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To cite this article: N G Burago and A I Fedyushkin 2021 *J. Phys.: Conf. Ser.* **1809** 012002

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Numerical solution of the Stefan problem

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Abstract. The paper describes an algorithm for solving the Stefan problem by the finite element method for modeling heat and mass transfer processes in a fluid with a phase transition. Modeling of heat and mass transfer is based on the solution of the Navier-Stokes equations for an incompressible fluid in the Boussinesq approximation and the heat conduction equation for a solid phase. The solution was made according to the explicit-implicit scheme of the matrixless finite element method 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 media, providing 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. The 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. An example of the application of the described finite element implementation of the Stefan problem for modeling of process for semiconductor single crystal growth by the Bridgman method taking into account the rotations of crystal, crucible and heater-vibrator is given.

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.

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2. Statement of the problem

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

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

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

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

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

where traditional notation is used. The problems were studied 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, μ, 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 Figure 1 where $R = 3.36 \text{ sm}$ - crucible radius, $\delta = 0.1 \text{ sm}$ - the size of the gap (3), $h = 0.8 \text{ sm}$, S_{SH} - area of immersed heater (1). $T_m = 937^\circ \text{ C}$ - 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:

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

2) on the wall of the crucible:

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

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

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:

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

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

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

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

time equations is implicit in diffusion terms, it is stable under the usual Courant condition for convection velocity $\Delta t^n \leq \min_k (h_k^n / \max(|u_k^n - w_k^n|, 1e^{-6}))$, 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

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

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 performed by calculating the well-known test problems of Val Davis [3] and Wheeler [4] on the melt flow in the Czochralski method. The unstructured moving grid was used to track the movement of the crystal – melt boundary. Grid nodes are numbered $(r_i, z_i, i = 1, \dots, n_1)$, the numbers of nodes forming three-node internal cells are determined $E(i, j)$ ($i = 1, \dots, n_2, j = 1, 2, 3$) and two-node boundary cells $G(i, j)$ ($i = 1, \dots, n_3, j = 1, 2$). 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.

The 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 the following equations were used:

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

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

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

The 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 ([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 $\delta(\Phi) = H(1 - |(\Phi)_i| / \Delta T_m) / (2.0 \Delta T_m)$.

4. The calculation results

Figure 1 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 1a. The influence of vibrations on the shape of the crystallization front of NaNO₃ are shown in Figures 1b, and 1c. Vibrations allow making 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.

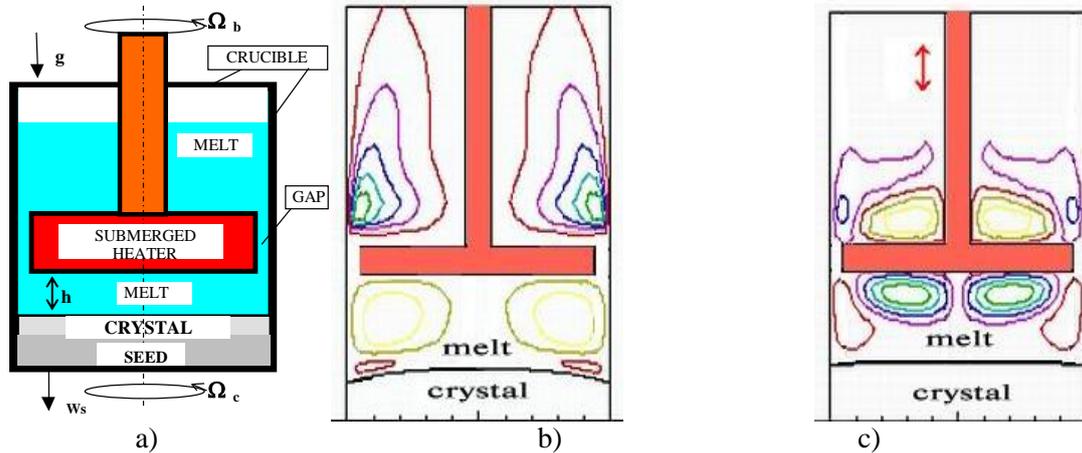


Fig. 1. a) Solution area b) Crystallization front without vibrations, c) with vibrations.

5. Conclusions

The 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.

6. Acknowledgements

The study was supported by the Government program (contracts # AAAA-A20-120011690132-4 and #AAAA-A20-120011690131-7) and was funded by RFBR, project number 20-04-60128.

7. References

- [1] Burago N G, Nikitin I S, Yakushev V L 2016 Hybrid numerical method for unsteady problems of continuum mechanics using arbitrary moving adaptive overlap grids *Computational Mathematics and Mathematical Physics* **56** (6) 1065-74 (ISSN print: 0044-4669) DOI: 10.7868/S0044466916060107.
- [2] Burago N G, Nikitin I S 2018 Matrix-Free Conjugate Gradient Implementation of Implicit Schemes *Computational Mathematics and Mathematical Physics* **58** (8) 1247–58 DOI: 10.1134/S0965542518080043
- [3] Samarskii A A, Moiseenko B D 1965 An economic continuous calculation scheme for the Stefan multidimensional problem *USSR Comput. Math. Math. Phys* **5** (5) 43–58
- [4] Davis de Vahl G, Jones I P 1983 Natural convection in square cavity: A comparison exercise *Intern. J. Numer. Meth. Fluids*. **3** 227
- [5] Wheeler A A 1990 Four test problems for the numerical simulation of flow in Chochralski crystal growth *J. Crystal Growth* **99** 910