

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 the 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 [11]), critical numbers for onset of instability are not systematically studied. The validation of the results and control of convection need a more detailed analysis of buoyancy-driven and Marangoni convection as main reason for instability 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 in Czochralski model.

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 $\Theta = 0$ on the crystal, $\Theta = 1$ on the

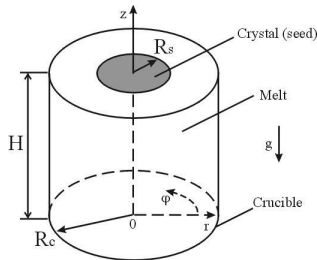


Fig. 1. Scheme of hydrodynamic Czochralski model.

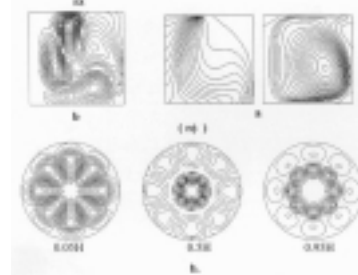


Fig. 2. Structure of three dimensional thermocapillary instability.

crucible wall, $\partial\Theta/\partial z = 0$ on the crucible bottom and different thermal boundary conditions on the melt surface are assumed. Even so idealized Czochralski model represents a nonlinear multi parametrical hydrodynamic system with wide range values of governing parameters. The flow pattern in the melt in the Czochralski model is extremely complex and not very well understood, especially the role of Marangoni and 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 FDM for specialized axisymmetric 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 for basic studies. 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,

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

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 $T_n(t \rightarrow \infty, r, z) \rightarrow T_n^1(r, z) \exp(\lambda_n^1 t)$, 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:

$$A = f(r, z, \varphi, Gr, Mn, Pr, Rs/Rc, H/Rc, \gamma_1, \gamma_2) \quad (1)$$

Here Gr , Mn - two natural convection criteria – Grashof and Marangoni numbers, Pr number- criteria of the physical properties, H/Rc , Rs/Rc – two geometrical parameters - non dimensional height of the melt and width of the seed, and γ_1, γ_2 – 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 convection and Marangoni convection including comparison of the impact of the thermal boundary conditions on the melt surface for the parameters of the benchmark configuration are done. The peculiarities of the flow and temperature instability for the low and high Pr melt for buoyancy-driven and Marangoni convection are also discussed. Fig.2 shows a typical "spoke-type" structure of three dimensional thermocapillary instability for a case of adiabatic melt surface for $Mn_c = 5.8 \times 10^5$ and low Prandtl ($Pr = 0.05$). Here a) basic temperature/flow fields, b) structure of 3D temperature disturbances.

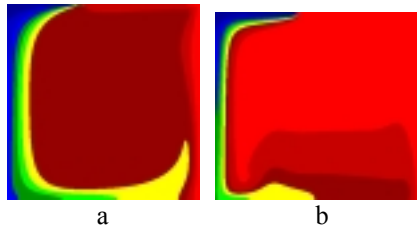


Fig.3. Steady state temperature fields for Marangoni (a) and buoyancy-driven (b) convection, $Pr = 6.5$.



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

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 $Gr = Gr_c = 4.4 \times 10^5$. Fig.4 shows typical instantaneous isotherms for developed buoyancy-driven convection in a supercritical case for $Gr \gg Gr_c$. Such kinds of structures were observed by Jones and Berdnikov in experiments with water (see ref. in [1, 7]). Note, that there is no similar change of instability for Marangoni convection for adiabatic bottom of crucible. Therefore for Czochralski growth with adiabatic melt surface and bottom the nature of Marangoni convection instability is different from buoyancy-driven one, and 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 multiparametric analysis of hydrodynamic Czochralski model needs additional efforts, education and tutorial course were developed [13].

References

- [1] Hurle D.T.J.: Crystal pulling from the melt, Springer, 1993.
- [2] Carruthers J.R.: Thermal convection instabilities relevant to crystal growth from liquids. In: Preparation and Properties of Solid State Materials. Ed. by W.R. Wilcox and R.A. Lefever. New York - Basel, Marcel Dekker, 1977, v. 3, . 1-121.
- [3] Polezhaev V.I.: Hydrodynamics, Heat and Mass Transfer During Crystal Growth, In: Crystals: Growth, Properties and Applications, V.10 (1981), Springer, 81.
- [4] Schwabe D.: Surface-tension driven flow in crystal growth melt. In: Crystals: Growth, properties and applications, v. 11, Springer, 1988., 75.
- [5] Müller G. and Ostrogorsky A.: Convection in melt growth. In: Handbook of Crystal Growth. Ed. by D.T.J. Hurle. Amsterdam, Elsevier, 1994, v. 2, p. 711-819.
- [6] Ristorcelli J.R. and Lumley J.L.: Instabilities, transition and turbulence in the Czochralski crystal melt. J. Crystal Growth, 1992, v. 116, N 3/4, p. 447-460.
- [7] Polezhaev V.I.: Modeling of Technologically Important Hydrodynamics and Heat/Mass Transfer Processes during Crystal Growth. In . Crystal Growth Technology (eds) Sheel H.J.,Fyukuda T., Wiley, (2003), 156-186.
- [8] Li You-Rong, Peng L. Akiyama Y., Imaishi N. J.: Crystal Growth, 259, (2003), 374.
- [9] N.V. Nikitin, V.I.Polezhaev.: J.Crystal Growth, 230, (2001), 30.
- [10] V.I. Polezhaev , O.A. Bessonov, N.V. Nikitin et al.: J. Crystal Growth, 230, (2001), 40.
- [11] Dupret F. and Van Den Bogaert N.: Modelling Bridgman and Czochralski growth. In: Handbook of Crystal Growth. Ed. by D.T.J. Hurle. Amsterdam, Elsevier, 1994. v. 2., 875-1010.
- [12] Koshmieder E.L.: Bernard cells and Taylor vortices. Cambridge University Press, 1993, 337 p.
- [13] M.K Ermakov, S.A. Nikitin, V.I.Polezhaev, V.P.Yaremchuk, 4rd International Workshop on modeling in Crystal Growth, Fukuoka, November 4-7, (2003), Abstracts., 99.