CONVECTIVE INSTABILITIES IN CZOCHRALSKI MODEL

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Summary Hydrodynamic Czochralski model as a combination of the classical models buoyancy-driven and Marangoni convection is studied on the basis of three dimensional unsteady Navier-Stokes equations in the Boussinesq approximation. Critical Grashof and Marangoni numbers for axisymmetrical and three dimensional fluid flow were found for different Prandtl numbers and boundary conditions on the melt surface. Role of the buoyancy–driven and Marangoni instabilities in the coupling flows are discussed.

Pulling crystal growth, which is well known as Czochralski growth is the widespread method for electronics and optoelectronics industry [1]. The temperature oscillations in the melt are the main reason of the striation defects in Czochralski crystal growth and studied during more than 25 years [1-5]. Last decade new round of activity was done due to possibility of 3D modeling in fluid dynamics (see [6-10] and references). Although direct three dimensional modeling taking into account all types of convection for the typical for industry high Grashof (Gr) and Marangoni (Mn) numbers are available now (see, for instance [7,11]), critical numbers for onset of instability haven't systematically studied. The validation of the results and control of convection needs more detailed analysis of buoyancy-driven and Marangoni convection, similar as for classical fluid mechanics models [12]. Experimental observations and three dimensional modeling of buoyancy-driven and Marangoni convection in the melt which discussed in above mentioned references show the spatial structures, which are of interest for basic fluid dynamics studies.

We study hydrodynamic Czochralski model (Fig.1), which represents a combination of the classical models of convection with side and bottom heating. The unsteady Navier-Stokes equations in the Boussinesq approximation and the equation for temperature were used. The boundary conditions for the velocity on the melt surface are no-slipping on the crucible wall and bottom and on the crystal. Temperature Θ = 0 on the crystal, Θ = 1 on the

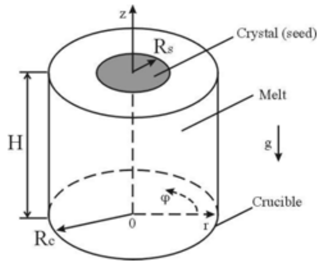


Fig.1. Scheme of hydrodynamic Czochralski model.

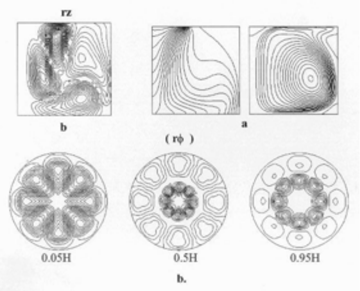


Fig.2. Structure of three dimensional thermocapillary instability.

crucible wall, ∂Θ/∂z = 0 on the crucible bottom and different thermal boundary conditions on the melt surface are assumed. Even idealized Czochralski model represents nonlinear multi parametrical hydrodynamic system with wide range values of governing parameters. Flow patterns in the melt in the Czochralski model is extremely complex and wasn't well understood, especially the role of Marangoni and it's coupling with buoyancy-driven convection.

A hierarchy of the models and computer codes were developed for the peer analysis of the problem including direct simulation of the transition and turbulent regimes on the basis of 3D Navier-Stokes equations [8-10]. However axisymmetric processes are still of interest in multiparametric analysis.

Three types of the FDM for axisymmertric Czochralski model are used here. The first type is based on the system «INTEX» and includes a variation of geometry, crystal and crucible rotation, gravity-driven and Marangoni convection in vorticity-stream function formulation. The second code is a basis of a novel Computer Laboratory [13]. It includes also 2D flat and axisymmetric problems in the ground-based and microgravity environments. The third type of the axisymmetric codes was used mainly for the calculation of a basic flow for linear stability analysis [9, 10]. For the stability analysis of the axisymmetric steady state flow with respect to 3D perturbations temperature field T is presented in the form,

$$T(t,r,\varphi,z)=T_{2D}(r,z)+\varepsilon T'_n, \qquad T'_n(t,r,\varphi,z)=\mathrm{Re}[T_n(t,r,z)\exp(in\varphi)], \quad n=1,2,\ldots$$

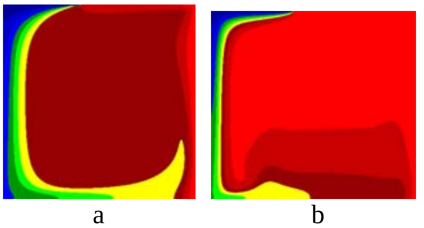
Here, T_{2D} is a given (previously calculated) steady solution of the 2D equations and $\varepsilon T'_n$ is a small 3D perturbation. Substituting this and similar expressions for the velocity components into the governing equations and neglecting $\sim\varepsilon^2$ terms we obtain a set of linear time-dependent problems for perturbations. A general solution for T_n for each azimuthal wave-number *n* has a following form

$$T_n(t,r,z)=\sum_{j=1}^{\infty} T_n^j(r,z)\exp(\lambda_n^j t)$$

Here, λ_n^j are the eigenvalues and T_n^j are the eigenfunctions of the corresponding spectral problem. Solving linear time-dependent equations with some random initial conditions we obtain $T_n(t \to \infty, r, z) \to T_n^1(r, z)\exp(\lambda_n^1 t)$, where λ_n^1 is eigenvalue with the maximal real part. In such a way we may determine the stability or instability of the axisymmetric flow as well as the spatial structure and temporal behavior (monotonic or oscillatory) of the most dangerous 3D perturbations. A focus of the concrete analysis in the paper is natural convection, which includes buoyancy-driven and gradient of the surface tension-driven (Marangoni) convection, which is the major cause of instability. The control function (for instance, amplitude of temperature oscillation, A) seems as follows:

$$A = f(r, z, \varphi, Gr, Mn, Pr, Rs/Rc, H/Rc, \gamma 1, \gamma 2) \qquad (1)$$

Here Gr, Mn – Grashof and Marangoni numbers - criteria of convection, Pr - criteria of the physical properties. Geometrical parameters - non dimensional height of the melt H/Rc = 1.0 and width of the seed Rs/Rc =0.4 for the parameters of the benchmark [7, 9], γ1, γ2 – thermal boundary and initial conditions. Analysis of the nature and comparison of the 2D and 3D instability phenomena in hydrodynamic Czochralski configuration for buoyancy-driven and thermocapillary convection is done. Systematically comparison of the buoyancy-driven and Marangoni convection including comparison of the impact of the thermal boundary conditions on the melt surface is done. The peculiarities of the convective instability for low and high Pr melt for buoyancy-driven and Marangoni convection are discussed. Fig.2 shows a typical "spoke-type" structure of three dimensional thermocapillary instability for a case of adiabatic melt surface for Mn_c=5.8x10^5 and low Prandtl (Pr=0.05). Here a) basic temperature/flow fields, b) structure of 3D disturbances.



a b

Fig.3. Steady state temperature fields for Marangoni (a) and buoyancy-driven (b) convection, Pr=6.5.

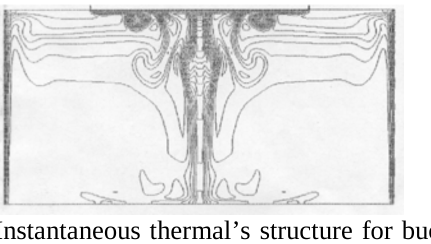


Fig.4. Instantaneous thermal's structure for buoyancy–driven convection, adiabatic melt surface, Pr=6.5, Gr=4.5 10^7.

Fig.3 shows structure of the temperature fields for high Pr number melt with adiabatic melt surface in axisymmetric case. Here Mn =10^5 (a) and buoyancy-driven convection for Gr < Gr_c (b). Critical Gr number for onset of the thermals was found here as Gr=Gr_c=4.4x10^5. Fig.4 shows change of the instability mechanism for high Pr melt: instantaneous isotherms for buoyancy-driven convection for Gr >>Gr_c seems as thermals. Such kind of the structures were observed by in experiments with water (see ref. in [1, 7]). Maximum of the Gr_c was found for Pr=0.25 in axisymmetrc case.
Note, that change of instability mechanisms for Marangoni convection in this case wasn't found.
Therefore the nature of Marangoni instability is different from buoyancy-driven one (case of adiabatic melt surface and bottom). It has to be taken into account for control of the temperature oscillations in the melt. Movies 6-8 in URL [http://www.ipmnet.ru/~yarem/paper3] illustrate dynamics of the temperature oscillations in axisymmetric case. Paper presents discussion of the governing parameters where these mechanisms are dominated and summary of the critical Mn and Gr numbers for parameters (1), comments of the coupling phenomena and possibilities for control of the temperature oscillations in the melt using thermal, dynamics (vibrations), magnetic actions as well as microgravity. Because multiparamertric analysis of hydrodynamic Czochralski model needs additional efforts, education and tutorial course were developed [13].

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