Eddy-resolving numerical simulation of silicon melt convection in a Czochralski crucible: effects of radiation from the free surface at various crucible rotation rates

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Abstract. The contribution covers results of numerical study based on conjugate heat transfer formulation of turbulent silicon melt convection in an industrial system for CZ Si-crystal growth of 100 mm diameter crystals. The computations have been performed using an eddy-resolving method treated as Implicit LES for two values of the emissivity from the melt free surface (0.25 and 0.3) and the crucible rotation rate of 2 and 5 rpm. The effects of these parameters on melt convection and characteristics of heat transfer are analyzed.

1. Introduction
The problems of investigating turbulent regimes of thermo-convection developing in confined enclosures provoke permanent interest of researchers. A highly demanded fundamental and applied area is the numerical simulation of convective flows and heat transfer in turbulent semiconductor melts in Czochralski (CZ) systems for Si-crystal growth.

In the 1980-1990s numerical studies of the problem were performed on the base of axisymmetric formulations using the RANS approach [1]. The accumulated computational experience allowed recognizing several principal drawbacks of the axisymmetric formulations and their fundamental inability to adequately reproduce flow structure and temperature distribution in the melt.

At the turn of the century, the first attempts were undertaken to carry out computations in enclosures with real crucible geometry of the CZ system and under practical thermal boundary conditions on grids consisting of tens of thousands of cells (see, for example, [2-5]). At the same time the LES and hybrid RANS/LES approaches began to be used in the studies at the Rayleigh numbers characterizing the real growth conditions [4, 5]. This served to reach an acceptable agreement with available experimental data for time-averaged flow fields and temperature fluctuations in time.

In recent years, under conditions of ever-growing computational capabilities, investigations based on refined eddy-resolving approaches, with more and more detailed computational grids, have come to the forefront [6-9]. An efficient computational method known as Implicit LES is increasingly applied to solve the CZ-growth problems in complex geometry.

Major numerical studies of 3D unsteady phenomena during the CZ crystal growth are based on segregated formulations for melt convection. These formulations require a definition of thermal boundary conditions at the melt-crucible interface. As a rule, an axisymmetric wall temperature distribution is assumed.
Solutions that are, as expected, closer to the reality can be obtained with a conjugate heat transfer formulation [10, 11]. Such problem statement originated from the suggestion that unsteady phenomena attributed to melt convection instabilities are concentrated in the hot zone including the melt, the quartz crucible and the graphite support.

It should be noted that the problem considered is characterized by a multiplicity of factors of the physical and chemical nature, which affect convection and heat transfer in the melt, and, as a consequence, the crystal quality. In the context of the existing uncertainties in setting the properties of liquid silicon and solid materials surrounding the crucible, it seems advisable to perform parametric computations aimed at quantitative evaluation of influence of individual factors on results of melt convection simulation.

In the present work, numerical solutions of the conjugate heat transfer problem formulated for the hot zone of the industrial EKZ 1300 system for CZ growth of 100 mm Si-crystal [4] are presented and discussed in detail. The coefficient of thermal radiation from the surface of the Si-melt and the crucible rotation rate are considered as varying parameters of the problem.

2. Computational model

The computational domain (see figure 1a) includes the quartz crucible of inner/outer radii $R_c$ and $R_q$, filled by molten silicon, and the support of radius $R_g$ made of graphite. A melt-crystal interface of radius $R_s$ occupies the central part of the melt upper boundary. The vertical distance from the lowest point of the bottom to the free surface $H$ was equal to 9.85 cm. The crystal and crucible rotate about the vertical axis with the angular velocities $\Omega_s$ and $\Omega_c$. The main geometrical parameters were taken as $R_s = 0.53H$, $R_c = 1.74H$, $R_q = 1.82H$, $R_g = 1.98H$, $H_g = 0.47H$, $L_q = 2.91H$, and $L_g = 2.54H$.

![Figure 1](attachment:image.png)

**Figure 1.** Computational domain geometry in the axial vertical section (a); multi-block computational grid (b).

3D unsteady Si-melt convection was computed based on the Navier-Stokes equations written in a rotating system (with the Boussinesq approach for incorporation of the gravity buoyancy effects) and added by the equation of convective-diffusive heat transport (diffusive-only in the solid regions).

Zero relative velocity conditions were imposed on the crucible wall, and the velocity distribution on the melt-crystal interface was given by $-\Omega_s r$. The dynamic effects associated with the flow of gas (argon) over the melt free surface in a real system were taken into account by setting the distribution of the tangential shear stress (see figure 2a) obtained from calculations based on the axisymmetric formulation [4]. Two values of the crucible rotation rate, $\Omega_c$, were used in the present computations (2 and 5 rpm). The crystal rotation rate $\Omega_s$ was fixed as $-20$ rpm.
Figure 2. Distribution of free surface shear stress produced by argon flow (a); distributions of radiative heat flux along the free surface (b), quartz (c) and graphite (d) walls.

The melt-crystal interface was maintained at a constant temperature equal to the Si crystallization temperature of 1685 K. On the other external boundaries the condition of radiative heat transfer was specified with the heat flux distributions adopted from the results of global heat transfer modeling in the CZ furnace [4]. Distributions of radiative heat flux on the free surface and along the quartz and graphite surfaces (see scheme in figure 1a) are shown in figures 2b-d (it should be noted that heat removal from the free surface due to convection is neglected). The central segment of the graphite body bottom wall of radius 0.45H was considered as thermally insulated.

The physical properties of the materials used in the present computations are as follows:

- **liquid silicon**: dynamic viscosity – 7.74·10^{-4} Pa·s, heat conductivity – 52.4 W/(K·m), specific heat – 1016 J/(K·kg), density – 2570 kg/m^3, thermal expansion coefficient – 1.45·10^{-4} 1/K;
- **quartz**: heat conductivity – 4.032 W/(K·m), specific heat – 1500 J/(K·kg), density – 2691 kg/m^3, emissivity – 0.85;
- **graphite**: heat conductivity – 35.3 W/(K·m), specific heat – 2000 J/(K·kg), density – 2030 kg/m^3, emissivity – 0.8.

Four cases have been computed: with two different values of the crucible rotational rate and for two values of free surface emissivity α, set as 0.25 or 0.3 (these values were chosen based on various literature data). The Prandtl number of Si-melt was set to be equal to 0.015.

The governing equations were solved using the computational approach treated as Implicit LES. The fractional-step method was applied, as implemented in the well-validated in-house finite-volume unstructured-grid CFD-code SINF/Flag-S developed at the SPbPU [12]. The third-order QUICK scheme was used for spatial discretization of the convective fluxes, and the diffusion terms were approximated by the second order central-difference scheme. Time advancing was carried out with the second-order Crank-Nicholson scheme.

Multi-block computational grid used in the computations (figure 1b) consisted of approximately 1.8 million cells, while about 1 million cells were located in the liquid zone; the vertical size of the first step near the crucible wall and near the free surface was about 10^{-3}H.

The time step was less than one thousandth of the characteristic convection time, t_b = (H/(gβΔT))^{0.5} ≈ 1 s, and the local Courant number did not exceed unity. The samples used for averaging, started after a transient period, amounted up to 200t_b.
3. Results and discussion

For the case of $\Omega_c = 5 \text{ rpm}$, figure 3 shows typical instantaneous temperature distributions over the central vertical section and the bottom wall of the crucible computed with two values of $\alpha$. It can be seen that a relatively small change in the free surface emissivity leads to a considerable reduction of the melt temperature and the temperature difference between the crucible wall and the crystal. Note also that, due to low thermal conductivity of the quartz wall, temperature pulsations developing in the melt do not penetrate into the graphite support, and the temperature field for this body distribution in it is almost stationary.

![Temperature fields](image)

**Figure 3.** Typical instantaneous temperature fields in the central vertical section (a) and on the crucible wall (b) for different $\alpha$ at $\Omega_c = 5 \text{ rpm}$.

The melt vertical velocity and temperature fluctuations, as well as data on power spectral density (PSD) of temperature fluctuations at a monitoring point placed at $r = 0.7H$, $z = 0.9H$ are shown in figure 4. One can see that fluctuations of vertical velocity and temperature are chaotic in time, so a turbulent regime of convection takes place and the Kolmogorov power law of $f^{-5/3}$ is observed at the PSD for the cases considered. Vertical velocity evolutions for different values of emissivity are very close for both the amplitude and the frequency. A comparison of the computational results for temperature pulsations with experimental data [3] shows that a good agreement for the mean temperature level is achieved in case of $\alpha = 0.3$.

Figure 5 shows radial distributions of the time-averaged melt temperature obtained for different sets of the varied parameters. A comparison of the Implicit LES results with the respective temperature thermocouple measurements [3] for $\Omega_c = 2$ and $5 \text{ rpm}$ is provided as well. The radial distributions are given for five values of the distance from the free surface ($z^*$). It can be seen that there are significant distinctions in the dependences obtained for different $\alpha$-values for both the crucible rotation rates. A satisfactory agreement with experimental data is registered at $\alpha = 0.3$, however, even in this case, the temperature values at small and middle radii are noticeably underestimated.
Figure 4. Vertical velocity and temperature fluctuations in the melt and the PSD of temperature fluctuations at monitoring point located at $r = 0.7H$, $z = 0.9H$: results obtained for different $\alpha$ at $\Omega_c = 5$ rpm.

Figure 5. Radial distributions of the time-averaged melt temperature.

Time-averaged temperature and heat flux distributions along the melt-crucible interface for all the cases computed are given in figure 6. One can see that the shape of the temperature profiles is the same in all the variants. However, as expected, the temperature level is significantly lower for the cases with higher value of the emissivity, and the difference exceeds 10 K. A better agreement with the experimental data reported in [3] for $\Omega_c = 2$ rpm is also achieved at $\alpha = 0.3$. In case of $\Omega_c = 5$ rpm, the computed and the measured temperatures agree well at the crucible bottom only, whereas the peak temperature values observed in the experiments at the crucible side wall are considerably underpredicted. An additional research work is needed to reveal possible reasons of this discrepancy.

Figure 6. Distributions of the time-averaged temperature and heat flux over the crucible wall.
The effective Rayleigh and the Rossby numbers evaluated using the maximum time-averaged temperature difference between the crucible wall and the crystal, as well as the surface-averaged heat flux at the crucible wall are given in table 1. The table shows, in particular, that the difference in values of $Ra_{\text{eff}}$ obtained at two emissivity values considered exceeds 50%, and the difference in the $Ro_{\text{eff}}$ numbers reaches 25%.

**Table 1.** The effective Rayleigh and the Rossby numbers, and the surface-averaged heat flux at the crucible wall.

| $\Omega_c$ (rpm) | $\alpha$ | $Ra_{\text{eff}}$ | $Ro_{\text{eff}}$ | $Q$ (W/m$^2$) |
|------------------|----------|--------------------|-------------------|--------------|
| 2                | 0.25     | $10.1 \cdot 10^6$ | 3.85              | $2.84 \cdot 10^4$ |
| 2                | 0.3      | $6.44 \cdot 10^6$ | 3.07              | $3.32 \cdot 10^4$ |
| 5                | 0.25     | $9.29 \cdot 10^6$ | 1.48              | $2.97 \cdot 10^4$ |
| 5                | 0.3      | $5.46 \cdot 10^6$ | 1.13              | $3.51 \cdot 10^4$ |

4. Conclusions

Based on the Implicit LES approach, numerical simulation of conjugate heat transfer at turbulent melt convection in an industrial system for CZ Si-crystal growth of 100 mm diameter has been carried out. The parametric computations were performed for two values of the emissivity from the free surface, $\alpha$, and with crucible rotation rates set at 2 or 5 rpm. A strong influence of these parameters on the flow field structure and the thermal state of the melt has been revealed. A satisfactory agreement with the experimental data for the melt temperature field has been obtained at $\alpha = 0.3$.

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