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Numerical simulation - an important tool for industrial processing of bulk semiconductor crystals

A. Seidl

Abstract

In this paper, the benefit of numerical simulation for the development of a special crystal growth technique for the processing of silicon wafers for photovoltaic applications on an industrial scale is demonstrated, as an example for the importance of numerical simulation for industrial processing of bulk semiconductor crystals in general. Depending on the complexity of the problems to be treated, 2D and 3D modeling of heat flow, temperature distribution, mass transfer, gas and melt flow are treated, and their impact on stress and plastic deformation are examined.

Introduction

The controlled crystallization of bulk semiconductor crystals on an industrial scale is basis of the complete semiconductor-related industry since it was recognized in the late 1940ies that the availability of semiconductor material of high crystalline quality and purity is essential for the realization of efficient electronic and optoelectronic devices on the micro- and macroscale [1]. Although a broad variety of semiconductors was found, only few of them (Ge and Si, and with some restrictions few III-V and II-VI compounds) are suitable for bulk mass production by controlled crystallization from the melt. Among these, Si evolved quite fast to be the leading material for the majoraty of applications, from microelectronics to photovoltaics and power electronics. Today, worldwide about 50.000 tons of high purity polysilicon are produced per year and crystallized by various methods into mono- and multi-crystalline bodies.

1. Modelling of industrial processing of bulk semiconductor crystals

Independent of the crystallization technique used, controlled crystallization of high-quality semiconductors of special properties is an inherently multi-scale challenge, with relevant length scales ranging from furnace dimensions to atomic-sized features in the grown crystal [2]. With increase of computational power of computers, only enabled by the very semiconductor crystals, process modeling for development and optimization of these crystallization techniques could be more and more supported by numerical simulation. Today, numerical simulation is a key tool for the industrial processing of bulk semiconductor crystals, ranging from global-scale furnace heat transfer models to local-scale mass transfer or defect formation models [3].

2. Modelling of induction heated Edge-defined Film-fed Growth (EFG)

Edge-defined Film-fed Growth (EFG) is an example for a cost-effective technology for the production of silicon wafers for photovoltaic applications [4]. By EFG, growth of thin-walled, polygonal silicon tubes takes place from a liquid meniscus film confined to the top of a capillary die wetted by the silicon melt. The wafers are cut from these tubes by laser cutting. EFG meets the demands of an economical material consumption since silicon losses are minimized: the thickness of the crystallized, hollow body is equal to the later wafer thickness.

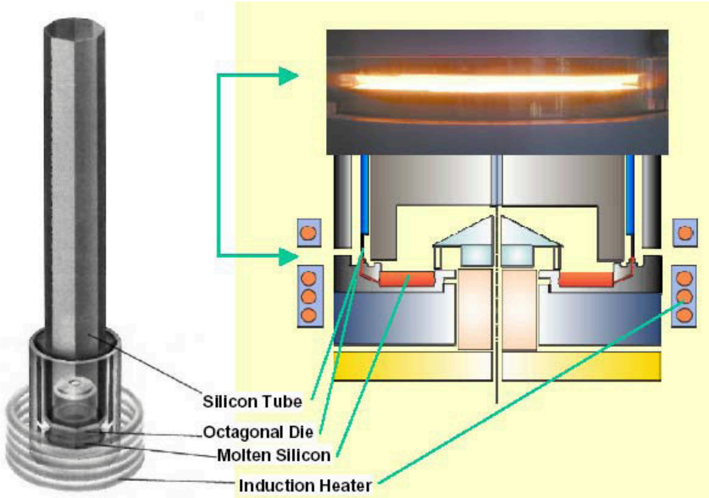

Fig. 1. Growing silicon tube and sketch of an EFG furnace geometry.

Fig. 2. Top-down view along a growing silicon tube.

The principle of the crystallization process is shown in Fig. 1. The crucible and other graphite components are heated by two induction coils. The polygonal tube is growing from an integrated capillary die, continuously replenished by molten silicon. The wall thickness of the silicon tube is controlled at thickness setpoints in the range from 200 to 300 µm. Today´s face width of the tubes is typically 125 mm; the tubes grow up to 7 m in length with a pulling speed of up to 2 cm/min [5]. A top-down view on the growth of an octagonal silicon tube is shown in Fig. 2.

The induction coils are supplied from two high frequency generators. The main induction coil is located in the region of the crucible. The secondary coil is responsible for setting the vertical temperature gradient along the tube. The close position of both induction coils leads to strong electromagnetic coupling. Additionally, the common magnetic flux strongly depends on the phase shift between the induction coil currents.

A special characteristic of EFG silicon tube growth is the very high vertical temperature gradient across the melt-crystal interface, necessary to dissipate the latent heat at high growth speed. The vertical temperature profile along the growing and cooling silicon tube is connected with thermal stresses and plastic deformation and it can cause undulation of the tube faces. Furthermore, horizontal (and azimuthal) temperature inhomogeneities lead to different thickness of single tube faces, which must be minimized. This requires detailed understanding how different graphite components are heated, how the different induction coils interact, and how this influences the temperature distribution. Many questions can be answered by 2D simulations, which treat the tube and the furnace as rotationally symmetric. But the real geometry of the crystallization process has strong impact on many issues of the temperature field of polygon shape and therefore requires 3D simulations for detailed analysis.

2.1. 2D axisymmetric modelling of heat and mass transfer

Operating conditions of an EFG process are given by induction heating of the hot zone, forming the quasi steady-state temperature field in the furnace. Therefore, numerical simulation of an EFG process requires both electromagnetic and thermal calculations. Electromagnetic analysis gives out the Joule heat distribution in the furnace as well as the induction coils currents. Electro-physical properties of the hot zone parts must be input to the electromagnetic analysis also. Due to temperature dependence of specific resistance and magnetic permeability, the temperature distribution must be known to correct the properties in electromagnetic analysis. On the other hand, the temperature field in the thermal model is formed by the Joule heat distribution calculated in electromagnetic analysis. This requires a coupling between electromagnetic and thermal analysis.

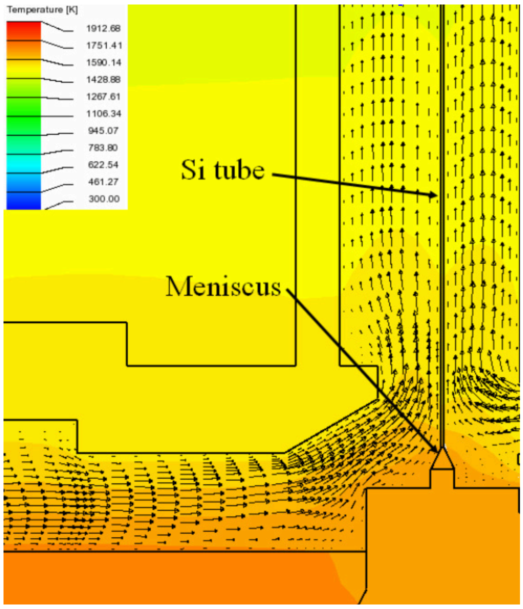

Fig. 3. T distribution and gas flow around the meniscus region of an EFG geometry.

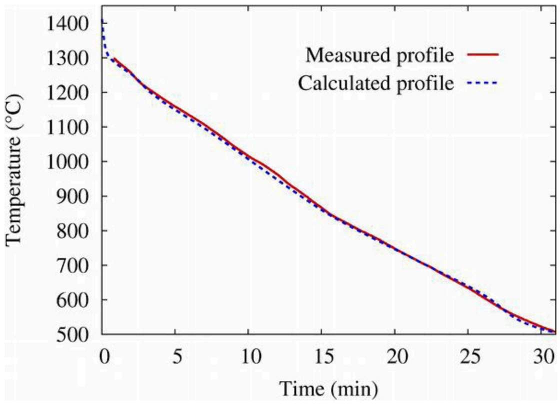

Fig. 4. T history of a growing Si tube (calucated, and measured by a moving thermocouple.

A 2D axisymmetric model of an EFG furnace constitutes the basis for proces s and furnace design optimization by numerical simulation. Such a reduced model, which represents a good approximation to the real polygonal shapes, was implemented in the software package CrysMAS [6], which allows a coupled computation of electromagnetic induction, distribution of generated heat, global temperature distribution, convection in the silicon melt, and inert gas flow. An example of a temperature distribution and inert gas flow obtained from CrysMAS is given in Fig. 3 [17].

For validation of the model, thermocouples were introduced at various positions within the chamber [7]. The discrepancies between model and thermocouple measurements in all relevant parts of the furnace are not more than 10 to 20 K, demonstrating that such a simplified 2D model is useful for obtaining global information on the temperature distribution within an EFG furnace. Of special interest is the axial temperature profile along the growing silicon tube. The temperature history experienced by the tube during cooling determines the evolution of stress and is the key parameter for optimizing tube quality by reducing buckling deformation, residual stresses, and dislocation density. Therefore, the significance of the numerical results was verified by comparing the axial temperature profile with measurements from a thermocouple attached to the growing tube [7, 17]. Such a comparison is shown in Fig. 4, where the very good agreement between calculations and measurement is demonstrated.

2.2. 3D coupled electromagnetic and thermal modelling

For all questions resulting from the non-axisymmetric symmetry, 3D modelling of the complex system is unavoidable. For some issues the n-fold symmetry can used in order to reduce the effort, but the more details has to be considered (e.g. the non-uniformity of thermal and electrical resistivity of graphite parts), the more a full 3D simulation is required.
For first 3D electromagnetic and thermal simulations, the eight fold symmetry of an EFG octagon process allowed for confining the geometry to 1/16 part in case of electromagnetic simulation by use of the commercial program package ANSYS, and to 1/8 part for temperature simulation performed with the program CASTS [8].

The numerical meshes used are different because the sensitive regions and the requirements are not the same in both calculations. The electrical conductivity is temperature dependent. Therefore, the simulation procedure used an iterative scheme. The electromagnetic field was calculated using temperature dependent electrical conductivity and the temperatures transferred from the thermal simulation to the electromagnetic FE-analysis. The calculated Joule heat was then transferred back to the thermal analysis, followed by the second iteration of temperature field simulation. Because the conductivity is not very temperature dependent within the process temperature range, two or three iterations were sufficient.

Fig. 5 shows on the left side the model of some graphite parts, the silicon melt and a part of the growing tube, which was considered in the calculation of the Joule heat together with the surrounding air. The inductors are not shown in this figure. In the middle, one example of Joule heat distribution is displayed. It shows clearly that there is no rotational symmetry. The thermal simulation considers heat conduction and heat transfer between the materials, the radiation, the latent heat, the water cooling and the continuous charging of silicon. It involves all components of the furnace as well as liquid and solid silicon. The region of high gradients in the vicinity of the die, the growth interface, and the lower tube region is meshed with high resolution. Fig. 5 shows on the right side the temperature field in this region [10].

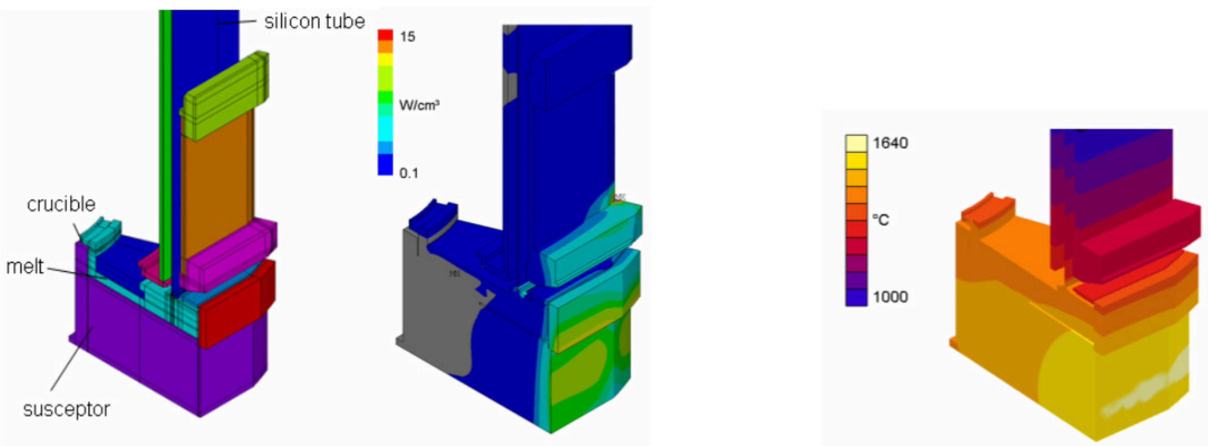

Fig. 5. Solid model for electromagnetic FE simulation (left), an example for Joule heat distribution, 1/16 geometry (middle), and resulting T distribution (right).

The simulation model was again validated by experimental measurements. Thermocouples were mounted at various positions within the EFG-furnace and the temperature measurements were done on the running system. The differences between experiment and simulation depend on the positions and are ±4°C in the region of crucible and die, and ±15°C in colder and remote regions. The relative deviations are less than 1.4%.

The simulations revealed that the current in the second inductor and the phase shift between the two inductors strongly influence the spacial distribution of Joule heat in the graphite components. Simulations for different combinations of current and phase were performed as they were measured on different furnaces. Fig. 6 shows some results of this parameter study [10]. The general temper profile along the tube is similar for all variations (Fig. 4). But the plot of differences between the profiles point up the effect of phase shift and current. The temperatures are locally shifted by up to 40°C. Because the edges are differently heated (see Fig. 5), the profiles along the edges differ locally by up to 6 K from the respective face profiles.

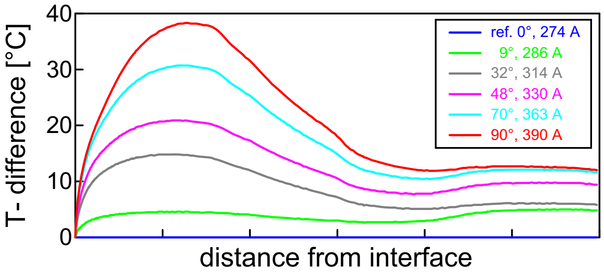

Fig. 6. Differences of the temperature profiles to a reference profile along the face center line.

2.3. 3D elastoplastic modelling of residual stress and crystal deformation

Unfavourable cooling profiles can lead to the presence of high residual stresses and can cause the tubes to develop a periodical deformation pattern, both effects being adverse for further processing. For optimizing the furnace design with respect to low residual stresses and buckling, the cooling profiles obtained from the axisymmetric calculations are used as input for a separate 3D finite element model that is capable of calculating the build-up of stress and plastic deformation during EFG growth [9, 10].

This model uses an elasto-plastic description of the deformation behaviour of Si, with temperature dependent expansion coefficient, Young's modulus and yield stress. The growth process is divided into discrete steps and each successive step is modeled by a strain-free addition of element sets at the growth interface, as scetched in Fig. 7. Each element set corresponds to a section of new-grown material of specified length, depending on the desired accuracy.

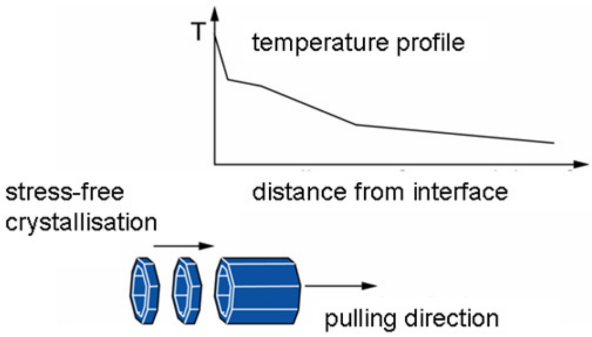

Fig. 7. Sketch of the deformation model.

In making use of the rotational symmetry, the 3D model can be reduced to a section of the tube. In most cases, the temperature profile is assumed to be homogeneous in the direction transverse to the growth direction. However, circumferential temperature variations may have an important influence on stress generation [11] and can also be addressed.

In order to use the model as a quantitative tool, adjustments of the Si material parameters are necessary. Starting from the yield stress data for single crystalline Si available from experiments as summarized in [12], the high temperature plastic deformation behaviour has been slightly adapted in order to reproduce the experimentally observed amplitudes of buckling.

An example of a deformation pattern obtained from the elasto-plastic model is shown in Fig. 8 [17], together with a comparison with measured deformation values. Both the amplitude and the length of the buckling period are in very good agreement. The regular buckling pattern that develops in the center part of the tube can be used to judge the quality of the underlying temperature profile.

Using this model of the tube deformation behaviour, the axial temperature profile of EFG furnaces can be successfully optimized towards a high degree of tube flatness.

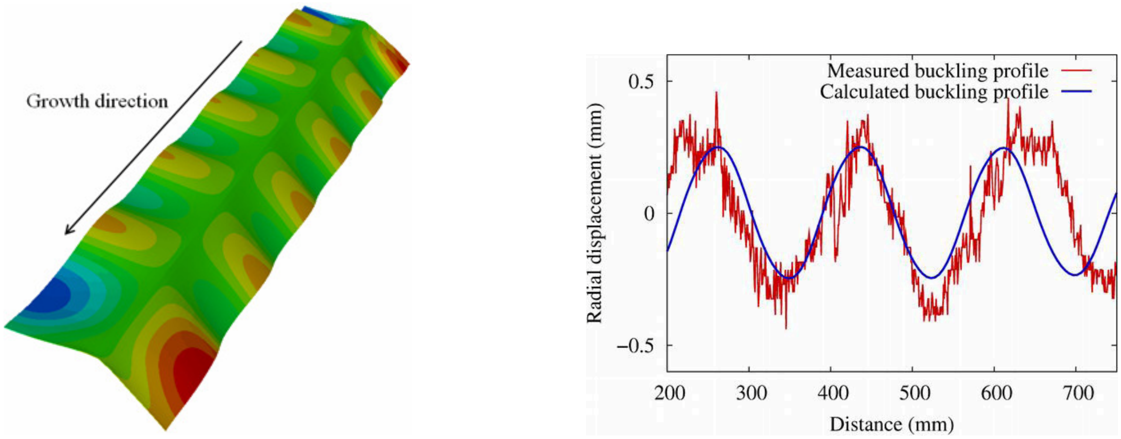

Fig. 8. Example of a calculated buckling deformation of an EFG silicon tube. On the right, a comparison of a measured and a calculated buckling profile is shown.

2.4. 3D modelling of melt flow and segregation phenomena

It is essential for the electrical quality of silicon wafers for photovoltaic applications (and for electronic applications in general), that segregated metallic impurities like iron or chromium are effectively removed from the phase boundary towards the melt, in order to prevent fast enrichment of such undesired impurities close to the phase boundary. In case of silicon, the segregation coefficients of metallic impurities are very small, in the range of 10^{-3} to 10^{-5} [13]. However, if they enrich within a small volume close to the crystallization front, this doesn´t help. Though it was well known that effective redistribution takes place in EFG systems used today, the mechanisms remained unclear for many years [14].

To clarify the reasons of the redistribution phenomenon, silicon melt flow and impurity transport within an dodecagonal EFG crucible were simulated by a 3D unsteady approach, including the transport of the melt towards the meniscus through a capillary system [15]. The computations accounted for natural convection in the bulk and the Marangoni flow on the free surfaces and along the meniscus. Melt convection was considered within a Large Eddy Simulation approach.

The 3D unsteady computations showed that there are large pulsating coherent structures on the melt free surface in the melt (Fig. 9 [15]). It has been found that the pulsations of the vortices in the melt result, due to local pressure gradients, in variations of the flow direction in the channel system connecting melt and shaper region: the flow periodically moves up and down (Fig. 10 shows two snapshots [17]). So, significant pulsations of metal concentration were found in the channel system, enabling an effective redistribution of segregated impurities.

For experimental validation, gallium was added to the melt as a model impurity [15]. The segregation coefficient of Ga is nearly as small as that of metals ($k_0 = 0.008$),

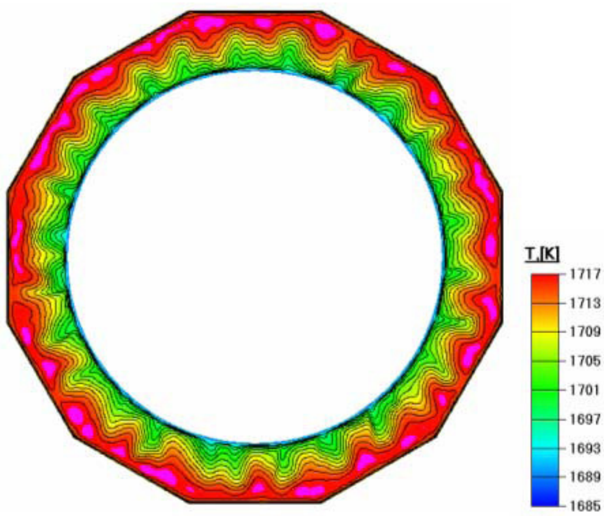

Fig. 9. The instantaneous temperature distribution on the melt free surface within a dodecagonal EFG crucible.

whereas it can be easily analyzed by resistivity measurements (in contrary to most iron-like metals, which do not act as donors or acceptors). These unique properties make Ga an ideal model impurity for segregation investigations.

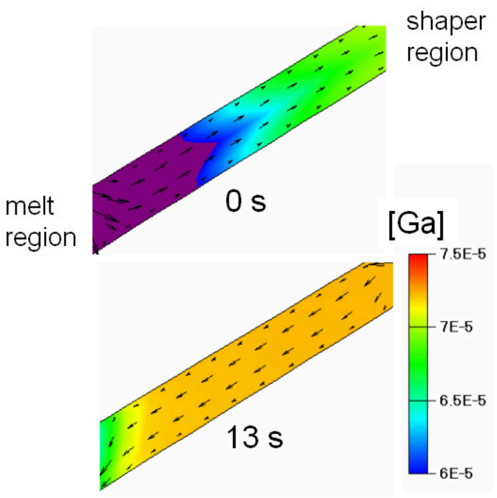

Fig. 9. Two snapshots of the fluctuating flow and impurity concentration within the capillaries connecting the melt shown in Fig. 8 with the shaper.

As predicted by the numerical simulation, no gradient of the Ga concentration along the first meters of the grown tube was found, while the concentration should radically increase in the die region with the time after growth start, if all segregated Ga would stay within the meniscus region. An effective segregation coefficient in the order of 0.01, was found for both the experimentally and the numerical attempt. The remaining difference to the theoretical value reveals that there is still potential for improvement.

Conclusions

The development of the EFG technique towards larger and thinner tubes is ongoing [16, 17]. A complete global 3D model of the non-axisymmetric growth furnace, including melt and gas convection together with the related mass transfer, including relevant chemical reactions, is still a challenge. Another challenge is defect modeling of such polycrystalline materials, including the formation and multiplication of dislocations as well as the grain formation. However, independent from the simulation stage reached, the aim of all simulation work has to be the coupling between the properties of the final product and the conditions of processing.

Acknowledgements

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Author

Dr.-Ing. Albrecht Seidl
WACKER SCHOTT Solar GmbH
Carl-Zeiss-Str. 4
63755 Alzenau, Germany
E-mail: albrecht.seidl@wackerschott.com