3D MODELLING OF HF EM, HD AND DOPANT CONCENTRATION FIELDS FOR THE FZ CRYSTAL GROWTH PROCESS

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Introduction. The analysis by computer modelling of 3D aspects of the industrial Floating Zone (FZ) process for large (up to 200 mm in diameter) silicon single crystal growth is necessary because a one-turn high frequency (HF) inductor is used. Due to the main slit of the inductor, current suppliers and other asymmetric elements, the inductor induces a magnetic field that causes asymmetric eddy currents on the surface of the polycrystalline feed rod, molten silicone and single crystal. As a consequence, the induced power density has no axial symmetry. To maintain symmetric melting of the feed rod and the crystallization process of single crystal, both of them are rotated.

One of the main quality criteria of silicon wafers is homogeneity of the radial resistivity distribution. In the FZ process, the silicon melt usually is continuously doped with boron or phosphorus. The melt flow influences the segregation process at the crystallization interface and, as a consequence, the dopant distribution in the melt along the crystallization surface. This causes variations of the concentration in the grown single crystal that leads to inhomogeneity in the crystal, e.g., rotational striations. To ensure better mixing of the melt, a low frequency rotating magnetic field can be used. Displacement of the rotation axis of the feed rod and of the single crystal is a known possibility, too. Nevertheless, experiments with large diameter crystals are very expensive, therefore, they have to be supported by computer modelling.

Various aspects of the axisymmetric (2D) mathematical modelling and the calculation methods for the shape of the molten zone and hydrodynamics during the radio-frequency needle-eye FZ growth of large crystals are described in [1] and [2]. The case of small crystals ($\leq$ 10 mm) is considered, e.g., in [3]. In [4] the calculation of the time-averaged dopant concentration fields and macroscopic resistivity distributions are given. Lüdge *et al.* in [5] compare the results for macroscopic resistivity distributions calculated by the model in [4] with spreading resistance and 4-point measurements. Some transient axisymmetric numerical calculations of the hydrodynamic and temperature fields in the melt are described in [6], considering 100-mm crystals. Transient dopant concentration fields are calculated in [6] and microscopic inhomogeneities are analyzed. The stationary and transient axisymmetric phase boundary calculations recently have been described in [7].

Since the pancake inductor has only one turn, the EM field and the distribution of heat sources and EM forces on the melt free surface have distinct asymmetric features. Since rotational striations are always originated by three-dimensional (3D) effects, they cannot be calculated within the limits of a two-dimensional model. Some 3D aspects of non-industrial FZ-processes (small crystal diameters)

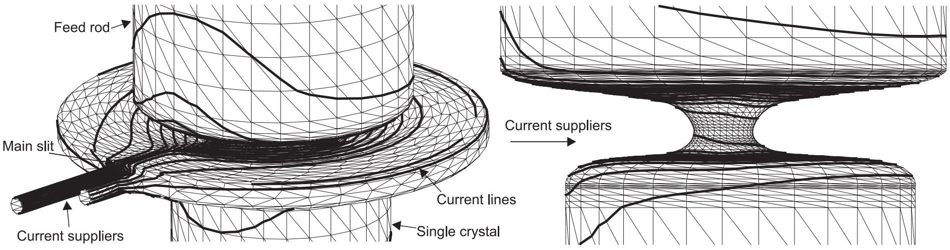

Fig. 1. BEM mesh for 3D HF EM field calculation. Current lines on the surfaces of the inductor and silicon.

are considered in [8]. 3D calculations of an industrial FZ-process have been carried out in [9], where the influence of the three-dimensional EM and Marangoni forces is taken into account. Analysis of rotational striations and a comparison with experiment is carried out in [10].

A new 3D model system for calculating the hydrodynamic and temperature fields in the melt for the industrial FZ growth process of large-diameter single crystals with a rotating magnetic field and a displacement of the crystal and the feed rod axis is described in details in [11]. This paper presents new results obtained by the 3D model system illustrating 3D features of the FZ crystal growth process.

1. The system of mathematical models. The current study is performed combining both 2D and 3D calculations. The shape of the molten zone is calculated with an axially symmetric approximation using a special program FZONE for phase interface calculation. Then a 3D EM field, both with and without displacement of the axis is calculated using a program based on BEM (calculation method is described in [12]). In these calculations the 3D form of the HF inductor is taken into account. The result – induced power density distribution and distribution of dopants on the free surface of molten silicon are interpolated on a 3D FEM grid for HD calculations, which are performed with the use of commercial package CFD-ACE for HD calculations. Forces induced by a low frequency magnetic field are calculated with the help of ANSYS package and imported in 3D HD calculation (the details see in [11]).

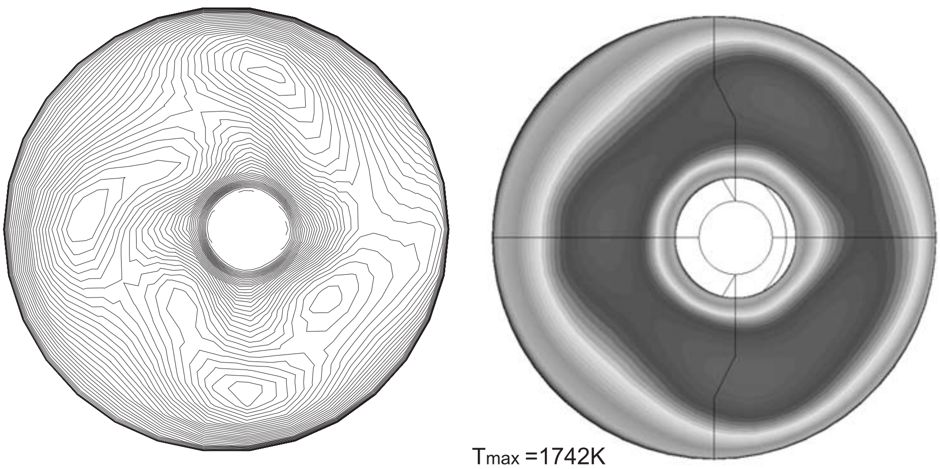

Fig. 2. Power isolines and temperature field on the free surface.

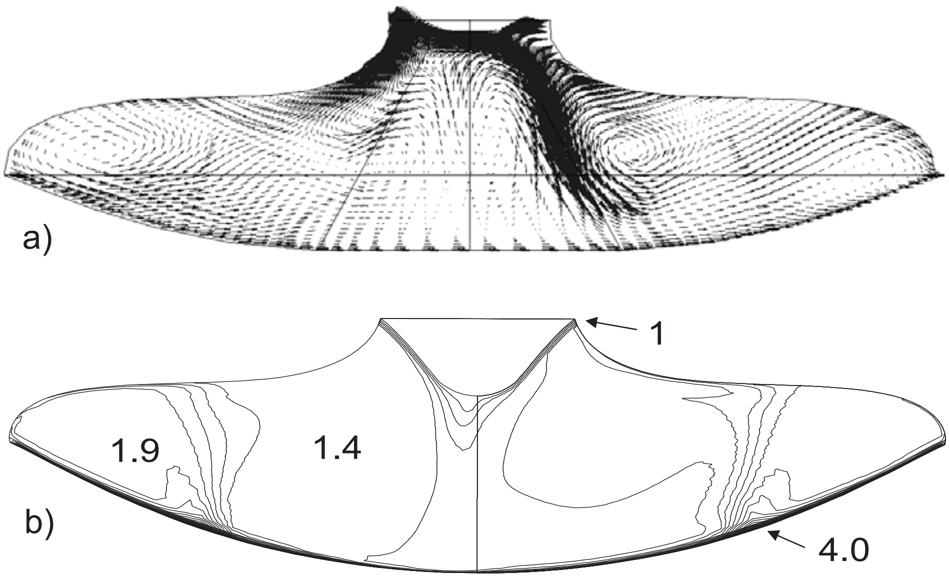

Fig. 3. (*a*) Velocity profiles in the vertical cross-section perpendicular to the plane of axis displacement. (*b*) Concentration field in the vertical cross-section perpendicular to the plane of axis displacement.

2. The calculation example. Current lines on the surface of the inductor and silicon are shown in Fig. 1. A distinct asymmetry can be observed near the main inductor slit. The power isolines and respective temperature distribution on the free surface of molten silicon are shown in Fig. 2. An example of calculated velocity concentration field in the vertical cross-section is shown in Fig. 3. Normalized resistivity radial distribution, e.g., rotational striations are shown in Fig. 4. The concentration field in the horizontal cross-section is shown in Fig. 5.

3. Conclusions. The 3D calculations of the HF EM field showed a distinct asymmetry of the magnetic field and induced power density on the surface of the silicon for the realistic FZ crystal growth process. HD calculations have shown that the asymmetry of power density leads to a distinct asymmetry of the velocity field pattern and dopant concentration field as well.

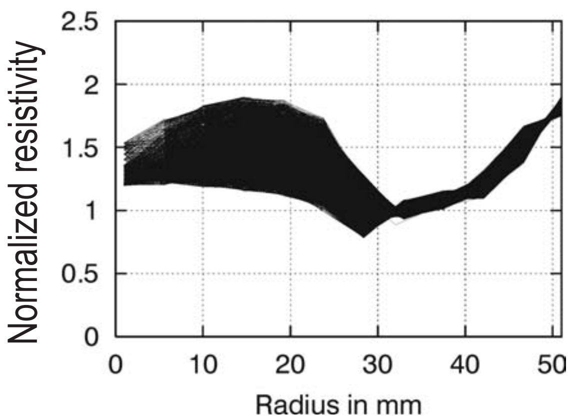

Fig. 4. Radial resistivity distribution - rotational striations.

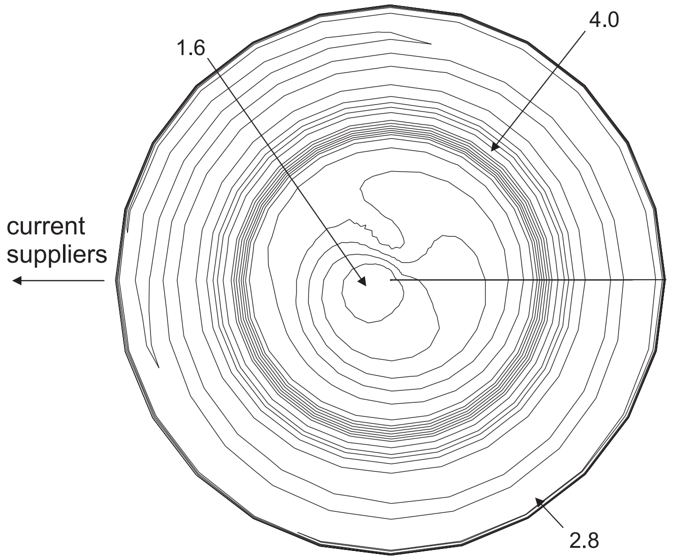

Fig. 5. Concentration field in the horizontal cross-section.

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