CRYSTAL GROWTH IN THE PROCESS OF MODIFIED CZOCHRALSKI

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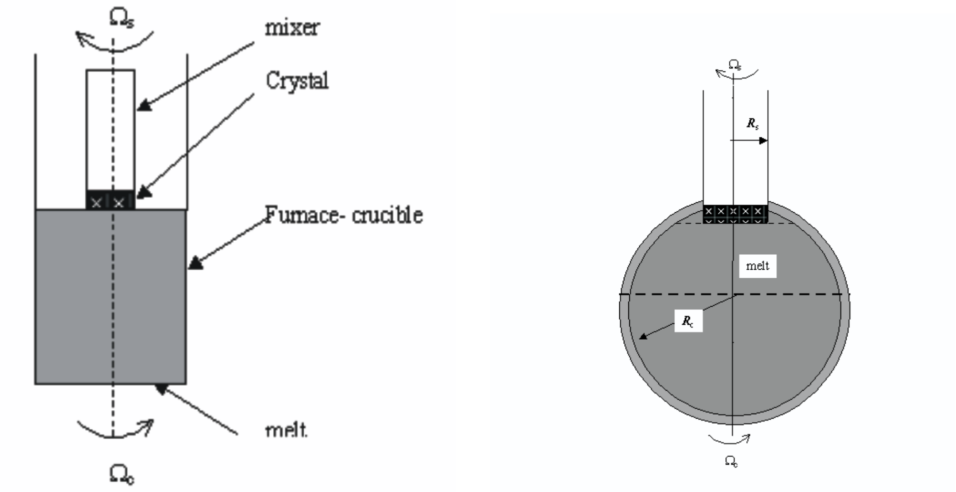
While basing oneself on the phenomenon of crystal growth in a cylindrical system, one proposes an alternative of this process, which is based on the modification of the crucible. This one is replaced by a sphere containing the molten phase of possibly variable material height, the cylinder carrying the germ of the crystal remains unchanged.

This work is thus justified by the study of the influence of the geometry for purposes to optimize the whole processes of transfer in action making it possible to homogenize the fields of temperature and to minimize the losses of masses having to take part in the development of the bulk-flow (traditional Czochralski process). The simulation of the phenomenon thus defined is considered within the framework of the assumption of Boussinesq to solve the equations of transfer of mass, heat, and momentum and written in a spherical frame of reference.

Introduction. The variation in temperature in the system of growth is at the origin of current of convection in the melt. It was shown that the flows play a significant role in the process of growth while acting on the form and the stability of the interface, like on the radial distribution of the doping agents in the crystal [1]. The increase in the variation in temperature induces the development of instabilities meadows of the interface. This bad effect to a good crystallization is eliminated due to the rotational movement, imposed on the crystal and/or the crucible, which are opposed to the natural convection. We passe thus from the mode of the free convection dominating to the mode of the forced convection controlled. Other types of forces can be used to attenuate the disturbances induced by the temperature like the magnetic field. Flows generated by forces, which had the gradients of surface stress, are also possible according to dimensions of the crucible. A compromise must be to adopt the size of the crystal and dimensions of the device [2].



(*a*) (*b*)

Fig. 1. (*a*) Device cylinder/cylinder. (*b*) Device cylinder/sphere.

1. Device. In a traditional device, the molten material is placed in a cylindrical furnace crucible, fixed at the temperature T_{c}, the mixer carrying the germ is of the same cylinder centers as the crucible (Fig. 1*a*). The two cylinders are caused by counter-rotating engines.

Anselmo *et al.* [3] showed by a numerical method that a crucible with a curved bottom has advantages for crystallization. This observationIt was taken into account that led us to replace the system cylinder/cylinder by a cylindro-spherical system.

It is thus about an alternative model represented in Fig. 1*b*, which one calls a cylindro-spherical system, made up of a cylinder carrying the germ of growth, of radius R_{c}. This one turns at an angular velocity Ω_{c} plunged in a spherical crucible which contains a melt of silicon of radius R_{s}, temperature T_{s}, and is laid out on a rotary table with an angular velocity Ω_{s}.

2. Formulation of the problem. Taking account of phenomenologic complexity, one is led to make assumptions of simplification, namely:

- The thermophysical properties of the fluid are constant.
- The molten melt is a Newtonian and incompressible fluid and satisfay the assumption of Boussinesq: it supposes that the effects of variations in density are significant for the forces of volume, the other variations are considered negligible.
- The flow of the liquid within the crucible is laminar.
- The shape of the liquid-solid interface is supposed to be spherical.
- Axial symmetry.
- At the melting point the temperature is constant.
- Calculations are carried out in a stationary mode.

The equations governing the dynamics of the flow result from the principles of conservation of mass, momentum, and the conservation equation of energy in the melt. One notes V the speed of the movement, and P is the associated pressure and T is the temperature, g is the field of gravity, Q is a source term coming from the radiation in the system.

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 V_r\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(V_\theta\sin\theta\right)=0$$

$$V_r\frac{\partial V_r}{\partial r}+\frac{V_\theta}{r}\frac{\partial V_r}{\partial\theta}-\frac{V_\theta^2}{r}-\frac{V_\varphi^2}{r}=-\mathrm{Gr}T\cos\theta-\frac{\partial P}{\partial r}+\Delta V_r-\frac{2}{r^2}V_r-\frac{2}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta V_\theta\right)$$

$$V_r\frac{\partial V_\theta}{\partial r}+\frac{V_\theta V_r}{r}+\frac{V_\theta}{r}\frac{\partial V_\theta}{\partial\theta}-\frac{V_\varphi^2}{r}\cot\theta=\mathrm{Gr}T\sin\theta-\frac{1}{r}\frac{\partial P}{\partial\theta}+\Delta V_\theta-\frac{1}{r^2\sin^2\theta}V_\theta+\frac{2}{r^2}\frac{\partial V_r}{\partial\theta}$$

$$V_r\frac{\partial V_\varphi}{\partial r}+\frac{V_\theta}{r}\frac{\partial V_\varphi}{\partial\theta}+\frac{V_\theta V_\varphi}{r}\cot\theta+\frac{V_r V_\varphi}{r}=\Delta V_\varphi-\frac{1}{r^2\sin^2\theta}V_\varphi$$

$$V_r\frac{\partial T}{\partial r}+\frac{V_\theta}{r}\frac{\partial T}{\partial\theta}=\alpha\left\{\frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)+\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial T}{\partial\theta}\right)\right]\right\}+Q$$

the boundary conditions are as follows:

$$\begin{array}{lll} r=1 & V=\mathrm{Re}_{\mathrm{c}}\sin\theta e_\varphi & T=1 \\ r=A & V=\mathrm{Re}_{\mathrm{s}}\sin\theta e_\varphi & T=0 \\ \theta=\dfrac{\pi}{2} & V_\theta=0 & \dfrac{\partial V_\varphi}{\partial\theta}=0 \end{array}$$

where A is the radius ratio; $\mathrm{Re}_{\mathrm{c}}=\dfrac{R_{\mathrm{c}}^2\Omega_{\mathrm{c}}}{\upsilon}$ and $\mathrm{Re}_{\mathrm{s}}=\dfrac{R_{\mathrm{c}}R_{\mathrm{s}}\Omega_{\mathrm{s}}}{\upsilon}$ are the Reynolds numbers associated with the crucible and the crystal.

We eliminate the pressure from the first and the second equations by deriving, following to θ and to r.

The Grashof number $\mathrm{Gr} = g\beta R_\mathrm{c}^3(T_\mathrm{s} - T_f)/\upsilon^2$ characterizes the effect of the natural convection.

The Prandtl number $\mathrm{Pr} = \upsilon/\alpha$ characterizes the importance of thermal diffusivity compared to molecular diffusivity.

We propose the expressions of the velocity and temperature fields, which verify the boundary conditions:

$$V_r = \sum_n \alpha_n (r-1)^2 (r-A)^2 r^{n-1} f(\theta)$$
$$V_\theta = \sum_n \beta_n (r-1)(r-A) r^{n-1}\, \Phi(\theta)$$
$$V_\varphi = \sum_n \gamma_n \left(ar + \frac{b}{r^2}\right) r^{n-1}\, \psi(\theta)$$
$$T = \sum_n \delta_n (r-A) r^{n-1}\, \Theta(\theta)$$

According to Galerkin method [5], we replace these expressions in the equations of movement, and we multiplies by $W_m = \sum_m \left(ar + \frac{b}{r^2}\right) r^{m-1}$ and integrate thereafter between A and 1.

By applying the boundary conditions to the form of V_φ, we can have the form of $\psi(\theta)$, a and b

$$\psi(\theta) = \psi_0 \sin\theta \qquad a = \frac{A^2\mathrm{Re}_\mathrm{s} - \mathrm{Re}_\mathrm{c}}{A^3 - 1} \qquad b = \frac{A^3\mathrm{Re}_\mathrm{c} - A^2\mathrm{Re}_\mathrm{s}}{A^3 - 1}$$

In the next step one is led to carry out an approximation of the order $n = m = 1$ to have an estimate of the solution:

$$\Phi = \frac{1}{\beta_1 \sin\theta^{1+N}} \left(\int_0^{\pi/2} \sin\theta'^{1+N} \mathrm{d}\theta' - \int_\theta \sin\theta'^{1+N} \mathrm{d}\theta' \right)$$
$$f = \frac{1}{\alpha_1} \left(2\frac{I_5}{I_3} - \beta_1 \frac{I_4}{I_3} C_2 \frac{\cot\theta}{\sin\theta^{1+N}} + I_5 \frac{I_1}{I_2} \frac{I_4}{I_3^2} \frac{\cot\theta}{\sin\theta^{1+N}} \int_\theta \sin\theta'^{1+N} \mathrm{d}\theta' \right)$$
$$\Theta = \cos\theta^p \left(-\int_\theta \frac{g(\theta)}{\cos\theta^{p+1}} \mathrm{d}\theta' + \Theta_0 \right)$$

The equation of the stream lines in the axisymmetric case is given by the relation

$$\left\{ \frac{(r-1)^A\, r^{(1-A)}}{r-A} \right\}^{-\frac{I_1}{I_2 A(A-1)}} = C\Phi \sin\theta$$

We fix the radius ratio $A = 0.25$; the complete definition of the velocity field requires the following data parameters: viscosity, radii of crystal and crucible and their respective angular velocities. Those are given close to those of Anselmo [4].

The evaluation of the integral $\int_\theta \sin\theta'^{1+N} \mathrm{d}\theta'$ is carried out using the Lanczos method [5].

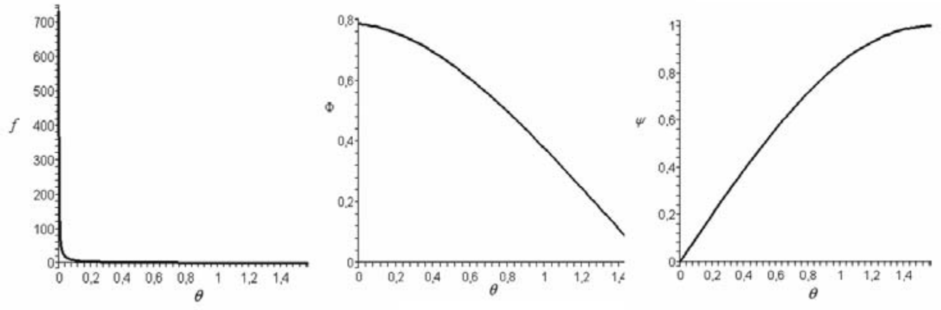


Fig. 2.

Therefore, the expression of the stream lines is given as the following transcendental relation:

$$\frac{(r-1)^{0.25}\, r^{0.75}}{r-0.25} = C\left(\frac{\pi}{4}\sin\theta^{0.288} - \frac{\theta}{2}\sin\theta\left(1-\frac{\theta}{6}\,0.712\cot\theta\right)\right)^{-4.8}$$

We obtain then the curves of f, Φ and ψ, Fig. 2

3. Conclusion. This study made it possible to verify the assumption concerning the importance of the spherical geometry in term of effectiveness of convective thermo exchange compared to the cylindrical configuration. Thus the process of growth is sensitive to the effect of spherical symmetry which induces the formation of a bulk flow of optimal size.

Indeed the distributions of the velocity and temperature fields are qualitatively comparable with the results found by Anselmo in the cylindrical geometry. However, it differs from it quantitatively in form and size from the configuration obtained due to the virtual non-existence of or not participative area of fluid died in dynamics in the geometry considered.

As a prospect with this work, one plans to examine the effect of the free surface or thermocapillarity effect on the flow when the height of the melt decreases compared with the radius of the hemispherical crucible.

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