Simulation of Industrial-Scale MCZ Process

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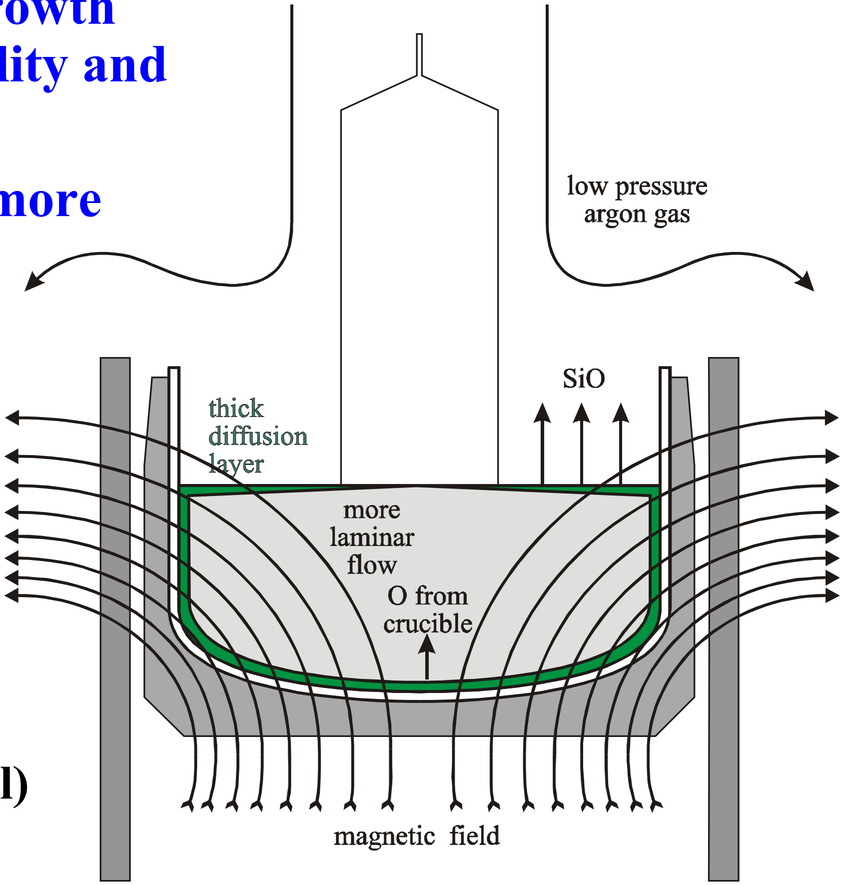
Outline

- Magnetic Czochralski crystal growth
- Mathematical model
- Simulation results (20” crucible)
- Validation of our 2D model (14” crucible)
- Summary
- Acknowledgements

Magnetic Czochralski crystal growth

- Silicon melt flow behavior during CZ growth plays an essential role in the crystal quality and yield
- With increasing melt sizes the need for more stable melt is evident
- Numerical simulations help one to understand the effect of various process parameters which influence the melt stability, and they offer an invaluable development tool
- Effect of magnetic field
  - crucible wear (yield, oxygen level)
  - crucible temperature (yield, oxygen level)
  - SiO evaporation (oxygen level)
  - melt stability, especially near the growth interface (yield, crystal quality)



Mathematical model (1/2)

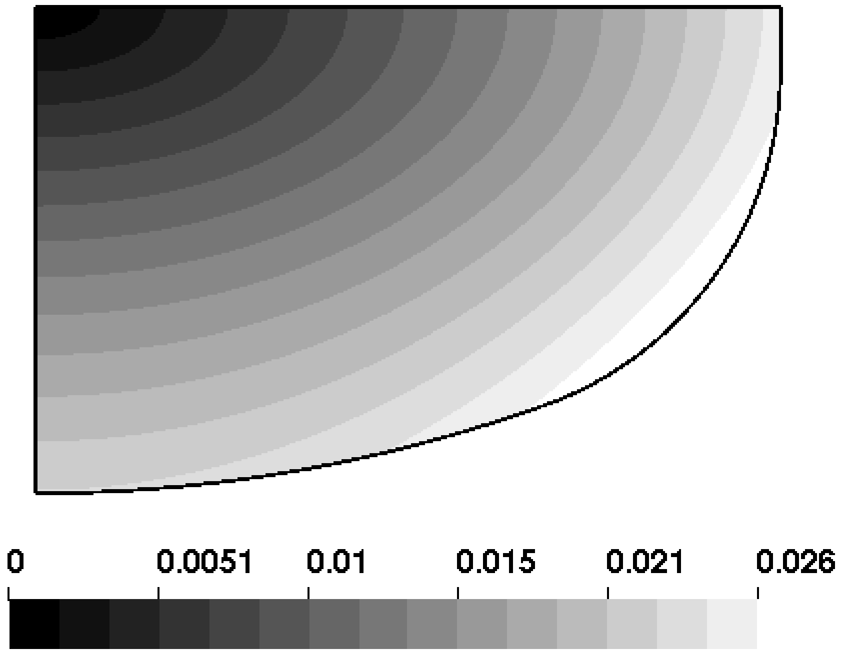
- We have modeled industrial-scale MCZ processes with realistic material parameters and boundary conditions
- Stabilized FEM (direct simulation, no turbulence model)
  - with small enough time step and refined mesh, converged solution is reached on each time step
- Melt flow is driven by
  - forced convection due to the rotations of the crucible and the crystal
  - Grashof and Marangoni convections due to temperature differences in the melt
  - Lorentz force due to both external and induced magnetic fields
- Cylindrically symmetric model is used in order to reduce CPU time
  - in modern PC 2D melt flow simulations can be carried out in a reasonable time frame (few days), parallel computing is required for 3D simulations
  - velocity and induced magnetic field have azimuthal components
  - validity of the 2D model will be discussed later in this presentation

Mathematical model (2/2)

- **Two main steps**
  - **applied axisymmetric steady state magnetic field (cusp field) is first solved in global geometry including coils of the magnet, iron shields, silicon melt and the intermediate space**
  - **then, the time-dependent magnetohydrodynamical (MHD) system for fully coupled velocity, pressure, temperature and induced magnetic fields is solved in the melt region**
    - **Navier-Stokes, heat and induction equations**
- **Model implemented in ELMER**
  - **multiphysics FEM software package, developed at CSC - Scientific Computing Ltd**
  - **collaboration between Okmetic and CSC since 1991 ⇒ ELMER has been tailored to meet specific requirements set by crystal growth modelling**
  - **more information available at http://www.csc.fi/elmer**

Simulation results, 20” crucible (1/4)

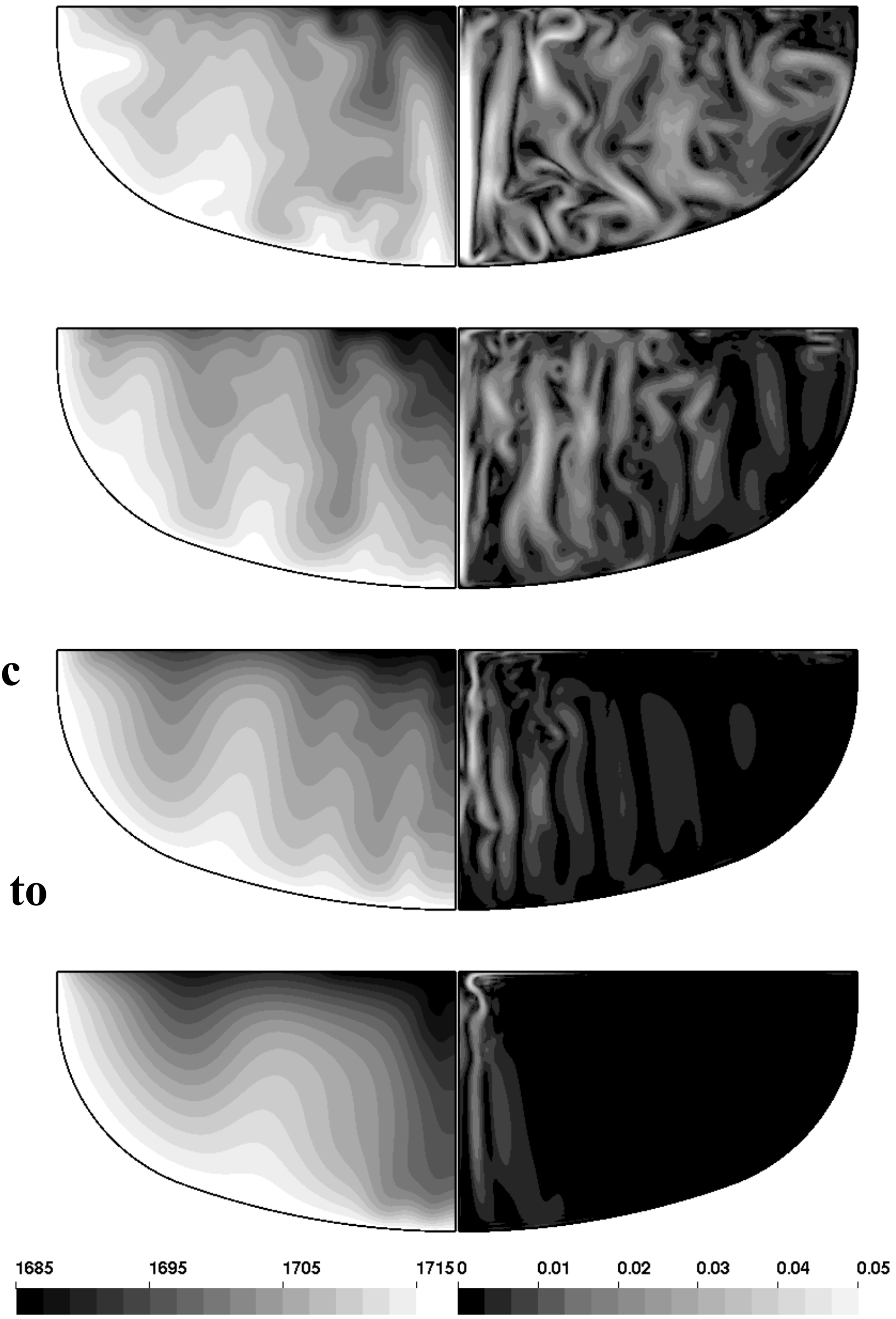
- **Results for 5 different cases are compared**
  - **case without a magnetic field**
  - **three different strengths of the cusp-field with its symmetry plane at the melt surface level (current in the coils 200 A, 500 A and 1000 A)**
  - **cusp-field with its symmetry plane 50 mm below the surface level (current 200 A)**



- **Magnetic flux density scales almost linearly with the applied current**
  - **maximum values of the field within the melt are about 25 mT (200 A), 65 mT (500 A) and 130 mT (1000 A)**
  - **actual fields used in industrial MCZ growth systems are usually lower than the highest fields simulated in this work**

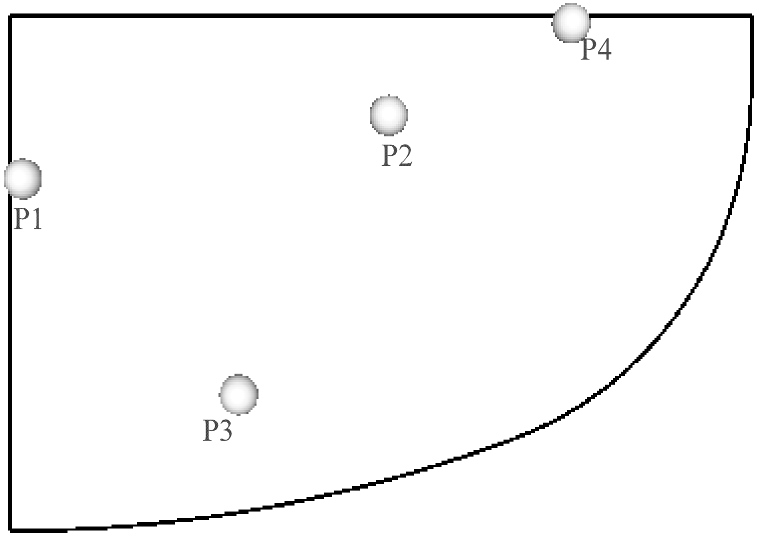
Simulation results, 20” crucible (2/4)

- No magnetic field vs. surface configuration, momentary temperature and perpendicular velocity fields
  - applied cusp-field damps the radial and axial components of the flow, stabilizing effect is strongest near the crucible wall where the magnetic field is highest
  - the larger the magnetic field is, the less there are convection rolls, the more stable they are, and the closer to the symmetry axis they are forced
  - maximum velocity is about 5 cm/s (with 1000 A, velocity is over 1 cm/s only in a narrow region near the symmetry axis)

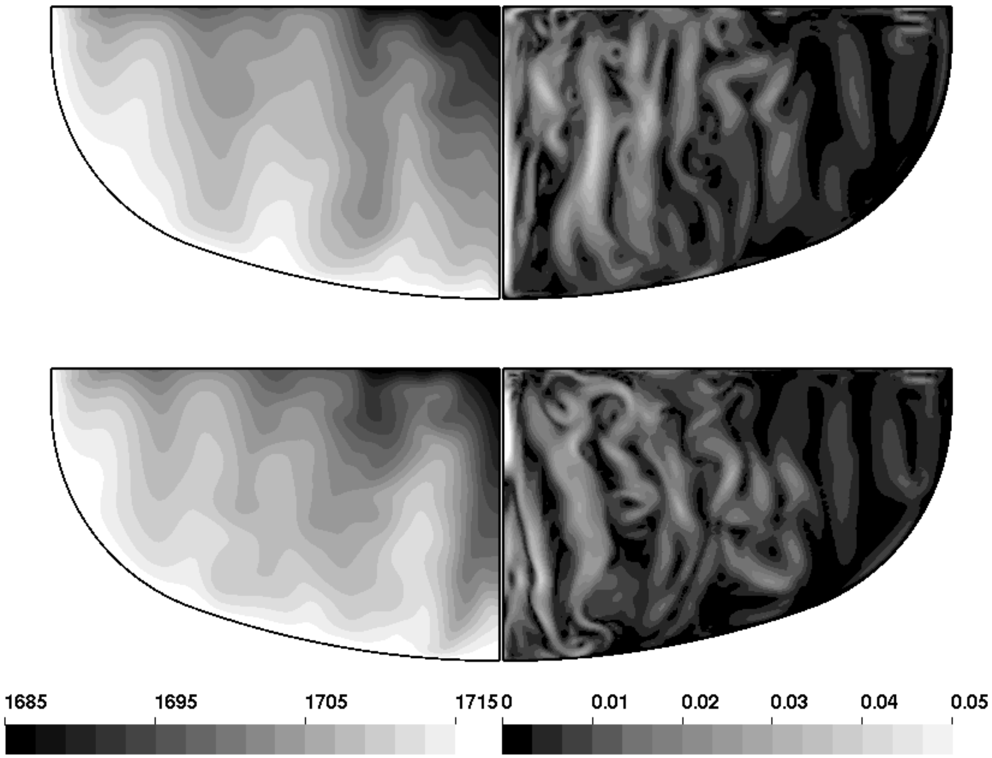


Simulation results, 20” crucible (3/4)

- Temperature time series
  - 100 s of real time, 0 A, 200 A, 500 A and 1000 A)
  - 4 analyzing points
  - without magnetic field temperature oscillations are about 10 K in P1, and about 6 K in P2-P4, period 10-20 s
  - 200 A field reduces faster components of oscillations in P2 and P4
  - 500 A and 1000 A fields strongly damp the temperature oscillations everywhere except in P1
  - in P1 only the 1000 A field slightly damps the oscillations
  - all three magnetic fields lower the average temperature near melt gas interface, as they slow down the transport of the heat from the crucible wall to the melt surface



Simulation results, 20” crucible (4/4)



- Surface (upper picture) vs. shifted (lower picture) configuration (both 200 A)
  - no consistent difference between time-dependent temperature and velocity fields, momentary fields naturally slightly different
  - also temperature time series are very similar
  - convection rolls are narrow and tall, and they are not much modified by shifting the field as long as the average magnetic field is of the same magnitude

Validation of the 2D model, 14” crucible (1/3)

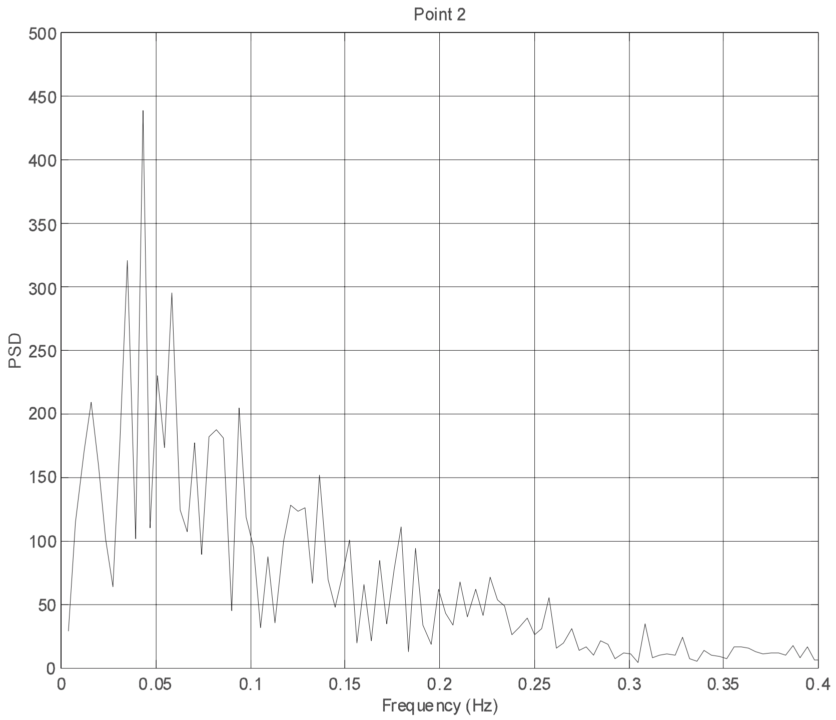
- With the industrial scale parameters silicon melt flow is turbulent and three dimensional
- Even though computer technology and numerical methods have developed rapidly during last few years, they do not enable direct 3D melt flow simulations without the turbulence models in a reasonable time frame
  - convenient duration of simulation is few days for those people who make development work in practical crystal growth
  - small errors are tolerable as long as 2D simulations catch the essential behavior of the melt flow, or they are, at least, capable of predicting the effect of different process changes
- Validity and consequences of the used 2D model have to be checked, but
  - no uncertainty due to the use of turbulence models (direct simulation)
  - effect of different time step and grid was studied

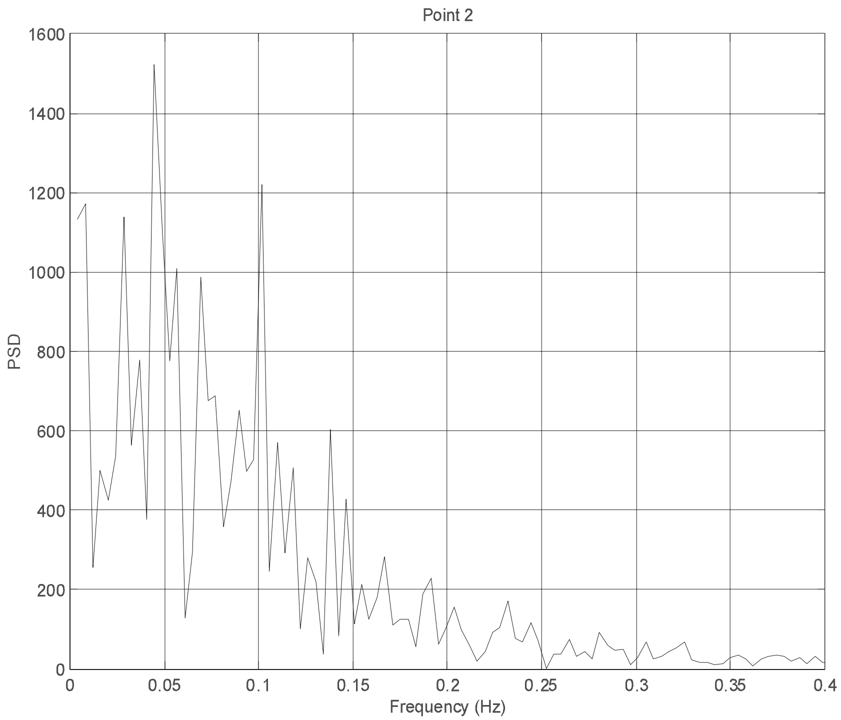
Validation of the 2D model, 14” crucible (2/3)

- Results computed using our 2D model were compared against three dimensional simulations and thermocouple measurements in identical setups
  - measurements by Wacker Siltronic AG (14” crucible, 4” crystal)
    - 3 comparison points: 30 mm from symmetry axis, 10, 20 and 40 mm below the crystal
    - crucible rotation rates 5 rpm and 2 rpm
    - crucible wall temperature measured for both rotation rates
  - 3D calculations by S. Enger, B. Basu, M. Breuer, F. Durst, (J. Crystal Growth 219 (2000) 144).
    - control volume method

Validation of the 2D model, 14” crucible (3/3)

- **PSD of temperature, 2D simulation vs. measured data (5 rpm case)**
  - **shape of power spectral densities in fairy good agreement in all cases ⇒ our model can be used to describe the time evolution of the flow**
  - **however, our model seems to underestimate the amplitude of the fluctuations**





Summary

- Numerical simulations can efficiently support the crystal growth process development by increasing the understanding of complicated physical phenomena and by reducing the economical investments required in the experimental work
- Industrial-scale MCZ processes was modeled with realistic material parameters and boundary conditions
- Melt velocity distributions and temperature time series for different cusp-type magnetic fields were presented
- Also, the validity of our cylindrically symmetric model was discussed
- It was found that a magnetic field of the order of 25 mT strongly stabilizes the melt outside about half the crucible radius, while a higher field of about 100 mT stabilizes the flow in most of the melt
- However, a very strong stabilization decreases the stirring of the melt and may result in large radial variation in oxygen and dopant concentrations in the crystal

Acknowledgements

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  - V. Savolainen, J. Heikonen, J. Ruokolainen, O. Anttila, M. Laakso, J. Paloheimo, “Simulation of large-scale silicon melt flow in magnetic Czochralski growth”, accepted for publication in Journal of Crystal Growth.

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