3D MODELING OF THE INFLUENCE OF THE INDUCTOR ON THE PHASE BOUNDARIES IN FZ CRYSTAL GROWTH

PLĀTE M., KRAUZE A., VIRBULIS J.
Department of Physics and Mathematics, University of Latvia
8 Zeļļu str., Rīga, Latvia
E-mail address of corresponding author: matiss.plate@lu.lv

Abstract: In a recent development, an improved mathematical model of the floating zone (FZ) silicon single crystal growth process takes into account main 3D aspects of the influence of a strongly asymmetric high frequency electromagnetic (HF EM) field. The model considers EM pressure acting on the free melt surface. 3D molten zone shape and the global heat exchange calculations are coupled. The influence of EM field asymmetry on the shape of phase boundaries and the meniscus angle is investigated for the FZ processes with 4” and 5” crystal diameter.

1. Introduction

In the FZ process, Fig. 1, a polycrystalline silicon feed rod is heated by a single-turn pancake-shaped HF induction coil. A molten zone is formed under the inductor, and a single crystal is pulled down from there at a constant rate.

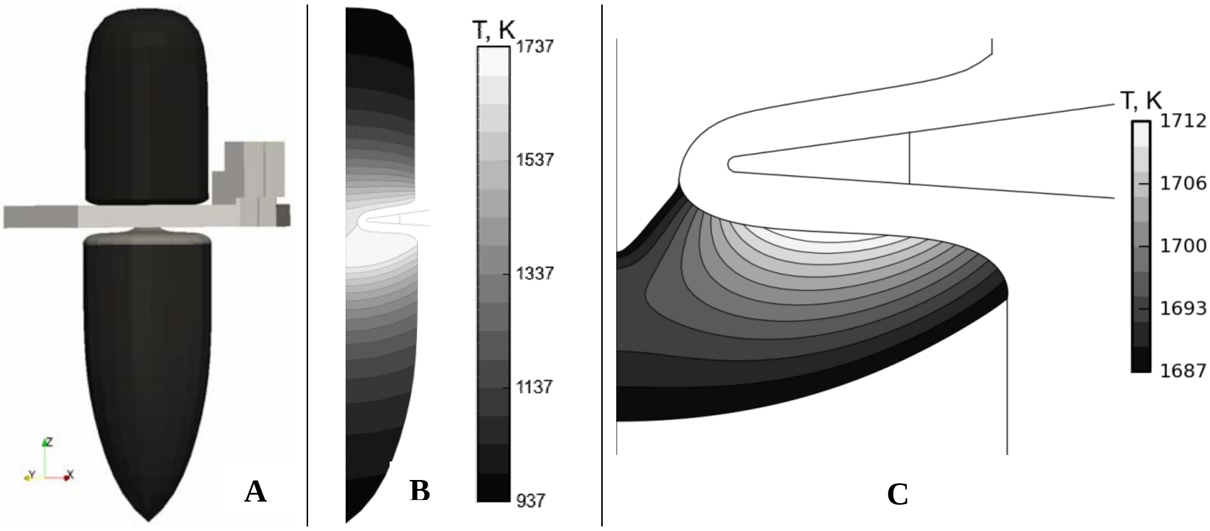

Figure 1: Mathematical modelling of the FZ process. Illustrative 3D scheme of the whole FZ system (panel A). The inductor (shown in grey) melts the feed rod, so that a molten zone develops below it. The crystal is pulled downwards from the bottom of the molten zone. Temperature field in the whole axisymmetric system (panel B) and in the melt (panel C).

Due to the crystal and feed rod rotation, FZ crystal growth systems are quite axisymmetric, and temperature distribution in the silicon, radiation exchange, and phase boundary shapes are usually modeled with 2D axisymmetric models, see [1] and Fig. 1-B, 1-C. For example, program FZone [1] uses this approach to obtain quasi-stationary states of FZ process via iteratively coupled calculations.

In FZone, 3D HF EM equations are solved to obtain 3D distributions of the EM pressure and power, which are azimuthally averaged and supplied to 2D axisymmetric models. Averaged EM pressure distribution is used to solve the equation for the 2D axisymmetric equilibrium shape of the free melt surface. The averaged EM power distribution together with the results from 2D radiation heat exchange calculations are used to formulate the boundary conditions for 2D heat transfer equations for the silicon. Finally, the calculated heat flow disbalances determine the rate of change of the solid-melt phase interfaces.

A significant drawback of this approach is the assumption that the shape of the free melt surface is axisymmetric. The shape of the free melt surface is affected by the distribution of the induced EM pressure, which has pronounced asymmetry because of the pancake-shaped form of the one-turn inductor and the presence of slits on it. Hence the shape of the free melt surface can also be expected to be asymmetric. The EM field distribution itself, however, is sensitive to the changes in the free melt surface shape, which means that modelling it as axisymmetric may introduce errors in the evaluation of the induced EM power.

To investigate the possible influence of asymmetry of the free surface shape, an improved model for the FZ process has been developed, based on the FZone program, in which modelling the 3D free surface shape is done explicitly and is iteratively coupled with calculations of the 3D HF EM field distribution. The improved model has been applied to a typical 4" FZ crystal growth process (data provided from IKZ, Berlin [2]) and a 5" process, and the calculation results have been compared with those from calculations with axisymmetric free surface shape.

2. Mathematical model

2.1. Model for 3D HF EM field. The EM field distribution in the FZ system is characterized by a distinct skin effect due to high field frequency (≈ 3MHz). The skin-layer depth varies between 0.038 mm for the Cu inductor and 1.30 mm for the solid silicon, much less than the characteristic dimensions of the FZ system (≈ 0.1 m). The EM field distribution is therefore determined by surface current density $\vec{i}$. Its distribution is obtained by solving an equation for the electric stream function Ψ , using a 3D boundary element method. See [2, 3] for details.

*2.2. Model for 3D free melt surface***.** The model for the free surface shape is based on the model implemented by Surface Evolver program [4]. The free surface is discretized with linear triangular elements, identical to the one used in 3D HF EM field calculations. A hydrostatic approach is used, in which the free surface form corresponds to its equilibrium shape, at which the sum of the surface tension ($\vec{F}_\sigma$), gravitational ($\vec{F}_g$), and constant pressure ($\vec{F}_0$) forces is zero on each non-fixed surface mesh node. By analogy with $\vec{F}_0$, we also add the electromagnetic force $\vec{F}_{EM}$, exerted by the EM pressure on the surface**:**

$$\vec{F}_\sigma = \sigma\frac{\partial S}{\partial \vec{r}},\ \vec{F}_g = -\frac{\partial E_g}{\partial \vec{r}},$$

$$\vec{F}_0 = p_0\frac{\partial V}{\partial \vec{r}},\vec{F}_{EM} = -p_{EM}\frac{\partial V}{\partial \vec{r}},$$

where $\vec{r}$ is a radius vector of a node, S and V denote surface area and volume of the melt, E_g is gravitational energy expressed as a surface integral, σ is a surface tension coefficient, p_0 is a constant pressure term, and p_{EM} is EM pressure distribution.

An algorithm iterates an initial surface shape with fixed triple point line positions by shifting the surface nodes proportionally to the normal component of total force until the equilibrium shape is reached. An iterative procedure chooses such a p_0 value, that the averaged meniscus angle at the crystal triple point line were equal to the silicon growth angle of 11°.

After the free surface shape is obtained, the EM calculations with the new free surface shape are repeated and the EM pressure distribution is updated. This cycle of 3D EM and free surface calculations is repeated until a stable free surface shape is obtained.

2.3. Coupling 3D EM and free surface model with 2D heat transfer model of FZone. To couple the EM-free-surface calculations with 2D heat transfer model of FZone, the EM power values are azimuthally averaged and provided to the heat transfer model. The result of the FZone calculations are a new geometry of the FZ system, including new positions of the triple point lines, and new inductor current strength.

The coupled EM-free-surface and 2D heat transfer calculations are repeated iteratively until a stable, quasi-stationary solution for the whole FZ system is found, i.e., the geometry of the FZ system and its parameters stop changing.

3. Calculation results

4” and 5” FZ crystal growth systems were modeled both with axisymmetric and 3D free surface models. 4” process data were provided by IKZ, Berlin [2]. 5” system was obtained by simply increasing the crystal and feed rod radii by 25%.

Table 1: Inductor current strength and deflection of the crystallization interface for 4” and 5” processes obtained by both models.

Process	Free surface model	Inductor current I, A	Deflection H_C, mm
4”	Axisymmetric	884.5	16.2
4”	3D	886.5	16.2
5”	Axisymmetric	1060.4	24.5
5”	3D	1062.6	25.7

The target zone height, defined as a vertical distance between the triple point line at the crystal and the lower outer point of the feed rod, was set to 32.5 mm for all cases. The inductor frequency was 3 MHz. The inductor had a main slot (1.5 mm width) and three additional slots of 2.0 mm width. The material properties of silicon were taken from [1]. The pulling velocity of the crystal was 3.4 mm/min for the 4” system and 3.0 mm/min for the 5” system. The feed rod was pulled at a constant rate to ensure mass conservation.

The calculations show that the inductor current strength, the deflection of the crystallization interface, and the shapes of the FZ system parts in general are practically the same in the results for the 4” system (Tab. 1), i.e., the 3D asymmetry of the free surface shape played no role for this system. However, there are significant differences in the 5” inch results: the deflection is higher, and a part of the feed rod melted away in the calculations with 3D asymmetric melt surface, see Fig. 2. The reason for this is the changes in the distribution of the azimuthally averaged EM power on the free surface, see Fig. 3, where it is shown as a function of the free surface arc length. The EM power increases near the neck for 5” process, which explains higher melting of the feed rod. There are practically no changes in the power distribution between axisymmetric and 3D cases for the 4” system.

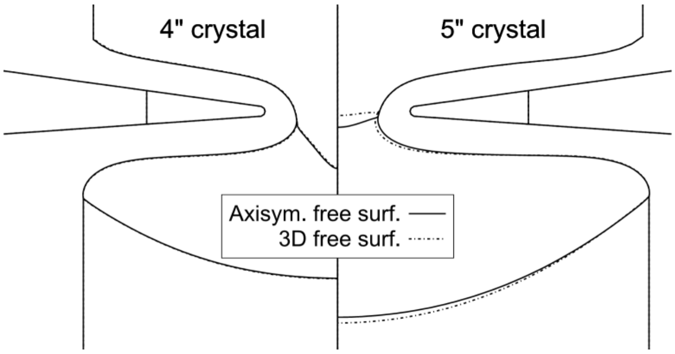

Figure 2: Shapes of the phase boundaries obtained by axisymmetric and 3D free surface models for 4” and 5” crystals.

Fig. 4 shows deviations of the 3D free surface shapes from the axisymmetric ones. The magnitude of the deviations is higher for 5” system, which explains the larger influence of these deviations. The free surface of the 5” system near the neck is, on average, elevated significantly above the axisymmetric surface. It is therefore closer to the inductor, which explains the increase of the received EM power at the neck. FZone uses azimuthally averaged pressure values internally to calculate phase boundary shapes, so its calculated axisymmetric free surface shape has actually a deflection near the neck, see Fig. 2, left, due to increased pressure. Increased EM power near the neck melts part of the feed rod and shifts upwards the triple point line at the feed rod rim. This leads to the free surface bending away from the inductor, thus counter-balancing the EM pressure influence.

Fig. 5 shows azimuthal distribution of the meniscus angle deviations from 11º at the crystal rim. One can see four distinct minima that are related to the EM pressure maximums on the free surface, created by the inductor slits. The main slit causes absolute minimum at 270º, and this minimum is lower for 5” system. The three side slit minima are higher, however, because the pressure maximums for 5” system lay at a greater distance from the crystal rim.

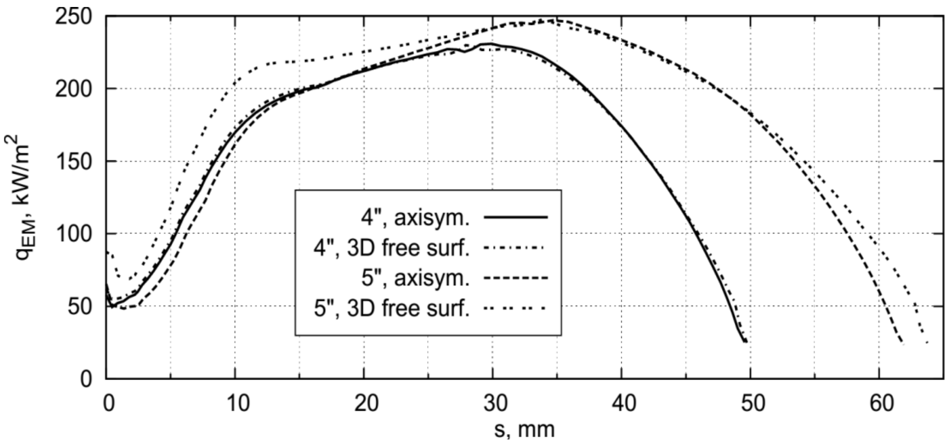

Figure 3: Azimuthally-averaged distributions of EM power density on the free melt surface as functions of arc length s along the free surface 2D profile for 4” and 5” processes. $s = 0$ corresponds to the triple point line at the feed rod (neck). Differences between axisymmetric and the 3D free surface models.

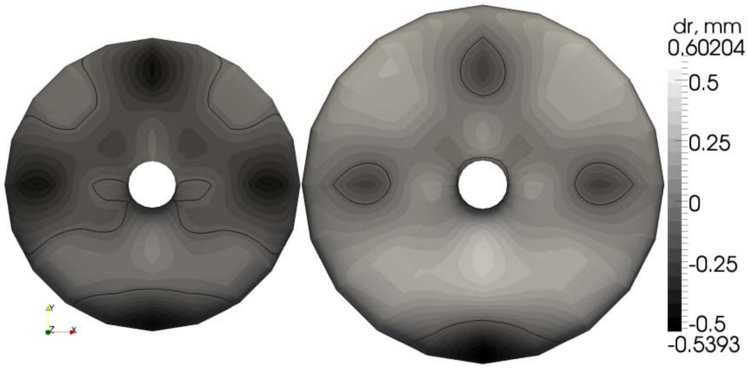

Figure 4: Deviation of the free surface in the normal direction from the axisymmetric free surface shape, 4” (left) and 5” (right) processes. Black line corresponds to dr = 0 mm.

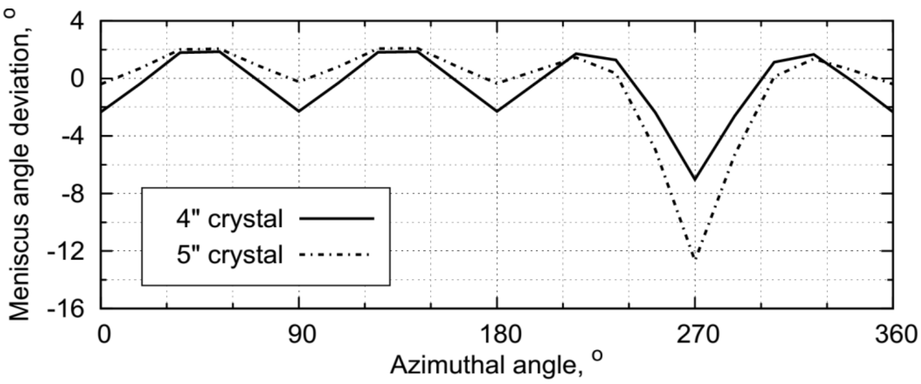

Figure 5: Azimuthal distribution of the meniscus angle deviation from the growth angle (11º).

4. Conclusions

The improved mathematical model with 3D free surface shape modeling has been successfully implemented in the program code for a quasi-stationary model of the FZ process. The calculations showed that the influence of 3D deformations in the free surface shape on the global heat transfer was negligible for the 4” crystal system, but significant for the 5” system. The EM power generation was increased in the area around the neck due to higher local elevation of the free surface. One can expect this effect to be more significant for FZ systems with larger crystal radii; therefore modeling full 3D shape of the free surface could be considered necessary for calculations of these systems.

5. Acknowledgements.
This work has been supported by the European Regional Development Fund, project contract No. 2013/0051/2DP/2.1.1.1.0/13/APIA/VIAA/009.

6. References

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