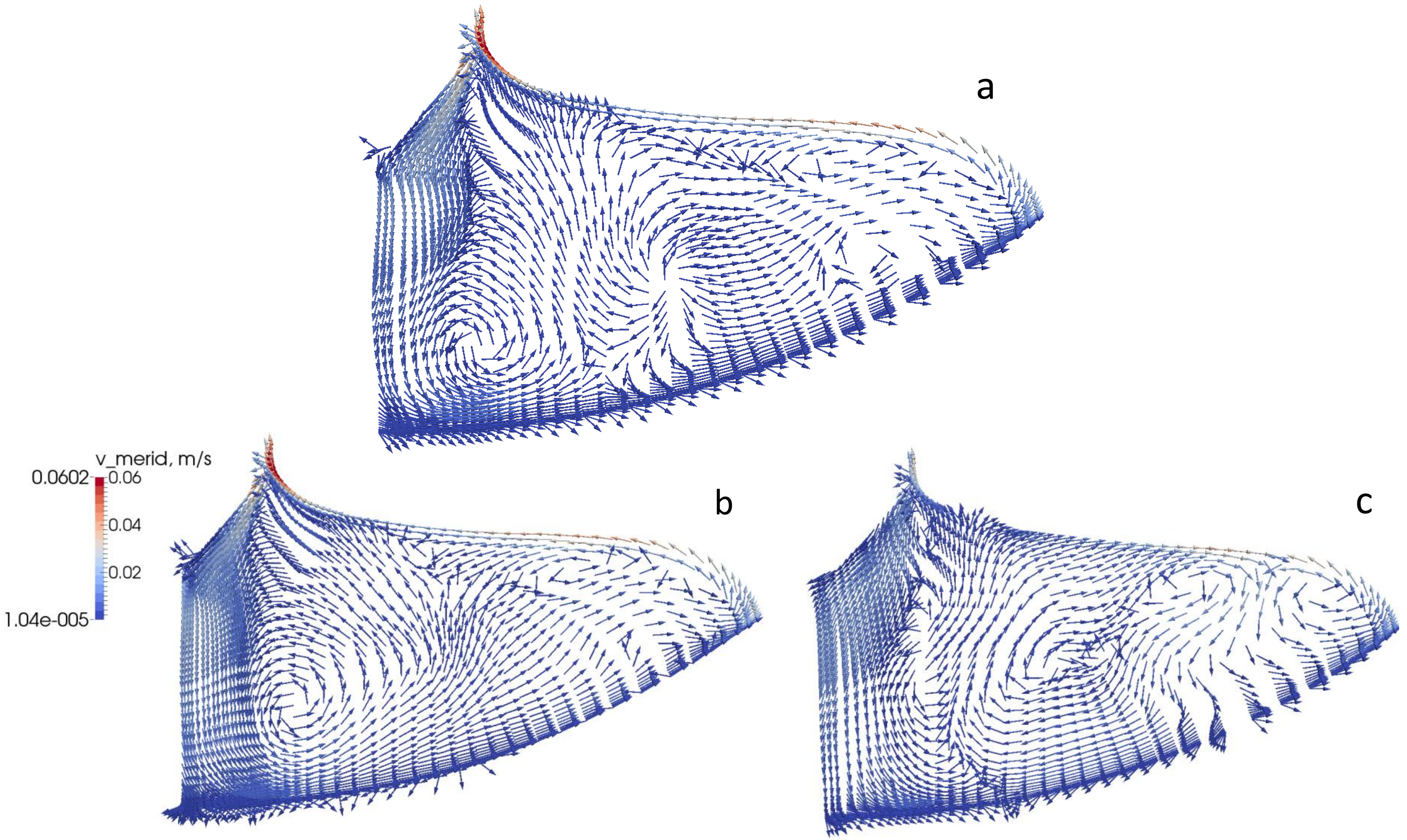


Current lines on melt free surface



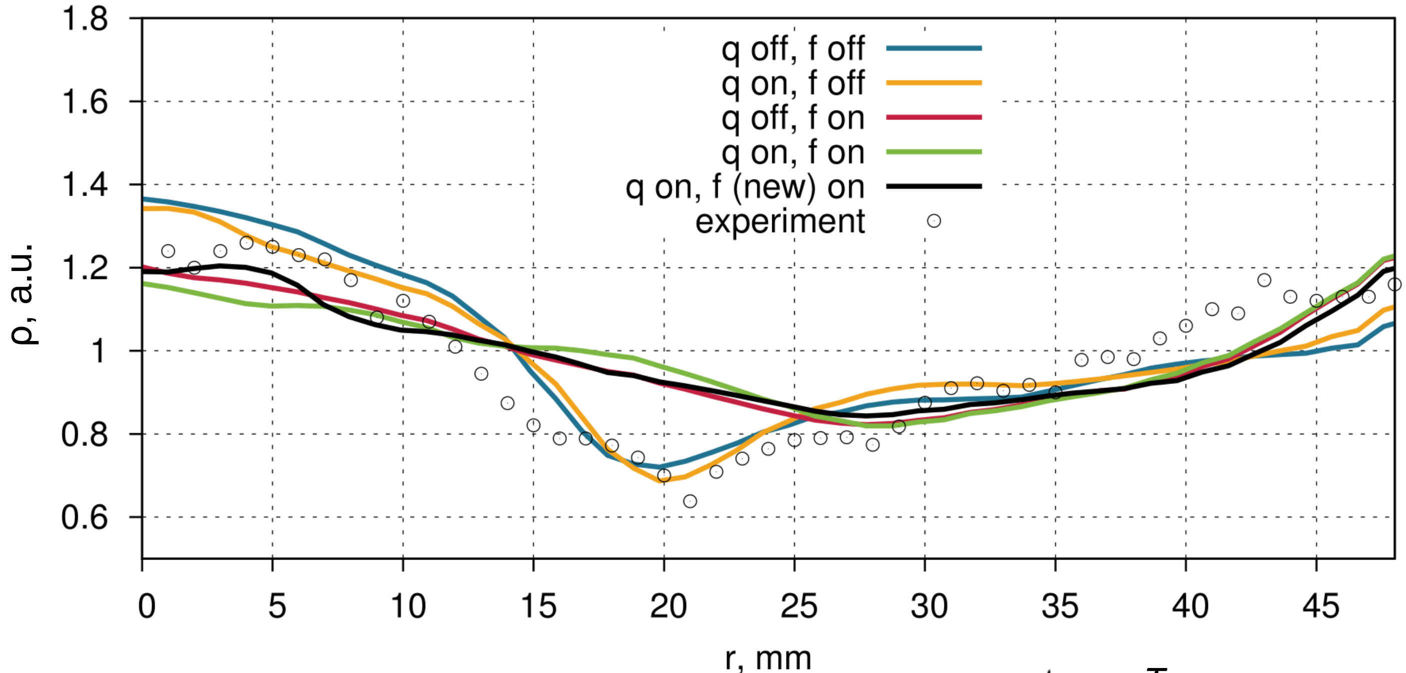
- Due to nonzero angle between current lines and ETP line, EM force correction should be different from heat source correction.
- Additional analysis was performed considering the case when current flows perpendicular to the surface between solid and liquid silicon. Results were included in 3D melt flow calculations.

Lorentz force correction

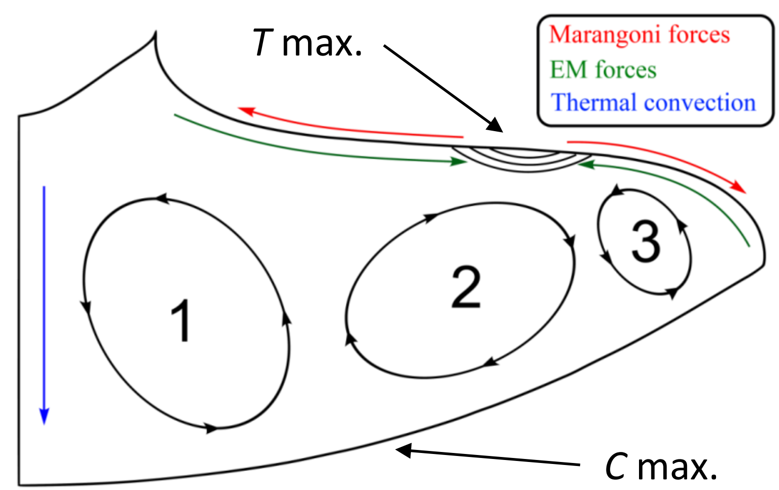


Time-averaged (5 s) meridional velocity in vertical slice for calculations with precized Lorentz force correction (a), «big» correction (b) and without Lorentz force correction (c).

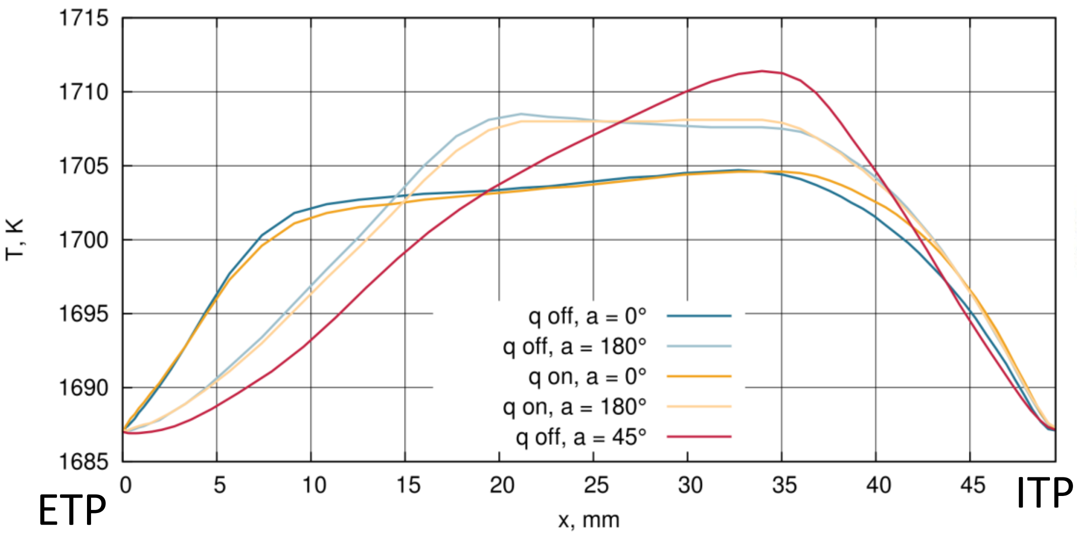
Results: crystal resistivity

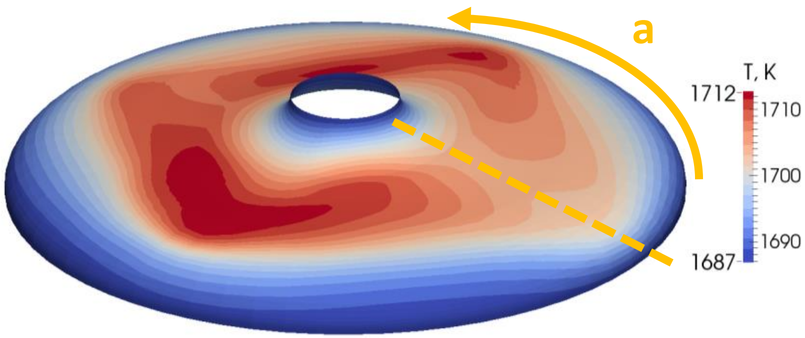


The more precise description of Lorentz force correction didn't improve correspondence to experiment. It can be explained with "threshold effect": when EM force is stronger than Marangoni force, it becomes principal in melt motion and further increase in it do not influence the flow so much.

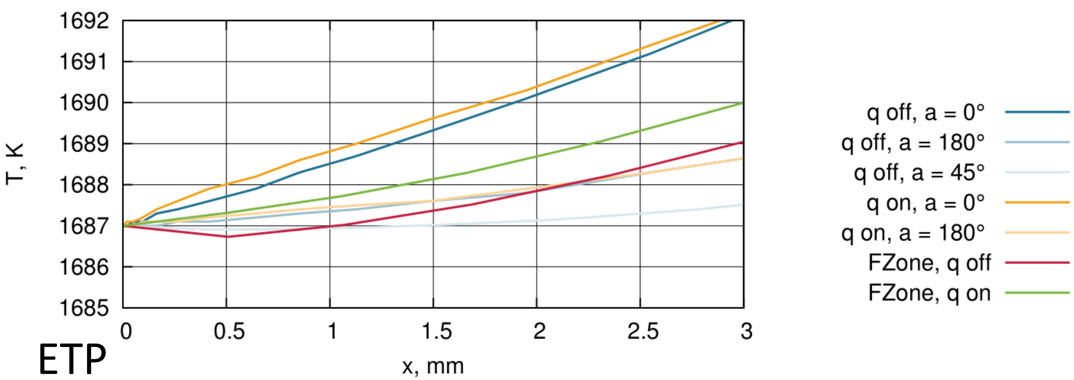


Results: melt temperature





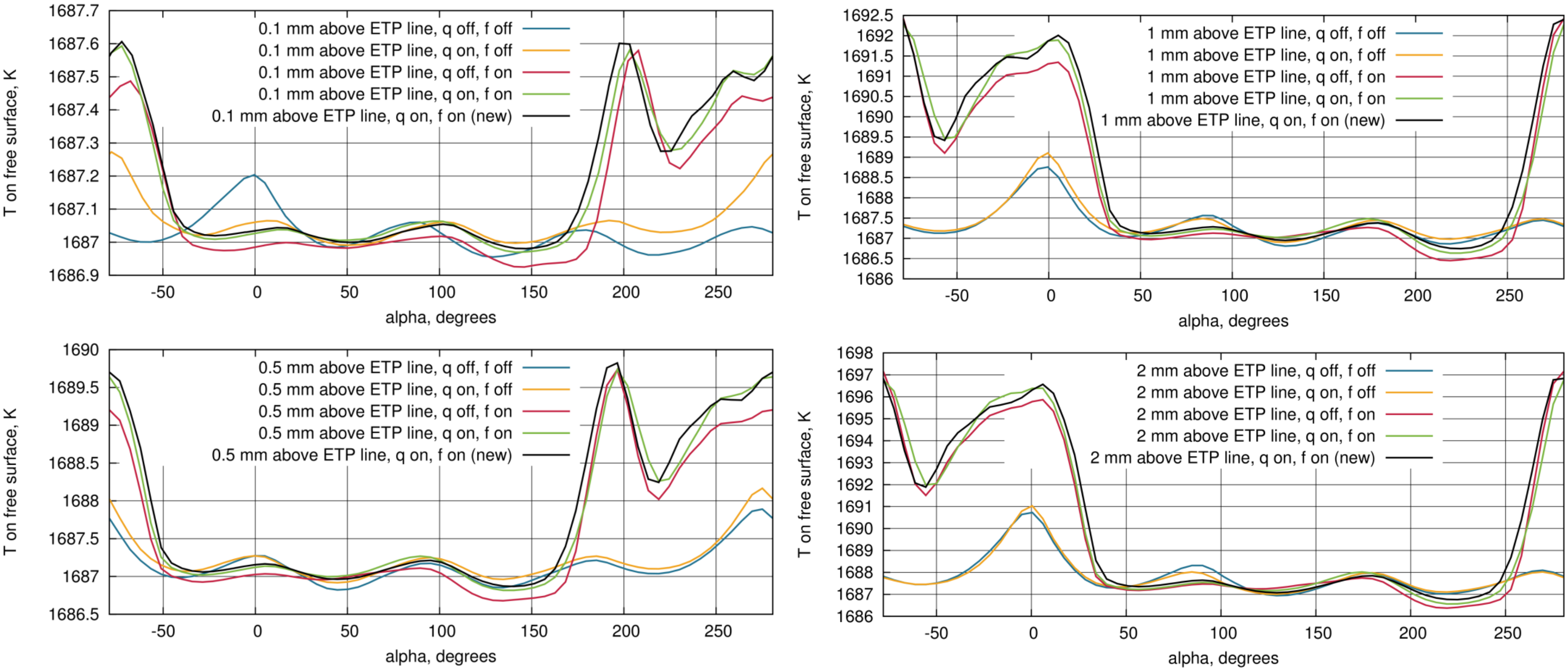
- EM correction of heat sources leads to small increase in temperature.
- EM correction has vanishing influence on T distribution on melt free surface, because it is integrally small.
- Distribution is very dependent on azimuthal direction.



x is radial coordinate, *x* = 0 at ETP

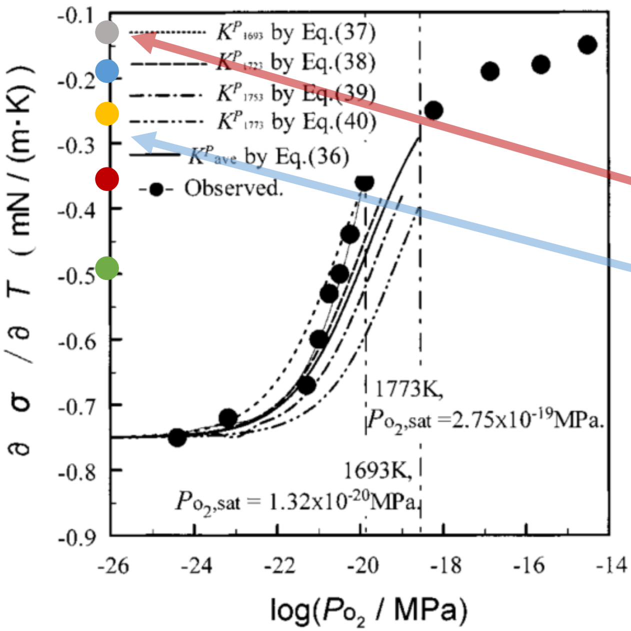
a is azimuthal coordinate, a = 0 below the main inductor slit

Results: melt temperature



Even with twice smaller force correction, temperature distribution remains highly distorted. Flow is very similar for different *f* corrections because the flow is determined by which of EM and Marangoni forces is stronger. For the cases with *f* correction, temperature maxima is shifted from the main slit due to intense convection. But still small undercooling of 0.2-0.3 K occurs.

Results: Marangoni coefficient

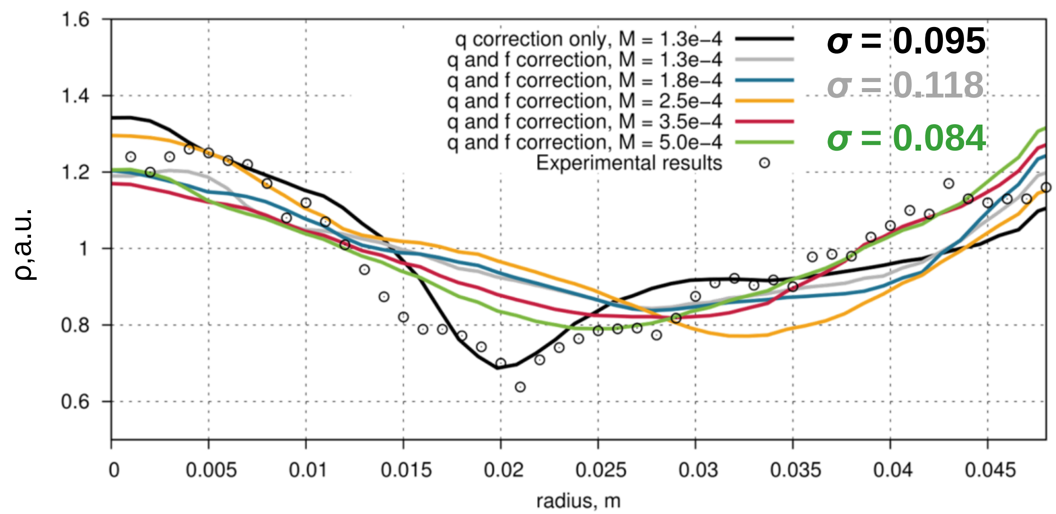


As Lorentz force correction do not improve model's correspondence to experiment, it is necessary to look at other details, that influence force balance in melt.

traditionally used, but non-realistic

parameter study

Z. F. Yuan, K. Mukai, and W. L. Huang. *Surface tension and its temperature coefficient of molten silicon at different oxygen potentials*. Langmuir, 18:20542062, 2002.

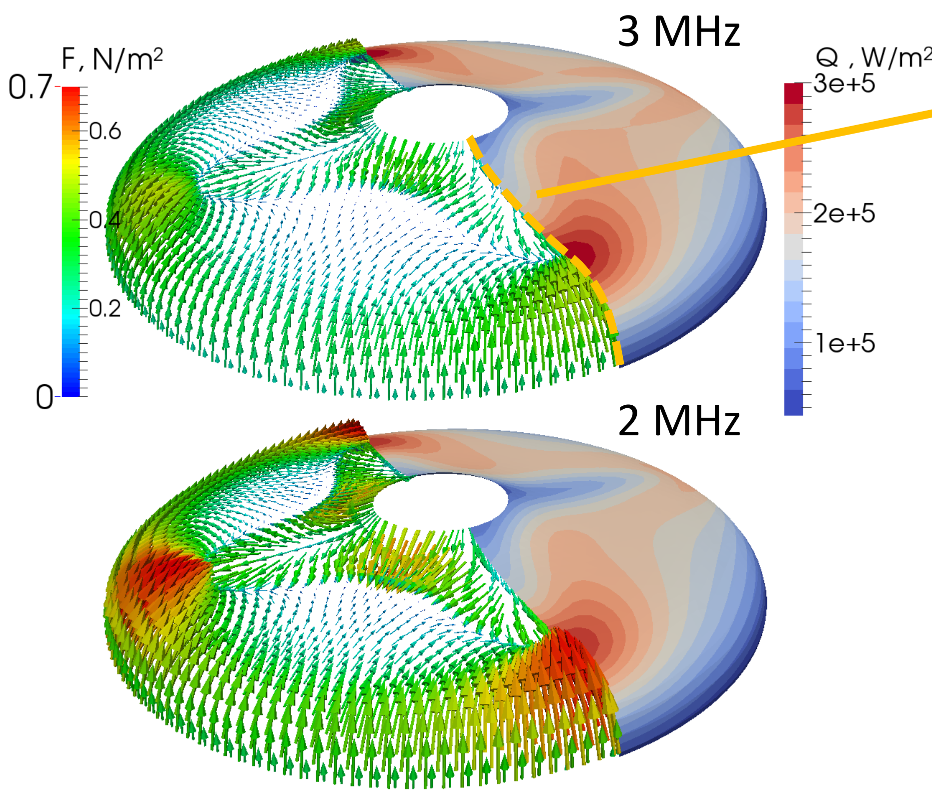


Mean square difference - to quantitatively check the correspondence

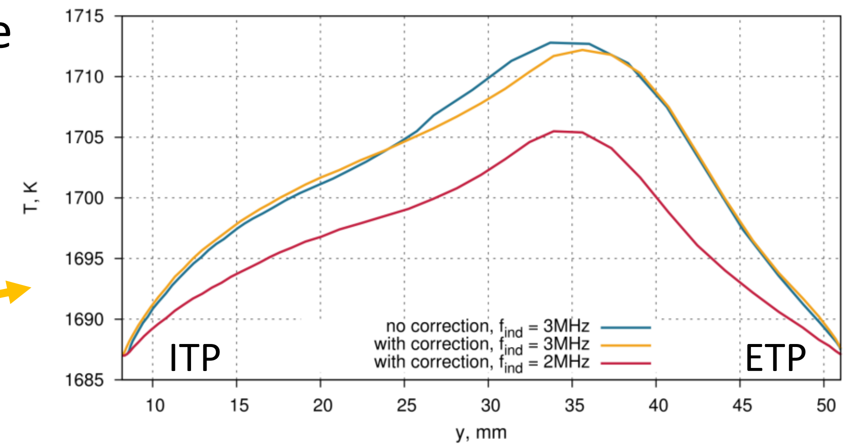
$$\sigma = \sqrt{\frac{\Sigma(\rho_i - \bar{\rho})^2}{n}}$$

Results: current frequency

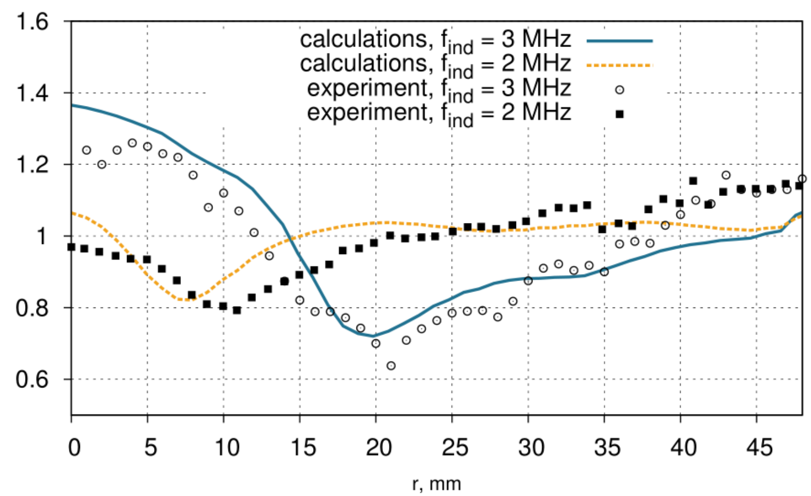
- To verify the program, calculations were performed for two different inductor frequencies.



Lorentz force (left) and heat sources (right) on melt free surface



Time-averaged temperature distribution on melt free surface



Radial resistivity distribution, averaged azimuthally and in time.

Conclusions

- Axially symmetrical EM correction in FZone allows to describe phase boundaries more precisely: it increases the deflection of the crystallization interface.
- 3D EM correction of heat sources eliminates (in 2D) and reduces (in 3D) undercooling near the ETP.
- 3D EM correction of heat sources only slightly improves correspondence between calculated and experimental RRV profiles.
- 3D EM correction of Lorentz force dramatically changes melt flow and makes this correspondence much worse (for traditional Marangoni coefficient).
- The use of heat source and Lorentz force corrections together with the increase of Marangoni coefficient to realistic values improve the correspondence between calculated and experimental RRV profiles
- Calculations with lower frequency clearly show experimental tendencies in radial resistivity profile – minima shifts closer to the axis and profile becomes more homogeneous.

Thank you for attention!