Effect of the temperature profile on the fluid flow and interface deflection in the case of crystals grown by Bridgman technique

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Abstract: A stationary, free boundary model describing the process of crystal growth in a vertical Bridgman installation is considered. The influence of the temperature profile in the furnace on the fluid flow and interface deflection, in terrestrial gravitational field, is investigated numerically by finite element method through FreeFem++ software.

Key–Words: free boundary problem, stationary problem, temperature profile, interface deflection, vertical Bridgman

1 Introduction

Bridgman technique allows growing compound materials that contain a volatile element, as in the case of the entire group III-V and II-VI semiconductor crystals. The method consists in movement of a crucible (ampoule) through a temperature gradient in a furnace. The crucible is charged with powder and with a seed. The ampoule is introduced in the hot region of the furnace until the powder is melted. Then, the ampoule is moved with a rate $u_{\text{translation}}$, such that it enters into the cold region and the solidification process begins [1].

The factors that influence the quality of the resulting crystal are:

- 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);
- the ampoules velocity of translation in the furnace;
- the shape of solid-melt interface.

In the case of alloys for which equilibrium segregation coefficient of the dopant is less than unity, a serious problem is the amount of dopant rejected at the solid-melt interface. This quantity depends on the velocity field in melt and on the shape of solidification interface. Both these parameters depend on the value of the gravitational field and on the temperature profile inside the furnace.

In literature, there are several numerical investigations of the solidification process in vertical Bridgman installations ([2], [3], [4], [5], [6], [7], [8]). However, as far as we know, the influence of the length of the adiabatic zone in the furnace on the resulting crystal was not investigated.

In this paper, the dependence of fluid flow and interface deflection on the temperature profile are investigated numerically in a vertical Bridgman furnace. The numerical simulations, based on a fixed-point algorithm, were performed using the FreeFem++ software.

2 Problem Statement

Let us consider the stationary, free boundary model proposed in [3]. Because the crucible presents axial symmetry, the three-dimensional problem could be reduced to a two-dimensional one. Denoting by $\Omega_s$ the domain occupied by melt, by $\Omega_t$ the domain occupied by crystal and the solidification interface by a function $h(r)$, we have [9]:

$$\Omega_s = \{(r, z) \in \mathbb{R}^2 | 0 < r < R \text{ and } 0 < z < h(r)\}$$

$$\Omega_t = \{(r, z) \in \mathbb{R}^2 | 0 < r < R \text{ and } h(r) < z < A\}$$

$$h(R) = \frac{A}{2}$$
A schematic representation of the computational domains is given in Figure 1. Here $A = 1$ represents

\[ \bar{u}_c \Gamma_1 \Gamma_2 = \bar{u}_{tr} \]  
\[ \bar{u} \cdot \bar{t} \Gamma_2 \Gamma_5 = Pe \cdot t_z \]  
\[ \sigma(\bar{u} \cdot \bar{n}) \Gamma_5 = Pe \cdot n_z \]  
\[ \theta_c \Gamma_1 = 0 \]

\[ \theta \Gamma_2 = \begin{cases} \frac{1}{L_g} z + \frac{L_g - A}{2L_g} , & z \in \left[ \frac{A}{2} , \frac{A + L_g}{2} \right] \\ 1 , & z > \frac{A}{2} + \frac{L_g}{2} \\ 0 , & z < \frac{A}{2} - \frac{L_g}{2} \end{cases} \] not $\tau$

\[ \theta_c \Gamma_2 = \begin{cases} \frac{1}{L_g} z + \frac{L_g - A}{2L_g} , & z \in \left[ \frac{A}{2} - \frac{L_g}{2} \right] \\ 1 , & z > \frac{A}{2} + \frac{L_g}{2} \\ 0 , & z < \frac{A}{2} - \frac{L_g}{2} \end{cases} \] not $\tau_c$

\[ \theta \Gamma_3 = 1 \]

\[ \theta \Gamma_5 = \theta_c \Gamma_3 = 0.5 \]

\[ [(\bar{n} \nabla \theta)_t - k (\bar{n} \nabla \theta)_s] \Gamma_5 = Sp e n_z \]  

where $\bar{u}_{tr} = -0.01 \bar{e}_z$ is the dimensionless velocity of translation of ampoule.

### 3 Numerical results and discussions

The numerical simulations were performed using FreeFem++, software developed at Universite Pierre et Marie Curie, Paris [10], dedicated to solve nonlinear two-dimensional and three-dimensional partial differential equations, using the finite element method.

The fixed point algorithm [9] used to obtain the free boundary takes as input data: $h^{(0)}(r) = \frac{A}{2}$, $\bar{u}^{(0)}(r, z) = \bar{u}_{tr}$, $\theta^{(0)}(r, z) = \tau$, $\theta_c^{(0)}(r, z) = \tau_c$, and computes the values for $h(r)$, $\bar{u}(r, z)$, $\theta(r, z)$, $\theta_c(r, z)$, as follows:

1. solve the heat equation with the boundary condition (11);
2. find the isotherm corresponding to (10);
3. construct a domain deformation in order to overlap the boundary to the isotherm found at the previous step;
4. solve the Navier-Stokes equation on the deformed domain;
5. repeat steps 1-4 until both variations of temperature field and velocity field become less than a sufficiently small value, $\varepsilon$. 

Figure 1: The computational domains and the temperature profile inside the furnace
In the following, the streamlines and temperature profiles, obtained for different values of the gradient zone length, \( L_g \), are presented.

Figure 2: Streamlines and temperature profile for \( L_g = 0.125 \).

Figures 2-7 show that, in terrestrial gravity conditions, the velocity fields present a convection cell. Also, if the gradient zone increases from 0.125 to 1, then the streamlines of the fluid flow have a maximum situated above the gradient zone. These maxima decrease as \( L_g \) increases (see Table 1).

<table>
<thead>
<tr>
<th>( L_g )</th>
<th>maximum value of streamlines of the fluid flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.125</td>
<td>0.152813</td>
</tr>
<tr>
<td>0.250</td>
<td>0.140295</td>
</tr>
<tr>
<td>0.375</td>
<td>0.123135</td>
</tr>
<tr>
<td>0.500</td>
<td>0.103699</td>
</tr>
<tr>
<td>0.750</td>
<td>0.0571388</td>
</tr>
<tr>
<td>1.000</td>
<td>0.000304688</td>
</tr>
</tbody>
</table>

The deflection of the interface for the considered \( L_g \) is presented in Figure 8. Figure 8 shows that variations of \( L_g \) in the range [0.125, 0.500] produce small variations on the melt-solid interface, but deflection of the interface is quit large. If \( L_g \) increases to 1, then the interface deflection decreases. Also, the shape of

Figure 3: Streamlines and temperature profile for \( L_g = 0.250 \).

Figure 4: Streamlines and temperature profile for \( L_g = 0.375 \).
Figure 5: Streamlines and temperature profile for $L_g = 0.500$.

Figure 6: Streamlines and temperature profile for $L_g = 0.750$.

Figure 7: Streamlines and temperature profile for $L_g = 1.000$.

Figure 8: The solidification interface corresponding to different values of $L_g$. 
the interface changes from "S"-shape to slight-convex shape when \( L_g \) increases.

4 Conclusions

In this paper, the influence of the temperature profile in a vertical Bridgman installation on the fluid flow and interface deflection was studied. The streamline maxim decreases and the shape of the solidification interface tends to flatten as the length of the grafiient zone in the furnace increases to 1.

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