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Crystal growth in heater-magnet modules - from concept to use

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Abstract

Many concepts of external magnetic field applications in crystal growth processes have been developed to control melt convection, impurity content and growing interface shape. Especially, travelling magnetic fields (TMF) are of certain advantages. However, strong shielding effects appear when the TMF coils are placed outside the growth vessel. To achieve a solution of industrial relevance within the framework of the KRISTMAG® project inner heater-magnet modules (HMM) for simultaneous generation of temperature and magnetic field have been developed. Global modelling was used to optimize the HMM configuration and process parameters. The successful growth of Ge and GaAs crystals in HMM-equipped VGF, LEC and VCz pullers demonstrate the industrial feasibility of this project.

1. Introduction

Further developments of industrial melt growth processes of semiconductors are focused on the increase of crystal output per run. This can be achieved by diameter enlargement and crystal lengthening. However, the buoyancy-driven convection, which changes its character to non-steady flows with increasing melt heights, must be controlled very accurately. The use of stabilizing high crucible rotation rates fails when growing from very large melt masses. Therefore, the induction of a magnetic field into the melt proves to be the most promising measure to damp the melt perturbations and to design the interface shape. Especially by applying a longitudinally TMF a favourable toroidal flow pattern can be generated, opposite to the natural convection streams. As a further advantage, within the melt only relatively low magnetic induction is needed (4 - 8 mT). However, there is a strong shielding effect when the TMF coils are placed outside the typical thick-walled high-pressure vessels. Therefore, the placement of the magnetic field generation as close as possible to the melt provides a promising solution to achieve maximum efficiency of flow driving.

Within the framework of the KRISTMAG® project (2005 - 2008), co-financed by the European Regional Developments Fund (EFRE), „Zukunftsfonds" Berlin and „Zukunftsagentur" Brandenburg, inner heater-magnet modules have been developed. Their design allows for coupled generation of temperature and travelling magnetic fields adjusted to industrial crystal growth equipments [1]. The induced TMF and its effect on the melt convection was studied for various growth systems, i.e. vertical gradient freeze (VGF), liquid encapsulated Czochralski (LEC) and vapour pressure controlled Czochralski (VCz), by global 2.5 and 3D modelling with codes CrysMAS [2], NAVIER, WIAS-HiTNIHS [3] and CFX [4]. The induced Lorentz force density was measured by the mass responses of a dummy made of stainless steel when the travelling magnetic field of given amplitude, frequency and phase shift were switched on. A good agreement with the numerical calculations has been observed.

To obtain a suitable magnetic field and to control the crystallization process effectively, amplitude, frequency and phase shift of the three-phase accelerated current (AC) are all adjustable and combined with a DC-component, respectively. To that end, a universal heater-magnet controller system has been developed and designed in collaboration with the industrial partners. Meanwhile, the first industrial application of the KRISTMAG® development has been installed at a Berlin company.

2. The HMM design

For the generation of vertically translating TMF the heater design has to be changed completely, i.e. from a conventional meander-like shape [5] to a hole-cylindrical body with an upwards-winding slit forming a single layered spiral- or staircase-shaped current path [1]. The path is subdivided in coil segments by contact points for the phase-shifted power supply in delta or star connection. The growth temperature and magnetic induction can be varied in wide ranges by adjusting the power P, current I, voltage U, frequency f and phase shift φ in the regions 0 - 40 kW, 0 - 330 A per coil, 0 - 40 V, 10 - 600 Hz and 5 -120 °, respectively.

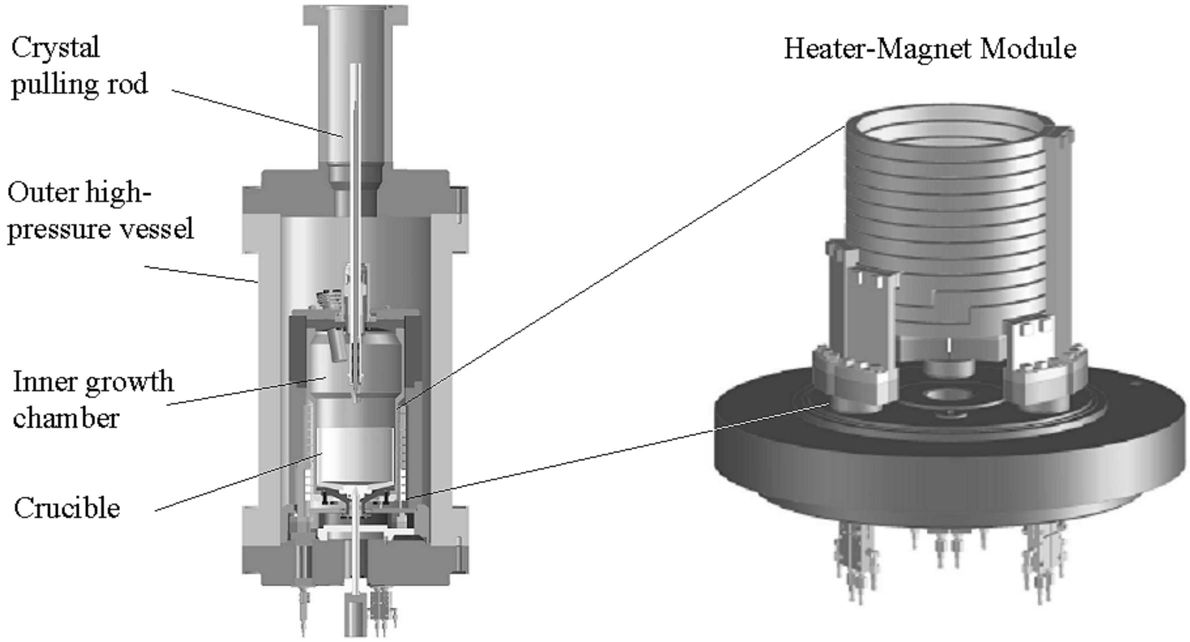

Fig. 1. Sketch of a HMM (right) installed in a vapour pressure controlled Czochralski puller (left). It replaces the conventional heater without complication.

Various HMM constructions have been first optimized by numeric modelling and then installed in a VGF furnace for directional solidification of 4 inch Ge crystals and in LEC and VCz pullers for 2-3 inch GasAs Czochralski growth. Fig. 1 shows such an HMM arrangement in a VCz high-pressure crystal growth puller.

A noteworthy advantage of such a combined heater-magnet module in close vicinity to the melt is the significant reduction of the power consumption needed for the generation of an effective magnetic field. It was determined that the power consumed by the HMM in a LEC puller for GaAs is only one sixth (10.5 kW) compared to a TMF setup with the same magnetic field characteristics with coils placed outside the growth vessel (60 kW). This demonstrates a clear effect of energy saving.

3. Modelling

The induced TMF and its effect on the melt convection were studied in each growth system by global 2.5 and 3D modelling. The code CrysMAS [6] was used for the analysis of the VGF growth process. The influences of gas convection and latent heat of crystallization were considered. The optimization of the solid–liquid interface shape during the crystallization was carried out by means of snap shots of different growth positions. As a result the interface morphology as function of the aspect ratio was obtained. Additionally, the transition value of the TMF force from steady-state situation to non-stationary melt flow was studied by 3D time-dependent simulations. In consequence, the flow velocity and temperature fields were obtained considering the Lorentz forces in 3D [2] (see Fig. 2 right).

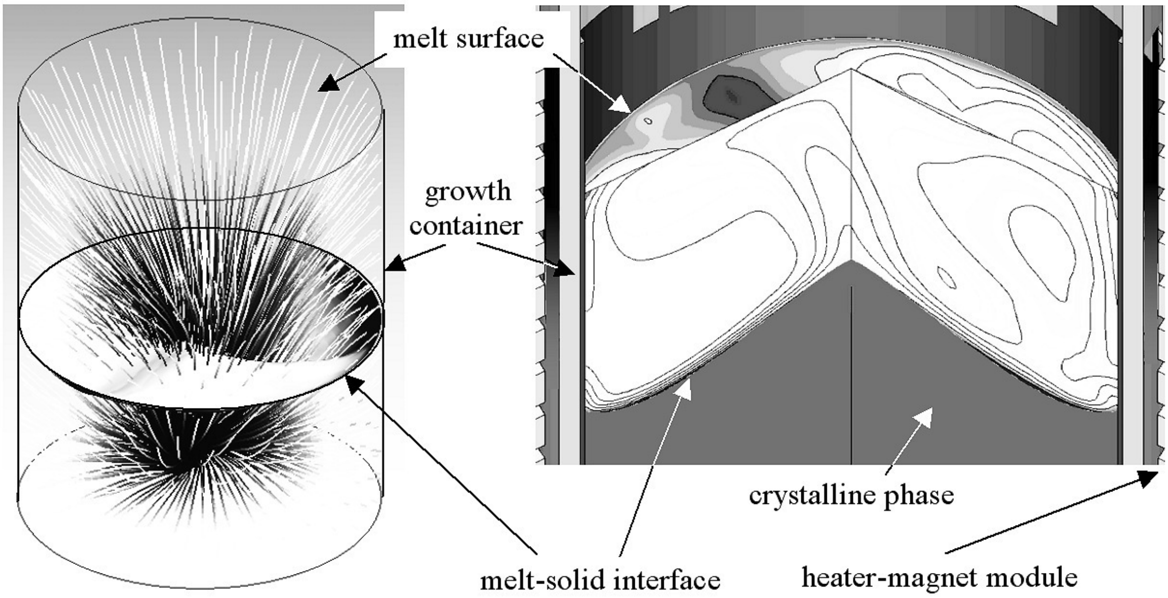

Fig. 2. Numerical 3D studies for VGF growth of 4 inch Ge crystals within HMM. Left: Virtuell particle tra-ces in the Lorentz force field computed by ANSYS (direction is from top to bottom). Right: Temperature distribution within the melt obtained by CrysMAS. For both examples exaggerated induced Lorentz forces were selected.

Possible 3D asymmetry effects generated by the electromagnetic field distribution using the HMM were analyzed by the commercial package ANSYS. Simulations of the melt flow were carried out with the commercial package CFX well adapting the interface to ANSYS. By using this combination, a simple transfer of the Lorentz force distribution data calculated with ANSYS into CFX was possible (see Fig. 2 left). It is noteworthy that the investigated effects of asymmetry require the use of the total system geometry without any simplifications by symmetry. Different connections to the three-phase power supply have been modeled considering the input of current or voltage with variable phases and frequencies [4]. An optimized bus bar configuration minimizing Lorentz force asymmetries has been ascertained.

The electro-magnetic fields and the temperature distribution in LEC and VCz growth apparatus were computed using software WIAS-HiTNIHS [7]. Its combination with the code NAVIER [8] allows to model important aspects of Czochralski crystal growth under the influence of a TMF, since WIAS-HiTNIHS is a suitable tool to simulate TMF and NAVIER allows to compute the melt flow under the influence of a Lorentz force [3].

Fig. 3 shows a numerical example of a Lorentz force configuration for effective damping of convection-driven temperature oscillations at the edge of a growing GaAs LEC crystal.

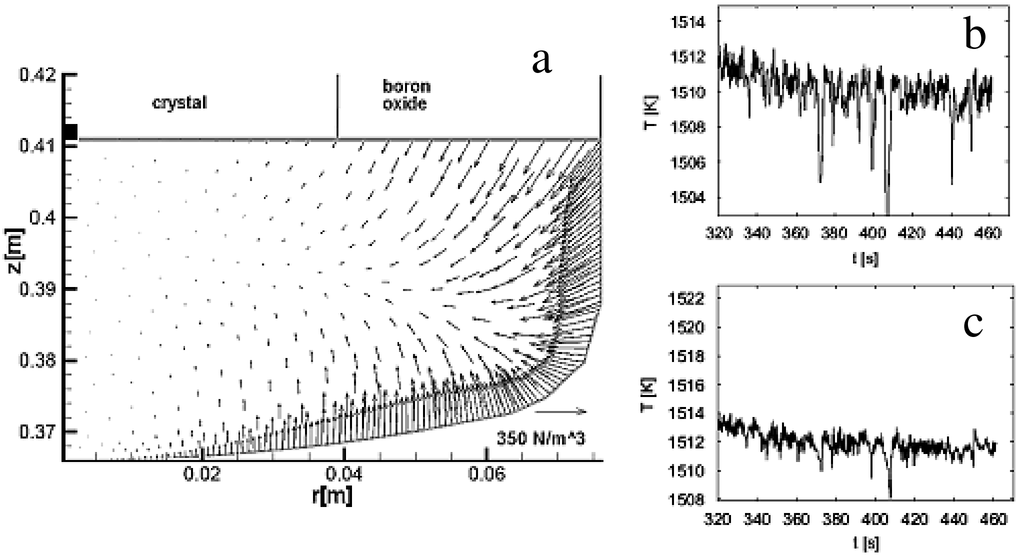

Fig. 3. a - simulated favorable Lorentz force configuration within the melt in a GaAs LEC crucible for effective damping of the convection-driven temperature oscillation (z - vertical axis, r - radius). Modeled temperature oscillations at the crystal edge without (b) and with travelling magnetic field generated in a heater-magnet module (c). More details are given in the present proceedings by the paper of O. Klein et al.

4. Growth results

4.1. Liquid Encapsulated Czochralski (LEC)

3-inch [001]-oriented GaAs crystals have been grown by the LEC method within an internal heater-magnet module placed inside the industrial LEC puller CI 358. A special multi-coil design was constructed to meet the optimized Lorentz field against buoyancy-driven temperature oscillations below the growing crystal (see Fig. 3). Fig. 4b shows an as-grown GaAs crystal obtained in such a travelling magnetic field with frequency f = 300 Hz and phase shift $\varphi = 70°$. The phase boundary curvature was analysed by striation technique. It has been found that a relatively strong Lorentz force field can be generated influencing the flow pattern and interface curvature very sensitively. Etch pit density measurements on (100) cuts revealed dislocation values of 5 x 10^4 cm^{-2}.

4.2. Vapour Pressure Controlled Czochralski (VCz)

A modified VCz version without boric oxide encapsulant has been developed for the industrial Czochralski puller LPA Mark 3 in order to grow near stoichiometric GaAs crystals from Ga-rich melts (Fig. 4a). The melt composition is controlled during growth by an arsenic source within the inner VCz chamber (see Fig. 1). For the first time VCz experiments in travelling magnetic fields have been performed. [001]-oriented 3-inch GaAs crystals were grown. The growth results indicate that the applied travelling magnetic fields influence the melt motion tremendously even in low aspect ration H/D configurations (H - melt height, D - melt diameter). Due to the missing boric oxide encapsulant a good visual observation of the stream

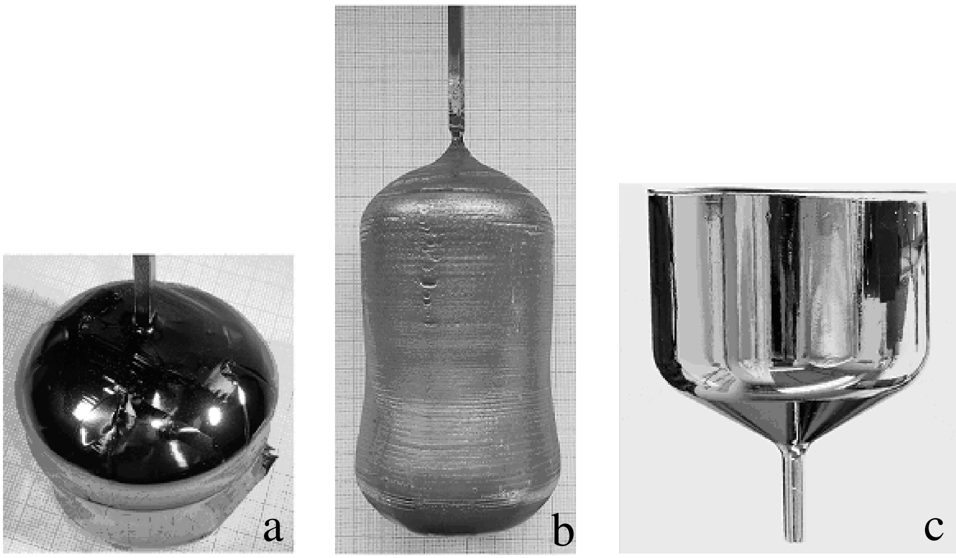

Fig. 4. Crystals grown within heater-magnet modules in industrial VCz (a), LEC (s) and VGF (c) growth equipments.

patterns as function of the magnetic field parameters was possible. For instance, in contrast to the conventional mode without magnetic field a controllable outwards directed stream away from the seed could be achieved. The striation analysis along longitudinal {100} cuts revealed significant differences between crystals grown without (Fig. 5a) and with magnetic field (Fig. 5b). Markedly reduced striation amplitudes and uniform interspaces were observed in crystals grown under TMF. A mean dislocation density of 1 x 10^4 cm^{-2} of enhanced radial distribution homogeneity was detected.

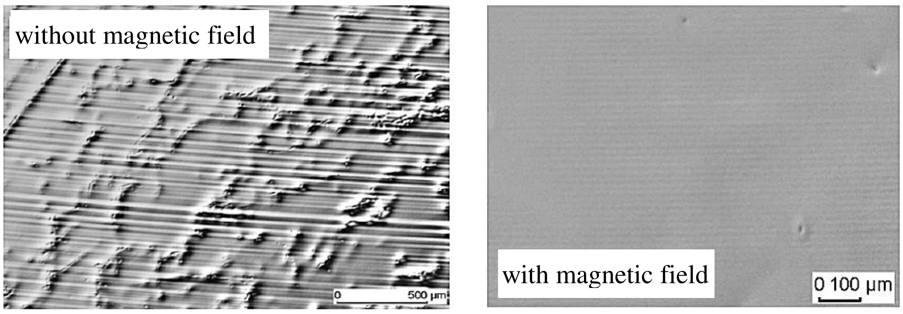

Fig. 5. Striations fluctuating in amplitudes and interspaces in a GaAs crystal grown without TMF (left). Reduced striation intensities when growing in TMF (right).

4.3. Vertical Gradient Freeze (VGF)

Growth experiments with germanium in travelling magnetic fields were carried out in the commercial VGF equipment Kronos. Also here the standard heater was replaced by a heater-magnet module. <111>-oriented Ge crystals of diameter 110 mm and weight of 6 kg were grown in pBN crucibles from a small seed crystal via conical bottom part (Fig. 4c). For the investigation of the interface curvature by the striation technique the as-grown crystals were longitudinally cut along the <211>- and <110>-directions and then analysed by etching and lateral photo voltage scanning. As can be seen from Figs. 6 nearly flat and slightly convex interface shapes can be achieved by using TMF. As it is well known such interface form cannot be obtained under conventional VGF growth conditions without magnetic field.

A mean EPD of (5 - 3) x 10^2 cm^{-2} and carrier mobility of μ = 2800 $cm^2V^{-1}s^{-1}$ were measured in as-grown crystals. An improved radial homogeneity of the electrical parameters, like carrier concentration, has been ascertained.

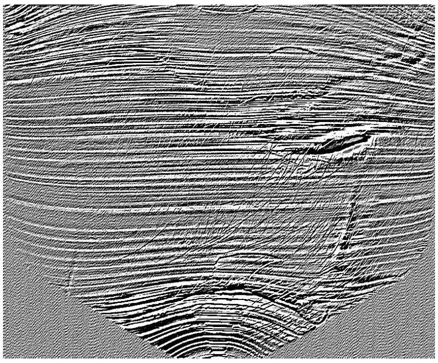

Fig. 6.
The morphology of the growing melt-solid interface in a VGF Ge crystal grown in a HMM revealed by striations which are analysed by lateral photo voltage scanning.

Conclusions

For the first time, in three industrial scale crystal growth pullers heater-magnet modules generating simultaneously well-controlled temperature and Lorentz force fields were successfully applied. Numerical modeling supported the optimization step very effectively.

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