Crystal Growth Laboratory

Your Competent Partner in Crystal Growth and Solidification Processes

Annual Report 2004

- Equipment and Process Development -
- Optical and Electrical Characterization -
- Numerical Modeling -

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Crystal growth processes provide basic materials for many applications and are for example one key technology in the chain of all manufacturing processes for (opto-)electronic devices. The research and development of crystal growth processes is driven by the demands which come from the specific applications; but in common there is a need for an increase of crystal dimensions, improved uniformity of the relevant crystal properties in the micro- and macroscale and materials with new properties.

Therefore, the focal area of research of the Crystal Growth Laboratory (CGL), is to develop – in close collaboration with industry - equipment and processes for the production of bulk crystals and thin films in order to meet the increasing requirements on crystal quality and cost reduction.

The strategy of CGL is to optimize the crystal growth processing by a combined use of experimental process analysis and computer modeling. These activities are based on a suitable experimental infrastructure and on highly efficient user friendly simulation programs named CrysVUn, STHAMAS and STHAMAS3D. These computer codes, which are continuously further developed, are used for and by the industrial partners to develop crystal growth equipment and processes.

CGL was founded at the Department of Materials Science of the University of Erlangen - Nuremberg by Prof. Dr. Georg Mueller in 1979. Since 1996 the Crystal Growth Laboratory has established the working group "Crystal Growth" at the Fraunhofer Institute for Integrated Systems and Device Technology (IISB) in Erlangen. This working group became the Department Crystal Growth in autumn 1999.

Since the foundation of CGL more than 200 papers in scientific journals and conference proceedings have been published. Furthermore, CGL has educated a lot of experts in this field. 117 "Study" theses, 86 diploma theses and 36 PhD theses may serve as a reference for this.

More than 90% of funding of CGL results from research contracts directly with industrial partners and with the German Ministry for Research and Development, the Bavarian Research Foundation, the Bavarian Government, the German Research Foundation (DFG). Since 1996, CGL has acquired almost 17 Mio. Euro from the different sources indicated above.

Today, CGL consists of more than 30 highly motivated coworkers. They are experts in...
different fields, e.g. systems engineering, metrology, computer simulation, physics, material science, mathematics.

In 2004 the CGL has consolidated its position as world-wide acknowledged center of competence in the field of crystal growth.

It was possible to produce reproducibly transparent GaN-quasi-substrates from Ga containing solutions at room pressure conditions. The structural and optical properties of the GaN, grown by that way, exceed partly the quality of GaN-layers with comparable thickness grown from the vapor phase.

In the field of optical crystals a new crystal growth facility was developed together with the industrial partner. This machine will allow for example to grow high melting oxide crystals to be used as detectors in medical applications.

In the field of microgravity research a space experiment was successful carried out during the rocket mission TEXUS 41, which was prepared from CGL by using computer simulation. Further more the thermal models of two furnace insert were validated, which shall be run on the International Space Station.

In the field of software development the basis was created that the software CrysVUn, which is the main product of the CGL, will be used in future also for turbulent melt and gas flows as well as for semitransparent media. In addition a flexible and robust framework called Orcan was developed, which is applied already by several external R&D partners for their software development projects.

The granting of the doctor honoris causa to Georg Müller, the organization of the International Summer School on Crystal Growth ISSCG12 in Berlin and of Erlangen’s 2nd Symposium on Crystal Growth and last but not least several invited talks during international conferences have contributed to strengthen the international reputation of CGL.

The department maintains national but also international co-operations to industry. The industrial partners are currently (in alphabetical order): AIM, Crystal Growing Systems, Deutsche Solar, EADS, Freiberger Compound Materials, Komatsu, LG Siltron, MEMC, Photonicmaterials, RWE Schott Solar, Schott Lithotec, Shinetsu, Sumco, Sumitomo Electrics, Tokuyama, Umicore, Wafer Technology.

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**Fig. 2:** CGL has organized together with the colleagues of the Institute of Crystal Growth in Berlin the 12th International Summer School in Crystal Growth (ISSCG12). Here, the 200 participants of ISSCG12 can be seen.

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Indium phosphide is a III-V compound semiconductor crystallizing in the sphalerite structure. The revolution in optical fiber communications has sweep InP into a promising position as substrate for opto-electronic devices. InP has a fortuitous lattice match to alloys with bandgaps coinciding with the 1.3µm and 1.55µm windows in optical fiber. For lattice-matched growth of ternary alloys InGaAs and InAlAs and quarternary InGaAsP and AlInGaAs, InP is the substrate of choice. Heterostructure devices based on these alloys, by virtue of their bandgaps, provide a strong driving force for bulk InP crystal growth development.

During the past twenty-five years, as the growth of InP single crystals has gone from a laboratory curiosity to a commercial process, many new applications for InP substrates have emerged. The main application continues to be in the field of telecommunications, but other uses for InP material involving high speed electronic and photonic circuits have arrived. In addition to high frequency, wireless communications, broadband gigahertz radar has been achieved using InP photoconducting antennas.

The state of the art for InP crystal growth is divided between three competing technologies; the Liquid-Encapsulated-Czochralski-Technique (LEC) and the Vapour-Pressure-Controlled-Czochralski-Technique (VCZ) with top seeding and vertical growth in a container with bottom seeding by the Vertical Gradient Freeze (VGF) or Vertical Bridgman (VB) Technique. The LEC method has generally been the most cost effective, but its disadvantage is the high dislocation density caused by high levels of strain during growth. On the other hand, vertical container growth offers a very low dislocation density because of its low-stress environment. But it is plagued by yield problems due to twinning and interface breakdown in heavily doped crystals.

One possibility to enhance the quality of the grown crystals is the usage of time dependent magnetic fields. So we investigated the influence of rotating as well as traveling magnetic fields on the crystal growth of InP by the VGF-technique by the aid of numerical simulations. From this study it turns out that rotating magnetic fields had no significant influence neither at the bending of the solid liquid interface nor on the resulting thermoelastic stress at the interface. In contrary traveling magnetic fields can reduce the bending of the interface up to 60 % and the thermoelastic stress up to 50 %.

In our laboratory undoped, S- and Fe-doped 2” crystals are grown by the VGF-technique in [001]-direction. To study the influence of crucible shape three different cone angles were selected. Processes for each crucible shape are developed by the aid of numerical modeling using the software package CrysVUn. The grown crystals were characterized by MD-PICTS, synchrotron white beam topography, microscopy and

**Figure 1:** X-ray topograms of vertical sections trough the seeding interface (marked by an arrow) a) seeding interface of a Fe-doped 2” InP crystal grown in a crucible with a conical part and a diameter of the seed crystal of 8 mm; b) seeding interface of a S-doped 2” InP crystal grown in a flat bottom container and a diameter of the seed crystal of 2”
PL-topography.

For the growth of semi insulating (Fe-doped) InP using a “flat bottom” container only semi insulating LEC-grown seed crystals with an EPD = 3·10^4 cm^-2 were available. In this case polycrystalline growth was observed a few centimeters above the seeding position. Polycrystalline growth can be avoided for the growth of S-doped InP crystals (n =2-8·10^18 cm^-3) by the same growth process and by the use of seed crystals with an EPD < 1000 cm^-2.

In experiments performed by using crucibles with a cone angle of 160° and seed crystals with a diameter of 8 mm only a small influence of the quality of the seed crystal is observed.

Investigations by synchrotron white beam topography shows a reduction of the dislocation density at the seeding interface for seed crystals with a diameter of 8 mm. In contrary a drastic increase of the dislocation density above the seeding position was observed for seed crystals with a diameter of 2” used for “flat bottom” containers.

In experiments that were carried out in crucibles with a cone of 160° Fe-doped InP crystals with a EPD < 2000 cm^-2 and a high lateral homogeneity of the dopant distribution were grown.

The main challenge in the growth of InP by the VGF-method remains the reproducible avoiding of twin formation.

**Recent Publications**

P. Schwesig, M. Hainke, J. Friedrich, G. Müller; Journal of Crystal Growth **266** (2004), 224-228

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**Fig. 2:** EPD- and PL-mappings of 2” substrates. Figure a) represents a substrate from the tail end of a Fe-doped crystal (EPD < 2000 cm^-2). In figure b) a PL-mapping of a substrate from the tail end of a Fe-doped crystal at 1124 nm is shown. The standard deviation is 0.03 %
The research in the field of nitride semiconductors was, national as well as international remarkably intensified during the last year.

Fortunately there have been substantial developments within Europe and Germany itself during the report period. Even through the big GaN crystal of relevant dimensions is still not in sight, there are more and more efforts being made, targeting the homoepitaxial growth of GaN on templates or so called quasisubstrates, in order to circumvent the disadvantages originating from epitaxy using non native substrates.

There has been ongoing research about the growth of GaN within the frame of the BMBF project (01BM158) at CGL during the last years. The main interest therein was the design of a growth process for the growth of GaN from a solution at ambient pressure and temperatures below 1100°C.

The first project period included the development of a growth facility, which proved suitable for the growth of GaN, such that it is now possible to reproducibly grow optical transparent GaN layers on larger surfaces by default.

Because this method generally works closer to the thermodynamic equilibrium, compared to a gas phase process, the solution grown GaN is expected to exhibit a lower defect density.

This defect reduction is indeed observed by TEM investigation of the material. If a GaN layer was grown from the solution, directly upon a GaN MOCVD layer, the typical c-directional dislocations emerging from the MOCVD layer, are recombining or bending away from the c-direction at the interface, such that a reduced dislocation density by about two orders of magnitude was found in the solution grown material. However the relevant mechanism for this observation is subject to detailed ongoing TEM studies, in order to achieve a deeper understanding and further optimization of the growth process as to this aspect.

The GaN grown by this manner is highly n-type conducting with a carrier density of 1-5\times10^{18}\text{cm}^{-3} (Fig. 1). The carrier density was determined by measuring the reflectivity spectra of the samples by means of FTIR spectroscopy. This method offers the advantage that the carries density as well as the mobility can be quantified contact less. The "state-of-the art" GaN, as grown from the solution growth process at CGL, showed a high room temperature.

![Figure 1: RT-PL Spectrum of solution grown GaN measured by Fraunhofer IAF, Freiburg.](image-url)
photoluminescence intensity. The wavelength of the near band edge luminescence compares well to that published from commercially available MOCVD GaN material. The typical yellow PL emission, often reported for GaN, is negligible for the solution grown material in relation to the intensity of the near band edge luminescence (Fig. 2). However locally, mainly close to the edges of the substrate, the peak wavelength can vary slightly, which is most likely due to small alterations in the surface morphology.

The surface of the GaN, grown by the solution growth method, was found to be Ga-terminated. The polarity of the material was determined by TEM investigations using a convergent beam electron diffraction technique.

Overall, the results of the characterization of the solution grown GaN collected so far, clearly showed, that the solution growth of nitrides is feasible and with good prospects in term of a production of low defect c-plane GaN with high structural quality.

Regularly the nitride devices are produced with a c-plane orientation. As a result of the polarity of the c-lattice direction in the wurzite structure of GaN the operation of the nitride based devices can be affected by polarization induced electrostatic fields along the c-axis. These internal fields can cause e.g. a redshift of the optical transitions. The growth along a non-polar axis of the GaN structure, like the a-lattice direction, would here be beneficial.

Within a collaboration with the University of Ulm, we could show for the fist time, that also the growth of a-plane GaN is possible by the solution growth method developed within this project. It was possible to deposit GaN with a-orientation on top of a MOCVD seeding layer. The thickness of the a-plane covered a surface area of 10X10mm². The electrical and optical properties of these materials will be studied in the near future.

The growth of GaN from a solution at low temperatures and ambient pressure will be prolonged in the future. For this purpose a new project proposal was submitted to the BMBF during summer 2004.

Figure 2: The carrier concentration 'n' of solution grown GaN (measured by Hall and FTIR) is 1-4 x 10¹⁹ cm⁻³ the mobility is around 80 cm² /Vs


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Analyses of the heat and mass transport during casting of photovoltaic silicon

Directional solidification of multi-crystalline photovoltaic silicon is the industrial production technique with the largest market share. For example, the ratio of multi-crystalline directionally solidified silicon is about 60%.

Directional solidification of photovoltaic silicon includes two methods (see figure 1): The Bridgman – method and the casting technique. In the Bridgman – method the melting and crystallization process takes place in one facility. After melting of the starting material, crystallization occurs due to a mechanical movement of the mould. In the casting process, the melting and crystallization process takes place in two different facilities. Thereby, the silicon melt is poured from the melting unit into the mould of the crystallization unit, where the melt solidifies by a controlled heat extraction. Today, silicon blocks with a weight of over 300kg, i.e. a volume of 70x70x25 cm³ are produced by the Bridgman or casting technique. In general, the advantages of directional solidification are the high productivity per run, the small energy amount needed for the production of 1kg silicon, the small costs and the good efficiency of the solar cells manufactured from the blocks.

In the previous experimental and numerical investigations of the heat transport during directional solidification of photovoltaic silicon, melt convection was often neglected. However, the results obtained so far in literature, show that radial temperature gradients are present in the melt, which can result in a curved crystallization front. Such radial temperature gradients are responsible for the occurrence of natural convection. The influence of convection of the heat and mass transport can be estimated as follows: For a typical length of $L = 300\text{mm}$, a typical temperature gradient of $1\text{K/cm}$ and a typical deflection of the crystallization front of $1\text{cm}$ a characteristic flow velocity of $2\text{cm/sec}$ result. By using this value of the flow velocity the thermal resp. solutal Peclet-number can be determined, which is the ratio between the convective to diffusive heat resp. mass transport. For the heat transport the Peclet-number is 10 whereas for the mass transport its value is 20 000. This means that a moderate influence of melt convection on the heat transport can be expected and a strong impact of melt convection on the mass transport should occur.

In order to investigate the influence of convection in more detail, a simplified three-dimensional model of the transport processes occurring during solidification is required. The model has to be developed and validated in comparision to experimental results.

Figure 1: Principle of the Bridgman-method (right) and the casting technique (left) for the production of photovoltaic silicon (after Woditsch, Kostenreduktionpotentiale bei der Herstellung von PV-Modulen, FVS 2000)
Analyses of the heat and mass transport during casting of photovoltaic silicon

during solidification of silicon in a mould with the dimension 55x70x23 cm³ was developed by using the code STHAMAS3D . With this model the influence of several process parameters such as axial temperature gradient in the melt, crystallization velocity, and radiation temperature at the free melt surface on the deflection of the crystallization front, on the flow pattern and on the maximum flow velocity in the melt was investigated.

In figure 2 typical flow pattern and shapes of the solid-liquid interface are shown. Depending on the process parameters used flat, concave or convex interface shapes are observed. In the case of the convex interface shape the flow is directed at the interface from the centre towards the wall of the mould, whereas in the other cases, the flow direction is vice versa. In the investigated parameter space the flow velocity is typically between a few mm/sec up to a few cm/sec. The deflection of the crystallization front varies from -2cm to +5cm.

The obtained results show, that convection is important for the considered mould dimensions and process parameters and has an influence on the heat transport and especially on the shape of the crystallization front. Therefore, convection in the melt should not be neglected when analysing the heat transport processes during directional solidification of photovoltaic silicon.

Figure 2: Typical, numerically calculated flow pattern and interface shapes in a vertical cross section through the mould during directional solidification of photovoltaic silicon.
Reaction model of the formation of CIS for thin film solar cells

Chalcopyrite semiconductors are promising absorber materials for thin film solar cell applications due to their high absorption coefficient. The most important compound is Cu(In,Ga)Se2 (CIS). In Germany the state of the art in CIS solar cell development is the installation of two pilot manufacturing sites for the production of modules with monolithically integrated cells.

It is expected that the fabrication of solar modules by thin film technology reduces significantly the production cost compared to the silicon technology dominating the market today. The material and labour costs are decreased because of the reduced material usage, the process technology simplified by integrated series connection, as well as the direct deposition of thin absorber layers on large glass or flexible substrates.

Since 1998, Shell Solar GmbH (formerly Siemens Solar) is the first manufacturer of commercial CIS solar modules with up to 40W. While presently more than 1MW of this first CIS-module generation have been tested successfully on the market, the expansion of this technology demands further development in three areas:

1. Reduction of the production cost by higher operational capacity of in-line manufacturing with modules larger than 1m² and more than 100W peak power compared to the present batch processes of smaller substrates (<0.5 m²).

2. Increased efficiency at maintained economic lifetime.

3. Development of cost-saving alternative processes for further reduction of cost of material and capital.

CGL has been working in the field of chalcopyrites for solar application since the FORSOL (Solar Energy Research Association) program which was established in 1995 with the support of a number of institutions throughout Europe.

This results in a direct cooperation of CGL and Siemens (now Shell Solar GmbH). The main topics of this project, which was supported by the Bavarian Research Foundation, were the first two R&D tasks mentioned above. The investigations concentrated on the characterization and optimization of the thin-film deposition and the absorber formation process. To achieve further insight in the involved chemical reactions in-situ methods are applied like Thin Film Calorimetry (TFC), in-situ resistivity measurements and X-ray-diffraction (in cooperation with the Institute of Crystallography and Structural Physics, FAU Erlangen - Nürnberg) during the semiconductor formation.

By the successful end of the project in April 2004 new insight into the absorber formation process had been gained. Fig 1 summarizes schematically the reaction processes and kinetic mechanisms which occur during the formation process of the PV absorber by the so-called Stacked-Elemental-Layer process developed by Shell Solar. Apart from such qualitative results quantitative reaction models have been developed. Moreover, several promising alternative processes – either by altering the deposition process or the thermal treatment of the absorber – with a potential for increased efficiency and reduced cost could be proposed.

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Reaction model of the formation of CIS for thin film solar cells

- This reaction determines kinetics of selenization
- Controlled by boundary reaction
- Extraction of Cu from Cu$_{11}$In$_9$ leads to release of elemental In which selenizes quickly

- Behavior of Cu-selenides only determined by thermodynamics:
  - Because of fast Cu-diffusion their formation and decomposition are not kinetically dominating
  - Transformations of Cu-selenides is either caused by Se deficiency or by peritectic reactions

- Formation of In$_3$Se$_3$ is kinetically limited by nucleation until 200-240 °C, depending on deposition parameters
- At higher temperatures the reaction is fast and not limiting the overall process

- Formation of InSe is a slow reaction at 260-350 °C
- Limited by kinetics of nucleation and growth of crystallites
  - Very dependent on heating rate

- Formation of CIS by two different mechanisms possible:
  - From CuSe + InSe
  - From Cu$_{2-x}$Se + InSe

The investigation of such alternative processes (the third above mentioned R&D task on the path toward mass-production of CIS PV-modules) is the goal of a new project which began in October 2004. Apart from the members of prior R&D projects – CGL, Shell Solar GmbH and the Institute of Crystallography and Structural Physics (FAU Erlangen - Nürnberg) – Atotech Deutschland GmbH is joining the cooperation. Their development of an electrodeposited chalcopyrite absorber promises a high potential of reducing CIS absorber production cost.

Two scientists and one technician will be involved in the R&D project at CGL. The planned duration is 3 years. The cooperation is supported by the German Federal Environment Ministry.

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Influence of convection on the microstructure development of alloys

Nowadays the effects of convective heat and mass transport during alloy solidification experience enhanced attention in the field of solidification research. IISB has initiated in 2000 the research program MICAST, which focuses on a systematic analysis of the effect of convection on the microstructure evolution in cast Al-alloys. One major goal of the MICAST project is the definition of microgravity experiments, which allow the performance of solidification experiments under purely diffusive conditions. Controlled convective conditions are achieved by the application of time-dependent magnetic fields.

The main task of the IISB is the support of the experimental investigations by global numerical simulations. The calculations are performed with the software package CrysVUn, which is developed at IISB since several years. The software was extended with appropriate models for columnar solidification of alloys, which differs in many ways from the solidification of semiconductor materials.

Usually, alloys solidify with a dendritic interface, revealing a complex growth morphology on a microscopic scale. On the macroscopic scale this region is usually termed the mushy zone, where solid and liquid phase are coexistent within a certain temperature interval. The resulting microstructure of the alloys is a consequence of capillarity effects, thermodynamic constraints and transport processes occurring inside this region.

The main goal of the numerical simulations is to support the preparation and the theoretical analysis of the experiments as performed within the MICAST project. This includes the determination of suitable magnetic field parameters and the evaluation of the solidification conditions like the growth velocity and local composition variations due to

Figure 1: Global thermal model of a furnace insert for material science experiments onboard the International Space Station (a) and a comparison of the model predictions with experimental measurements: temperature at a thermocouple inside the cartridge (b) and heater power for a heating element located in the cold zone of the furnace (c).

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Influence of convection on the microstructure development of alloys

macrosegregation.

IISB is additionally responsible for the development of thermal models of the furnace inserts, which are foreseen for the material science experiments onboard the International Space Station.

The implemented models have been systematically validated in the last year. A typical result for one furnace is shown in figure 1. Regarding the complexity of the model a remarkable agreement for the predicted temperatures and especially for the predicted heater powers was obtained.

In the MICAST experiments performed so far a significant influence of convection on the microstructure development was observed. Due to the changed heat and mass transfer lower values for the primary arm spacing and increased values for the secondary arm spacing result. Numerical results at CGL illustrated the tremendous segregation effects due to the magnetically controlled flow. The predictions were qualitatively confirmed by experimental results.

Usually, industrial relevant castings are solidifying partly with an equiaxed microstructure. For this reason, the solidification model of CrysVUn is currently further developed to treat also this important solidification type. Equiaxed solidification is in many ways different from columnar solidification. For this type of solidification, the solutal undercooling ahead of the solidification front has to be taken into account and the solid phase is non-stationary. This makes the numerical treatment difficult and even today several modeling issues are still unresolved. The current model is restricted to the pure diffusive case (figure 2).

IISB is financially supported by ESA and the DLR.

Figure 2: Multiscale modeling of alloy solidification. One of the latest developments of CrysVUn is the incorporation of a dendrite growth model, based on a multi-scale approach. The introduction of different physical phases (a) allows modeling the undercooling in the liquid zone ahead of the solidification front (b). Test calculations show a good agreement with previously published results (c).
Modelling the dynamics of dislocations during growth of semiconductors and optical crystals

Structural defects, like dislocations have a big importance for the application of semiconductor crystals as substrates for device manufacturing. In many cases, these dislocations have negative effects on the quality of the manufactured devices. The main cause to generate dislocations is the plastic deformation of the crystal. During the growth process of the crystal from the melt or from the gas phase thermo elastic stress is generated as a result of an inhomogeneous temperature field in the growing crystal. This can cause the generation and the movement of dislocations.

As a result of the mentioned problems the Crystal Growth Laboratory develops a numerical model to describe the dislocation dynamics during the growth of semiconductors and optic crystals in the framework of a research fellowship of the "Förderkreis für Mikroelektronik e.V." After the verification of the model with experimental data, the model will be used to analyze the influence of different process parameters on the formation and on the distribution of dislocations in the crystal.

The dynamics of the dislocations is a physically extremely complex process. Thus, the development and the verification of the dislocation model take place step-wise. In order to get from a qualitative description of this problem to a quantitative one, additional physical effects will be added step-by-step. With this iterative procedure it is possible at every step of this development to perform parameter studies with the corresponding model.

The first assumption for the development of the dislocation model is the possibility to calculate the thermal stress considering the plastic deformation. In the first step, the thermo elastic stress model already available in the software packet CrysVU n is extended taking into account the plastic deformation.

To describe the dependency between plastic deformation in the crystal and the motion of dislocations the classical Alexander-Haasen model (AH-model) is used. First, the implementation of the AH-model was done in an axisymmetric quasi-stationary approximation. For specific physical conditions, for example constant effective stress, the equations of the AH-model can be analytically solved. The implemented AH-model in CrysVUn is verified with this analytical solution. The outcome is a good agreement between the analytically calculated values and the results obtained from the model implemented in CrysVUn.

The quasi-stationary approximation of the available AH-model gives information about the dislocation dynamic.

![Figure 1: With CrysVUn computed temperature field (left) and dislocation density N (right, max. \(N_{\text{max}} = 2000 \text{cm}^{-3}\)) in a GaAs-crystal with 8cm diameter.](image.png)
Modelling the dynamics of dislocations during growth of semiconductors and optical crystals

during the crystal growth process, not during the cooling process or during the subsequent annealing steps. Therefore, the existing implemented model was extended to be able to calculate time-dependent phenomena. With the implemented time-dependent model it is possible to compute the dislocation dynamics and the plastic deformation during the cooling and/or annealing process. For the verification of the implemented model, the dislocation density was computed for short time interval. These results can be compared with analytic estimations. This analysis gives a good agreement between the computed and the estimated results. So far, this time-dependent implemented model is only applicable for constant crystal geometries. For the time-dependent calculation of the dislocation density during the growth process the available model will be extended.

The dislocation dynamic is in reality a three dimensional process, in which each slip plane and slip direction has importance. Therefore, in the second development phase it is planned to extend the model further in order to be able to calculate the dislocation density in each slip plane. The sums of the density from each slip plane give then the density of dislocations in the crystal. Such calculations are only possible in the three dimensional description of the crystal. Thus, a program for 3D stress calculations was developed and verified, which can be transferred to the dislocation on model in the future.

Parallel to the development of the model the study of the effect of the growth conditions on the dynamic of the dislocations for the growth of III-V semiconductors and optical crystals are continued.

Figure 2: with CrysVUn simulated temperature field (left) and final dislocation density (right) in an InP-crystal after 500sec annealing in a constant temperature field. On the right side, the evolution of the dislocation density and the second invariant of the stress at the point marked with the arrow are shown.
The efficient solution of the convective heat and mass transport in the melt and in the gas atmosphere remains a big challenge for modeling of crystal growth processes. For example the spatial resolution of the numerical mesh has to cover 4 to 5 orders of magnitude ranging from the global dimension of the growth facility down to the diffusion boundary layer in the vicinity of the solid-liquid interface. In order to compute efficiently and robustly the convective heat and mass transport a new hybrid-model was developed for the computer program CrysVUn. The hybrid-model combines the advantages of the two existing simulation packages CrysVUn and STHAMAS2D. Both codes are applied for the global simulation of crystal growth processes, but they are using different numerical methods.

The goal of the current development was to combine the strengths of CrysVUn, which are the automatic mesh generation, the inverse modeling capability and the user friendly graphical user interface with the main advantage of STHAMAS which is the fast solution of fluid dynamic problems.

In the hybrid version a new method is implemented using overlapping grids. Heat conduction, thermal surface radiation and inductive heating are treated on the unstructured grid using the methods existing in CrysVUn already. Convection, turbulence and species transport are solved on the block structured grid. Therefore, the corresponding algorithms for the block structured grid are incorporated into the code CrysVUn. A comfortable preprocessor for the automatic creation of the block structure and for the structured grid was developed. The corresponding features of the graphical user interface were extended. This includes also the visualisation and the numerical analysis of the results obtained on the hybrid mesh.

The new hybrid code CrysMAS can compute laminar and turbulent convection in the melt and in the gas in the stationary and in the transient mode. The fluid dynamics calculations can be performed simultaneously in multiple connected fluid domains with different fluids. The species transport can be analysed correspondingly in the multiple fluid domains. The

Figure 1: The global numerical model of a Cz puller. On the left the hybrid grid is shown. On the right the computed temperature distribution is shown for an Ar gas pressure of 3bar.

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Efficient solution of fluid dynamic problems with the aid of a new hybrid-model

fluid-fluid interaction on the common fluid interfaces are described by means of automatically set boundary conditions. The phase transition between the crystal and the melt is computed by the phase tracking method. The inverse modelling can be done now without any restriction for the combined unstructured and block structured grid.

This hybrid approach consisting of the simultaneous use of unstructured and block structured grids allows now an efficient, robust and user friendly solution of fluid dynamic problems which occur in the daily work during modeling of crystal growth processes.

A first example for the application of the new hybrid model is the calculation of the gas convection occurring during growth of GaAs crystals by the Liquid Encapsulated Czochralski method (LEC, see figure 1). While the computation of the turbulent gas convection takes a half day or even longer by using CrysVUn, a converged solution is now obtained within a few hours. In addition, the time for the preprocessing which requires a few hours by using STHAMAS reduces now to a few minutes only.

Another example is the computation of the melt and gas convection during growth of silicon tubes by the EFG-method (Edge-Defined-Film-Fed-Growth). The EFG-technique is a cheap method for the production of photovoltaic silicon. In this technique the shape of the crystal is defined by a capillary supplied with silicon from a melt pool. The multicrystalline crystal is pulled vertically out of the top of the facility.

By using the new hybrid model the convective heat transport can be treated now within a few hours starting from the formulation of the problem until the visualization of the obtained results.

The presented developments were financially supported by Freiberger Compound Materials and RWE Schott Solar.

Figure 2. The global numerical model of an EFG facility: Left temperature field, right flow pattern in melt and gas. The insert shows the z-component of the flow velocity of the gas and the melt in the vicinity of the melt meniscus.
Innovative methods for describing the heat transport through radiation in semitransparent materials

Optical crystals are of great importance for lasers, scintillators, non-linear optics, windows, lenses and other applications. In order to simulate the growth process of such materials we decided to implement a new numerical model for describing the interaction between thermal radiations and participating media in CrysVUN is a software package for global modeling of crystal growth processes having either translation symmetry or a rotational symmetry (cylindrical symmetry).

As the name says, participating media is interacting in many ways with the thermal radiation. When the radiation enters such a material many physical phenomena occurs such as absorption, reflection, refraction, volume emission, and dispersion. So this material behaves quite different from opaque (where the radiation travels unaffected through the material). Taking into account this and the difficulties when trying to numerically best describe the participating media we decided to implement a model based on the ray tracing technique. There are many models developed for the treatment of radiation in participation media but in order to get higher numerical accuracy one should consider in such models higher order approximations which rise many difficulties such that: huge equation systems to be solved, longer computation times, finer numerical grids. Taking also into account the symmetry of our problem we have chosen to implement a model based on the ray tracing technique which has the advantages of being grid

Figure 1. The axial temperature profile computed with our model (red line) as opposed to a benchmark solution (blue dots) for the case of two neighbor materials (one opaque and one semitransparent). For reference also the solution for the case of opaque material is given.
Innovative methods for describing the heat transport through radiation in semitransparent materials

independent, not requiring us to solve huge equation systems, allowing us to implement boundaries in a simple way and requiring less memory than other approximations.

The most important physical measure for our model is the intensity of the radiation coming from a given direction. To compute this we send rays in many directions (based on a given spatial discretization scheme) and follow them until a given stopping criteria is met. Whenever a surface is intersected we decide if the ray is reflected or refracted or absorbed based on the material properties. So we end up with a lot of ray paths which are used later on to compute the source term in the global temperature equation. By solving this equation the temperature field in every point is known.

The model is implemented in our software package CrysVUn and the solution provided is in good agreement with a benchmark solution we have used to test the model (see Figure 1).

In figure 2, the influence of the absorption coefficient on the axial temperature profile in a semitransparent medium is presented which is placed in a typical VGF-furnace. It can be seen that the absorption coefficient has a big influence on the thermal field.

Figure 2. The axial temperature profile along the symmetry axis in a typical VGF furnace, in which a semitransparent crystal is grown in the crucible. The plots are done for different values of the absorption coefficients of the participating medium.
ORCAN – An efficient framework for scientific computation

The numeric group of the Crystal Growth Laboratory (CGL) at Fraunhofer IISB has been developing software for simulation of crystal growth and related processes in complex geometries for several years. Up to now, complex growth apparatus have been modeled using two-dimensional or axisymmetric approximations.

However, there is a strong demand to perform fully three-dimensional simulations, and to include additional physical models. We arrived at a point where it became obvious that it is impossible to develop everything by ourselves. Thus, there was a need for some environment which would allow to use existing packages for some parts of the software in order to focus the development efforts on that parts where the CGL has the expertise.

The Open Reflective Component Architecture (ORCAN) was designed to build the basis for rapid incorporation of existing software packages into large-scale software projects - including the ability to replace packages with a minimum of effort. It consists of a collection of libraries implemented in portable C++ classes.

To make it ‘easy to use’ it is designed to present as little framework overhead as possible to the application developer. The user is isolated from all framework specific operations like loading components, identifying their content and resolving symbols.

Components in ORCAN do not implement any functionality, they solely define a set of interfaces. A realization of a component implements one or more interfaces and builds up the actual functionality of the component.

Due to a strict component/interface specification it is possible to replace the implementation of a component, even at runtime. The cost of integrating an existing software package as a component realization is limited to interface adaptation.

ORCAN components are reflective, thus, the application can query the implementation for its intrinsic parameters. This reflectivity property is also used for the automated generation of a component’s graphical user interface (GUI).

While ORCAN itself can be used for arbitrary applications, a set of components named ORCAN/Sim has been defined especially for standard simulation purposes. Existing components include mesh management, mesh generation, FEM discretization, linear equation system solving, and visualization toolkits.

This predefinition of components for simulation applications enables different groups to exchange their implementation of a specific component without any integration overhead.

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Another benefit of the component architecture is the ability of rapid application prototyping. A program can easily be assembled by using existing realizations of ORCAN/Sim components. The developer can write an application in a fractional of time and with the automated GUI generation of ORCAN/wx with a certain amount of user-friendliness.

An example of the successful application of the ORCAN framework is CrysVUn3D, a program for fully three-dimensional simulation of global heat transfer in crystal growth and related processes. The focus of this project is on the realistic modeling of thermal radiation under consideration of participating media and different reflection models.

Before we could start to work on the actual project, we had to setup an application environment. For example, the geometry of the furnace must be imported and approximated, a mesh generator was necessary to create tetrahedron meshes for the FEM discretization and a solver for linear equation systems must be included. Thus, a good deal of time must usually be spend to prepare for the real task. With ORCAN as the base system of CrysVUn3D, together with the already available realizations of components, the expenditure of time to setup the application could be reduced dramatically.

With the definition of simulation specific components in ORCAN/Sim and the collection of ready-made realizations, this framework is also applicable by other groups in the simulation software area. The entire ORCAN framework and a number of additional utilities, as well as most of the realizations, are open source.

Up to now, different research organization in Germany are already using or plan to use the ORCAN framework for their simulation software. They all profit from the use of prefabricated component realizations and can address their research problems. Their developments in turn may lead to new component realizations, hopefully available as free software.

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Recent Publications:


Figure 2: The program CrysVUn3D is an ORCAN based simulation software to calculate coupled head conduction and heat radiation.
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Publications

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in Computational Modelling and Simulations of Materials (eds. P. Vincenzini, A. Lami) 2003 Techna Srl. 267-278

V. Socoliuc, D. Vizman, B. Fischer, J. Friedrich, G. Mueller
3D numerical simulation of Rayleigh-Bénard convection in an electrically conducting melt acted on by a travelling magnetic field
Equipment

Laboratory space
200 m² laboratory space in total at university and Fraunhofer IISB plus offices

Crystal growth
- several multi-zone furnaces for vacuum and high pressure conditions (for 2" - 6" crystal diameter)
- several multi zone furnaces for sample preparation and growth of small diameter crystals
- 1 liquid phase epitaxy facility

Analysis and characterization of materials
- Several optical/infrared microscopes
- Access to high resolution microscopes
- Mapping system for optical spectroscopy of semiconductor wafers
- Interferometric profilometer for surface analysis of semiconductor wafers
- X-ray Laue camera
- Hall-measurement-system (temperature dependent 15K-650K)
- Measurement system for characterization of deep and shallow levels by capacitance techniques (CV, DLTS) and by conductance techniques (TSC, PICTS)
- Differential Thermal Analysis for determination of phase diagrams
- Differential Scanning Calorimeter for thermodynamic and kinetic studies
- Thermogravimetry

Preparation and metallography
- Facilities for preparative work related to wafer preparation (grinder, annular and wire saws, lapping and polishing equipment)
- Several evaporation systems
- Sputtering systems (DC, 6" target diameter)
Contact and travel information

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By plane
From Nürnberg (Nuremberg) airport use taxi (15 minutes) or bus 32 to Nürnberg-Thon and then bus 30/30E to Erlangen-Süd (30 minutes).

By train
From Erlangen station, use taxi (15 minutes) or bus 287 to Stettiner Straße (30 minutes). Convenient train services from Nürnberg Hauptbahnhof (central station) to Erlangen station.

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