Scientific Cooperation between Hanover University, Latvian University and Wacker Siltronic AG on the Field of Mathematical Modeling in Crystal Growth

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At the beginning of 1983 I received a letter from a young Latvian scientist in which he ask me to host him in Hanover to carry out his scientific continuous education work, offered by the German- Soviet- Exchange-Agreement. It was very clear to us that only excellent physicists were assigned for that program. Therefore, we could expect a highly qualified person, who would be able to contribute substantially to our R&D work in Hanover, as he had been working in a quite similar scientific area: The electromagnetic and hydrodynamic investigation of metallurgical installations.

Of course, I supported that application, a DAAD scholarship was granted, a working scheme was agreed on and in December 1985 (2 1/2 years after), just before Christmas, Dr. Andris Jakovics arrived in Hanover. This was the actual beginning of our scientific cooperation, and he was the first Latvian in our Institute and he has supported our work very effectively.

Although the subjects of research in Riga and Hanover were very similar, differences existed as far as the customers and the approaches were concerned: For the Latvians the work was focused on the physical analysis and the mathematical modeling, for us in Hanover the engineering methods, including numerical process modeling, and experimental investigations were in the center of interest. Those different approaches facilitated our mutual work and the development of our cooperation significantly. A very fruitful period of collaboration began.

In the second half of the eighties it became possible to activate mutual visits and real common research. In 1988, the first contract was formulated and signed some time later by the Universities of Latvia and Hanover. Subject of the joint work was the wide field of Electrothermal Processes in Metallurgical Devices. For our partner university it was the first agreement of such kind with a Western- German university. The actual Latvian performers of the research work were at that time the lecturers, the staff- members and the students of the Chair for Electrodynamics and Continuous Mechanics and from the Hanover side the staff of the Institute for Electroheat, today Institute for Electrothermal Processes.

The following years were characterized by a big mobility flow mainly from Riga to Hanover, although parts of the mutual projects were worked out in each of the home universities. The financing of the short- term and long-term visits of all the Latvian researchers was critical, because even a German academic institution like ours was not able to provide such a substantial support. But with the help of different German foundations, associations and industrial partners it became possible to grant the necessary funds. I would like to mention here some of our long-term guests and part-time staff- members by name and also name the sources of the funds received:
Dr. Andris Jakovics**:** Sponsored by DAAD, the Alexander von Humboldt-Foundation and the Robert-Bosch-Foundation, in total about 4 years.
Dr. Andris Muiznieks**:** Sponsored by the Electroheat-Association EWH, the DAAD and the VW-Foundation. He has been a fellow of EWH since 1996, and been with us about 10 years.
Dr. Janis Virbulis**:** Sponsored by the Electroheat-Association for about 3 1/2 years.
Dr. Sandris Lacis**:** Sponsored by DAAD (10 month).

Moreover, many other researchers have visited our institute and they were also fully integrated in our team. Their contribution to our R&D work was very important and highly appreciated by our industrial partners. On the other hand staff- members from Hanover have visited our partner university in Riga, taking part in different activities such as internal seminars, lectures, workshops, conferences, but especially collaborating with the Latvian colleagues on our joint projects.

The cooperation has made it possible for the Latvian researchers to take part at several international congresses and conferences with their reports, not only in Germany but also in other countries:
A.Muiznieks has been in Canada, several times in USA, in Italy, in Belgium, …
A.Jakovics several times in France, in Sweden, in England, in Italy,...
L. Buligins in Israel, in Sweden,...
J. Virbulis in USA.
This list is not complete because some other persons from Riga have traveled to foreign countries as well.
We Germans have taken part in MHD- conferences in Riga, in MAHYD- and Heat-Transfer conferences as well as in some "Modeling Colloquia" , taking place in Riga. The contributions to all those international conferences reflects the wide spectrum of topics of our mutual work, whereas The Electromagnetic Processing of Materials and the Modeling of Crystal Growth Processes have been in the focus of our efforts.

Besides other activities, the Semiconductor Material SILICON has been in the center of the research work in the Hanover Institute since I have taken over the management in 1979. In the eighties, together with Siemens, we have carried out projects devoted to the carbothermic production of Solar-Grade Silicon, the energy conversion in such processes, the modeling of the directional solidification of solar-grade silicon, and we undertook first steps to model the electrodynamic convection in silicon floating zones. At that time not much had been known about the mathematical modeling of real FZ growth under industrial conditions. Though the needle-eye technique enabled the crystal growers at that time to produce rods with diameters of 50mm, 75mm and more, but the knowledge was mainly based on experience and not so much on a deeper physical understanding. A common saying was (and is): *We are glad if the process runs, even we do not know exactly why!*

And then, the very well educated, young physicist from Riga, the very best in electrodynamics and hydrodynamics, highly motivated, were in the starting position in Hanover to contribute effectively to our research work. It was an obvious choice to assign the FZ modeling project to them among other tasks, because all necessary prerequisites were fulfilled. In this way first joint investigations of the FZ problems began. The main target was the development of mathematical models and numerical codes for the determination of the electromagnetic field distribution, the connected thermal field including the calculation of melting and solidification interfaces as well as the free surface of the melt. Finally, the fluid flow motion under the different acting driving forces had to be calculated as well. Step by step a system of coupled mathematical models and useful numerical tools was developed. The obtained results were reported and many detailed problems were studied intensively. In the first half of the nineties Andris Jakovics, Andris Muiznieks and Janis Virbulis essentially contributed to that topic. First common reports were given in Toronto ('90), San Francisco ('94), Miami ('94), Riga ('95), Berlin ('95), and several papers were published. Janis' master thesis under the supervision of Dr. Jakovics was also devoted to the FZ modeling (1992), and after that, he has prepared his PhD thesis in Hanover on the same topic. He did this very successfully, described the complete FZ process, i.e. he developed a complete chain of models that enables us to calculate not only the already mentioned fields, but also the dopant distribution and in a first approximation the mechanical stresses in the crystal. Andris Muiznieks has taken part in this activities after having moved to Hanover more and more in a key position. The first complete description of the FZ process was presented in a paper which was of special interest to the industrial crystal growers. The title is "*Interface shape, heat transfer and fluid flow in the floating zone growth of large silicon crystals with the needle-eye technique*" . Its authors were beside others Dr. Anke Lüdge and Dr. Helge Riemann. They belong to the Institute for Crystal Growth (IKZ) in Berlin, and they have thoroughly validated our calculated results experimentally. Many discussions in Berlin and in Hanover have brought out a deeper understanding of the problems and have supported the further development of models for the FZ process.

The obtained results showed the expertise and the special qualifications of our Latvian friends in Hanover and gave us the chance to cooperate on a contractual basis with one of the biggest manufacturers of Electronic Grade Silicon in the world, the Wacker Siltronic AG (WSAG) in Burghausen, Germany. In the field of FZ-Silicon, which comprises about 5% of the total Si-Market, WSAG is first worldwide. Our cooperation started with the first formal agreement end of 1994. The cooperation based on mutual trust has also included the IKZ, and all groups together have forwarded the project remarkably. The success achieved lead to an job-offer to Janis from Wacker and since 1996 he has been a member of the working group "Modeling". In this function he is now sitting on the other side of the desk when we are meeting Wacker in Burghausen, giving instructions to us. Approximately six years of close, fruitful and intensive working together with Wacker in FZ growth have yielded a lot of new results and deeper knowledge. But the modeling of a fairly well operating process only is not enough. Industrial partners expect distinct suggestions to improve their processes. Therefore, Andris Muiznieks, Georg Raming and some others have given very useful proposals, for example, how to reduce the radial dopant variations in a macroscopic and microscopic scale. It has been possible to show that the application of external magnetic fields during the growth of large diameter crystals helps to make these profiles more uniform. Other important challenges have been linked with the so called "Ziehbarkeit", i.e. the increase of the growth rate without loosing stability, with the formulation of a criteria for the dislocation generation and cracking conditions, especially in large rods of 150mm and 200mm diameter. I'm sure that the reports given later will discuss those problems in detail.

All the time, our colleagues from the Wacker FZ group, namely Dr. Grundner, Dr. Knobel and Mr. Altmannshofer, have been providing a very open atmosphere and given us valuable inspiration for our work, influenced by their enormous practical experience. Only a close and confident cooperation between groups can lead to such good results as we have worked out together. And the person who has especially guaranteed the smoothly running of our mutual work has been our good old friend Janis Virbulis, forming the bridge between Burghausen, Hanover and Riga.

Up to now I have reported rather detailed about the FZ activities which we are dealing with as academic and industrial partners. However, besides FZ growth, we are cooperating with Wacker in crucible pulling of 300 mm diameter CZ crystals as well. Since 1998 we have been working together closely in this field within a formal agreement. Dr. Wilfried von Ammon, head of the development division of WSAG, a well known expert in crystal growth and defect engineering, has asked us to contribute to the 300mm project. The increase of crystal diameter up to 300mm and crucibles up to 36" in silicon CZ growth during recent years has led to several problems that cannot be solved with the conventional technology. That serious challenge has led to the idea to apply external magnetic fields to influence the hydrodynamics independently to facilitate the necessary control of the growth process. However, the development of magnetic systems and the required growth experiments in industrial CZ pullers are very expensive and time consuming. The numerical modeling of the melt behavior has grown to become a powerful tool. It can shorten design cycles, reduce development costs, and demonstrate how to use the installed magnet system. Although the turbulent CZ melt-flow is characterized by a 3D time dependent flow and temperature distribution, we have used an axisymmetric 2D model, because a fully 3D transient simulation of large melt volumes of up to 300kg is a very time and resource consuming task. On the other hand, for a successful application of magnetic fields in an industrial surrounding it is necessary to reveal trends and to develop a qualitative understanding of melt behavior under field induced convection. More information about the results of the influence of magnetic fields on the crystal growth will be given in the next report by Janis Virbulis.

Anyway, we have performed numerous simulation runs with several parameter combinations to investigate aspects that are of particular importance for industrial process development. Andris Muiznieks and Thomas Wetzel have carried out the model development as well as the numerical calculations in Hanover, assisted by Latvian students in Hanover and in Riga. The attainable accuracy must be evaluated using experimental data and has to be considered when using the simulation results. The experimental investigation of the CZ process of large diameter silicon under the influence of magnetic fields has been carried out by Prof. Y. Gelfgat and Dr. L. Gorbunov at the Institute of Physics in Salaspils, University of Latvia. They revealed excellent experimental results for the fluid flow motion and the temperature distribution in the GaInSn-model-melt of a big laboratory setup. The 20" diameter crucible allows the several measurements without disturbing the fluid flow and temperature field to much by the probes used. The characteristic similarity numbers of both, the 20" laboratory setup and a typical 28" silicon puller, demonstrate that the results of the physical modeling system are useful. They can serve not only as reference to compare simulation results, but they make clear that the model setup models the situation in an real CZ puller with a large crucible very well. Moreover, it shows that the simulation models tested experimentally are transferable to the simulation of the actual silicon CZ process. The verification shows acceptable results.

The comparison of such a high number of calculated and measured values with all the possible errors and misunderstandings requires a very intensive and confident collaboration between the groups involved. Fortunately, all the groups in Riga, Hanover and Burghausen and that in Salaspils have communicated very openly and successfully. This is an eminent advantage for any further cooperation.

I think, it is obvious that it is not possible to touch adequately all important and interesting aspects of such an excellent scientific cooperation between the Universities of Hanover and Latvia and the Wacker Siltronic Company. Because all of us know that working together successfully is mainly based on the people involved and, therefore, I am convinced that all conditions for a further close cooperation are fulfilled. Another good reason is that meanwhile 3 researchers from Hanover have entered Wacker. After Dr. Janis Virbulis, Dr. Thomas Wetzel and Dr. Georg Raming have taken over interesting positions 1 1/2 years ago. All of them are active in the 300mm project and partially engaged in the FZ technology. These are good reasons to be sure that our mutual effort to push the development of the FZ and CZ processes further will yield new and attractive future projects.