Mathematical Modelling of the Industrial CZ Crystal Growth:
Melt Hydrodynamics Control by Imposed Magnetic Fields∗

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Abstract

The paper describes a numerical simulation tool for heat and mass transfer processes in large diameter CZ-crucibles under the influence of several non-rotating AC and CUSP magnetic fields. Such fields are expected to provide an additional means to influence the melt behaviour, particularly in the industrial growth of large diameter silicon crystals. The simulation tool is based on axisymmetric 2D models for the AC and CUSP magnetic fields in the whole CZ-facility and turbulent hydrodynamics, temperature and mass transport in the melt under the influence of the electromagnetic fields. The simulation tool is verified by comparisons to experimental results from a laboratory CZ set-up with eutectics InGaSn model melt.

Introduction

The increase of crystal diameters up to 300 mm and crucible diameters up to 36” in silicon CZ crystal growth during recent years has lead to several problems that cannot be solved with the conventional pulling technology [1]. The use of CUSP- and especially AC-electromagnetic (EM) fields to influence melt hydrodynamics promises to facilitate the necessary control of the growth process [2, 3]. However, the development of magnet systems and corresponding growth experiments in industrial scale CZ pullers is very expensive. Several authors have indicated that the highly complex mechanisms in turbulent CZ-melt flows are characterised by three-dimensional time dependent flow and temperature distributions, e.g. [4]. However, a fully 3D transient simulation of large melt volumes of up to 300 kg is a very time and resource consuming business. On the other hand, for a successful application of the magnetic fields in an industrial environment it is necessary to reveal trends and to develop a qualitative understanding of the melt behaviour under the field influence. For that purpose performing numerous simulation runs with several parameter combinations is indispensable in order to investigate a number of aspects that are of particular importance for industrial process development. The attainable accuracy must be evaluated using experimental data and has to be considered in using the simulation results. The purpose of this paper is to present a complete numerical simulation tool based on axisymmetric 2D models for the simulation of AC and CUSP magnetic fields in the whole CZ facility as well as turbulent hydrodynamics and temperature distribution in the melt under the influence of different electromagnetic fields. The main part of the paper is focused on the verification of the 2D simulation tool by comparisons to experimental data from a laboratory CZ set-up with eutectics InGaSn model melt.

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1. Mathematical Model and Numerical Implementation

1.1. Electromagnetic Field

The axisymmetric electromagnetic (EM) field is calculated using a complex equation for the azimuthal component of the magnetic vector potential. It is implemented in a FEM formulation that considers regions with eddy currents and magnetic cores [5]. The feedback of the moving melt on the AC and CUSP magnetic field can be neglected, therefore the FEM program for the calculation of the EM fields delivers the distributions of force density and magnetic flux density in the melt for further use in the hydrodynamic simulation. In the case of the CUSP field the interaction of the magnetic field and the velocity is considered.

1.2. Heat and Mass Transfer

The calculation of the axisymmetric turbulent flow field is based on the simultaneous steady state solution of the Reynolds averaged equations for continuity, momentum and energy for an incompressible fluid, as given e.g. in [6] and [7]. Buoyancy is considered using Boussinesq’s approximation. Standard hydrodynamic boundary conditions are used for the equations, e.g. fixed velocities along crucible and crystal, and symmetry or slip conditions along axis and free surface. The simultaneous calculation of heat and mass transfer as well as the current density due to CUSP magnetic fields are carried out using the commercial code CFD-ACE that is a finite volume (FVM) code, based on a structured multi-domain grid approach. For the present model this code had to be customised, in particular to incorporate the force density and the heat sources due to the AC magnetic fields etc.

1.3. Turbulence Modeling

Crucibles used for the industrial growth of 300 mm silicon crystals reach diameters between 28” and 36”. With rotation rates of about 3 rpm for the crucible and of about 10 rpm for the crystal, these diameters lead to local Reynolds numbers of several $10^4$. The Rayleigh number is on the order of $10^7$. According to these figures the melt flow can show areas of strong and weak turbulence. Therefore we propose the extension of the LowRe-k-ε model that takes into account the direct damping of turbulent eddies due to a DC field.

2. Laboratory Set-up

Because the melt flow in large diameter CZ-crucibles is known to be turbulent and to show three-dimensional features it is necessary to carefully check the applicability of the 2D model by comparisons to experimental results. However, temperature measurements in molten silicon are a very difficult task, especially when temperature distributions, e.g. a complete cross section, should be determined. Velocity measurements are also a very useful means to check the turbulence modeling, but are practically impossible in molten silicon. Consequently, a physical model of the industrial CZ-puller was designed and implemented. It uses eutectics InGaSn as model melt. This alloy has a melting point of 10.35°C, which enables long time measurements and the determination of temperature and velocity fields. Fig. 1 shows the main parts and some important dimensions of the laboratory setup. The central part is a 20” standard CZ crucible, filled with the model melt that is covered by a HCl layer to protect it against oxidation on the free surface. Within this layer lies a surface cooler that models the radiation heat losses which occur during silicon CZ growth. The crystal model is made of stainless steel and is strongly cooled from inside to simulate the isothermal crystallisation front. The crucible is heated from outside by NiCr-heaters that are attached to the outer surface of the silica wall in a meandric pattern to prevent induction effects. The inductor coils also shown in Fig. 1 offer the possibility of using different AC and CUSP magnetic fields and combinations of them.
The temperature is measured in the experiments by thermocouples and the velocity components are determined using a conductive anemometer. All temperature values were transformed into temperature differences with respect to a reference point. It is the point closest to the minimum temperature along the crystal wall and so all the calculated temperature differences can be regarded as overheating temperatures. In addition to the averaged quantities, the standard deviations of temperature and velocity components are calculated. Several measuring runs were carried out for different operation conditions and purposes. The results used for the verification of the simulation tool were determined during experiments with different field types, rotation rates, etc., but with fixed heat flux densities along the heater sections on the crucible wall. These heat flux densities were used as thermal boundary conditions for the simulation.

3. Some Examples of the Verification of the Results of Numerical Calculations and Analyses

3.1. AC Side Inductor

Fig. 2 shows the calculated and measured radial temperature distribution 5 mm below the melt free surface in the laboratory set-up for a case with acting AC side inductor. The most significant difference between the reference case (without AC field) and this case is the lowered temperature level in the melt, in particular in the outer melt region towards the crucible wall. This effect is caused by the enhanced mixing of the melt due to the electromagnetic force density. The AC field causes a two-vortex structure in the outer melt region, but leaves the inner region underneath the crystal almost unaffected.

3.2. AC-bottom Inductor

Some examples of the influence of the AC bottom inductor (total current 2 kAw) on the meridional flow are shown in Fig. 3 and 4. Here the field causes a flow cell in the outer region near the crucible wall which is rotating opposite to the original buoyancy driven convection. As an example for the measured velocity distributions in the laboratory set-up Fig. 3 shows the axial velocity component at a depth of 60 mm along a radial line without heating and crystal rotation, leaving the field of the acting bottom inductor as the only driving force. The comparison with the calculated velocity distribution indicate a less exact matching of experimental and simulation results compared to the temperatures, but in general the agreement is sufficiently good. The simulation was done using the Low-Re-k-ε model. The Fig. 4 illustrates the influence of the AC-bottom inductor for two crucible rotation rates on the flow structure and on the radial temperature derivative at the crystal rim.

3.3. CUSP Field

An example of the calculated flow structure and the corresponding values of the radial temperature derivative at the crystal rim and the content of oxygen in the crystal in the case of CUSP field are shown in Fig. 5. It can be seen that only one large single vortex remains in the vertical cross-section. This result is supported by experimental observations of the temperature distributions that show a strong curvature of the isotherms that would be caused by a single vortex flow [8]. The one vortex structure of the flow correspond qualitatively to the reduced oxygen content in the crystal (Fig. 5) also.
Fig. 1. The scheme of the experimental setup of the laboratory facility with 20” crucible. The electromagnetic system contains: AC-bottom inductor, AC-side inductor and two inductors for the CUSP field.

Fig. 2. Influence of the AC-side inductor. Comparison of the measured and calculated radial temperature distribution on the line 5 mm below the free surface of the melt. Crystal and crucible rotation rates are correspondingly –15 and 5 rpm.
Fig. 3. Comparison of the measured and calculated radial distribution of the vertical velocity component in the case of the AC-bottom inductor. Below: calculated stream function for the considered case.

Fig. 4. Influence of the AC-bottom inductor on the stream function and on the radial temperature derivative $G_{RS}$ at the crystal rim at two different crucible rotation rates: 2 and 4 rpm. Crystal rotation rate is –9 rpm.
Fig. 5. Influence of the CUSP-field on the stream function, on the radial temperature derivative \( G_{RS} \) at the crystal rim and on the oxygen content \( C_{OZ} \) in the crystal. Crystal and crucible rotation rates are correspondingly –9 and 4 rpm.

References

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