MATHEMATICAL STUDY OF DOPANT DISTRIBUTION IN SUBMERGED HEATER CRYSTAL GROWTH IN MICROGRAVITY AND TERRESTRIAL ENVIRONMENT

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ABSTRACT

Present paper is devoted to numerical simulation of crystal growth by using submerged heater method (A. G. Ostrogorsky (1991), V. D. Golyshev and M. A. Gonik (1994)). Influence of thermo-mechanical parameters on Gallium dopant distribution in the Germanium melt and in Germanium crystal invrstigated. Modes of crystal growth, which provide almost homogeneous dopant distribution, are found in numerical experiment for terrestrial environment.

INTRODUCTION

A. Ostrogorsky and Z. Dragojlovic (1994) investigated the dopant distribution in melt in a frame of steady Navier-Stokes formulation. In most cases steady state does not take place during crystal growth. Therefore we use here unsteady Navier-Stokes formulation and determine dopant distribution not only in the melt but also in the crystal. Existence of almost optimal modes of crystal growth is found in numerical experiment.

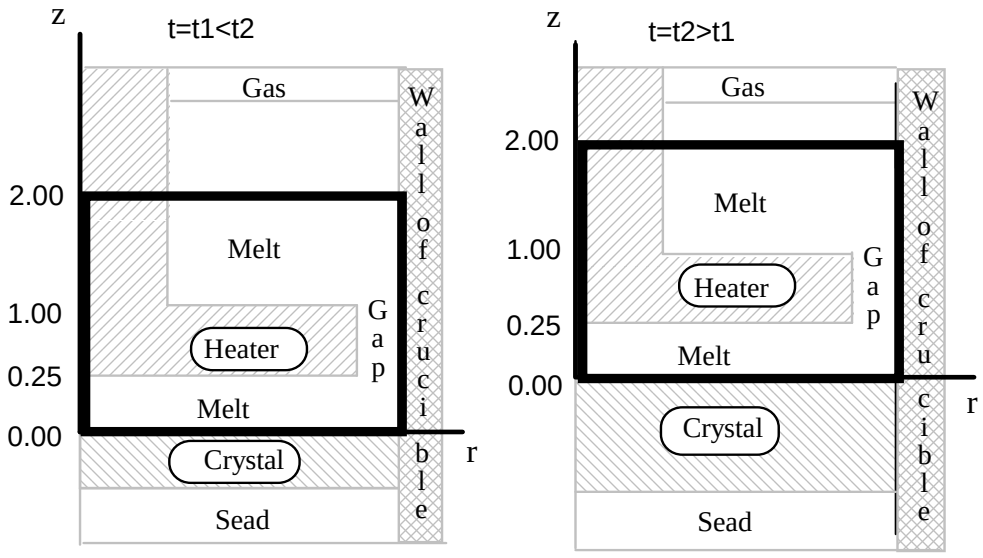

Fig. 1 Schematic of Bridgman crucible. Configuration is shown for two instants: t_1 and $t_2 > t_1$. Fat lines show moving computational domain. Dimensionless radius of the domain $r = 1.00$, size of gap $\delta = 0.015$.

FORMULATION OF PROBLEM

Solution domain is shown in Fig. 1. The problem is axisymmetrical, height of work zone between growth interface (z=0) and heater (z=0.25), growth rate and thermal boundary conditions are constant. Flow of the melt is subjected to the system of Navier-Stokes-Boussinesq equations which consists of continuity equation, of momentum equations for r, z directions, of heat transfer equation and of equation for dopant. Dimensionless equations read:

$$\frac{\partial u}{\partial r} + \frac{u}{r} + \frac{\partial w}{\partial z} = 0$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r} + w\frac{\partial u}{\partial z} + Ha^2 u = -\frac{\partial p}{\partial r} + Pr\left(\Delta u - \frac{u}{r^2}\right)$$

$$\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial r} + w\frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} + Pr\,\Delta w - Pr^2\left(Gr \cdot T + Gr_C \cdot C\right)$$

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial r} + w\frac{\partial T}{\partial z} = \Delta T$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial r} + w\frac{\partial C}{\partial z} = \frac{Pr}{Sc}\Delta C$$

where u, w - velocities, T - temperature, C - dopant concentration, p - pressure, Gr - Grashof number, Gr_C - solutal Grashof number, Pr - Prandtl number, Sc - Schmidt number, Ha - Hartman number, which represents given axial constant magnetic field. Boundary conditions read:

(i) axis of symmetry:

$$r = 0: \; u = 0, \; \frac{\partial w}{\partial r} = 0, \; \frac{\partial T}{\partial r} = 0, \; \frac{\partial C}{\partial r} = 0$$

((ii) side wall of crucible:

$$r = 1: \; u = 0, \; w = -V_s, \; \frac{\partial T}{\partial r} = 0 \;\; (0 \le z < 1), \;\; T = 1 \;\; (1 \le z \le 2), \;\; \frac{\partial C}{\partial r} = 0$$

(iii) top inlet boundary:

$$z = 2: \; u = 0, \; \frac{\partial w}{\partial z} = 0, \; T = 1, \; C = 1$$

(iiii) surface of heater (S_H):

$$(r, z) \in S_H: \; u = 0, \; w = 0, \; \left[\frac{\partial T}{\partial n}\right] = 0 \;\; (0.25 < z < 2.0), \; T = 0.7 + \frac{0.3r}{0.95} \;\; (z = 0.25), \; \frac{\partial C}{\partial n} = 0$$

(iiiii) growth interface:

$$z = 0: \; u = 0, \; w = -V_s, \; T = 0, \; \frac{Pr}{Sc}\frac{\partial C}{\partial z} = V_S C(1 - k)$$

Initial conditions read:

$$t = 0: \; u = 0, \; w = 0, \; T = T_m, \; C = C_{01} \;\; (0 \le z \le 1), \; C = C_{02} \;\; (1 \le z \le 2)$$

RESULTS

We used code ASTRA (N. G. Bourago (1994)). The code was tested on known test problems of Wheeler [1991] for diffusion-convection flow in a cavity. For grids 20x20 the error was not greater then 5%. Also we repeated calculations of steady state of submerged heater crystal growth (SHCG) and very good coincidence of our results with results of A. G. Ostrogorsky (1995) was established.
Then simulation of unsteady SHCG has been done.

The duration of crystal growth is about several hours, and during this time steady state does not take place. After several minutes the temperature field is stabilized (due to big value of temperature conductivity of the melt). Soon after in about 10-15 minutes the velocity field also becomes almost steady. But the concentration of dopant varies during hours due to segregation of dopant on growth interface and due to convection-diffusion flow in the melt. Following input data are used: $C_{01} = 1$; Results of parametric calculations are presented in Fig. 2 and in table 1, where N is a number of run; V_S - growth rate; $n = C_{01} / C_{02}$ - ratio of initial concentrations, C_{01} -initial dopant concentration below heater, C_{02} - initial dopant concentration above heater, $\mathrm{sign}(\partial_t C)$ - calculated sign of time derivative of dope concentration for $z = 0$ and $t = t_{max}$, ΔC - relative deflection of dopant concentration from its maximum for radial distribution and for maximal time.

The goal of the parametric calculations was to find conditions under which the distribution of dope on the solid-liquid interface becomes permanent while radial dope distribution stays so homogeneous as possible.

Case of absence of natural convection (run 1) does not lead to homogeneous distribution of dope because forced convection (a melt flow from region 2 through the gap δ into the region 4 caused by relative motion of crucible and heater) violates homogeneity of dope distribution near solid-liquid interface. Fortunately it is possible to find some optimal conditions of balance between natural and forced convection flows when they compensate each other and provide almost homogeneous distribution of dope in the crystal. These conditions depend on growth rate, on size of the gap δ, on thermal boundary conditions and on values of initial concentrations C_{01} and C_{02}. The influence of all mentioned conditions can be seen in Fig. 3 and in Table 1. In calculations almost optimal conditions have been found: they are represented by run 5.

Table 1

N	Gr/Gr_0	V_S cm/hour	n	sign(dC/dt) r=1, z=0, $t=t_{max}$	t_{max} hour	$\Delta C = (C_{max} - C_{min}) / C_{max}$
1	0.00	1.00	10.0	1	3.29	1,000
2	1.00	0.01	16.7	-1	8.20	0.005
3	1.00	10.0	16.7	-1	1.32	0.800
4	1.00	1.00	1.67	1	1.29	0.190
5	1.00	1.00	10.0	0	1.09	0.180
6	1.00	3.60	10.0	-1	1.16	0.550

CONCLUSION

The mode of submerged heater crystal growth which provides almost homogeneous dopant distribution in Ge crystals doped by Ga is found numerically for crucible of definite geometry and under defined thermal conditions by means of choice of growth rate and initial distribution of dopant concentration. At current stage of research it seems impossible to get the general answer on question how to get optimal modes of crystal growth for all cases of geometrical and physical conditions. But the use of numerical modeling in every particular case can help to find such modes and to improve the quality of growing crystals.

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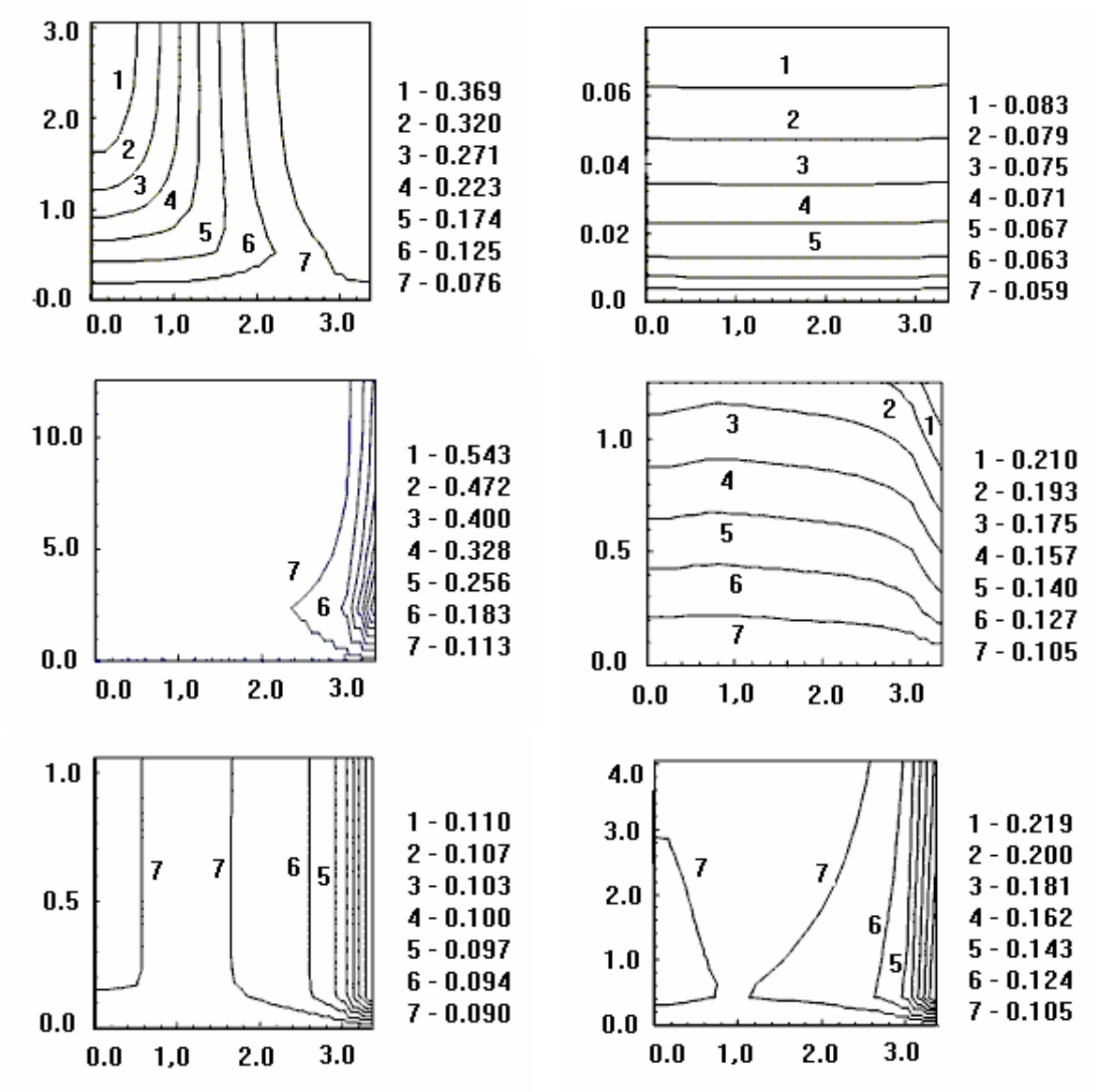

Fig. 2. Contours of dopant in the crystal.

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