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Тематика сборника охватывает широкий спектр актуальных исследований в области физической гидродинамики, перспективных материалов и технологий, физики мягких конденсированных сред.

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Численное решение задачи Стефана

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В работе описан алгоритм решения задачи Стефана методом конечных элементов для моделирования процессов кристаллизации методом Бриджмена с погружным нагревателем-вибратором.

Ключевые слова: задача Стефана; МКЭ; рост кристаллов

Numerical solution of the Stefan problem

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The paper describes an algorithm for solving the Stefan problem by the finite element method for modeling crystallization processes by the Bridgman method with an immersed heater-vibrator.

Keywords: Stefan problem; FEM, crystal growth

1. Introduction

This paper presents the results of numerical modeling by the finite element method of convective heat and mass transfer during the growth of single crystals by the vertical Bridgman method with a submerged heater. Numerical calculations were performed using the implicit matrixless finite element method based on the iterative process of conjugate gradients and significantly reducing the requirements for RAM and computer speed. The effects of gravity, rotation, crystallization rate and vibration on heat and mass transfer in the melt, the geometry of the crystallization front, and the thickness of the boundary layers were studied. It is shown that the above effects can be effectively used to control the distribution of impurities in crystals grown by the vertical Bridgman method.

2. Statement of the problem

The melt flow is described by the Navier-Stokes equations for an incompressible fluid in the Boussinesq approximation:

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho_0 d\mathbf{u}/dt + \nabla p = \nabla \cdot \left(\rho_0 \nu \nabla \mathbf{u}\right) - \rho_0 g \beta (T - T_0)\mathbf{e}_z$$

$$\rho_0 c_V dT/dt = \nabla\cdot(k_T \nabla T)$$

$$dC/dt = \nabla\cdot(D\nabla C)$$

where traditional notation is used. The problems were considered under conditions of axial symmetry. Therefore, it is convenient to write the boundary conditions in a cylindrical coordinate system r,θ,z, then u,v,w are radial, circumferential and axial velocity projections, $\mu, k_T . k_C$ are dynamic viscosity, heat conduction and diffusion coefficients, β is the buoyancy coefficient, T_0 is a reference temperature, ρ_0 is a reference density, g is the gravity acceleration along z. The state of the growing crystal is subject to the following relations: $u = 0$, $w = 0$, $v = \Omega_0 r$, $\rho_0 c_V dT/dt = \nabla\cdot(k_T \nabla T)$

The calculation domain is shown in Fig. 1 where $R = 3.36 sm$ - crucible radius, $\delta = 0.1 sm$ - the size of the gap (3), $h = 0.8 sm$, S_{SH} - area of immersed heater (1). $T_m = 937^o C$ - melting point germanium - concentration of gallium impurity. On solid walls, adhesion conditions are specified, Ω_{CR} - crucible rotation speed (bottom - crystal (5) and vertical crucible walls), Ω_0 - rotation speed of the immersed heater (1).

The boundary conditions were adopted as follows:

1) On the axis of symmetry:

$$r = 0,\ 0 \le z \le H\ :\ u = 0,\ v = 0,\ \partial w/\partial r = 0,\ \partial T/\partial r = 0,\ \partial C/\partial r = 0$$

2) On the wall of the crucible:

$$r = R,\ 0 \le z \le h\ :\ u = 0,\ v = 0,\ w = 0,\ \partial T/\partial r = 0,\ \partial C/\partial r = 0$$

$$r = R,\ h < z \le H\ :\ u = 0,\ v = 0,\ w = 0,\ T = T_{CR}(z),\ \partial C/\partial r = 0$$

3) At the crystal boundary:

$$r = R:\ u = 0,\ v = 0,\ w = 0,\ k_T \partial T/\partial r = q_R^*(z,t),\ \partial C/\partial r = 0$$

4) Based on the crystal:

$$z = 0:\ u = 0,\ v = 0,\ w = 0,\ T = T_1,\ C = C_1$$

5) At the upper boundary:

$$z = Z:\ \partial u/\partial z = 0,\ \partial v/\partial z = 0,\ \partial w/\partial z = 0,\ \partial T/\partial z = 0,\ C = C_2$$

6) at the melt-crystal interface $z = \eta(r,t)$ Stefan conditions were set:

$$z = \eta(r,t):\ (T)_S = (T)_L = T_m(1+\alpha_1(C)_L)$$

$$(u)_S = (u)_L = (w)_S = (w)_L = 0$$

$$(v)_S = (v)_L = 2\pi\Omega_0 r\ \ u_n \Delta H = \left(k_T \partial T/\partial n\right)_S - \left(k_T \partial T/\partial n\right)_L$$

$$u_n (C)_L (1-k_*) = \left(D\partial C/\partial n\right)_L$$

$$(C)_S = k_* (C)_L$$

where u_n - rate of propagation of the crystallization front, $z = \eta(r,t)$, ΔH - latent heat of crystallization absorbed / released at the front. In the above formulas, the indices S and L note the solid and liquid phases, respectively, α_1 - coefficient of dependence of the hardening / melting temperature on the concentration of impurities in the melt, k_* - coefficient of equilibrium distribution (rejection) of the impurity. The initial conditions were:

$t = 0:\ u = 0,\ v = 0,\ w = 0,\ T = T^*(r,z),\ C = C^*(r,z)$

$t = 0:\ \eta(r,0) = z_0,\ T^*(r,z_0) = T_m C^*(r,z_0)$

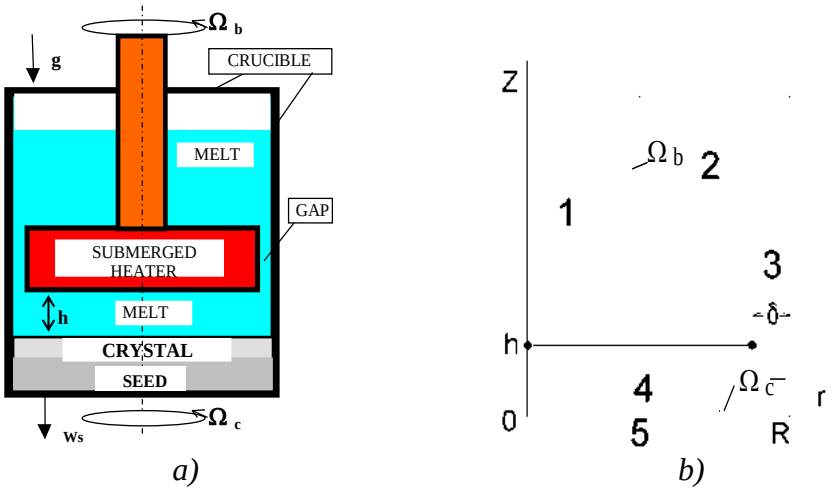


Fig. 1. *Schematic of Bridgman method with submerged heater (a) and solution domain (b).*

At the crystallization front, the condition of mass transfer of the third kind (8) is set taking into account the crystallization rate W_s and with the equilibrium extrusion coefficient of impurity k_*, $\mu, k_T . k_C$ are dynamic viscosity, heat conduction and diffusion coefficients, β is the buoyancy coefficient, T_0 is a reference temperature, ρ_0 is a reference density, g is the gravity acceleration along. Vibrations were specified as a harmonic function of time for movement or speed on a submerged vibrator. The task is characterized by the following similarity numbers: Reynolds number associated with the crystal growth rate $Re_s = W_S R / \nu$; vibrational Reynolds number $Re_{vibr} = A\omega R / \nu$, where A is the amplitude, $\omega = 2\pi f$ is circular frequency of translator's vibrations; Prandtl number $Pr = \mu c_p / k_T$; Grashof number $Gr = g\beta\Delta T R^3 \rho_0^2 / \mu^2$ (or Rayleigh number $Ra = Gr \cdot Pr$), where ΔT is the temperature range, c_p is the heat capacity.

2. Solution Method

The solution was made according to the explicit-implicit scheme of the matrixless finite element method [1] using a moving finite element mesh. The mobility of the grid nodes is due to the variable geometry of the solution region due to the motion of the melt-crystal interface. The new positions of the nodes of the moving mesh were calculated by the model of elastic networks [1], supporting the approximate equality of the volumes of the mesh cells. The grid nodes belonging to the moving boundary between the melt and the growing crystal moved in accordance with Stefan's conditions. Since the integration of time equations is implicit in diffusion terms, it is stable under the usual Courant condition for convection velocity $\Delta t^n \le \min_k (h_k^n / \max(|\ u_k^n - w_k^n\ |, 1e^{-6}))$, where h_k^n - the size of the neighborhood of the node k,

values u and w are velocities of the material and coordinate media. The motion of the interphase boundaries is calculated by using the economical Samarsky-Moiseenko pass-through method [2]. The position of the border was determined from the condition

$$\Phi(r,z,t) = T(r,z,t) - T_m - \alpha_1 C(r,z,t) = 0$$

The heat generation / absorption during the phase transition was taken into account by the equation

$$\rho_0 c_V dT/dt = \nabla \cdot \left(k_T \nabla T\right) - \Delta H \delta(\Phi) dT/dt$$

The delta function was approximated by the expression $\delta(\Phi) = H(1-|(\Phi)_i|/\Delta T_m))/(2.0\Delta T_m)$. The verification of the algorithms was done by calculating the well-known test problems of Val Davis [3] and Wheeler [4] on the melt flow in the Czochralski method. An unstructured moving grid was used to track the movement of the crystal – melt boundary. Grid nodes are numbered $(r_i, z_i, i = 1,...,n_1)$, the numbers of nodes forming three-node internal cells are determined $E(i,j)$ $(i = 1,...,n_2,\ j = 1,2,3)$ and two-node boundary cells $G(i,j)$ $(i = 1,...,n_3,\ j = 1,2)$. The first index of information arrays $E(i,j)$ и $G(i,j)$ corresponds to the cell number, the second to the node number in the cell.

Generalized solution of the problem is determined by the variational equations of the Bubnov-Galerkin method, that are derived in a known manner from the original differential equations. Each moving grid node placed to a central position relative to its neighbors. The grid nodes belonging to the moving interface boundaries moved in accordance with Stefan's conditions. To monotonize the artificial viscosity was used:

$$\nu_*^n = \nu + 0.5((u^n - u_g^n)^2 + (w^n - w_g^n)^2) * \Delta t^n$$

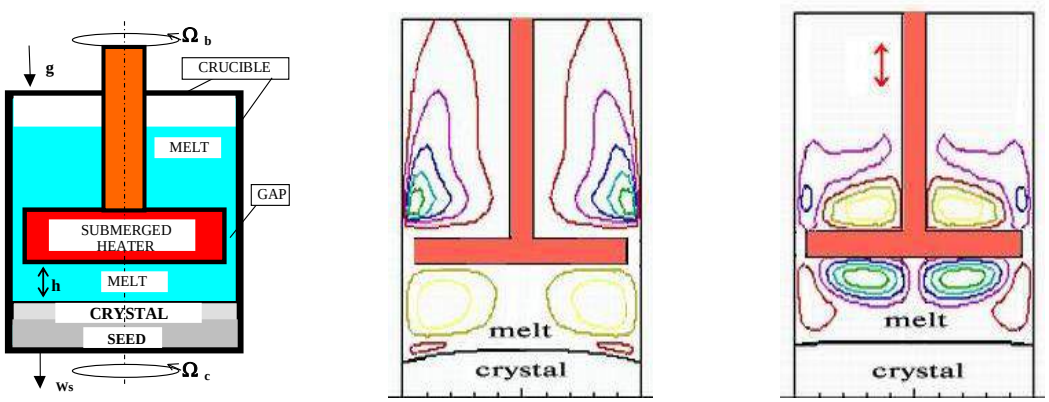
$$D_*^n = D + 0.5((u^n - u_g^n)^2 + (w^n - w_g^n)^2) * \Delta t^n$$

$$k_*^n = k + 0.5((u^n - u_g^n)^2 + (w^n - w_g^n)^2) * \Delta t^n$$

Auxiliary systems of algebraic equations for the nodal values of the desired functions were solved by the matrixless conjugate gradient method with preconditioning by using the diagonal approximation of the stiffness matrix (see [1]). Since the time difference scheme is implicit only for diffusion terms and uses physical processes splitting, it is stable under usual Courant restriction for time step. To calculate the motion of interphase boundaries, the A.A. Samarsky method of through counting was used [2]. In the numerical implementation, the delta function was approximated by the expression $\delta(\Phi) = H(1-|(\Phi)_i|/\Delta T_m))/(2.0\Delta T_m)$.

3. The calculation results

Figure 2 shows the simulation results of the hydrodynamics of the melt and heat transfer during the growth of gallium arsenide single crystals by the vertical Bridgman method with an immersed vibrator. The computational domain is shown in Figure 2a. The influence of vibrations on the shape of the crystallization front of NaNO3 are shown in Figures 2b, and 2c. Vibrations allow us to make the shape of the crystallization front more flat It was assumed that the immersed vibrator or crystal oscillates according to the law: with a frequency f and a small amplitude A. The vibration amplitudes were constant with values in the range from 0 to 400 μm, and the frequencies were in the range from 0 to 100 Hz.



a) b) c)

Fig. 2. *a) Solution area b) Crystallization front without vibrations, c) with vibrations.*

4. Conclusions

Comparison of the calculations with the test data showed good accuracy of the described algorithm for solving the Stefan problem. Using this method, the authors obtained the results of modeling the hydrodynamics of melt and heat transfer during the growth of gallium arsenide single crystals by the vertical Bridgman method with rotation.

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References

1. *Burago N. G., Nikitin I.S., Yakushev V. L.* Hybrid numerical method for unsteady problems of continuum mechanics using arbitrary moving adaptive overlap grids // Computational Mathematics and Mathematical Physics. 2016. Vol. 56. N.6. P. 1065-74. DOI: 10.7868/S0044466916060107.
2. *Burago N G, Nikitin I. S.* Matrix-Free Conjugate Gradient Implementation of Implicit Schemes // Computational Mathematics and Mathematical Physics. 2018. Vol. 58, No. 8, P. 1247-58. DOI: 10.1134/S0965542518080043
3. *Samarskii A. A., Moiseenko B. D.* An economic continuous calculation scheme for the Stefan multidimensional problem // USSR Comput. Math. Math. Phys. 1965. Vol. 5 (5). P. 43–58
4. *Davis de Vahl G., Jones I.P.* Natural convection in square cavity: A comparison exercise // Intern. J. Numer. Meth. Fluids. 1983. Vol.3. P.227.
5. *Wheeler A. A.* Four test problems for the numerical simulation of flow in Chochralski crystal growth // J. Crystal Growth, 1990. Vol. 99. P. 910.