

Numerical simulations of the influence of a traveling magnetic field, generated by an internal heater-magnet module, on Czochralski crystal growth

O. Klein, Ch. Lechner, P.-É. Druet, P. Philip, J. Sprekels, Ch. Frank-Rotsch, F.-M. Kießling, W. Miller, U. Rehse, P. Rudolph

Abstract

Numerical simulations of liquid encapsulated Czochralski crystal growth of GaAs under the influence of a traveling magnetic field will be presented. As described in Rudolph 2008 (Proceedings for ICCG-15), the magnetic field is generated by an internal heater-magnet module, replacing the usual heater units inside the pressure chamber in the growth arrangement.

The numerical results show the influence of the Lorentz force on the melt, e.g. the damping of the temperature oscillations in the Taylor cell below the crystal.

This work is conducted in the project KRISTMAG®, see <http://www.kristmag.com/>.

1. Introduction

Time-dependent magnetic fields have successfully been used to improve crystal growth processes from the melt. Typically, the magnetic fields are generated by magnets or induction coils placed outside of the growth apparatus. Hence, producing a field of sufficient magnitude in the melt requires much energy, especially during the growth of III–V compounds, where the thick walls of the pressure chamber significantly diminish the magnetic field generated by coils outside of the chamber. In the project KRISTMAG®, an internal heater-magnet module (HMM) has been developed, consisting of several coils that generate heat due to resistance heating and produce simultaneously a traveling magnetic field (TMF), see references [1-4]. 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.

Numerical simulations of liquid encapsulated Czochralski (LEC) crystal growth of GaAs will be presented, showing the influence of the TMF. It will be investigated, how the magnetic field can be used to modify the temperature oscillations in the melt, appearing since the flow in the melt is transient and the eddies therein change size and position. Temperature fluctuations at low frequencies arising near the crystal melt interface can cause faceting and, eventually, twinning, and have, in consequence, a negative impact on the quality of as-grown crystals, see [5]. Therefore, one would like to damp the oscillations and increase their frequencies by using magnetic fields. This is important if one aims increasing the melt volumes, and can therefore not damp this oscillations by rotating the melt.

2. Global simulation of an LEC growth configuration

For the global simulation, i. e., the computation of electro-magnetic fields and the temperature distribution in the entire pressure chamber, the software WIAS-HiTNIHS is used, see references [3, 4]. Dealing with an axisymmetric approximation of the growth vessel, WIAS-HiTNIHS solves the energy balance equation in the whole growth apparatus, taking heat conduction and radiative heat transfer between the surfaces of cavities into account. Moreover, WIAS-HiTNIHS determines the magnetic flux field, the heat sources, and the Lorentz forces by solving an appropriate formulation of Maxwell's equations, which is derived under the additional assumption that the involved electro-magnetic quantities are axisymmetric in space and have a sinusoidal time dependence. WIAS-HiTNIHS is based on the finite volume method and it was implemented in the framework of the program package pdelib. It uses the grid generator Triangle and the sparse matrix solver PARDISO.

Fig. 1 and Fig. 2 show a computed temperature distribution for an LPA Mark 3 in a configuration for liquid encapsulated Czochralski crystal growth of GaAs. The 4 kg GaAs melt has a diameter of 15.2 cm, a height of 4.5 cm, and is covered by a boric oxide layer with a height of 1.35 cm that is assumed to be opaque. The considered HMM contains a total of 3 coils, surrounding the crucible with the melt and being placed above each other. The HMM produces a downwards moving TMF, generating the Lorentz force density shown in Fig. 3. This density has its maximum near the crucible wall and is almost vanishing near to the bottom of the melt. The input power P was chosen such that at the given trijunction between melt, crystal, and boric oxide, the melting temperature of GaAs, i.e. 1511 K, was attained.

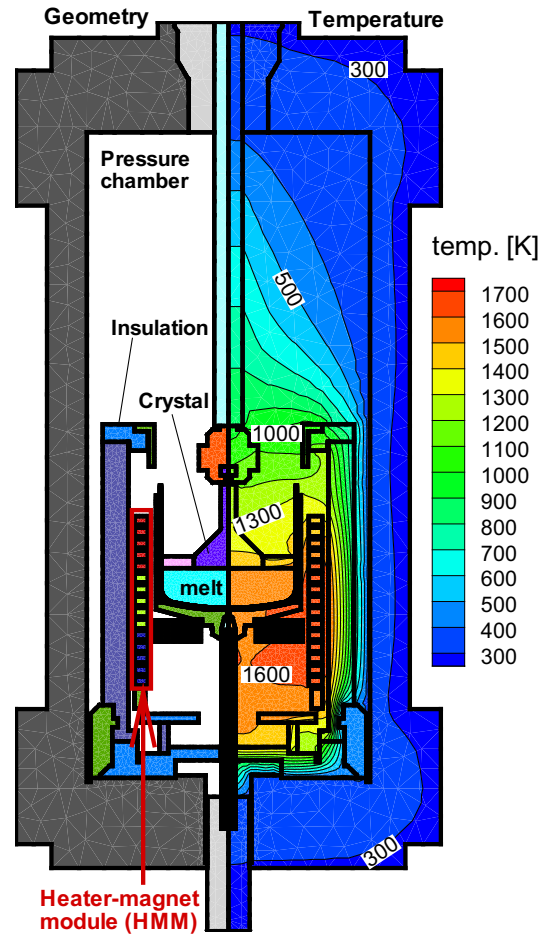


Fig. 1: An LEC growth configuration with an HMM and a computed temperature distribution. The isotherms on the right-hand side are spaced at 100 K.

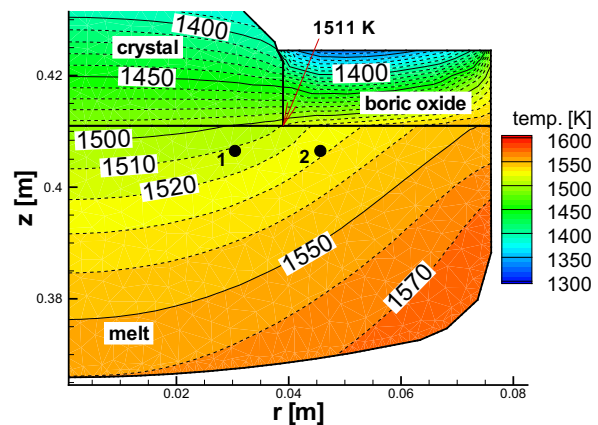


Fig. 2: Temperature distribution in melt, crystal, and boric oxide encapsulation. The solid isotherms are spaced at 50 K, the dotted isotherms in between are spaced at 10 K. The points 1 and 2 mark the points used for the temperature evaluation in here and in Section 3.

3. Local simulation of an LEC growth configuration

The temperature, heat fluxes, and Lorentz force fields computed by the global simulation, see Figures 2 and 3, are used as input data for the local direct transient simulation of the melt. For this simulation, we use the finite element code NAVIER developed by E. Bänsch [7] to solve the Navier Stokes equations together with the energy equation in the Boussinesq approximation, see [3,4]. We assume that the crystal rotates with 5 rpm and that the crucible performs a counterrotation with the same rate. We impose no-slip and non-penetration boundary conditions for the velocity. The temperature at the melt-crystal interface is fixed, and on the remaining boundary we prescribe the normal heat flux, using the results from the global simulation. It is assumed that the melt flow is axisymmetric.

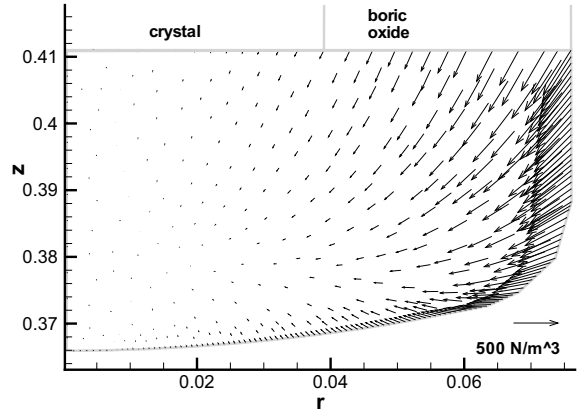


Fig. 3: Lorentz force density in the melt. The reference vector shown corresponds to a force density of 500 N/m^3 the maximum of the density is around 600 N/m^3 .

Due to convective effects in the melt, the temperature difference of 85 K within the melt arising during the global simulation is reduced to 1/3 of its value in the local simulation.

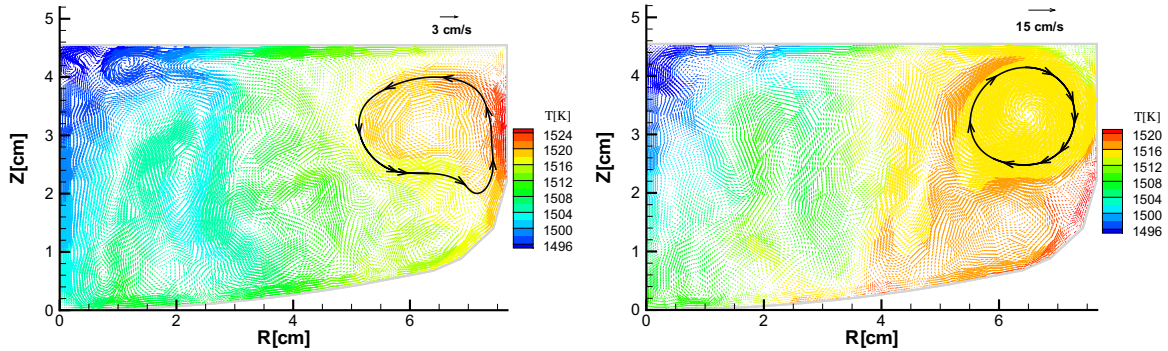


Fig. 4: Snapshots of velocity and temperature distribution from the local simulation of the LEC configuration without Lorentz force (left-hand side) and with Lorentz force (right-hand side). Note the different scales for temperature and velocity.

In Fig. 4, we show snapshots of the velocity and the temperature distribution computed in the local simulation, comparing a simulation result obtained without taking the influence of the Lorentz force into

account (left-hand side) to a result obtained with taking this influence into account (right-hand side). Without Lorentz force, the natural convection generates a roll in the outer part of the

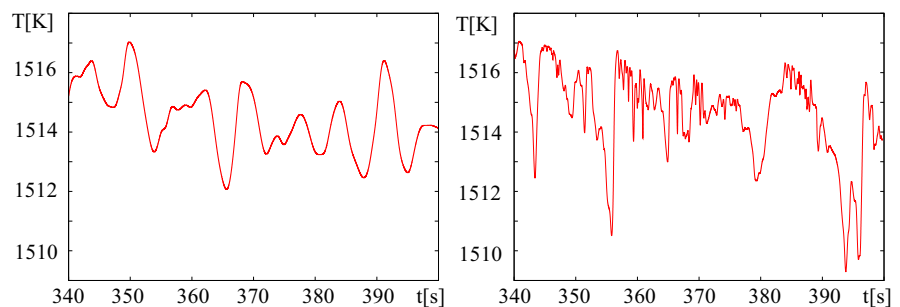


Fig. 5: Temperature oscillations in the monitor point 2 from the local simulation of LEC configuration, without Lorentz force (left-hand side) and with Lorentz force (right-hand side).

crucible. The Lorentz force generates in the same region a roll that rotates in the opposite direction. This roll persists if one considers the evolution of the flow in the melt, while one can observe generation and vanishing of rolls in the lower part of the melt. Moreover, the Lorentz force increases the maximal velocity of the melt by a factor of almost 5 and decreases the temperature difference in the melt.

As pointed out in the introduction, one would like to damp the oscillations by using magnetic fields. Therefore, we investigated the transient behavior of the temperature at the point near the trijunction that is marked as “2” in Fig. 2. Comparing the normal behavior at point 2 shown on the left-hand side of Fig. 5 with the behavior under the influence of the Lorentz force shown on the right-hand side of Fig. 5, one observes that the Lorentz force increases the main temperature variation from approximately 5K to approximately 8K and increases the frequency of the oscillation. This shows that this Lorentz force is not suitable to damp the oscillation. This seem to follow from the fact that the Lorentz force does not influence the region near to the bottom of the crucible, wherein the melt flow changes significantly in time.

4. Result for an LEC growth configuration with an extended HMM

Having in mind results like the one above indicating that TMF generated by coils surrounding the melt may not be appropriate to influence the lower part of the melt, further considerations lead to the idea that one should place additional coils below the crucible, see patent [6]. The HMM shown in Fig. 1, consisting of three coils surrounding the crucible, has been extended by adding two additional coils below the melt, see Fig. 6. This HMM has been considered for the LPA Mark 3 in the configuration discussed in Section 1, and

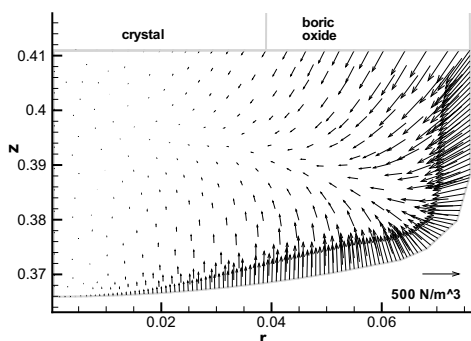


Fig. 7: Lorentz force density in the melt. The reference vector shown corresponds to a force density of 500 N/m^3 . The maximum of the density is around 570 N/m^3 .

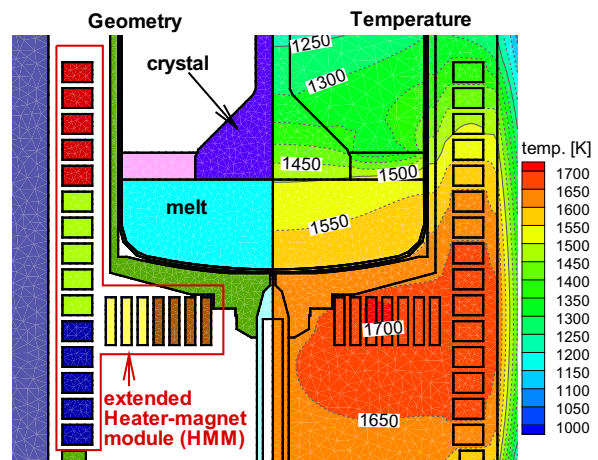


Fig. 6: An LEC growth configuration with an HMM extended by two additional coils below the melt crucible, and a computed temperature distribution. The isotherms on the right-hand side are spaced at 100 K.

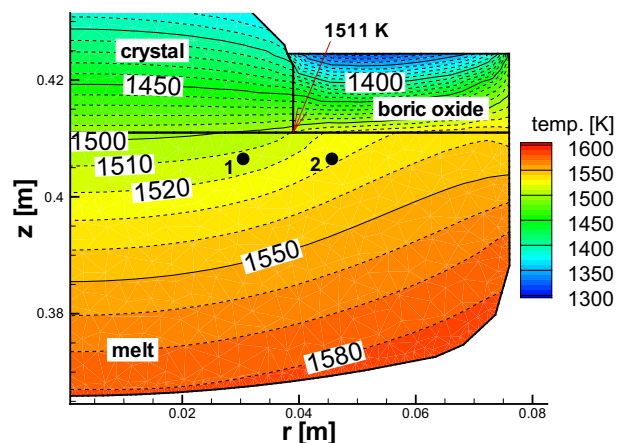


Fig. 8: Temperature distribution in melt, crystal, and boric oxide encapsulation. The solid isotherms are spaced at 50 K, the dotted isotherms in between are spaced at 10 K. The points 1 and 2 mark the points used for the following temperature evaluation.

the additional coils are used to produce an outward moving TMF. Combined with the downwards moving TMF generated by the other coils, a Lorentz force density is generated, shown in Fig. 7, that is at the bottom of the melt of the same order of magnitude as at the outer boundary of the melt. As in Section 1, the input power P was chosen such that at the given trijunction the melting temperature of GaAs, i.e. 1511 K, was attained.

As in Section 3, the temperature, heat fluxes, and Lorentz force fields computed by the global simulation, see Figures 7 and 8, are used as input data for the local direct transient simulation of the melt.

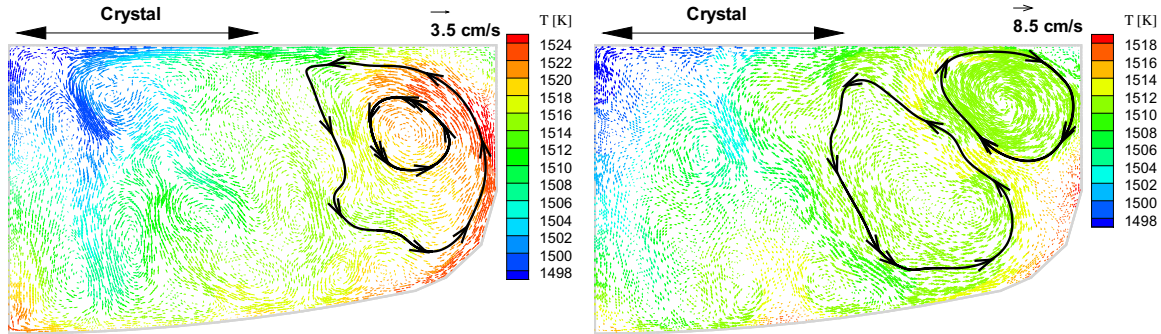


Fig. 9: Snapshots of velocity and temperature distribution from the local simulation of the LEC configuration without Lorentz force (left-hand side) and with Lorentz force (right-hand side). Note the different scales for temperature and velocity.

In Fig. 9, we show snapshots of the velocity and the temperature distribution in the melt without (left) and with influence of the Lorentz force (right) computed by local simulations. Without Lorentz force, the natural convection generates a roll near to the crucible wall. The Lorentz force generates a roll in the outer corner of the melt, rotating in the opposite direction, which pushes the convections generated roll downwards and towards the center. Moreover, the Lorentz force stabilize the convection generated roll, increases the maximal velocity of the melt, and decreases the temperature difference in the melt.

Figs. 10 and 11 show the temperature evolution in the two points near the trijunction that are marked as “1” and “2” in Fig. 8. Comparing the normal behavior at point 1 shown on the left-hand side of Fig. 10 with the behavior under the influence of the Lorentz force shown on the right-hand side of Fig. 10, one observes

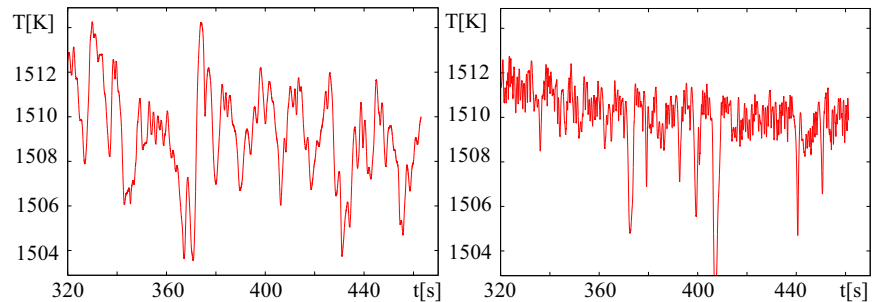


Fig. 10: Temperature oscillations in the monitor point 1 from the local simulation of LEC configuration, without Lorentz force (left-hand side) and with Lorentz force (right-hand side).

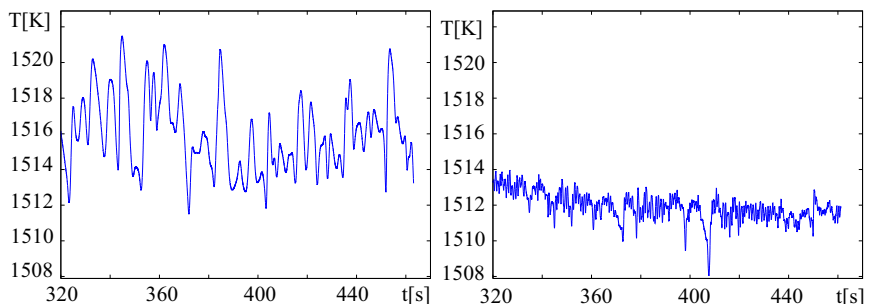


Fig. 11: Temperature oscillations in the monitor point 2 from the local simulation of LEC configuration, without Lorentz force (left-hand side) and with Lorentz force (right-hand side).

that the Lorentz force reduces the main temperature variation from approximately 10K to approximately 4K and increases the frequency of the oscillation. In Fig. 11, it is shown that the Lorentz force reduces in point 2 the main variation from 8K to 2 K and increases its frequency.

Conclusions

It has been shown that Lorentz forces generated by an internal HMM can be used to influence the melt flow during crystal growth, and to improve the growth conditions. Experiments and numerical simulations are necessary to find further suitable conditions, fields, and HMM configurations.

Acknowledgements

The authors wish to thank W. Dreyer from the WIAS for fruitful discussions. This work is done within the project KRISTMAG® (2005-2008) supported by the German Federal State of Berlin in the framework of the “Zukunftsfonds Berlin” and the Technology Foundation Innovation center Berlin (TSB). It is co-financed by the European Union within the European Regional Development Fund (EFRE). The authors are responsible for the content of this paper.

References

- [1] Rudolph, P.: *Travelling magnetic fields applied to bulk crystal growth from the melt: The step from basic research to industrial scale*. J. Crystal Growth, Vol. 310, 2008, Issues 7-9, pp.1298-1306.
- [2] Rudolph, P., Frank-Rotsch, Ch., Kiessling, F.-M., Miller, W., Rehse, U., Klein, O., Lechner, Ch., Sprekels, J., Nacke, B., Kasjanow, H., Lange, P., Ziem, M., Lux, B., Czupalla, M., Root, O., Trautmann, V., Bethin, G.: *Crystal growth in heater-magnet modules - from concept to use*, Proceedings of the International Scientific Colloquium Modelling for Electromagnetic Processing (MEP 2008), Hannover, October 27-29, 2008.
- [3] Lechner, Ch., Klein, O., Druet P.-É.: *Development of a software for the numerical simulation of VCz growth under the influence of a traveling magnetic field*. J. Crystal Growth, Vol. 303, 2007, pp. 161-164.
- [4] Klein, O., Lechner, Ch., Druet, P.-É., Philip, P., Sprekels, J., Frank-Rotsch, Ch., Kießling, F.-M., Miller, W., Rehse, U., Rudolph, P.: *Numerical simulation of Czochralski crystal growth under the influence of a traveling magnetic field generated by an internal heater-magnet module (HMM)*. J. Crystal Growth, Vol. 310, 2008, pp. 1523–1532,
- [5] Hurle, D.T.J., Rudolph, P.: *A brief history of defect formation, segregation, faceting, and twinning in melt-grown semiconductors*. J. Crystal Growth, Vol. 264, 2004, pp.550-564.
- [6] Frank-Rotsch, Ch., Rudolph, P., Lange, P., Klein, O., Nacke, B.: Patent application DE 10 2007 028 548, submitted June 18th 2007.
- [7] Bänsch, E.: *Simulation of instationary, incompressible flows*: Acta Math. Univ. Comenianae, LXVII, Vol. 101, 1998. pp. 101 –114.

Authors

P.-É. Druet, O. Klein, Ch. Lechner,
J. Sprekels,
Weierstrass Institute for Applied
Analysis and Stochastics (WIAS),
Mohrenstraße 39,
10117 Berlin, Germany
E-Mail: druet@wias-berlin.de,
klein@wias-berlin.de,
lechner@wias-berlin.de,
sprekels@wias-berlin.de

P Philip,
Department of Mathematics,
Ludwig-Maximilians University
(LMU) Munich,
Theresienstrasse 39
80333 Munich, Germany.
E-Mail: philip@math.lmu.de

Ch. Frank-Rotsch, F.-M. Kießling,
W. Miller, U. Rehse, P. Rudolph,
Leibniz Institute for Crystal
Growth (IKZ),
Max-Born-Straße 2,
12489 Berlin, Germany
E-Mail: frank@ikz-berlin.de,
kiessling@ikz-berlin.de,
miller@ikz-berlin.de,
rehse@ikz-berlin.de,
rudolph@ikz-berlin.de