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3D Transient LES Modeling of Turbulent Melt Flow in a Laboratory Model for Large CZ Industrial Silicon Crystal Growth Systems

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Abstract

Czochralski method of single crystal growth is the backbone of the industrial silicon crystal growth, and numerical modeling of the silicon melt flow in the crucible has tremendous importance for the industrial process development. The axisymmetric 2D turbulence models provide limited ability to model 3D turbulent melt flow in CZ crucible, and nowadays 3D LES turbulence modeling has become a practical tool for silicon melt flow modeling. However, as 2D turbulence models, LES models also need verification. We present the first results of 3D LES modeling of melt flow for a laboratory Czochralski facility with low temperature metallic eutectic melt and compare these results with 2D modeling results and with temperature measurements in the melt.

Introduction

The Czochralski (CZ) crystal growth method is the most widely used method for the single silicon crystal growth in the microelectronic industry, and it accounts for about 95% of the total silicon single crystal production. Typically, a CZ crystal growth system consists of a silica crucible filled with silicon melt, graphite heaters, heat shields, and the whole system is enclosed in a vessel that protects it from the outside environment, see Fig. 1. The crystal is grown from a seed, and both the crystal and crucible can rotate. Various electromagnetic systems can be implemented for additional influence on the melt flow.

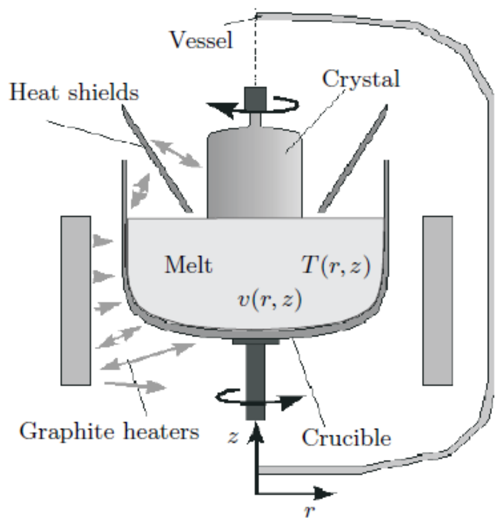

Fig. 1. A schematic layout of a CZ silicon single crystal growth system.

In the course of the time, the size of grown crystals has significantly increased, and nowadays 300 mm crystals are standard in the industry. The large dimensions of CZ systems have significantly complicated the control over the growth process and quality of the grown crystals, and for this reason the numerical modeling have become extremely important in understanding the processes in CZ systems and reducing the development costs.

A very important aspect of the CZ system modeling is the modeling of the melt flow in the crucible. The melt flow distribution determines, for example, distribution of oxygen in the melt at the crystallization interface and therefore affects the oxygen distribution in the crystal. Similarly the melt flow determines temperature distribution at the crystallization interface, which determines the point-defect distribution in the crystal. The melt flow distribution may also affect the crystal growth stability.

Different models have been used to model the melt flow in CZ systems. Several authors used the steady-state axisymmetric laminar flow model to model the melt flow in CZ growth facilities, see, for example, [1, 2]. This model considered the the oxygen transport, Marangoni convection, and other processes. However, the steady-state axisymmetric laminar flow model can only be used for small CZ systems like systems in [2] (Re $\approx 10^3$). In cases with larger crystals, the flow becomes turbulent, and therefore the steady-state laminar flow model can not be used. One possibility is to artificially increase the viscosity of the melt, see, e.g. [3]. Another possibility is, see e.g. [4], to apply un-steady axisymmetric laminar flow models.

The typical values of Reynolds numbers for the silicon melt flow in modern industrial CZ systems is about 10^5, and the melt flow can certainly be considered as turbulent; therefore turbulent melt flow models have to be applied in the numerical modeling. Among the most widely used turbulence models are the Reynolds-averaged Navier–Stokes equations (RANS) turbulence models, see [5, 6, 11], for example.

One of the most and still widely used turbulence models are 2D axisymmetric k-ε turbulence models, which can be applied due to axial symmetry of the CZ crystal growth systems. For example, Chien low-Re-number k-ε turbulence model has been applied to model various melt flow regimes both in the laboratory models (see [5,11]) as well as in the real CZ systems. 2D axisymmetric k-ε turbulence models are robust and relatively fast, so large series of calculations can be carried out with modern computers in very short time. However, comparisons between 2D calculation and temperature measurement results for the laboratory model of CZ systems have shown that 2D Chien turbulence model has several problems with correct modeling of the melt flow in CZ systems. Particularly, an artificial symmetry axis as well as the deficiencies of k-ε models can be blamed for the discrepancies.

Alternatives to 2D axisymmetric k-ε turbulence models are 3D transient melt flow models such as Large Eddy Simulation turbulence models (LES) and "quasi-DNS" approach. "Quasi-DNS" approach is, in fact, modeling the laminar melt flow using relatively rough 3D grids (several hundreds of thousands of cells). This model has been applied to model silicon melt flow in CZ crucibles in [7]. The problem of this approach is the dependence of the solution on the grid roughness, which is insufficient for modeling small scale turbulence. Therefore LES models are more preferable since they model the small scale eddies and directly solve only the transient 3D melt flow equations for large eddies. LES modeling requires greater numerical meshes and is more time-consuming than the 2D axisymmetric turbulence models. However, using clusters of modern computers makes 3D LES modeling a practical alternative to 2D turbulence models, and 3D LES models have been already successfully applied in modeling the silicon melt in CZ crystal growth systems [8, 9]. Nevertheless, due to complicated character of turbulent flow in CZ systems, 3D LES modeling of melt motion in the crucible needs greater experimental verification.

In this paper we summarize the characteristic discrepancies between the temperature measurements in the CZ laboratory system (which works with low temperature eutectic melt) and the results of 2D axisymmetric turbulence model, and we also present first, preliminary results of 3D LES simulation of the turbulent melt flow in the laboratory model.

1. Description of the low temperature laboratory model of industrial CZ silicon crystal growth systems

Very high silicon melt temperatures and aggressive environment complicates the temperature and velocity measurements in industrial CZ silicon crystal growth system. For this reason, the team of Prof. Gelfgat and Dr. Gorbunov at the Intitute of Physics of the University of Latvia (Salaspils) developed a laboratory model for CZ silicon single-crystal growth systems, in which InGaSn eutectic with melting point of about 10º C was used as melt, see Fig. 2. The laboratory model [10] consists of a silica crucible filled with the eutectic and a crystal model which is a metal can cooled by water. A layer of hydrochloric acid solution covers the free surface of the melt to prevent oxidation, and a system of water-cooled pipes is immersed in the acid to model the radiation heat losses from the free melt surface. The crucible is heated by resistance heaters at the crucible.

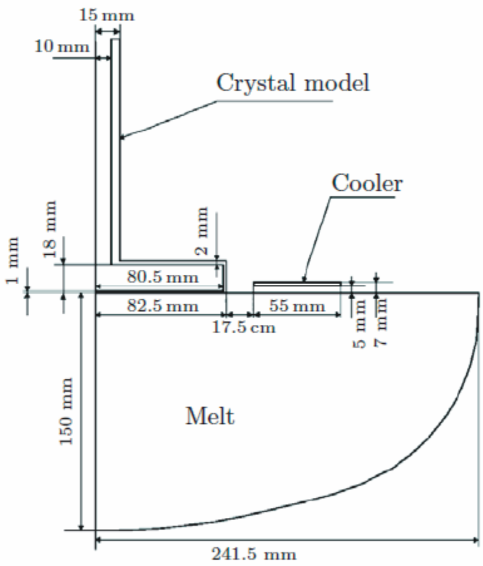

Fig. 2 Scheme of the laboratory model

A system of 32 thermo-pairs has been used to measure temperature and temperature fluctuation distributions in meridional and horizontal planes in melt, see Fig. 3. Temperature measurements are read from each thermo-pair with high frequency and stored on a computer; later average temperature and temperature fluctuation values are calculated for each measurement point. Afterwards the distributions of averaged in time temperature and the characteristic value of temperature fluctuations (standard deviation) are interpolated using the sets of measured values at all 32 points.

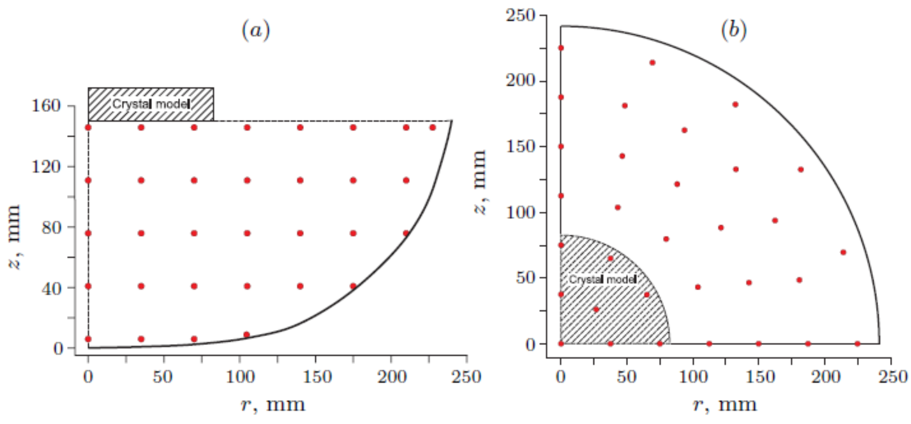

Fig. 3. Placement of thermo-pairs for temperature measurements in the CZ laboratory model: a) measurement points in the meridional plane; b) measurement points in the horizontal plane.

2. 2D turbulence modeling problems

In [11, 12] we have carried out a series of numerical modeling of the melt flow in the CZ laboratory model for different crystal and crucible rotation rates and we have investigated also the influence of various EM fields on the melt flow. The “CFD-ACE 2003V” program package for 2D HD turbulent melt flow modeling was used, and the Chien low-Re number k-ε turbulence model was chosen.

Here we present the calculation results for the melt flow in the CZ laboratory model with the crucible rotation $\Omega_{crucible}$ = -5 rpm and the crystal rotation $\Omega_{crystal}$ = 15 rpm to show the characteristic problems that arise in calculations of the CZ systems with 2D axisymmetric k-ε turbulence models. Fig. 4 shows the calculated and measured temperature and temperature fluctuation distributions. To derive the standard deviation δT of temperature fluctuations from the calculated turbulent melt flow quantities, we use the following estimation, see [11]:

$$\delta T = \frac{0.5|\nabla T|\lambda_{turb}}{\rho c_p \sqrt{k}} , \tag{2.1}$$

where k is turbulence kinetic energy and λ_{turb} is turbulent heat conductivity.

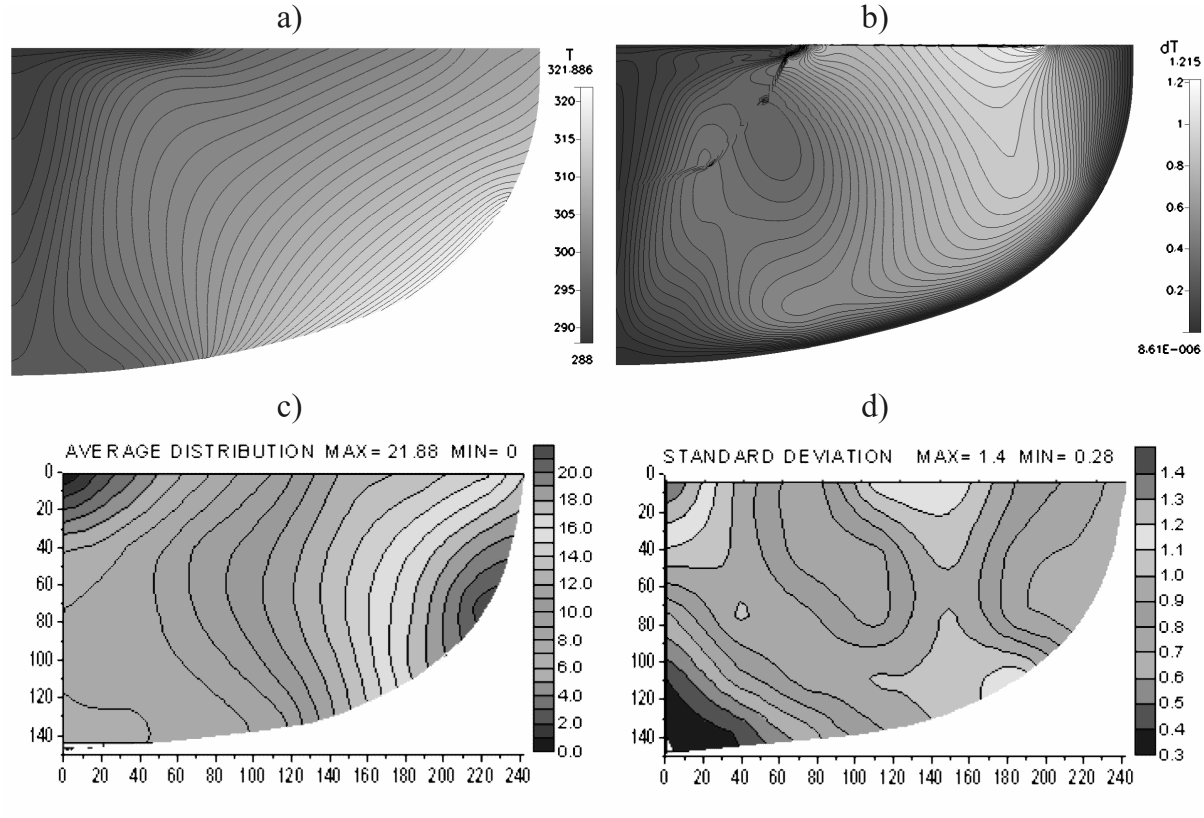

Fig. 4. Comparison between the numerically modeled (top) and measured (bottom) temperature and temperature fluctuation (standard deviation) distributions for the case with $\Omega_{crucible}$ = -5 rpm and $\Omega_{crystal}$ = 15 rpm: a) and c) averaged temperature distribution; b) and d) temperature fluctuations (standard deviation) distribution.

From Fig. 4, the following main discrepancies between calculated and measured results can be seen: 1) Calculations show a long “tongue” of low temperatures under the crystal, while there is no such a “tongue” in the measured distribution; 2) In the outer zone of the melt (the melt region under the free melt surface), the calculated isotherms are more sloping than measured isotherms, and the calculated temperature maximum is positioned lower than the measured maximum; 3) In the outer zone, the calculations and measurements show similar temperature fluctuation distributions but under the crystal the measured fluctuations are much higher than the calculated fluctuations.

All these discrepancies can be attributed to the deficiencies of the 2D axisymmetric k-ε turbulence models: 1) artificially imposed symmetry axis on the melt flow; 2) the inability of the low-Re k-ε turbulence model to correctly describe large scale turbulent melt flow fluctuations.

The calculations show a strong downward flow along the symmetry axis and low level of velocity fluctuations there, which contradicts to temperature measurements. It seems that the applied 2D axisymmetric turbulence models do not model correctly the fluctuations across the axis; i.e. the fluctuations appear to be reduced. Similarly, it can be assumed that the average meridional flow in the outer zone in the experiment is more intense than the 2D modeling results imply, which would explain the discrepancy of the slope of the isotherms.

3. Short description of Large Eddy Simulation method for turbulence modeling

LES method allows modeling the basic turbulent melt flow features on the grids with the same resolution level as in RANS modeling. LES model is based on distinguishing two scales in flow fluctuations: 1) large scale fluctuations that are calculated directly; 2) small, grid scale fluctuations which are modeled indirectly. Mathematically it can be represented by filtering operation:

$$\bar{f}(x,t) = \int f(x',t)G(x-x',t,\overline{\Delta})dx', \qquad (3.1)$$

where $\bar{f}$ represents the filtered value of a field variable f, G is a symmetric filtering function, and $\overline{\Delta}$ is filter (grid) width. Applying this filtering operation to the Navier-Stokes equations, one obtains the equation for the filtered flow field, which differs from the original equations by an additional stress term $\tau_{ij} = \bar{u}_i \bar{u}_j - \overline{u_i u_j}$, which appears due to filtering non-linear convection terms. This stress term is known as subgrid scale stresses.

One of the most popular LES models is Smagorinsky-Lilly model. In this model, the deviatory part of the subgrid scale stresses is modeled via Bussinesq hypothesis (as in RANS turbulence models):

$$\tau_{ij} - \frac{1}{3}\tau_{kk}\delta_{ij} = -2\mu_T \overline{S}_{ij}, \quad \mu_T = \rho(C_s\overline{\Delta})^2 \left|\overline{S}\right|, \qquad (3.2)$$

where $\overline{S}_{ij}$ is the rate-of-strain tensor, μ_T is the subgrid-scale turbulent viscosity, and the constant C_3 has the value in the interval 0.05 – 0.2.

4. Preliminary results of 3D LES modeling of the turbulent melt flow in the laboratory system

Fig. 5 presents first, preliminary 3D LES simulation results obtained with program package "FLUENT 6.0.20" for the melt in the ELMATEC laboratory system with the crucible rotation rate $\Omega_{crucible}$ = -5 rpm and the crystal rotation rate $\Omega_{crystal}$ = 15 rpm. As one can see the LES modeling results agree with the measured temperature distributions much better than the 2D axisymmetric modeling results. For example, the narrow low temperature "tongue" under the crystal has disappeared, and the temperature distribution in the outer zone has become closer to the measured distribution, i.e., isotherms have become more vertical and the position of the temperature maximum also is closer to the measured position. Similarly, 3D LES modeling results show more intense temperature fluctuations under the crystal (with the exception of a thin layer under the crystal), which is in better agreement with the measurements.

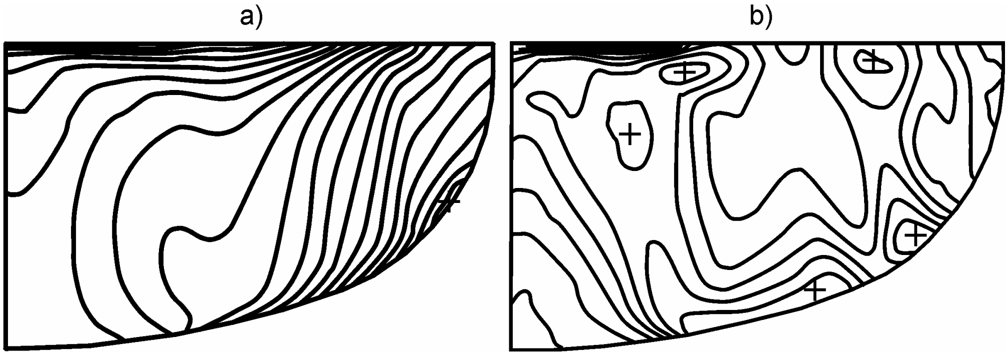

Fig. 5. Meridional temperature (a) and temperature fluctuation (b) distributions calculated with LES for the case with $\Omega_{crucible}$ = -5 rpm and $\Omega_{crystal}$ = 15 rpm.

Conclusions

Our first preliminary results of 3D LES modeling of the melt flow in the CZ system laboratory model have shown that 3D LES modeling results agree better qualitatively with temperature measurements as the 2D modeling results.

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