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Influence of Ultrasonic Treatment on Crystal Growth From Melt

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Abstract

Ultrasonic treatment can be a powerful tool to influence the fluid convection in crystal growth processes from melt in a favorable way. Especially in the vicinity of solid-liquid interfaces it helps to reduce the harmful diffusion boundary layer. In this paper the effect of ultrasonic treatment is calculated for three different waveguide measurements.

Introduction

The future challenge in the fabrication of semiconductor bulk crystals will be the improvement of the quality with a simultaneous decrease of the production costs. This difficult task can only be achieved by increasing the size of the crystals. As a consequence, bigger melt masses have to be handled. This involves the danger of convective streaming, because of the increasing melt column, especially in Czochralski arrangements. External force fields can be applied to control this non-steady flow [1]. In addition, forced convective flow can help to reduce the harmful diffusion boundary layer having increased dimension in vertical Bridgman methods where near buoyancy-stable conditions do exist. In this paper the influence of ultrasonic treatment to the streaming inside of the melt container is investigated. As has been already shown by Zharikov [2] the application of vibrations during melt growth of $NaNO_3$ crystals improved both radial dopant and stress distribution homogeneity. Furthermore was demonstrated that the curvature of the solid-liquid interface can be reduced markedly. According to Kozhemyakin [3-10], the striations in the central part of various crystals disappear after an ultrasonic treatment in the range of 0,5 to 5 MHz. In addition, resulting standing waves affected the convective flow in the vicinity of the solid-liquid interface. In the present work the influence of three different ultrasonic waveguide set-ups on the melt-flow and their comparison have been studied in detail by numerical simulations.

1. Numerical Simulations

The numerical simulations were realized with the commercial software packages ANSYS® and FLUENT®. The used model of a vertical gradient freeze (VGF) system is shown in Fig. 1. The inner radius and wall thickness of the crucible are 57 and 5 mm, respectively. The melt column has a height of 69 mm. It is assumed that already a bulk height of 7 mm is crystallized. The ultrasound with frequency of 1 MHz is centrally injected by a waveguide from above. The influence is analyzed for three different waveguide diameters, i.e. 10, 20 and 40 mm. ANSYS® was used to calculate the acoustic field. It was computed with a 2D model, because of the cylindrical set-up symmetry.

The numerical model includes the crucible and the crystal as solid parts and the melt and a thin layer of surrounding media as liquid parts. The model is also shown in Fig. 1. As a boundary condition the pressure at the outside of the surrounding media is set to zero. In place where the waveguide touches the melt surface a displacement with a harmonic excitation is default. The supplied acoustic power is inversely proportional to the radius of the waveguide. To hold the acoustic power still constant up to 100 W the excitation amplitude is adapted for the three different waveguides. The preconditioned material properties for the liquid parts are density ρ and sound velocity *c*. For the solid parts of the system the density ρ, Young´s modulus *E*, Poisson´s ratio σ and damping coefficient α have to be considered. As a result, the sound pressure distributions *p* is calculated in every point of the melt and surrounding media by:

$$\frac{1}{c^2}\frac{\partial^2 p}{\partial t^2} - \nabla^2 p = 0\,, \qquad (1)$$

with *t* the time.

The displacement *u* in every point of the crystal and crucible has been obtained by using the equation of motion:

$$M\ddot{u} + C\dot{u} + Ku = F^a\,, \qquad (2)$$

where *M* indicates the mass matrix, *C* the damping matrix, *K* the stiffness matrix and F^a the vector of the apposed forces, like the excitation forces. Both equations are coupled in such a way that the displacement is converted into a pressure at all solid-liquid interfaces and vice versa. The computed acoustic velocity v_A can now be used to calculate the velocity v_S of the Schlichting streaming at the solid-liquid interface affecting the diffusion boundary layer

$$\vec{v}_S = -\frac{1}{2\omega}\left\{\frac{1}{2}(\vec{v}_A\nabla)\vec{v}_A + \vec{v}_A(\nabla\vec{v}_A) + \frac{3}{2}(\vec{v}_A\nabla\varphi)\vec{v}_A\right\}, \qquad (3)$$

with φ the phase shift and ω the angular speed $2\pi f$, whereby *f* is the ultrasonic frequency being in our case 1 MHz.

Finally, the obtained Schlichting velocity can be used as boundary condition for the hydrodynamic calculation. Usually, for this type of simulation a non-slip boundary condition is set at all solid-liquid interfaces. To take the ultrasonic treatment into account the Schlichting velocity is set instead. The simulation was provided with the commercial software package FLUENT® including melt flow and temperature distribution calculations.

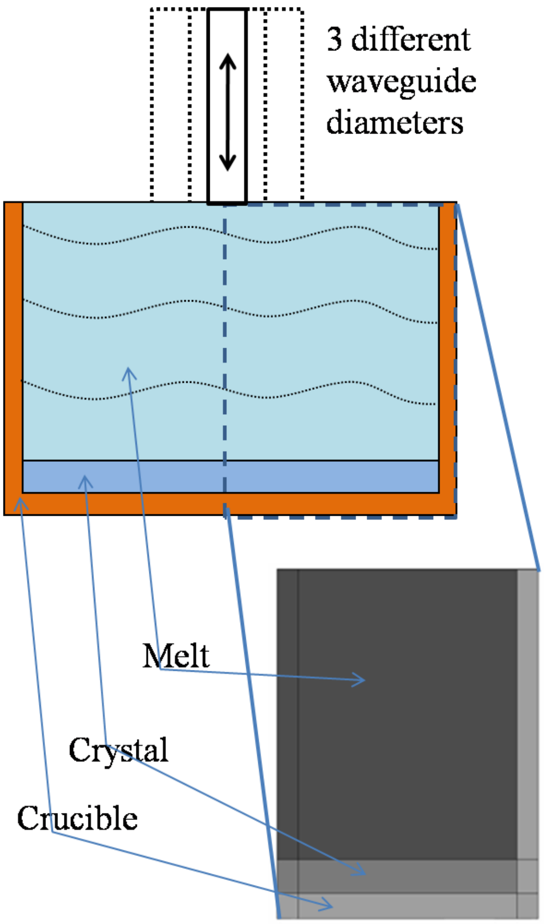

Fig. 1. Sketch of the treated VGF process with ultrasonic waveguide (above) and numerical model for calculating the sound field (below)

2. Results and Discussion

Fig. 2 shows the induced acoustic field for the three different waveguide diameters. It can be seen that the peak values of pressure and displacement decrease with increasing waveguide diameter. Especially in the vertical part across the symmetry axis between waveguide and solid-liquid interface the acoustic field seems to be more homogenized. The structures of the occurring standing waves are clearly visible first of all for the waveguide with 40 mm diameter. The distance between two pressure peaks is around 1,86 mm. This complies exactly to a half wavelength of the longitudinal pressure waves, when the ultrasonic frequency of 1 MHz and the sound velocity for germanium of 3716 m/s is considered. In the solid parts of the system like crucible and crystal the acoustic waves propagate in terms of displacement waves. They are able to distribute in longitudinal and transversal directions leading to their superimposition in these parts. The sound speed in solids is 4517 m/s and 2602 m/s for transversal and for longitudinal translation directions, respectively. As results different wave lengths and acoustic association patterns are appeared.

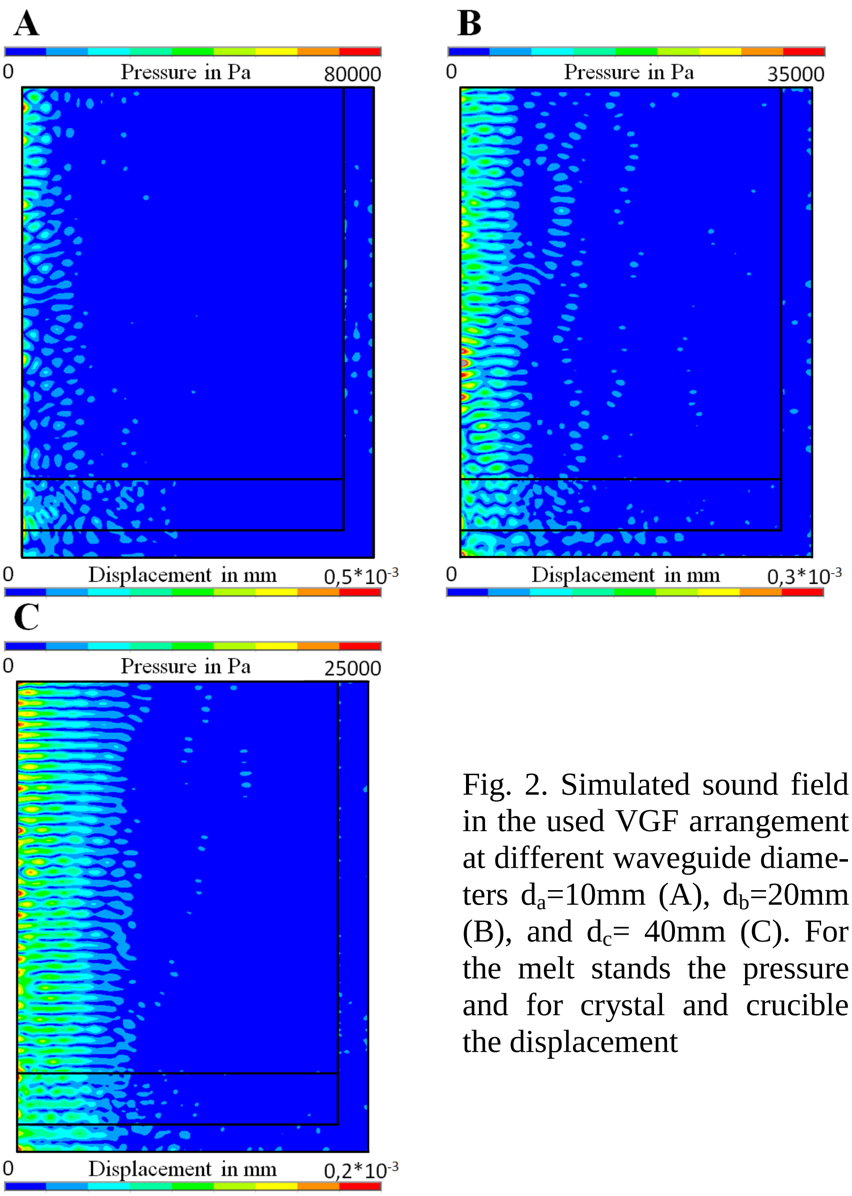

Fig. 2. Simulated sound field in the used VGF arrangement at different waveguide diameters d_a=10mm (A), d_b=20mm (B), and d_c= 40mm (C). For the melt stands the pressure and for crystal and crucible the displacement

The results of the acoustic simulation can now be used to calculate the Schlichting streaming. The Schlichting streaming occurs at the interfaces between crystal and melt in a very thin layer and the velocity direction is parallel to it. The acoustic boundary layer, in which the Schlichting streaming acts, has a thickness of around only 1 µm. Equation 3 is used to calculate the Schlichting velocity for the three different waveguide diameters plotted in Fig.3.

In the next step a global hydrodynamic simulation is provided. For that the Schlichting streaming across the solid-liquid interface was set as boun-dary condition taking into accound the ultrasonic treatment. Usually a no-slip condition is default for all walls of the liquid. The acoustic boundary layer proves to be so thin that the Schlichting streaming acts inside the hydrodynamic boundary layer. Therefore, the assumption of a moving wall as the boundary condition is acceptable.

This procedure shows very useful for easy calculation of the ultrasonic influence. It allows to add an ultrasonic treatment to all kinds of hydrodynamic simulations by using a simple boundary condition. It allows also to calculate the superimposition of an acoustic field with other external force fields, like electric or magnetic ones.

The comparison between hydrodynamic calculations for the three different waveguide diameters and case without any ultrasonic treatment is shown in Fig. 4. As it is visible the Schlichting velocity produces little vortices across the solid-liquid interface being of very effective mixing ability.

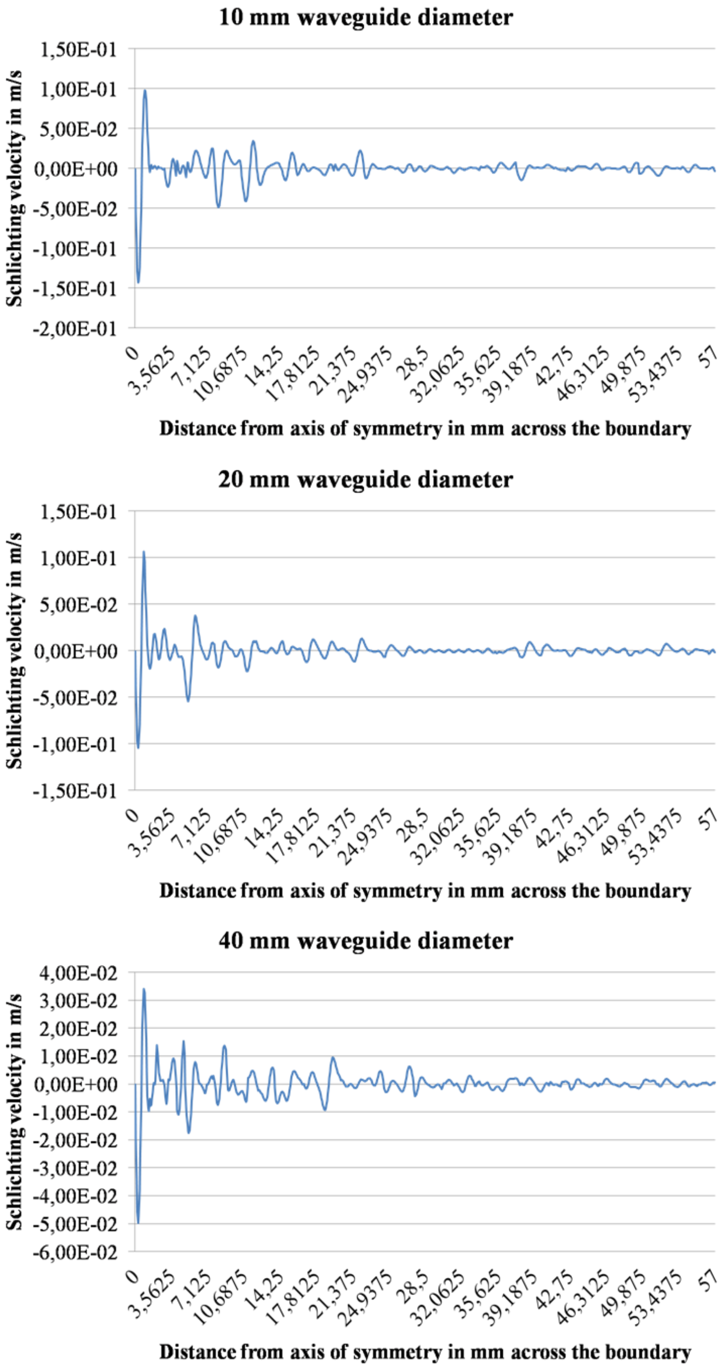

Fig. 3. Schlichting velocity at the solid-liquid interface parallel to the boundary for the three waveguide cases specified in Fig. 2

It is noteworthy that the high ultrasound frequency does not affect the crystal micro-homogeneity due to the low-pass filter behaviour of the melt-solid interface [1].

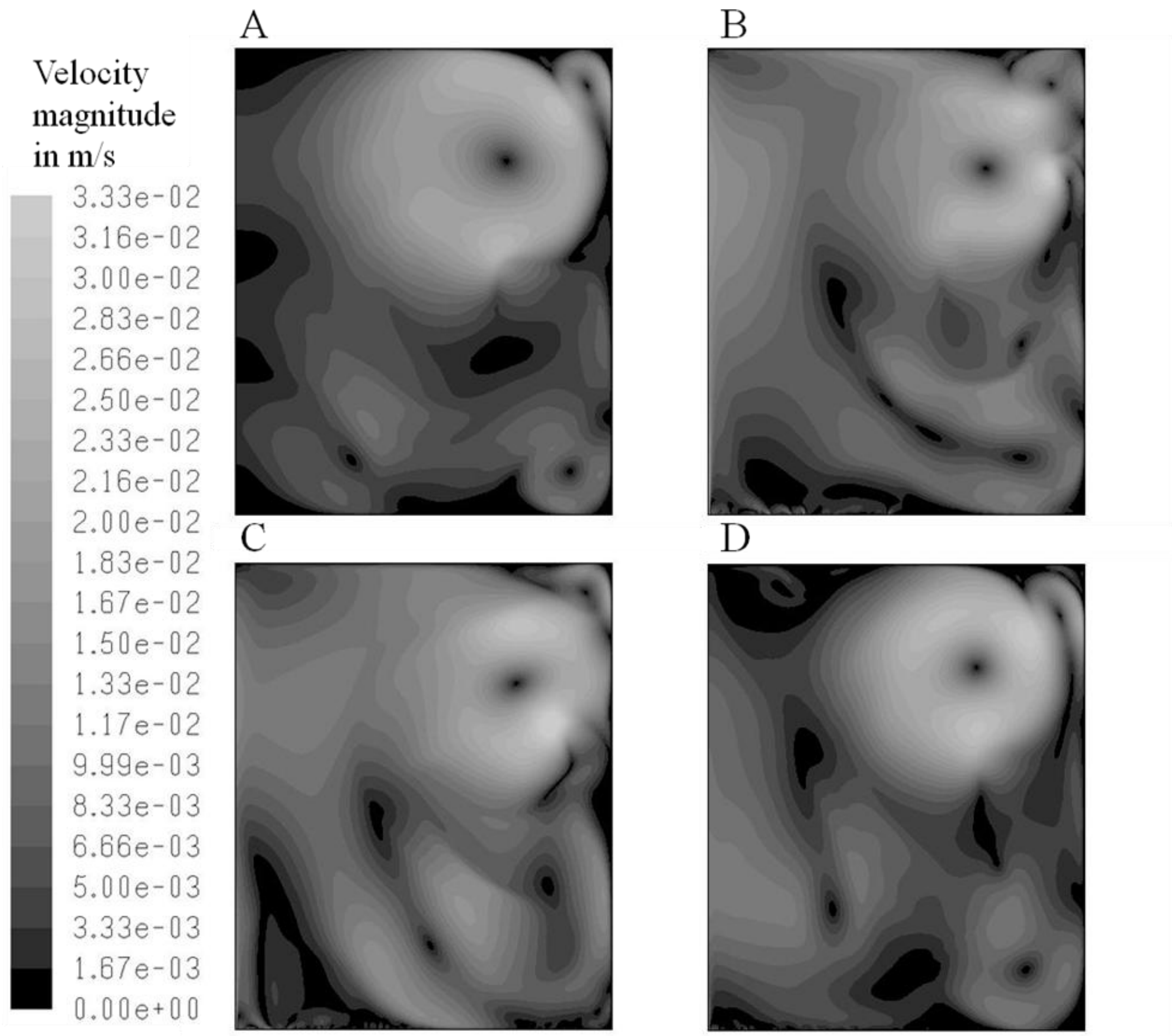

Fig. 4. Simulated flow patterns in germanium melt. (A) - without ultrasonic treatment, (B) - waveguide diameter d_1 = 10mm, (C) - d_2 = 20mm, and (D) - d_3 = 40mm

Conclusions

It has been analyzed numerically that the ultrasonic treatment is of positive influence on the crystallization process. The occurring Schlichting streaming produces vortices in the vicinity of the solid-liquid interface. These streams help to reduce the harmful diffusion boundary layer very effectively. The generated ANSYS® and FLUENT® models are able to be extended for further variances and upgrades.

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