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Hydrodynamical aspects of the floating zone silicon crystal growth process

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ABSTRACT

3D numerical modeling of dopant transport in the melt is carried out for the 100 mm floating zone silicon single crystal growth process. The axis-symmetric shape of the molten zone is calculated with the program *FZone* considering the coil and the high frequency (HF) electromagnetic (EM) field in 3D. Time dependent melt flow, temperature and dopant concentration fields are modeled using a specialized solver based on the open source code library OpenFOAM®. The influence of the Marangoni coefficient in the boundary conditions on the melt velocity field is analyzed. The obtained shapes of the crystallization interface and resistivity profiles in the grown crystal are compared with experimental results. Differences between axis-symmetric and non-symmetric models are analyzed.

1. Introduction

There are two main methods of growing silicon (Si) single crystals for microelectronics – the Czochralski (CZ) method and the Floating zone (FZ) method. The experiments of Si single crystal growth process carried out for the process development are very expensive therefore numerical modeling is frequently used to support the process improvement. Computational resources allow to model many physical aspects of a FZ system, e.g., hydrodynamical (HD) processes in liquid silicon, that cannot be revealed by performing experiments.

In this study the calculations of phase boundaries are performed with the previously developed program *FZone* [1], where all interfaces and fields are calculated in axially symmetrical approximation (2D), except the 3D HF EM field of non-symmetrical inductor. The influence of the melt flow on 2D shape of phase boundaries can be investigated using *FZone* as well. The other program used — 3D solver *FZSiFOAM* for the melt flow, temperature and dopant concentration distribution based on the open source code library OpenFOAM® is described in [2]. However, the results of this program were not verified by experiments, e.g., compared with measured radial resistivity variations (RRV).

Although many numerical models are successfully used to describe the FZ crystal growth process it is necessary to improve them using new available experimental data. In the present work HD modeling is used to obtain a more precise shape of phase boundaries and for the calculation of RRV profiles from the dopant concentration field in the melt. This allows to investigate the influence of the temperature coefficient of surface tension $M = \partial\gamma/\partial T$ (i.e., Marangoni coefficient), which has strong dependence on the oxygen content in growth chamber [3].

2. Description of experimental FZ system

The experiments have been carried out in the Leibniz Institute for Crystal Growth by Robert Menzel who investigated the influence of a lower frequency of the induction coil on the FZ process [4]. The parameters of the experimental system are listed in Table 1 and the inductor used is shown in Fig. 1.

Table 1
Parameters of the experimental system.

Parameter, unit of measurement	Value
Radius of crystal R_C, mm	51
Radius of feed rod R_F, mm	49
Zone height H_Z, mm	34.87
Pull rate of crystal v_C, mm/min	3.4
Pushing rate of feed rod v_F, mm/min	3.68
Frequency of current in inductor f_{ind}, MHz	3
Rotation speed of crystal ω_C, rpm	6
Rotation speed of feed rod ω_F, rpm	0.8

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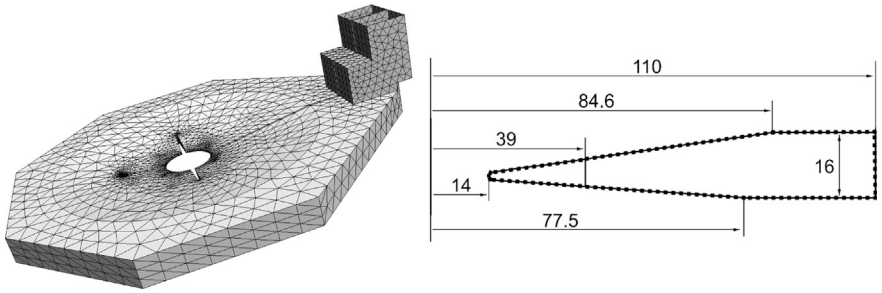

Fig. 1. Overall view of the HF inductor (left) and its geometrical dimensions of the vertical cross-section (right).

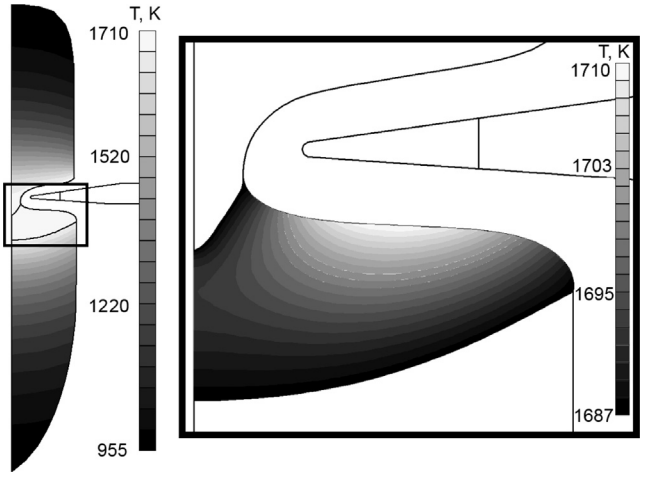

Fig. 2. Calculated phase boundaries and obtained temperature field using the program *FZone* [1].

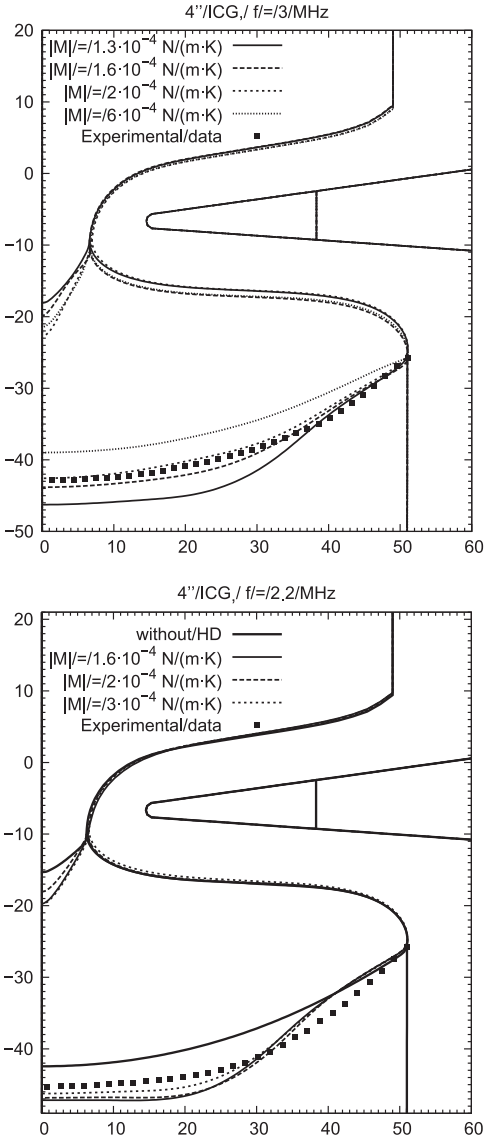

Fig. 3. Phase boundaries in the 4 inch FZ system for $f_{ind} = 3$ MHz (top) and $f_{ind} = 2.2$ MHz (bottom).

3. Mathematical models and software

3.1. Phase boundaries

The first step of the numerical modeling of the FZ crystal growth process is 2D axis-symmetric calculations of phase boundaries using a specialized program *FZone* [1]. The calculations of the HF EM field are done considering the 3D HF inductor [5]. The obtained induced power surface density values are averaged in the azimuthal direction so that they can be used as a heat source for the 2D axis-symmetric phase boundary calculations. Melt motion (incompressible, laminar, buoyancy-driven flow) can be taken into account. The position of the phase boundaries is found iteratively starting from some initial approximation. The direction and magnitude of the movement of any interface point depends on the equations of heat balance where temperature gradients are obtained from the calculated temperature field [1]. An axially symmetrical approximation of melt flow is used due to the large number of iterations required — for every shape of phase boundaries the temperature field must be solved (Fig. 2).

3.2. Melt flow

The unsteady 3D numerical modeling of the melt flow in the FZ process is performed with the solver *FZSiFOAM* which is based on the open source code library OpenFOAM. For the calculations a structured mesh of 160,000 hexahedral elements was used. The melt flow is considered as laminar as the characteristic Reynolds number is approximately 1500. The detailed description of the used mathematical models is given in [6], only the most important equations are listed here:

$$\rho_0\frac{\partial \mathbf{v}}{\partial t}+\rho_0(\mathbf{v}\nabla)\mathbf{v} = -\nabla p+\eta\Delta\mathbf{v}-\rho_0\mathbf{g}\beta(T-T_0),$$

$$\nabla\mathbf{v} = 0,$$

$$\rho_0 c_p\frac{\partial T}{\partial t}+\rho_0 c_p(\mathbf{v}\nabla)T = \lambda\Delta T,$$

where ρ_0 is the density of liquid silicon at melting temperature, $\mathbf{v}$ — melt velocity, t — time, p — pressure, η — dynamic viscosity, $\mathbf{g}$ —