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Unsteady 3D LES modeling of turbulent melt flow with AC traveling EM fields for a laboratory model of the CZ silicon crystal growth system

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Abstract

A series of 3D LES calculations of turbulent melt flow and temperature distributions in a InGaSn laboratory model with a 20” crucible for industrial Czochralski silicon single-crystal growth is presented, in which the influence of the traveling AC EM field and crystal and crucible rotations on the melt flow is shown. The applied program package was developed on the basis of the open-source code library OpenFOAM. The calculated temperature and temperature fluctuation distributions give better agreement with previously obtained experimental results than in the formerly published calculations with 2D axisymmetric RANS turbulence models.

1. Introduction

The numerical modeling of the industrial Czochralski (CZ) Si single-crystal growth is an important part in the optimization of the growth process and understanding its physics. One of the key physical processes that affect the crystal growth is the turbulent melt flow in modern 24”-32” crucibles; therefore it is crucial to correctly model it.

Nowadays, Large Eddy Simulation (LES) methods have proved to be very effective in modeling the turbulent flows in various systems. They require relatively modest computer resources and allow modeling the most essential 3D unsteady turbulent melt flow motion features. LES turbulence models were used also to model melt flow in CZ crystal growth systems for many materials. For example, CZ Si crystal growth was modeled in [1-5], GaAs crystal growth in [6,7], InP crystal growth method in [8], and GeSi crystal growth in [9].

In some calculations, different variations of Smagorinsky LES model were applied. In [1], a Smagorinsky LES model with wall-function boundary treatment for velocity, temperature, and concentration and a damping function for turbulent viscosity was used. [2] presents a LES/RANS hybrid model with a mixing length model with near-wall turbulence damping. This model also includes modeling the DC magnetic field influence on the large scale melt flow for regimes with $\mathrm{Re}_m << 1$.

Non-Smagorinsky LES/RANS hybrid model is presented in [3], where one-equation model for unresolved turbulence kinetic energy is used, and its dissipation rate is used to switch between LES and RANS models. This model also includes DC magnetic field influence, both on large scale motion and on the unresolved turbulence kinetic energy. The LES model presented in [3] was also used in [4-7]. In [8], a Spalart-Allmaras model extended for LES is used.

The mentioned models were partly verified by comparisons with experimental data, see [1-9], such as temperature measurements in the melt and on the melt-crucible interface and crystallization front deflection. In [1], the LES turbulence model was verified also with DNS calculations. Besides, the mentioned papers also show that 3D LES models practically always outperform 2D RANS turbulence models.

Nevertheless, 3D LES modeling for the industrial Si CZ growth systems requires additional verification, for example, for modeling the AC traveling EM field influence on the melt flow. We present 3D LES modeling results for an InGaSn eutectic flow in a laboratory model with a 20" crucible for the industrial CZ Si single-crystal growth systems, in which the influence of the AC EM fields and crucible and crystal rotation on the melt flow is examined. The calculation results are compared with experimental averaged temperature and its fluctuation distributions that were measured in the Institute of Physics of the University of Latvia and in ELMATEC Ltd, see [10].

2. Model description

The Institute of Physics of the University of Latvia and ELMATEC Ltd have conducted a large series of experiments in a low-temperature laboratory model of the industrial CZ Si single-crystal growth systems. The model consisted of a 20" silica crucible with InGaSn eutectic as a working material. The crystallization interface presence and the radiation heat losses from the free melt surface were modeled with a special cooling system. The crucible heating was modeled by electric resistance heaters mounted directly on the crucible. A detailed description of the laboratory model can be found in [10]. The melt flow dependence on the crystal and crucible rotation rates and various AC EM fields was measured in this model.

In our calculations for the laboratory model, only the melt region was considered in 3D LES modeling. The LES modeling was carried out with a self-developed program CZLESFOAM written using open-source code OpenFOAM program library, see [11,12]. For turbulence modeling, three LES models were used: Smagorinsky, Smagorinsky model with van Driest damping function for the wall regions, and dynamic Smagorinsky model with van Driest damping function.

In the standard Smagorinsky model, see [13], the equations for the filtered flow have the form of the unsteady Navier-Stokes equations with effective viscosity $\nu_{eff}=\nu+\nu_t$, where ν is laminar kinematic viscosity, and ν_t is turbulent viscosity that models subgrid turbulence. It is modeled as $\nu_t = C_s^2\delta^2\sqrt{2S_{ij}S_{ij}}$, where S_{ij} is mean rate-of-strain tensor, $C_s = 0.13$, and the filter width δ is defined as a cubic root from the mesh cell volume.

In OpenFOAM, van Driest damping, [11], is applied by calculating the filter width as $\delta = \min(\delta_{mesh}, (k / C_{delta}) y(1-\exp(-y^+ / A^+)))$, where δ_{mesh} is cubic root of the cell volume, $k = 0.4187$ is von Kármán constant, $C_{delta} = 0.158$, $A^+ = 26$, y is distance to the wall, and y^+ is a dimensionless distance to the wall, calculated from the wall shear stress.

In the dynamic Smagorinsky model, the value of coefficient C_s is calculated dynamically from the flow properties using Germano procedure, see [14,15]: $C_s^2 = -1/2 < L_{ik}M_{ik} > / < M_{ik}M_{ik} >$, where L_{ik} and M_{ik} are special tensors calculated from velocity field, and this expression is obtained using the least square method proposed by Lilly, [15]. To increase calculation stability, OpenFOAM averages C_s^2 expression for the whole flow area (hence $<>$), so that a single C_s value is obtained.

The heat transfer was modeled by temperature transfer equation with subgrid heat conductivity with turbulent Prandtl number $\Pr_t = 0.85$. The non-slip boundary condition was applied for the solid boundaries, and the free slip condition for the free melt surface. The buoyancy forces were modeled in Boussinesq approximation. The constant temperature (288 K) boundary condition was applied for the crystal-melt interface, and special distributions of heat flow densities were used for other boundaries with total heat flow 2730 W from the crucible and -2080 W from the free surface. The applied heat flow density distributions were obtained in 2D axisymmetric turbulent flow calculations, see [16], in which various distributions were tried out to fit the experimental data better.

The following material properties for the InGaSn eutectic were used: density ρ=6350 kg/m^3, specific heat c_p=363.5 J/(kg·K), dynamic viscosity 0.0019 Pa·s, heat conductivity λ=22.6 W/(m·K), and volumetric expansion rate $\alpha=7\cdot10^{-5}$ 1/K. The reference temperature for buoyancy forces in the Boussinesq approximation was T_b=288 K.

137000-cell 3D mesh was used as a basic mesh in the calculations, although control calculations with 80000 and 450000-cell meshes were also conducted. For the basic mesh, 0.02 s time step was used. The characteristic time that was needed for the melt flow regime to stabilize was about 3000-3500 s. The temperature and its fluctuation averaging was carried out for 500 s of the real melt flow time. The calculations were carried out on a computer cluster using four to eight processors for parallel computations. One calculation took around five days on eight processors of quad-core Intel® Xeon® X5355 CPUs with 2.66GHz speed.

The EM field calculations were carried out with a self-written 2D axisymmetric EM field calculation program. Two EM fields were considered: a traveling magnetic field (TMF) upwards ("up") and downwards ("down"). The EM fields were generated by a system of three ring inductors with 60° phase shift for 1667 Aw inductor currents, see also [10]. The calculated in the melt induced force densities were read as momentum sources for the Navier-Stokes equations by CZLESFOAM. The in the melt induced heat sources were ignored, because they were relatively unimportant.

3. Calculation results

Tab. 1. Comparison between calculated and measured temperature drops in the melt: D - TMF „down"; U - TMF „up"; „Exp" – experiments; „Sm" - Smagorinsky model; „Sm van Driest" – Smagorinsky model with van Driest damping; „Dyn" – dynamic Smagorinsky model with van Driest damping.

Crucible rotation	Crystal rotation	EM field	Exp	2D low-Re Chien k-ε [16]	Sm	Sm van Driest	Dyn Sm.
-5 rpm	15 rpm	-	23.5 K	33.9 K	45 K	33 K	31 K
0	25 rpm	-	6.3 K	20.7 K	13 K	12 K	15 K
-6 rpm	0 rpm	-	18.6 K	45.4 K	47 K	34 K	-
-5 rpm	15 rpm	1667 D	10.7 K	14.5 K	35 K	13 K	15 K
-5 rpm	15 rpm	1667 U	7.6 K	14.7 K	38 K	10 K	10 K

The calculations have shown that standard Smagorinsky model without turbulence damping at the solid walls performs quite poorly. For example, it significantly overestimates the characteristic temperature drop in the melt (the difference between maximum and minimum temperatures), see Tab. 1. A better agreement between the experiments and calculations has been obtained with Smagorinsky model and van Driest turbulence damping near the solid walls, see also Fig. 1 and Fig. 2. Especially good agreement is in the cases with applied AC traveling EM fields. Nevertheless, the LES calculations still overestimate the temperature drop values. A possible explanation is that, the measurements inside melt could have missed high temperature gradients that can be seen in the LES calculations near the crucible wall and under the crystal. One can estimate that up to 4 K could have been lost due to measurement imprecision. Therefore actual discrepancies could be lower, and qualitative agreement is good both for the averaged temperature and for its fluctuations. Nevertheless, the calculated temperature drop in the cases without EM fields still seems too high in comparison with experiments. The calculations with dynamic Smagorinsky model and van Driest damping do not differ significantly from the calculations with the non-dynamic model, see Tab. 1.

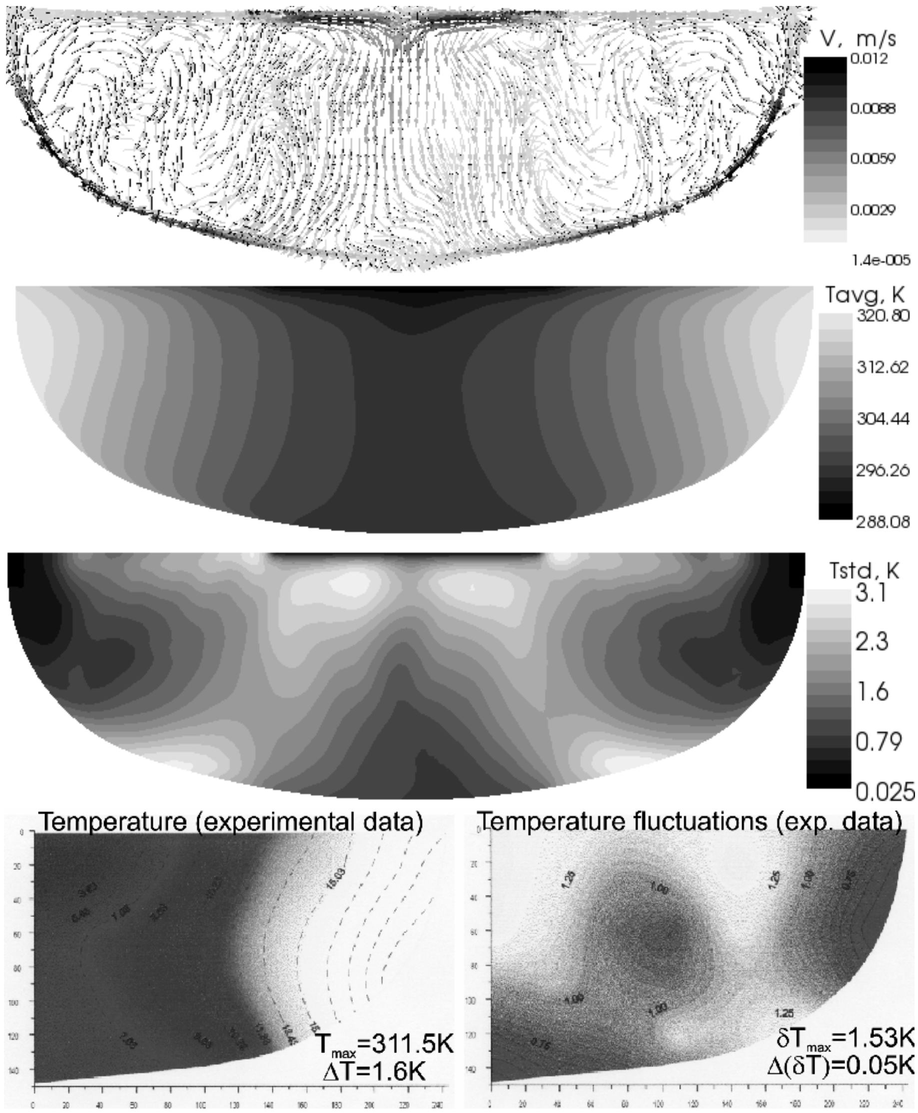

Fig. 1. 3D LES calculations with Smagorinsky model and van Driest damping for crucible rotation -5 rpm and crystal rotation 15 rpm. From top to bottom: averaged velocity, temperature, and root mean square temperature fluctuation distributions, experimental averaged temperature and its fluctuations distirbutions.

Conclusions

The 3D LES calculations have shown that the results of calculations of the temperature and its fluctuations with the standard and dynamic Smagorinsky models, both with van Driest damping, agree well with experimental results, especially in the cases with AC EM field application. However, 3D LES modeling overestimates the temperature drop in the cases without EM fields.

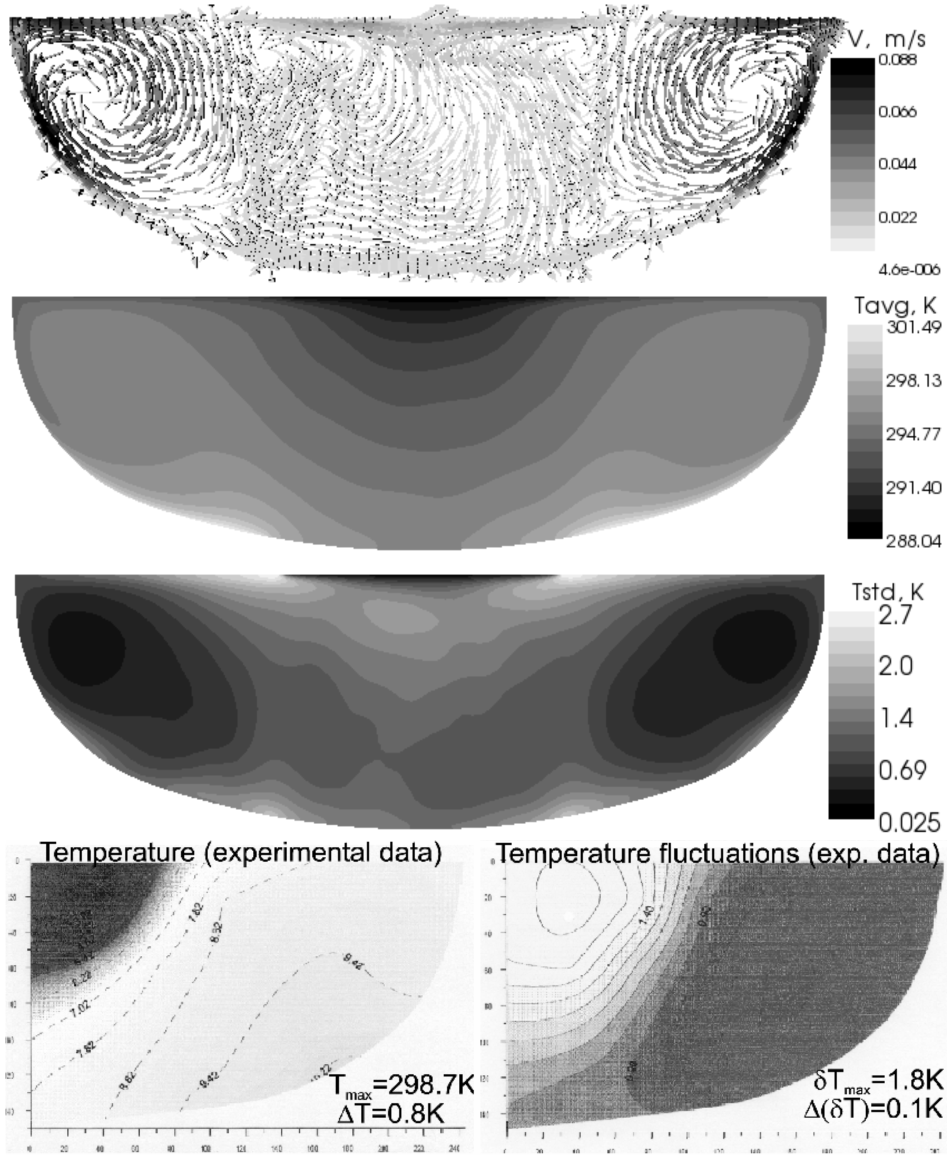

Fig. 2. 3D LES calculations with Smagorinsky model and van Driest damping for crucible rotation -5 rpm and crystal rotation 15 rpm and TMF „down". From top to bottom: averaged velocity, temperature, and root mean square temperature fluctuation distributions, experimental averaged temperature and its fluctuations distirbutions.

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