Weierstrass Institute for
Applied Analysis and Stochastics

Leibniz Institute for
Crystal Growth

Leibniz Association

Modeling and numerical simulation of the application of traveling magnetic fields to stabilize crystal growth from the melt

O. Klein (WIAS + MATHEON, Berlin)

DFG Research Center MATHEON
Mathematics for key technologies

joined work with:

Ch. Grützmacher, P.-E.-Druet, J. Sprekels (WIAS + MATHEON, Berlin),

Ch. Lechner (TU Vienna), P. Philip (LMU, Munich),

Ch. Frank-Rotsch, F.-M. Kießling, W. Miller, U. Rehse, (IKZ, Berlin),

P. Rudolph (CTC, Schönefeld)

Magnetic fields and crystal growth processes

- Semi-conductor mono-crystals are important for high-technology devices
- Many of the crystals: grown from the melt by growth processes of Czochralski type
- To improve the growth processes, one needs to stabilizes the melt movement
- (Time-dependent) magnetic field can stabilizes the melt movement
- Typically, the magnetic fields are generated by induction coils placed outside of the growth apparatus
- Growth of III–V compounds requires to use pressure chambers with thick steel walls ⇝ walls diminish the magnetic field generated by external coils

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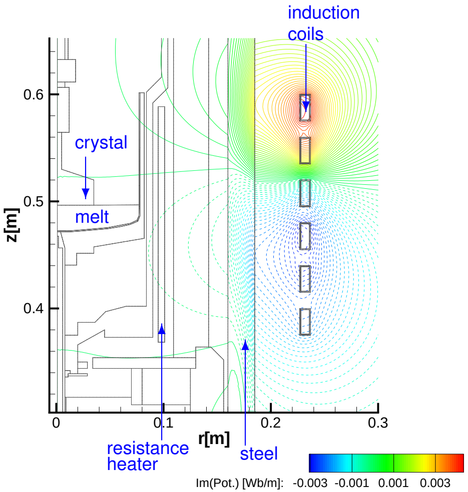
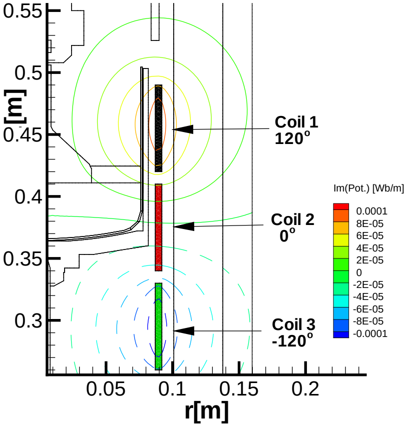


⇝ producing a field of sufficient magnitude in the melt requires much energy

- **Cooperation of :**
  - Leibniz Institute of Crystal Growth (IKZ)
    - ETP (Hannover)
    - IISB (Erlangen)
  - WIAS
  - *Steremat Elektrowärme GmbH, Berlin*
  - *AUTEAM Industrie-Elektronik GmbH, Brandenburg*
- Internal *heater-magnet modules (HMM)*, i.e. coil–formed resistance heaters, and electrical components to use them have been developed
- Replacing the usual meander-formed resistance heater units in the growth vessel by an HMM

  ⇝ one can generate appropriate fields in the melt with moderate power consumption



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Innovation award Berlin-Brandenburg 2008

given to the project

Full Model of Magneto-Hydrodynamics

- Navier-Stokes equations in Boussinesq approximation: for melt in Ω_1

$$\rho_1 \left(\frac{\partial u}{\partial t} + (u \cdot \nabla) u\right) = -\nabla p + \operatorname{div}(2\,\eta(\theta)\, D\, u) + f(\theta) + j \times \mu\, H,$$
$$\operatorname{div} u = 0 \qquad \text{in }]0,T[\times\Omega_1\,.$$

- Maxwell's equations

$$j = \operatorname{curl} H = 0\,, \quad \operatorname{div}(\sigma_c\, E) = 0, \qquad \text{in }]0,T[\times\tilde{\Omega}_{nc}\,,$$
$$j = \operatorname{curl} H = \sigma_c(\theta)\,(E + u \times \mu\, H) \quad \text{in }]0,T[\times\tilde{\Omega}_c$$
$$\operatorname{curl} E + \mu\,\frac{\partial H}{\partial t} = 0\,, \quad \operatorname{div}(\mu\, H) = 0\,, \qquad \text{in }]0,T[\times\tilde{\Omega}\,.$$

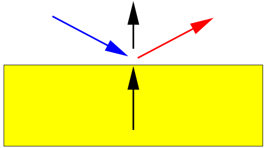
- Energy balance

$$\rho_1\, c \left(\frac{\partial \theta}{\partial t} + u \cdot \nabla\theta\right) = \operatorname{div}(\kappa(\theta)\,\nabla\theta) + \eta(\theta)\, D(u,u) + \frac{|j|^2}{\sigma_c(\theta)} \text{ in }]0,T[\times\Omega_1,$$
$$\rho\, c\, \frac{\partial \theta}{\partial t} = \operatorname{div}(\kappa(\theta)\,\nabla\theta) + \frac{|j|^2}{\sigma_c(\theta)} \qquad \text{in }]0,T[\times\Omega_i \;\; (i \neq 1)\,.$$

Radiative heat transfer between surfaces of cavities:

$$-\kappa_{\text{gas}}(\theta_{\text{gas}})\nabla\theta_{\text{gas}} \bullet \vec{n}_{\text{gas}} - R + J = -\kappa(\theta)\nabla\theta \bullet \vec{n}_{\text{gas}}$$

- $\vec{n}_{\text{gas}}$: outer unit normal w.r.t. gas phase,
- total outgoing radiation $R = \sigma\epsilon T_{\text{glo}}^4 + (1-\epsilon)J$
  - σ Boltzmann radiation constant, ϵ emissivity
- incoming radiation
  $J(x) = \int_\Gamma \Lambda(x,y)\,\omega(x,y)R(y)dy$
  - Γ boundary of cavity
  - $\Lambda(x,y) = 1$ if y is "visible" from x, 0 otherwise
  - $\omega(x,y)$ view factors



$$\omega(x,y) := \frac{\big(\vec{n}_{\text{gas}}(y) \bullet (x-y)\big)\,\big(\vec{n}_{\text{gas}}(x) \bullet (y-x)\big)}{\pi\big((y-x) \bullet (y-x)\big)^2}$$

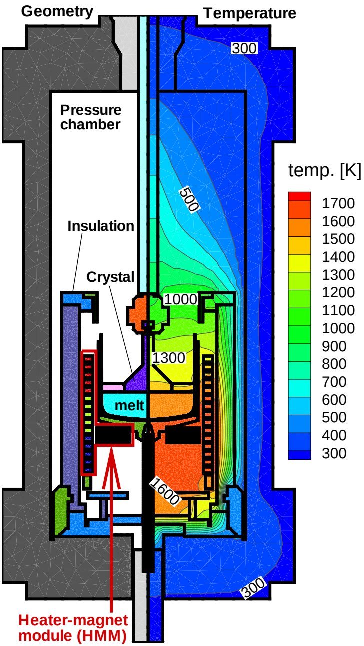
Publications

- Concept of HMM: Rudolph JCG 2008
- Modeling and Simulation: Lechner–K.–Druet JCG 2007
  K.–Lechner–Druet–Philip–Sprekels–Frank-Rotsch–Kießling–Miller–Rehse–Rudolph JCG 2008, MHD 2009
  Rudolph–Czupalla–Dropka–Frank-Rotsch–Kiessling-K.-Lux-Miller-Rehse-Root JKCGC 2009
  Dropka–Miller–Rehse–Rudolph–Buellesfeld–Sahr–K. –Reinhardt JCG 2011
  Dreyer–Druet–K.–Sprekels WIAS 2012
- Existence of solutions: Druet Thesis 2009, MMAS 2009, CzMJ 2009, NA-RWA 2009, ApM 2010,
- Optimal control problem: Druet–K.–Sprekels–Tröltzsch–Yousept SIAM JCO 2011
- Free Boundary Problem: Druet WIAS 2011, WIAS 2012,
  Contributed Talk Wed. 11.00

P.-É. Druet is researcher in the project C9 “Simulation and Optimization of Semiconductor Crystal Growth from the Melt Controlled by Traveling Magnetic Fields” in the DFG-Research Center FZT 86, MATHEON, (Heads: O. Kl., J. Sprekels, F. Tröltzsch)

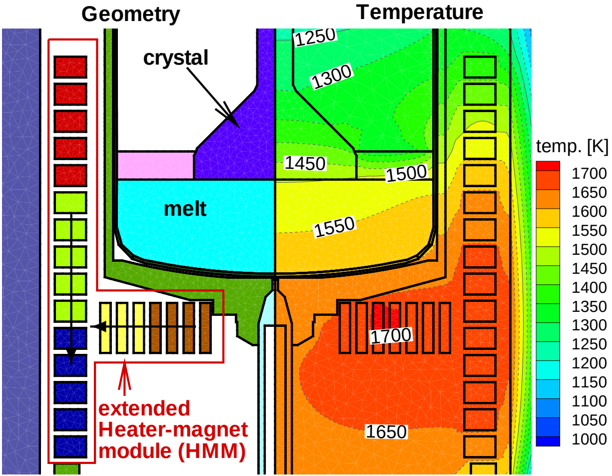
Global simulations

- main parts of crystal growth device are simulated, axially symmetric approximation of real geometry is considered
- melt motion is ignored
- time-harmonic version Maxwell equation
- stationary heat equation
- Software `WIAS-HiTNIHS` (P. Philip, O. Kl.) WIAS-High Temperature Numerical Induction Heating Simulator (partially developed in MATHEON Project C9)
- LPA Mark 3 in a configuration for LEC crystal growth of GaAs
  4 kg GaAs melt, diameter=15.2 cm, height=4.5 cm
  GaAs melt covered by a boric oxide layer with a height of 1.35 cm
  Control T at triple point by adapting power used in simulation



Special HMM following the patent DE 10 2007 028 548 by Ch. Frank-Rotsch, P. Rudolph, O. Kl., R.-P. Lange, B. Nacke:

- 3 coils surrounding the crucible, each having 5 rings, producing a downwards moving TMF,
- 2 additional spirals below the crucible, producing an outward moving TMF



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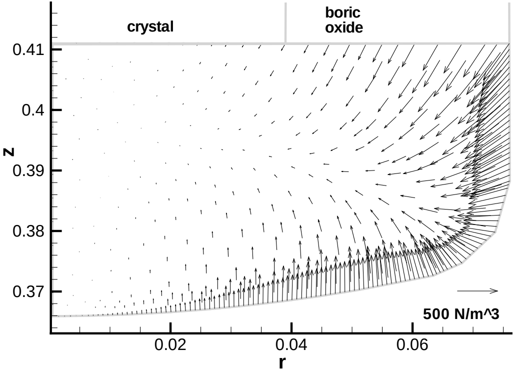
- time average over one period of electromagnetic fields, computed form time-harmonic representation $\mapsto$ Lorentz-force density for local simulation
- Lorentz force density in melt generated by the HMM in the LPA Mark 3:

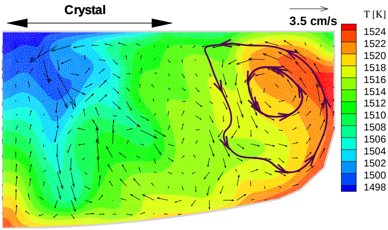


- Temperature and heat fluxes in the melt computed by **global** simulations are also used as initial and boundary data for local simulation in the melt

- only domain filled with melt is considered.
- heat sources by induction current ignored
- motion induced current $\vec{u} \times \vec{B} = \vec{u} \times \mu \, \vec{H}$ neglected $\rightsquigarrow$ Maxwell equation are decoupled from melt motion
- Implementation by Ch. Lechner in the framework of NAVIER (E. Bänsch)

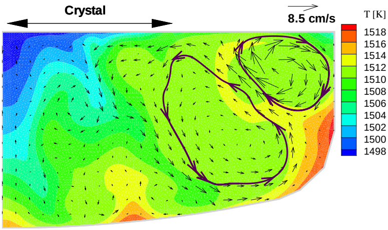
Snapshots of computed velocity and temperature distribution

without Lorentz force



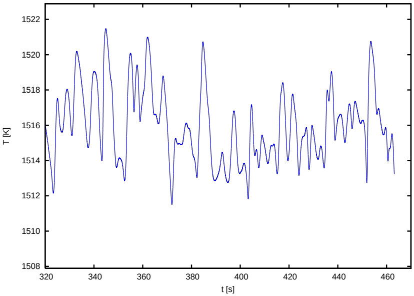
maximal velocity $\approx 3.5 \frac{\text{cm}}{\text{s}}$

with Lorentz force



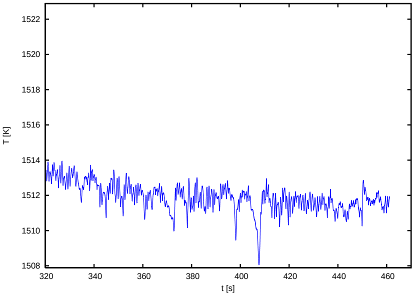
maximal velocity $\approx 8.5 \frac{\text{cm}}{\text{s}}$

Temperature oscillations in a monitor point (Ch. Lechner using `NAVIER`)



without Lorentz force

main temperature oscillations ≈ 8K



with Lorentz force

main temperature oscillations ≈ 2K

frequency increased

Project KRISTMAG® / Project AVANT*SOLAR* (2008-2011)

- Conclusion project KRISTMAG®:
  - Numerical simulations + crystal growth experiments show
    - Lorentz forces generated by an internal HMM can influence the melt flow during crystal growth
    - using an extended HMM and appropriate TMFs, we can improve the growth conditions
  - an extended HMM has successfully been used for LEC crystal growth at the IKZ
- Project AVANT*SOLAR* (2008-2011):
  - KRISTMAG® project partners + SCHOTT Solar Wafer GmbH + two other research institutes
  - using traveling magnetic fields generated by an internal HMM to improve directional solidification of solar-grad silicon
  - successfully growth of 640 kg Si ingots

Funding

- Projects KRISTMAG® (07/2005–06/2008) and AVANT*SOLAR* (07/2008–06/2011) were supported by
  - the German Federal State of Berlin in the framework of the "Zukunftsfonds Berlin",
  - the Technology Foundation Innovation Center Berlin (TSB),
  - cofinanced by the European Union within the European Regional Development Fund (EFRE). Investing in your future.

Berlin EFRE TSB TECHNOLOGIESTIFTUNG BERLIN

- Project C9 "Simulation and Optimization of Semiconductor Crystal Growth from the Melt Controlled by Traveling Magnetic Fields" (05/2002–05/2014) is supported by:

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