Growth of semiconductor bulk single crystals

Olaf Klein and Jürgen Sprekels

Semiconductor materials like silicon or gallium arsenide constitute the heart of modern technology. Without them, achievements such as iPods, LED screens, digital cameras, solar energy, or electronic parking assistants would not be possible. However, it would not be sufficient to have the semiconductor materials to hand in just any form: they are needed as high-purity single crystals, a form that is hardly to be found in nature and has to be manufactured.

In industrial practice, the most important class of production techniques runs under the name of *Czochralski type* growth. In such a process, the semiconductor material (silicon, say) is first melted in a rotating crucible; then, a small silicon seed crystal is dipped from above into the melt and very slowly pulled upwards. In this way, a liquid silicon film is lifted upwards – just as if you dipped a spoon into a glass of honey and pulled it up slowly. The liquid silicon film is cooled by the surrounding gas and solidifies – and a single crystal comes into being. With this technique, silicon single crystals of enormous size can be grown; they may reach diameters of forty centimeters and a length of more than one meter.

A typical growth apparatus for gallium arsenide is depicted in Figure 1; here, on the left side the overall furnance is presented, and on the right side its center is shown in more detail. Therein, the geometry (left-hand side) and the temperature distribution (right-hand side) during a growth run calculated with the software package `WIAS-HiTNIHS` are presented.

In many growth processes of Czochralski type, the melt flow is turbulent, which creates the problem that impurities can find their way into the crystal, lowering its quality. However, if the melt is electrically conducting then time-dependent elec-

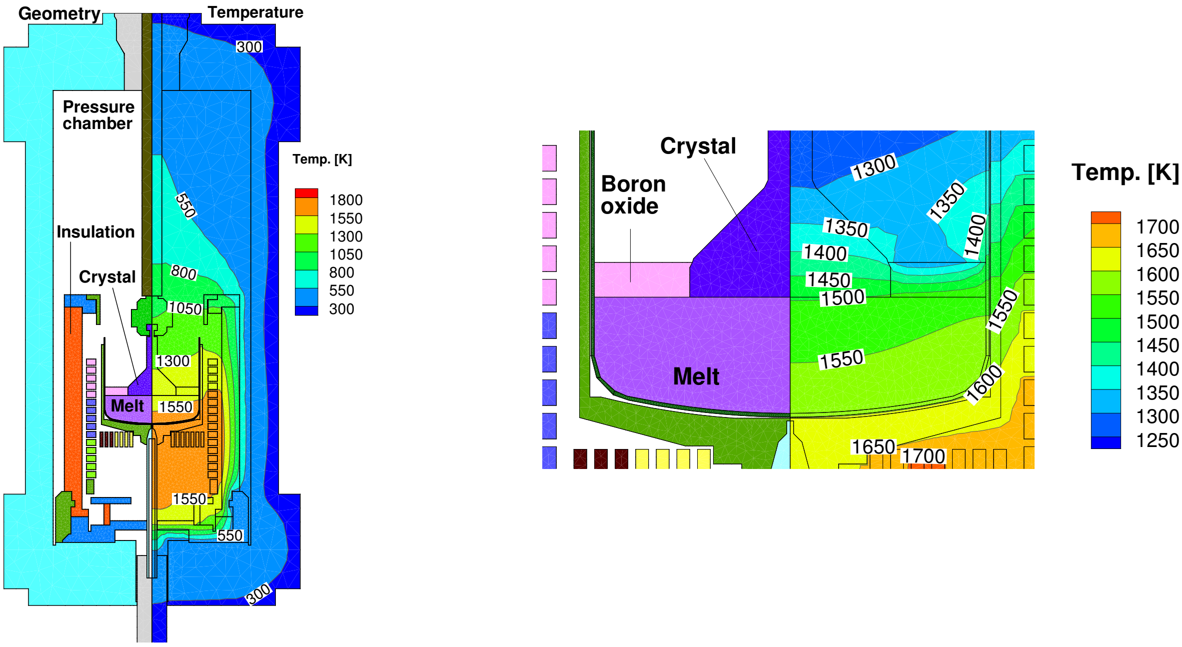

Figure 1. *A cut through the overall cylindrical furnance (left-hand side) and a zoom to its central part (right-hand side). In both cuts the left side shows the configuration and the right side shows the computed temperature field.*

tromagnetic fields can be applied to control the melt flow. In the past, various kinds of magnetic fields have been employed for this task with some success, until in the project KRIST*MAG*® a consortium led by the Leibniz Institute of Crystal Growth (IKZ) achieved a major technological breakthrough: a so-called *internal heater-magnet module* was developed, which operates as a resistance heater while simultaneously generating a *traveling magnetic field*. Such traveling magnetic fields turned out to be very effective tools for controlling the melt flow, which resulted in high-quality single crystals. Within the project, several patents were granted, and all over the world crystal growth machines have been equipped with the new technology. As a recognition of this success story, the KRIST*MAG*® consortium was awarded the Innovation Prize Berlin-Brandenburg 2008.

What did all this have to do with mathematics and MATHEON? As a matter of fact, mathematical modeling and simulation played a crucial role for the success of the KRIST*MAG*® project, to which the WIAS project heads of the MATHEON project *Simulation and Optimization of Semiconductor Crystal Growth from the Melt Controlled by Traveling Magnetic Fields* belonged. To avoid expensive time- and energy-consuming experiments, the entire growth process was modeled and eventually cast into a complicated system of highly nonlinear partial differential equations. To solve this system, the software package WIAS-HiTNIHS, originally developed in the MATHEON project for other crystal growth processes, was adapted. In this way, a *virtual* crystal growth furnace was created in which different growth configurations could be simulated very efficiently. Using this virtual growth furnace, promising scenarios could be identified and proposed to the crystal growers, which contributed a lot to the eventual success of the project.

Within MATHEON, the project permanently dealt with crystal growth technology. Besides developing the simulation software WIAS-HiTNIHS, many important mathematical questions were addressed over the years (cf. [1]). In particular, systems of partial differential equations governing the growth process were studied analytically. The outstanding theoretical work was the PhD thesis of the project coworker P.-É. Druet, which was honored with the Young Scientists Award 2010 of the Leibniz Association. And, last not least, a whole hierarchy of optimization problems of ever increasing complexity was studied in order to optimize various aspects of the growth process.

Further reading

[1] W. Dreyer, P. Druet, O. Klein, and J. Sprekels. Mathematical modeling of Czochralski type growth processes for semiconductor bulk single crystals. *Milan J. Math.*, 80:311–332, 2012.