Determination of the stationary solution in the case of solidification using Bridgman technique

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Abstract— A stationary free boundary model of solidification in the case of the vertical Bridgman crystal growth technique is considered. The Navier-Stokes and heat equations are employed and upper bounds for the velocity and temperature fields are determined theoretically. Then the determined properties are validated through numerical simulations in an axi-symmetric domain, based on a fixed point algorithm, performed using FreeFem++ software.

Keywords— Free boundary problem, Stationary problem, Vertical Bridgman

I. INTRODUCTION

In 1924, Bridgman developed a method for growing crystals in a cylindrical crucible. The crystal grows as the crucible moves in a certain temperature configuration and layout of the furnace [1]. Most known temperature configurations are Grenoble (corresponding to adiabatic insulation among the ampoule's sidewall) and MIT (corresponding to three zones of temperature among the ampoule's sidewall). As for the layout of the furnace, it can be vertical or horizontal.

The Bridgman technique is used to grow single crystals of As, Ag, LiI, SiAs, GaAs, GaGe, etc.

The properties of the resulting crystal depend on:

- the temperature gradient in the furnace;
- the value of the gravitational field;
- the properties of the material (such as specific heat, density, kinematic viscosity, thermal expansion coefficient, solidification temperature, and initial dopant concentration in case of binary alloys);
- the ampoule's velocity of translation in the furnace;
- the shape of solid-melt interface, which is given by two conditions: constant temperature and constant heat flux.

In the case of binary alloys, the rejection of the dopant at the solidification interface represents a serious problem for practical crystal growers. Hence, the properties of the semiconductor crystals are strongly dependent of the dopant rejection which is controlled by the shape of the solid/liquid interface. On the other hand, the interface is a free boundary, unknown apriori, reason for which this kind of problems request more theoretical investigations. In literature, there are

some investigations based on the model proposed in [2], but they were made under the assumption that the solidification interface is apriori known [3]-[7].

In this paper the free boundary model proposed by Chang and Brown is considered [2]. The furnace configuration is of MIT type, i.e., the furnace presents three zones: (i) the hot zone; (ii) the gradient zone; and (iii) the cold zone.

Some properties of the solution for the considered boundary value problem are established. These are validated through numerical simulations, based on a fixed point algorithm, performed using FreeFem++ software.

II. PROBLEM STATEMENT

A. Dimensional governing equations for the process

Consider the Bridgman method for growing crystals in a MIT furnace. A schematic representation for the ampoule's transition and heat profile in the furnace is given in Fig.1.



Fig. 1: Configuration of the MIT furnace

The equations governing the process are:

for the velocity field in melt: $\nabla \overline{v} = 0$ $\rho_l \frac{\partial \overline{v}}{\partial t} + \rho_l (\overline{v} \nabla) \overline{v} =$

$$= -\nabla p_l + \rho_l v \Delta \overline{v} + \rho_l g \beta_l (T - T_r) \cdot \overline{e}_z$$

- for the temperature in melt:

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$$\frac{\partial T}{\partial t} + \overline{v}\nabla T = \alpha_l \Delta T$$

- for the velocity field in crystal $\overline{v}_s = \overline{V}_s$
- for the temperature in crystal $\frac{\partial T_s}{\partial t} + \overline{v}_s \nabla T_s = \alpha_s \Delta T_s.$

Cl The corresponding boundary conditions are:

- the walls of the ampoule are no-slip surface:
 - $\overline{v} = \overline{V}_{s}$

 $\overline{v}_{s} = \overline{V}_{s}$

- the solid/melt interface is no-slip surface: $\overline{v} \cdot \overline{t} = Pe \cdot (\overline{e_z} \cdot \overline{t})$ $\sigma(\overline{v} \cdot \overline{n}) = Pe \cdot (\overline{e_z} \cdot \overline{n})$
- the temperature for the upper and the lower side of the ampoule is equal to the temperature of the furnace;
- the temperature of the sidewall of the ampoule is equal to the temperature of the furnace in the hot zone and in the cold zone and decreases linearly in the adiabatic zone;
- at the solid/melt interface the following two conditions for temperature hold:

a) constant temperature:

$$T = \frac{T_c + T_r}{2}$$

b) constant heat flux:

$$k_{l}(\overline{n}\nabla T)_{l}-k_{s}(\overline{n}\nabla T)_{s}=\Delta H\rho_{l}\overline{n}\cdot\overline{u}_{tr}$$

The initial conditions are:

$$v_0 = u_1$$

$$T_0 = T_c$$

The signifiance of the symbols involved in previous equations and conditions is:

 \overline{v} - velocity field in melt

- ρ_l density of melt
- p_l pressure in melt

v-kinematic viscosity of melt

- g-gravitational constant
- β_t thermal expansion coefficient

T - temperature field in melt

- T_r temperature of cold zone
- α_l thermal diffusivity in melt
- \overline{v}_s velocity field in crystal
- \overline{V}_s pulling rate
- T_s temperature field in crystal
- α_s thermal diffusivity in crystal

- Pe-Peclet number
- \overline{n} outward normal unit vector
- \bar{t} tangent unit vector
- $\sigma\operatorname{-ratio}$ of the solid and melt densities
- k_l thermal conductivity of melt
- k_s thermal conductivity of crystal
- ΔH latent heat of melt
- ρ_l density of melt

B. Dimensionless governing equations

In order to obtain the dimensionless equations describing the process, the dimensional parameters are scalled as follows:

$$\overline{u} = \frac{L}{\alpha_l} \overline{v}$$
$$\overline{u}_c = \frac{L}{\alpha_l} \overline{v}_s$$
$$p = \frac{L^2}{\rho_l \alpha_l^2} p_l$$
$$\overline{x} = \frac{\overline{X}}{L}$$
$$\theta = \frac{T - T_r}{T_c - T_r}$$
$$\theta_c = \frac{T_s - T_r}{T_c - T_r}$$

In this way, the dimensionless velocity field in the melt (\overline{u}), the dimensionless velocity field in the crystal (\overline{u}_c), the dimensionless pressure field in the melt (p), the dimensionless coordinate (\overline{x}), the dimensionless temperature in the melt (θ), and the dimensionless temperature in the crystal (θ_c) are obtained.

Since the crucible presents axial symmetry, the threedimensional problem describing the solidification process is reduced to a two-dimensional one.

In the following, the domain occupied by the melt is denoted as Ω_{l} , and the domain occupied by the crystal as Ω_{r} , i.e.,

$$\begin{split} \Omega_s &= \left\{\!\!(r,z) \in R^2 | 0 \leq r < R \text{ and } 0 < z < h(r) \right\}\\ \Omega_l &= \left\{\!\!(r,z) \in R^2 | 0 \leq r < R \text{ and } h(r) < z < A \right\} \end{split}$$

where h(r) is the function describing the solidification interface. Note that the function h(r) satisfies $h(R) = \frac{A}{2}$. A schematic representation of the domain $\Omega = \Omega_1 \cup \Omega_s$ is given in Fig. 2.



Fig. 2: The domains occupied by melt and solid, the corresponding boundaries, and the temperature profile in the furnace.

Hence, the dimensionless form of the Navier-Stokes and heat equations in the liquid and crystal is given by:

$$\begin{cases} \nabla u = 0 \text{ in } \Omega_1 \\ (\overline{u}\nabla)\overline{u} = -\nabla p + Pr\Delta\overline{u} + Ra \ Pr \ \theta\overline{e}_z \text{ in } \Omega_1 \\ \overline{u}\nabla \theta = \Delta\theta \text{ in } \Omega_1 \\ \overline{u}_c = -Pe \ \overline{e}_z \text{ in } \Omega_s \\ \overline{u}_c \nabla \theta_c = \gamma \Delta \theta_c \text{ in } \Omega_s \end{cases}$$
(1)

where the following dimensionless parameters are introduced:

- Rayleigh number

$$Ra = \frac{\beta_t g(T_c - T_r)L^3}{\alpha_s V}$$

- Prandtl number

$$Pr = \frac{v}{\alpha_1}$$

- Péclet number

$$Pe = \frac{V_s L}{\alpha_l}$$

and γ is the ratio of the solid and melt thermal diffusivities.

The boundary conditions corresponding to problem (1) are: $\overline{u}|_{\Gamma_2,\Gamma_2} = \overline{u}_{tr}$ (2)

$$\overline{u}_c |_{\Gamma_1, \Gamma_2} = \overline{u}_{tr} \tag{3}$$

$$\overline{u} \cdot \overline{t} \Big|_{\Gamma_{5}} = Pe \cdot t_{z} \tag{4}$$

$$\sigma(\overline{u}\cdot\overline{n})|_{\Gamma_5} = Pe \cdot n_z \tag{5}$$

$$\theta_c \mid_{\Gamma_1} = 0 \tag{6}$$

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$$\theta \mid_{\Gamma_{2}} = \theta_{c} \mid_{\Gamma_{2}} = \begin{cases} 0 & , z < \frac{A}{2} - \frac{L_{g}}{2} \\ \frac{1}{L_{g}} z + \frac{L_{g} - A}{2L_{g}} & , z \in \left[\frac{A}{2} - \frac{L_{g}}{2}, \frac{A}{2} + \frac{L_{g}}{2}\right]^{not} \\ 1 & , z > \frac{A}{2} + \frac{L_{g}}{2} \end{cases}$$

$$\theta \mid_{\tau_{2}} = 1 \qquad (7)$$

$$\theta|_{\Gamma_3} = 1 \tag{8}$$

$$\theta|_{\Gamma_5} = \frac{T_t - T_r}{T_c - T_r} = 0.5$$
(9)

$$\left[\left(\overline{n}\nabla\theta\right)_{l}-k\left(\overline{n}\nabla\theta\right)_{s}\right]_{\Gamma_{5}}=SPen_{z}$$
(10)

where:

- $\overline{u}_{tr} = u_{tr} \cdot \overline{e}_z$ is the dimensioneless velocity of translation,
- \bar{t} tangent unit vector to the solidification interface,
- \overline{n} outward normal unit vector,
- σ ratio of the solid and melt densities,
- A dimensionless length of the ampoule,
- L_{σ} dimensionless length of gradient zone,
- k ratio of the solid and melt thermal conductivities,
- $S = \frac{\Delta H_l}{\rho_l c_{pl} (T_c T_r)} \text{dimensionless Stefan number}$

 $(\Delta H \text{ is the latent heat of melt, } c_{pl} \text{ - heat capacity of melt).}$

The translation of the ampoule in the furnace is simulated by supplying melt into the ampoule at z = A, and pulling crystal at z = 0.

III. SOME PROPERTIES OF THE BVP'S SOLUTION

A. Homogenization of the boundary conditions

In order to determine the solution's properties for problem (1)-(10), the boundary conditions for the Navier-Stokes equation are first homogenized. After that, a global equation for the temperature field is considered (based on the heat equations in melt, solid and the corresponding boundary conditions).

Let $(\overline{u}, \overline{u}_c, \theta, \theta_c)$ be a solution of the problem (1)-(10), $\overline{u}_1 = \overline{u} - \overline{u}_t$ and $\overline{u}_{1c} = \overline{u}_c - \overline{u}_t$ the velocity fields obtained after homogenizing the Navier-Stokes' boundary conditions. Denoting by

$$\Theta(r,z) = \begin{cases} \theta, \text{ for } (r,z) \in \Omega_l \\ \theta, \text{ for } (r,z) \in \Omega_s \end{cases}$$

the "global temperature", and defining the coefficients $\overline{\alpha}$

and β as follows:

$$\overline{\alpha}(r,z) = \begin{cases} \overline{u}_{1}, \text{ for } (r,z) \in \Omega_{l} \\ 0, \text{ for } (r,z) \in \Omega_{s} \end{cases}$$
$$\beta(r,z) = \begin{cases} 1, \text{ for } (r,z) \in \Omega_{l} \\ \gamma, \text{ for } (r,z) \in \Omega_{s} \end{cases},$$

the problem (1) becomes:

$$\begin{cases} \nabla \overline{u}_{1} = 0 \text{ in } \Omega_{1} \\ (\overline{u}_{1} \nabla) \overline{u}_{1} = -\nabla p + Pr \Delta \overline{u}_{1} + Ra Pr \Theta |_{\Omega_{l}} \overline{e}_{z} - \\ -(\overline{u}_{1} \nabla) \overline{u}_{tr} - (\overline{u}_{tr} \nabla) \overline{u}_{1} - (\overline{u}_{tr} \nabla) \overline{u}_{tr} \text{ in } \Omega_{1} \\ \overline{\alpha} \nabla \Theta = \beta \Delta \Theta - \overline{u}_{tr} \nabla \Theta \text{ in } \Omega \\ \overline{u}_{1c} = 0 \text{ in } \Omega_{s} \end{cases}$$
Note that $\Omega = \overline{\omega}$ and α are continuous functions defined as

Note that Θ , $\overline{\alpha}$ and β are continuous functions defined on Ω . The corresponding boundary conditions are:

$$\overline{u}_1 \mid_{\Gamma_2, \Gamma_3} = 0 \tag{12}$$

$$\overline{u}_{l_c}|_{\Gamma_1,\Gamma_2} = 0 \tag{13}$$

$$\overline{u}_1 \cdot \overline{t} \mid_{\Gamma_5} = (Pe - u_{tr}) \cdot t_z = 0 \tag{14}$$

$$\sigma(\overline{u}_1 \cdot \overline{n})|_{\Gamma_5} = (Pe - \sigma u_{tr}) \cdot n_z = 0$$
⁽¹⁵⁾

$$\Theta|_{\Gamma_1} = 0 \tag{16}$$

$$\Theta|_{\Gamma_2} = \tau \tag{17}$$

$$\Theta|_{\Gamma_2} = 1 \tag{18}$$

$$\Theta|_{\Gamma_5} = \frac{T_t - T_r}{T_c - T_r} = 0.5$$
(19)

$$\left[\left(\overline{n}\nabla\Theta\right)_{l}-k(\overline{n}\nabla\Theta)_{s}\right]_{\Gamma_{5}}=SPe\,n_{z}$$
(20)

B. An upper bound for the temperature

Multiplying equation

$$\overline{\alpha}\nabla\Theta = \beta\Delta\Theta - \overline{u}_{tr}\nabla\Theta$$

by Θ and integrating over Ω , we get: $\int_{\Omega} \overline{\alpha} \nabla \Theta \cdot \Theta = \int_{\Omega} \beta \Delta \Theta \cdot \Theta - \int_{\Omega} \overline{u}_{tr} \nabla \Theta \cdot \Theta \,.$

Because

$$\begin{split} &\int_{\Omega} \overline{\alpha} \nabla \Theta \cdot \Theta = 0, \\ &\int_{\Omega} \beta \Delta \Theta \cdot \Theta = -\beta \int_{\Omega} |\nabla \Theta|^2 + \frac{1}{2} \beta SPe \int_{\Gamma_5} n_z, \\ &\int_{\Omega} \overline{u}_{tr} \nabla \Theta \cdot \Theta = \frac{Ru_{tr}}{2} + \frac{1}{8} u_{tr} \int_{\Gamma_5} n_z, \end{split}$$

we obtain the inequality

$$\int_{\Omega} |\nabla \Theta|^{2} = \frac{1}{\beta} \left[\frac{Ru_{tr}}{2} + \frac{1}{8}u_{tr} \int_{\Gamma_{5}} n_{z} + \frac{1}{2}\beta SPe \int_{\Gamma_{5}} n_{z} \right] \leq \frac{1}{\beta} \left[\frac{Ru_{tr}}{2} + \frac{4\beta SPe + u_{tr}}{8} l(\Gamma_{5}) \right]$$

or

$$\|\nabla\Theta\| \leq \sqrt{\frac{1}{\beta} \left[\frac{Ru_{tr}}{2} + \frac{4\beta SPe + u_{tr}}{8} l(\Gamma_5) \right]} =$$
(22)
$$\stackrel{\text{not}}{=} M_{\Theta} < \infty.$$

Relation (22) implies that the growth of the temperature field is finite in Ω . Since $\Theta|_{\Gamma} = 0$, it follows that Θ is finite, and hence $\|\Theta\|_{L^2} \leq C_1$, with C_1 a real positive constant.

C. An upper bound for the velocity field
Let
$$X_0 = \{\overline{u} \in (H_0^1(\Omega_l))^3 | \nabla \overline{u} = 0\}$$
. Multiplying equation
 $(\overline{u}_1 \nabla) \overline{u}_1 = -\nabla p + Pr \Delta \overline{u}_1 + Ra Pr \Theta|_{\Omega_l} \overline{e}_z - (\overline{u}_1 \nabla) \overline{u}_{tr} - (\overline{u}_{tr} \nabla) \overline{u}_1 - (\overline{u}_{tr} \nabla) \overline{u}_{tr}$

by $\overline{u}_1 \in X_0$, and integrating over Ω_l we get:

$$\int_{\Omega_l} (\overline{u}_1 \nabla) \overline{u}_1 \overline{u}_1 = -\int_{\Omega_l} \nabla p \overline{u}_1 + Pr \int_{\Omega_l} \Delta \overline{u}_1 \overline{u}_1 + Ra Pr \int_{\Omega_l} \Theta \Big|_{\Omega_l} \overline{e}_z \overline{u}_1 - \int_{\Omega_l} (\overline{u}_1 \nabla) \overline{u}_{tr} \overline{u}_1 - \int_{\Omega_l} (\overline{u}_{tr} \nabla) \overline{u}_{tr} \overline{u}_1 - \int_{\Omega_l} (\overline{u}_{tr} \nabla) \overline{u}_{tr} \overline{u}_1$$

or

$$Pr \int_{\Omega_l} \Delta \overline{u}_1 \overline{u}_1 + Ra Pr \int_{\Omega_l} \Theta \Big|_{\Omega_l} \overline{e}_z \overline{u}_1 = 0.$$
(23)
This leads to

This leads to

$$\begin{aligned} \left\|\nabla \overline{u}_{1}\right\|_{L^{2}} &\leq \int_{\Omega_{t}} \left|\nabla \overline{u}_{1}\right|^{2} = Ra \int_{\Omega_{t}} \Theta \Big|_{\Omega_{t}} \overline{e}_{z} \overline{u}_{1} \leq \\ &\leq Ra \left\|\Theta \Big|_{L^{2}} \left\|\overline{u}_{1}\right\|_{L^{2}} \end{aligned}$$

Applying the Friedrichs inequality, which in our case is written $\left\|\overline{u}\right\|_{L^{2}} \leq \sqrt{A^{2} + R^{2}} \left\|\nabla\overline{u}\right\|_{L^{2}}$

we get

(21)

$$\left\|\nabla \overline{u}_{1}\right\|_{L^{2}} \leq \sqrt{A^{2} + R^{2}} \operatorname{Ra} C_{1} < \infty.$$
(24)

Inequality (24) implies that the growth of the velocity field is finite in Ω . Since $\overline{u}_1 \mid_{\partial\Omega} = 0$, it follows that \overline{u}_1 is finite, or $\overline{u} = \overline{u}_1 + \overline{u}_{tr}$ is finite.

IV. NUMERICAL EXAMPLE

In the following, numerical simulations, based on a fixed point algorithm, are performed using FreeFem++ software [8].

FreeFem++ is a software developed at the Universite Pierre et Marie Curie, Paris, under freeware license, dedicated to solve two-dimensional and three-dimensional partial differential equations using the finite element method.

The values for the parameters involved in (1)-(10), corresponding to Ga-dopped Ge grown in two distinct gravity conditions: terrestrial ($Ra = 10^6$) and zero-gravity (Ra = 0), are given in Table I.

Table I: Values of the parameters

Symbol	Value	Symbol	Value
Α	1	u_{tr}	0.01
L_g	0.125	γ	1
Pr	0.01	k	1
Ra	0, 10 ⁶	S	1
Pe	0.01	σ	1

The algorithm for solving problem (1)-(10) consists in the following:

INPUT DATA:

- $h^{(0)}(r) = \frac{A}{2}$
- $\overline{u}^{(0)}(r,z) = \overline{u}_{tr}$
- $\Theta^{(0)}(r,z) = \tau$

OUTPUT RESULTS:

- h(r)
- $\overline{u}(r,z)$
- $\Theta(r,z)$

STEPS:

- 1. Solve the "global" heat equation with the boundary condition (20).
- 2. Find the isotherm corresponding to condition (19).
- 3. Construct a domain deformation, in order to overlap the boundary to the isotherm found at step 2.
- 4. Solve the Navier-Stokes equation on de deformed domain.
- 5. Repeat steps 1-4 until both the variations of temperature field and velocity field become less than a sufficiently small error, ε .

A schematic representation of the computed free solid-melt interface, following the described algorithm is given in Fig. 3.

Following the steps described previous, first the "global" heat equation with constant heat flux as boundary condition on Γ_5 is solved, and a temperature profile on Ω is found.

Because the isotherm corresponding to condition (19) is not necessarily overlapping the boundary Γ_5 , its position should be determined. For this aim:

- (i) the points $P_i(r_i, z_i)$ (with $i = \overline{1,7}$) for which $\Theta(P_i) = 0.5$ are found, and
- (ii) the Bezier curve $h_{\theta}(r)$ determined by the computed points $P_i(r_i, z_i)$ is constructed.

Once determined the parametric equation of the isotherm corresponding to $\Theta = 0.5$, the next step consists in domain's deformation, in order to overlap the isotherm to the inner boundary (solidification interface). It is not necessarily to

construct another analytic curve for the inner boundary, because this is exactly the Bezier curve computed at the previous iteration.



Fig. 3: The computed solid-melt interface deformation

The deformation of the domain must satisfy the following conditions:

- the horizontal displacement must be zero on the domain and its boundaries;
- on Γ_1 and Γ_3 the vertical displacement must be zero;
- on Γ_5 the vertical displacement must be equal to the difference $h_a(r) h(r)$.

Thus, the deformation must satisfy the following system: $(\nabla \delta = 0 \text{ in } \Omega)$

$$\begin{cases} \delta \big|_{\Gamma_1} = \delta \big|_{\Gamma_3} = 0 \\ \delta \big|_{\Gamma_5} = h_{\theta}(r) - h(r) \stackrel{not}{=} dif \\ \frac{\partial \delta}{\partial \overline{n}} \big|_{\Gamma_2} = \frac{\partial \delta}{\partial \overline{n}} \big|_{\Gamma_4} = 0 \end{cases}$$
(25)

Once the position of the solidification interface is determined, the Navier-Stokes equation is solved.

The values of the temperature and velocity field depend on the domain on which the corresponding equations are solved. The shape of this domain depends on the position of the solidification interface. This implies that it is not sufficient that the solidification interface overlap the isotherm $\Theta = 0.5$, but it requests also that the values for the temperature and velocity fields have a sufficiently small variation.

The computed temperature and velocity fields for two Rayleigh numbers ($Ra = 10^6$, corresponding to terrestrial

conditions, and Ra = 0, corresponding to zero-gravity conditions) are presented below.



Fig. 4: Flow field in the stationary case for Ga-dopped Ge grown in terrestrial conditions ($Ra = 10^6$)



Fig. 6: Temperature in the stationary case for Ga-dopped Ge

grown in terrestrial conditions ($Ra = 10^6$)



Fig. 7: Temperature in the stationary case for Ga-dopped Ge grown in zero-gravity conditions (Ra = 0)

Fig. 5: Flow field in the stationary case for Ga-dopped Ge grown

in zero-gravity conditions (Ra = 0)

Computations show that the behaviour of the flow field in the melt is strongly determined by the Rayleigh number.

For $Ra = 10^6$, two convection cells are observed: a strong one, in the lower part of the melt, and a weaker one in the upper part. The computed streamlines are equally spaced between the maximum (0.1526) and the minimum (-0.0118) values (Fig. 4).

For Ra = 0, there is no convection. The computed streamlines are equally spaced between the maximum (0.000304) and the minumum (7.81 · 10⁻⁶) values (Fig. 5).

In case of the temperature field, for $Ra = 10^6$, it can be observed that the shape of the isotherms tend to flatten in melt toward the solidification interface. Because the velocity in crystal is constant, and equal to the growth rate, the shape of the isotherms in crystal is not affected by the gravity condition. The computed isovalues for temperature are equidistant between a minimum (0) and a maximum (1) value (Fig. 6).

For Ra = 0, the shape of isotherms in melt is similar to the shape of isotherms in crystal. This is due to the absence of convection. The computed isovalues for temperature are equidistant between a minimum (0) and a maximum (1) value (Fig. 7).

A larger view of the region containing the computed solidification interface is presented in Fig. 8 and Fig. 9.



Fig. 8: The solidification interface for $Ra = 10^6$



Fig. 9: The solidification interface for Ra = 0

It can be observed that in case of $Ra = 10^6$ the shape of the solidification interface tends to lower at r = 0, due to the strong convection in melt. Thus, the difference between the computed interface and the input data $(h^{(0)}(r) = \frac{A}{2})$ is significant. For Ra = 0, the absence of convection causes no significant deviation of the computed interface and the input

significant deviation of the computed interface and the input data.

It can be also observed that in case of zero-gravity

conditions (Ra = 0), a straight line of equation $z(r) = \frac{A}{2}$ represents a good approximation for the shape of the solidification interface, but in case of terrestrial gravity conditions ($Ra = 10^6$), it is no longer possible to approximate solidification interface as a straight line.

In conclusion, a larger Ra number, corresponding to a stronger gravitational field, produces a stronger convective flow in the melt. This influences the shape of isotherms in melt: a stronger convective flow causes flattened isotherms toward the solidification interface. Since the shape of solid-melt interface is determined by the isotherm $\Theta = 0.5$, it follows that the interface shape is affected by the value of the gravitational field.

It should be underlined that in previous investigations [3]-[7], the numerical solution of the problem (1)-(10) was computed under the assumption that the solidification interface is a straight line, on which a constant temperature is imposed, but the heat flux at the interface was neglected. The approach proposed here is more realistic because it considers both conditions of constant temperature and prescribed heat flux at the interface.

V. CONCLUSIONS

A free boundary stationary model for the Bridgman crystal growth technique was considered. From the properties of the considered BVP's solution, upper limitations for the velocity field and temperature were estimated. Numerical simulations, based on a fixed point algorithm, were performed using FreeFem++ software.

Further investigations of the present work will focus on the non-stationary case able to give more useful information for optimizing crystal growth processes.

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