International Scientific Colloquium
Modelling for Material Processing
Riga, September 16-17, 2010

Instabilities in Silicon Czochralski Crystal Growth Process in Different geometries

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Abstract

The flow and heat transfer of molten silicon during Czochralski growth under the interaction buoyancy and crucible rotation in the Czochralski process are studied numerically. In this work we present a set of computational simulations using the finite volume package in order to analyse different instabilities induced by buoyancy, and centrifugal forces that occur in silicon Czochralski crystal growth in a traditional and a new systems.

Introduction

The Czochralski crystal growth is one of the most important methods of producing single crystals from the melt. The quality of these crystals depends on heat and mass transfer in the melt during growth, due to complex interactions of many driving forces including buoyancy, centrifugal, thermocapillary and Coriolis forces. Nearly all crystals have inhomogeneities and growth bands called striations [1]. Melt grown elements like silicon show striations due to impurities, in the case of silicon-oxygen striation from partial dissolution of quartz crucible. A time dependent melt flow causes the temperature fluctuation at the crystal/melt interface, leading to undesirable inhomogeneities such as doping striations and crystallographic defects in the crystal [2].

In this work we present a set of computational simulations using the finite volume package Fluent in two different geometries, a new geometry [3-7] as cylindro-spherical and the traditional configuration as cylindro-cylindrical in order to analyse different instabilities induced by buoyancy and centrifugal forces that occur in silicon Czochralski crystal growth.

1. Physical and Mathematical Model

1.1. Physical Model

Schematic diagrams adopted in the present simulation are shown in Fig.1. The crucible contains silicon melt with height H and radius R_c and rotates at the angular velocity Ω_c in the clockwise direction. The crystal has a constant radius R_s. The melt/crystal interface is assumed flat with the melting temperature T_m.

1.2. Mathematical Model

To facilitate the procedure of modeling related to the considered problem, we admit some assumptions; the molten silicon is assumed to be a viscous, Newtonian and incompressible fluid satisfying the Boussinesq assumption. We assume the solid liquid interface and the free surface to be flat initially. The thermo physical properties of the fluid are constant except for the density variation in the buoyancy force term. The flow is symmetric in the axial direction. Fixed temperatures are imposed on the walls of the melt crucible and the crystal melt interface. Considering the preceding assumptions, the resolution of the problem will be done in two-dimensional geometries, limited to axisymmetric sections of the crucible [5,6].

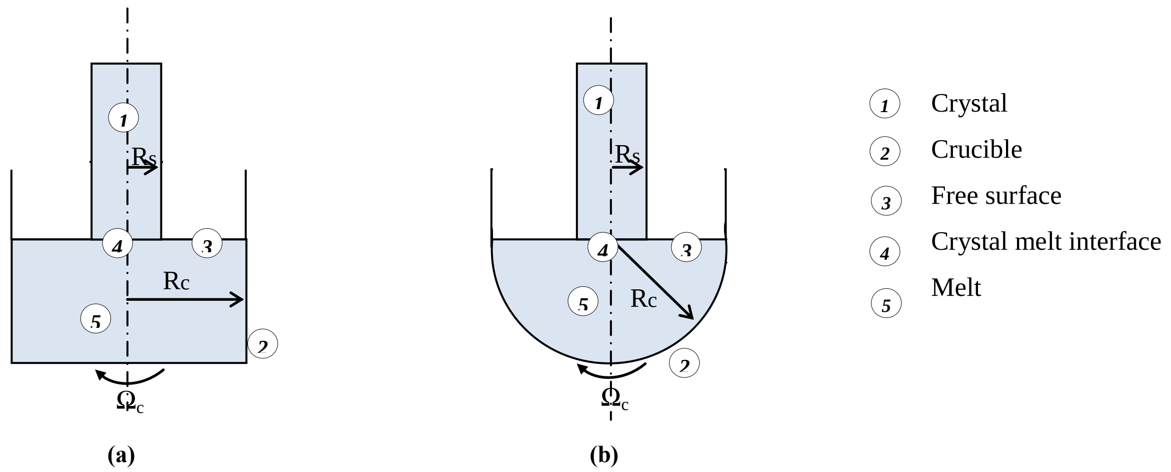

Fig. 1. Traditional (a) and modified (b) Czochralski crystal growth systems

The dimensionless governing equations for the fluid motion and temperature field derived under the above assumptions are

Continuity

$$\frac{\partial V_r}{\partial r}+\frac{V_r}{r}+\frac{\partial V_z}{\partial z}=0 .$$

Momentum

$$\frac{\partial V_r}{\partial t}+V_r\frac{\partial V_r}{\partial r}+V_z\frac{\partial V_r}{\partial z}=-\frac{\partial P}{\partial r}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial V_r}{\partial r}\right)-\frac{V_r}{r^2}+\frac{\partial^2 V_r}{\partial z^2}\ ;$$

$$\frac{\partial V_\varphi}{\partial t}+V_r\frac{\partial V_\varphi}{\partial r}+V_z\frac{\partial V_\varphi}{\partial z}+\frac{V_r V_\varphi}{r}=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial V_\varphi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 V_\varphi}{\partial \varphi^2}+\frac{2}{r^2}\frac{\partial V_r}{\partial \varphi}+\frac{\partial^2 V_\varphi}{\partial z^2}\ ;$$

$$\frac{\partial V_z}{\partial t}+V_r\frac{\partial V_z}{\partial r}+V_z\frac{\partial V_z}{\partial z}=-\frac{\partial P}{\partial z}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial V_z}{\partial r}\right)+\frac{\partial^2 V_z}{\partial z^2}\text{-Gr.T} .$$

Energy

$$\frac{\partial T}{\partial t}+V_r\frac{\partial T}{\partial r}+V_z\frac{\partial T}{\partial z}=\frac{1}{\mathrm{Pr}}\left\{\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)+\frac{\partial^2 T}{\partial z^2}\right\},$$

where Grashof number $Gr=\frac{g\beta R_c^3\left(T_c-T_f\right)}{\upsilon^2}$ characterizes natural convection effect. Prandtl number $\mathrm{Pr}=\frac{\upsilon}{\alpha}$ measures the relative importance of heat transfer by conduction and convection. The non dimensional boundary conditions are as follows

Crucible wall and bottom $V_\varphi = r.\mathrm{Re}\ \ V_r = V_z = 0$, $T=1$;

Crystal melt interface $\quad V_r = V_\varphi = V_z = 0 \;, \quad T = 0 \,,$

where $Re = \dfrac{\Omega_c R_C^2}{\upsilon}$ is Reynolds number associated to the rotating crucible.

Axis of symmetry $\quad \partial V_z / \partial r = 0 \;, \quad V_r = 0 \;, \quad \partial T / \partial r = 0 \,;$

Free surface: $\quad V_z = 0 \;, \quad \dfrac{\partial V_r}{\partial z} = \dfrac{Ma}{\Pr}\dfrac{\partial T}{\partial r} \,.$

The properties used in simulation are dimensionless parameters. The Prandtl number characterizing silicon is *0.0113*. We propose to maintain the Grashof number to 10^7.
The problem is solved using the finite volume package Fluent. The steady segregated axisymmetric swirl solver was used with the first order upwind discretization for convection, SIMPLE algorithm for pressure-velocity coupling and the PRESTO (PREssure STaggering Option) scheme for pressure interpolation. The convergence is handled by monitoring residuals of continuity, momentum and energy equations.

2. **Results and Discussions**

The aim of this work is based on the numerical study of the barocline instability effect induced by natural and forced convection (induced by crucible rotation) on flow pattern, temperature and pressure field in silicon Czochralski crystal growth process. By carrying out the convergence test of grid and residuals, we find a grid of *200*200* and residuals of 10^{-6}. We maintain the Grashof number value to 10^7, we modify the crucible rotation rate by increasing Reynolds number value. For the different analyzed cases we represent the corresponding streamlines, azimuthal velocity, vorticity, isotherms, and isobars contours.

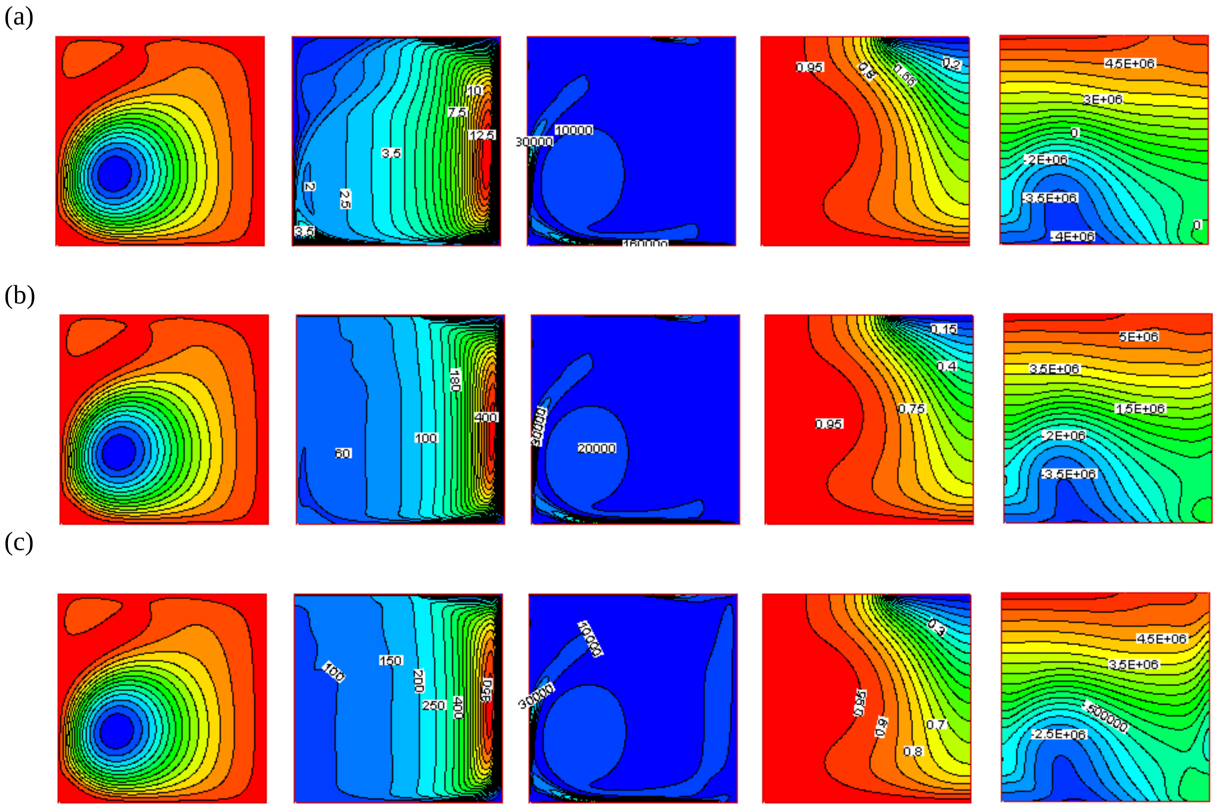

Fig. 2. Streamlines, azimuthal velocity, vorticity, isotherms and isobars respectively for (a) Re=0, (b) Re=50, and (c) Re=100

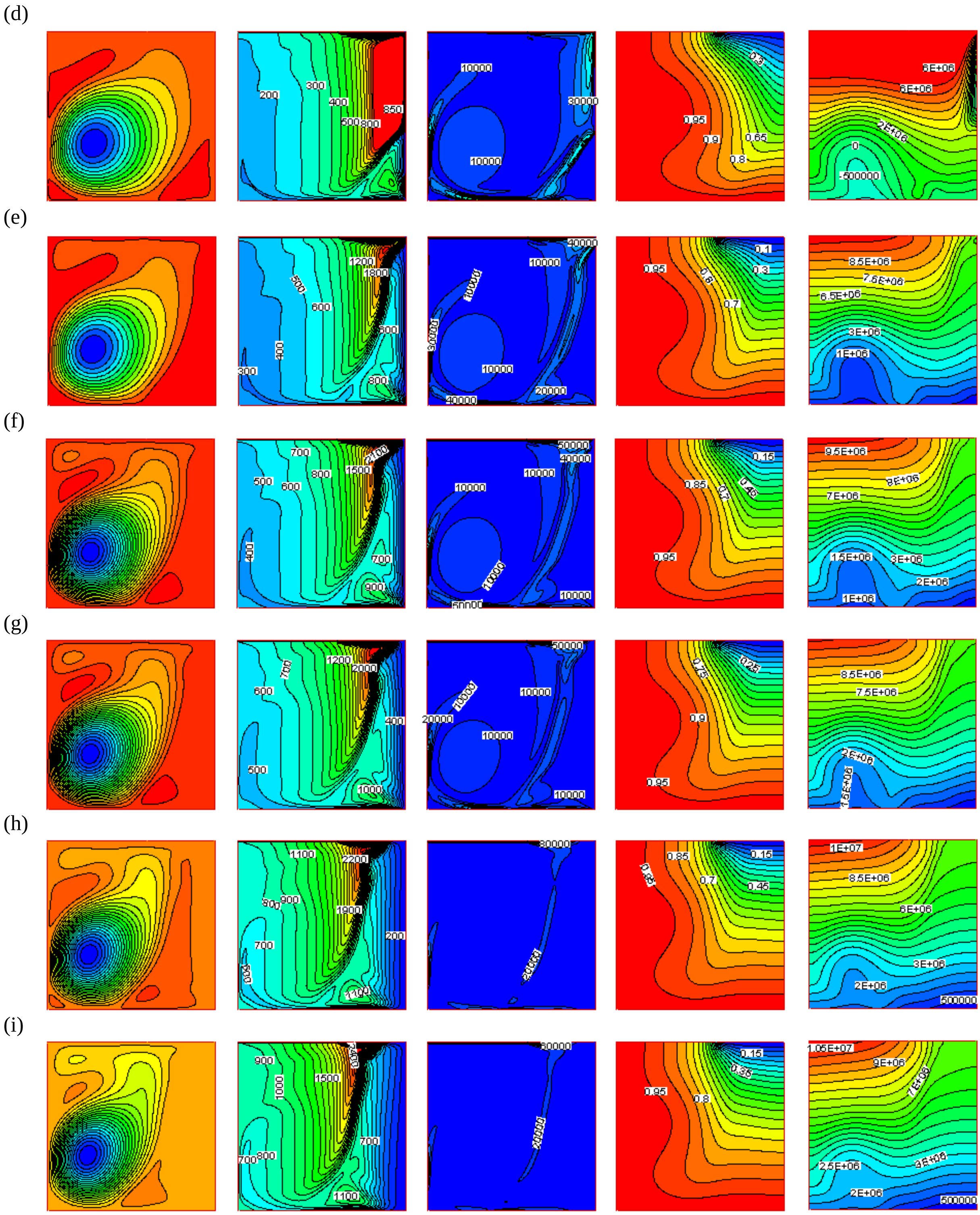

Fig. 3. Streamlines, azimuthal velocity, vorticity, isotherms and isobars respectively for (d) Re=200, (e) Re=400, (f) Re=700, (g) Re=700, (h) Re=800 and Re=900

For the low values of Reynolds number, we note the presence of only one big vortex occupying all the melt volume, it is induced by natural convection (buoyancy force), the melt is cooler near the surface of the crystal than along the crucible walls, causing the fluid to drop along the axis and rise on the outside. We note that the streamlines remain unchanged in the range of *Re* between *0* and *100*. From *Re=200*, we note the appearance of an additional vortex below the free surface near the axis of symmetry, this bifurcation is caused by the presence of a second convection mode in the silicon melt, it is the forced convection induced by rotation of crucible. By further increasing the rotation rate, the main vortex due to the natural convection becomes weak in intensity and volume and the forced convection becomes more dominant. We note that for higher values of Reynolds number as $Re=900$, the melt column beneath the crystal has the same intensity of stream function.

By analyzing the contours of the azimuthal velocity, we note in all studied cases, the value of the azimuthal velocity at the crucible wall is equal to the value of the associated Reynolds number.

By changing Reynolds number from $Re=0$ to $Re=10$, we note that these contours become almost parallel to the crucible wall. From $Re=10$ to $Re=100$, their shape is almost identical, and from the crystal rotation rate corresponding to the Reynolds value $Re=200$ which corresponds to a transition, we note the appearance of a new inclusion near the axis of symmetry, this value can be called value of transition that corresponds to a Richardson number, $Ri=250$. We remind that the Richardson number $Ri=Gr/Re^2$ is defined by the ratio of intensities of natural convection to forced convection. By increasing crucible rotation rate, we note that the line corresponding to the maximum azimuthal velocity moves toward the solidification interface. The shape of the azimuthal velocity lines becomes conical from the Reynolds number value $Re=300$, the basis of these cones is located on the upper surface and its vertex is near the bottom of the crucible.

We note also that the high azimuthal velocity moves from the area near the axis of symmetry to the triple point, this latter plays an important role in crystal growth, it is defined by the coexistence of three phases (solid, liquid and gas) [5,6]. We also note that the number of azimuthal velocity lines increases under the free surface for large values of Reynolds number, then the radial gradient of this velocity is very high as the forced convection is dominant.

By analyzing the contours corresponding to vorticity, we note that the overall shape remains the same from Reynolds number $Re=0$ to $Re=50$. In the region between the axis of symmetry and the triple point the vorticity becomes variable up to $Re=100$. From $Re=700$, we note the disappearance of the main vortex and the vorticity is nearly uniform throughout the melt.

We note a slight change in isotherms, such that, for large values of Reynolds number, the shape of the isotherms becomes less sinuous, flattened in the column beneath the crystal by increasing the crucible rotation rate. The axial temperature gradient becomes uniform on the axis of rotation for higher values of Reynolds number.

Unlike the temperature field, the pressure changes significantly, it increases in the melt while increasing the crucible rotation rate.

Near the crucible bottom, the isobars are concave; we notice that this concavity disappears by increasing the rotation rate of the crucible until these isobars are evenly stratified at the upper surface of the melt. The radial pressure gradient increases, it appears clearly near the triple point. We note also that for $Re=200$ corresponding to Richardson number value $Ri=250$, new isobars appear near the axis of symmetry at the top of the melt, it is present with the main changes noted in the vorticity, which enables us to confirm the relationship between the vorticity and pressure field [7].

Now, in order to compare the traditional geometry to the hemispherical one, we calculate the velocity, temperature and pressure fields for the same Grashof number value $Gr=10^7$ and Prandtl number $Pr=0.0113$ and for Reynolds number $Re=200$ that represents a value of transition. We note there is not a region of stagnation in the spherical crucible corner as for the cylindrical process. The convective vortex is bigger and near to the top in this case and there is only one small additional vortex under the free surface of the melt.

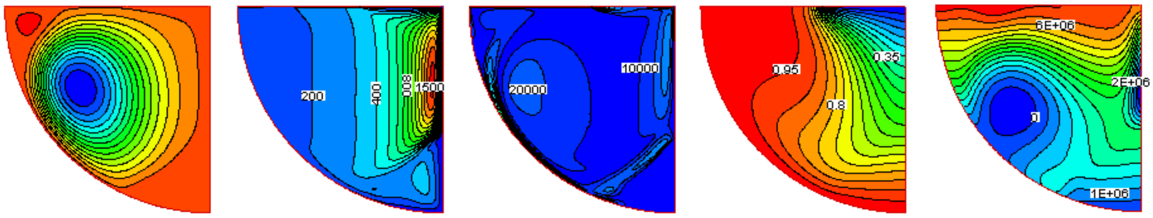

Fig. 4. Streamlines, azimuthal velocity, vorticity, isotherms and isobars respectively for Re=200

Conclusion

In this work we present a set of computational simulations using the finite volume package Fluent in order to analyse the barocline instability induced by buoyancy, and centrifugal forces that occur in silicon Czochralski crystal growth.

The velocity, temperature and pressure fields are calculated for a Grashof number value $Gr=10^7$, Prandtl number $Pr=0.0113$ and different Reynolds number values that correspond to crucible rotation rates in the cylindrical and hemispherical systems.

We found that for the low values of Reynolds number the buoyancy force is acting on melt flow so only one big vortex is present in the melt. For bigger values of *Re* there are several vortices. The value of the azimuthal velocity at the crucible wall is equal to the value of the associated Reynolds number. Near the triple point the vorticity becomes variable by increasing the velocity rate and it reaches its maximum at this point.

We showed that the pressure field is more sensitive that the temperature to the centrifugal and Coriolis forces induced by the crucible rotation.

Finally, the hemispherical crucible shape is found to be advantageous for crystal growth than the cylindrical one.

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