INFLUENCE OF VIBRATIONS ON HEAT AND MASS TRANSFER DURING CRYSTAL GROWTH IN GROUND-BASED AND MICROGRAVITY ENVIRONMENTS

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ABSTRACT

The results of mathematical and physical modeling of heat and mass transfer in vibrating flows are presented for Bridgman crystal growth with submerged vibrator. The shadow system and computer processing of photographs is used to observe the melt motion in the experiments. Mathematical modeling is performed on the basis unsteady Navier-Stokes-Boussinesq equations for incompressible fluid. The finite element code ASTRA used for calculations. In numerical simulation the calculated instantaneous flows were averaged in time to evaluate averaged vibrational flow.
The numerical and experimental results illustrate the influence of the vibration and the crucible arrangement as well as the vibration amplitude/frequency on the averaged vibrational flow.

INTRODUCTION

In present paper the influence of the vibrations on the melt flow is considered for the vertical Bridgman crystal growth. The vibrations are initiated by the submerged vibrator. It should be mentioned that big variety of different kinds of vibrations exists [1]. The vibrations can be of the following types: 1) progressive (linear, circular, non-circular etc.); 2) rotational, (circular and non-circular); 3) swinging; 4) total volume vibrations and/or submerged body vibrations; 5) harmonic and non-harmonic; 6) low and high frequency vibration. We consider here only progressive vertical vibrations induced by the submerged body. The applied vibrations are assumed to be of small amplitude, therefore the vibrator displacements are negligible, and the velocity of the vibrator is predefined as a harmonic function $v = A\omega\sin(\omega t)$, where A - an amplitude, ω - a frequency. Some of results were calculated on the basis of the direct solution of the axisymmetrical unsteady Navier-Stokes-Boussinesq problem, some of the results were obtained in the physical experiments by using the laser shadow method. A lot of issues should be taken into account to get deep understanding of the mechanisms acting in the AVF. Here only some of them are in question. In particular the following features are under study here: influence of vibrations on boundary layers in melts with various Prandtl numbers; influence of frequency of the vibrations on the structure of the AVF; influence of the amplitude of the vibrations on the shape of the solid-liquid interface; influence of the arrangement of the vibrator and crucible on the AVF; and, finally, the influence of the rotation on the AVF. The presented results should be

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treated as preliminary and far not complete. We are just making first steps on the way to understanding the possible outcomes from using the vibrations as a handling tool in crystal growth production techniques.

STATEMENT OF THE PROBLEM

Numerical modelling was conducted on the basis of the unsteady axisymmetrical 2D Navier-Stokes-Boussinesq equations including the balance equations for heat and mass transfer:

$$\frac{\partial u}{\partial r}+\alpha\frac{u}{r}+\frac{\partial w}{\partial z}=0 \quad (1)$$

$$\frac{du}{dt}-\alpha\frac{v^2}{r}=-\frac{1}{\rho}\frac{\partial p}{\partial r}+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\nu\frac{\partial u}{\partial r}\right)+\frac{\partial}{\partial z}\left(\nu\frac{\partial u}{\partial z}\right)-\alpha\nu\frac{u}{r^2} \quad (2)$$

$$\frac{dw}{dt}=-\frac{1}{\rho}\frac{\partial p}{\partial z}+\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\nu\frac{\partial w}{\partial r}\right)+\frac{\partial}{\partial z}\left(\nu\frac{\partial w}{\partial z}\right)+g\beta(T-T_0) \quad (3)$$

$$\frac{dv}{dt}+\alpha\frac{uv}{r}=\alpha\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\nu\frac{\partial u}{\partial r}\right)+\frac{\partial}{\partial z}\left(\nu\frac{\partial u}{\partial z}\right)-\nu\frac{u}{r^2}\right] \quad (4)$$

$$\frac{d\rho c_p T}{dt}=\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha\lambda\frac{\partial T}{\partial r}\right)+\frac{\partial}{\partial z}\left(\lambda\frac{\partial T}{\partial z}\right) \quad (5)$$

$$\frac{dC}{dt}=\frac{1}{r^\alpha}\frac{\partial}{\partial r}\left(r^\alpha D\frac{\partial C}{\partial r}\right)+\frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z}\right) \quad (6)$$

Here and farther the following notation is used: r and z - radial and axial coordinates, t - time, u and w - velocity vector components in r and z directions, v - azimutal velocity, T - a temperature, C - a dopant concentration, p - a pressure, ρ - a density, g - gravity acceleration, β_T, ν, λ, c_p, D - coefficients of thermal expansion, kinematic viscosity, heat conductivity, heat capacity and dopant diffusivity, α - a geometry factor, which is equal to 0 for flat geometry and to 1 for axisymmetrical problems, A and ω - an amplitude and a frequency of vibrations, Ω - an angle velocity of rotating crucible, a - thermal conductivity coefficient, W_S - rate of the crystal growth, ΔT - a temperature scale, k_0 -dopant segregation factor, **n** - normal unity vector.

The boundary conditions read:

axis of symmetry ($r=0$): $u=0$, $\frac{\partial w}{\partial r}=0$, $v=0$, $\frac{\partial T}{\partial r}=0$, $\frac{\partial C}{\partial r}=0$; (7)

solid-liquid interface $z=0$: $u=0$, $w=-W_S$, $v=2\pi r\Omega_C$, $T=T_m$, $D\frac{\partial C}{\partial z}=W_S C(1-k_0)$; (8)

side wall of crucible $r=R$: $u=0$, $w=0$, $v=2\pi R\Omega_C$, (9)

$\frac{\partial T}{\partial r}=0$ $(0<z<h)$, $T=T_h$ $(h<z<H)$, $\frac{\partial C}{\partial r}=0$; (10)

vibrator: $u = 0,\ w = A\ \omega \sin(\omega t),\ v = 2\pi r\Omega_{vibr},\ \frac{\partial C}{\partial n} = 0,\ \frac{\partial T}{\partial n} = 0$ (11)

upper opened boundary ($z = H$): $u = 0,\ \frac{\partial w}{\partial z} = 0,\ v = 0, T = T_h,\ C = C_0$ (12)

Initial conditions t=0 : $u = 0,\ w = 0,\ v = 0,\ T = T_m,\ C = C_0$ (13)

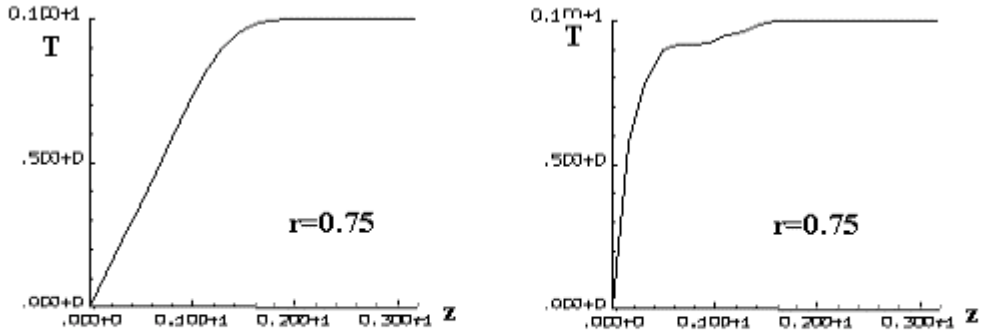
All calculations were conducted for the initial temperature field, which corresponds to the thermal regimes with temperature boundary conditions pointed above. The crystal growth rate was the same in all runs: W_S = 0.3 sm/h and the amplitude of vibrations was constant A=100mm. The problem is characterized by the following similarity numbers: rotational Reynolds number $Re_\Omega = \Omega_C R^2/\nu$, Reynolds number $Re = W_S R/\nu$, vibrational Reynolds number $Re_{vibr} = A\omega R/\nu$, Grashof number $Gr = g\beta\Delta T R^3/\nu^2$, (or Rayleigh number Ra = GrPr), Prandtl number $Pr = \nu\rho c_p/\lambda$ and Schmidt number $Sc = \nu/D$.

NUMERICAL AND EXPERIMENTAL RESULTS

The initial boundary value problem (1-13) was solved by the finite element method by using the code ASTRA" [5,6].

It is known [1], that under effect of vibrations depending on the time scale two types of the flow can be selected: instantaneous vibrational flow and averaged vibrational flow (AVF). These flows can lead to significant additional mixing and redistribution of the temperature [1-3] and dopant.

1. Influence of vibrations on boundary layers



a) b)

Fig. 1 Vertical profile of the temperature for follow different cases:
a)without vibration (f=0 Hz, Gr= 2 10^6,Pr =5.43)
b) with vibration (f=50 Hz, Gr= 2 10^6, Pr = 5.43)

Fig.1 shows the calculated vertical temperature profiles (r=0.75) for the following four cases: a) - thermal convection without vibrations (Fig.1a), b) - thermal convection with vibrations under high Prandtl number (Fig. 1b, g/g_o =1, Pr=5.43), c) - vibrational flow without thermal convection (Fig. 1c, g/g_o =0, Pr=5.43), d) - thermal convection with vibrations under low Prandtl number (Fig. 1d, g/g_o =1, Pr=0.01). These results show that the vibrations strongly decrease the thickness of the temperature boundary layers (Fig. 1a and Fig. 1b). The results show that the influence of the

vibrations on the temperature in terrestrial and microgravity environment is practically the same, i.e. the effects of the vibrations and the gravity are practically independent. Of course, the influence of the vibrations on the temperature field depends on the amplitude and the frequency of the vibrations, on the heat conductivity and the viscosity (on the Prandtl numbers).

2. Influence of Prandtl number

The temperature field in case for Pr=0.01 as well as in the case of microgravity is not practically changed by the vibrations. In such a case of low Prandtl numbers the vibrations of increased amplitude and frequency should be applied to get the effect of thin boundary layers.

3. Influence of frequency

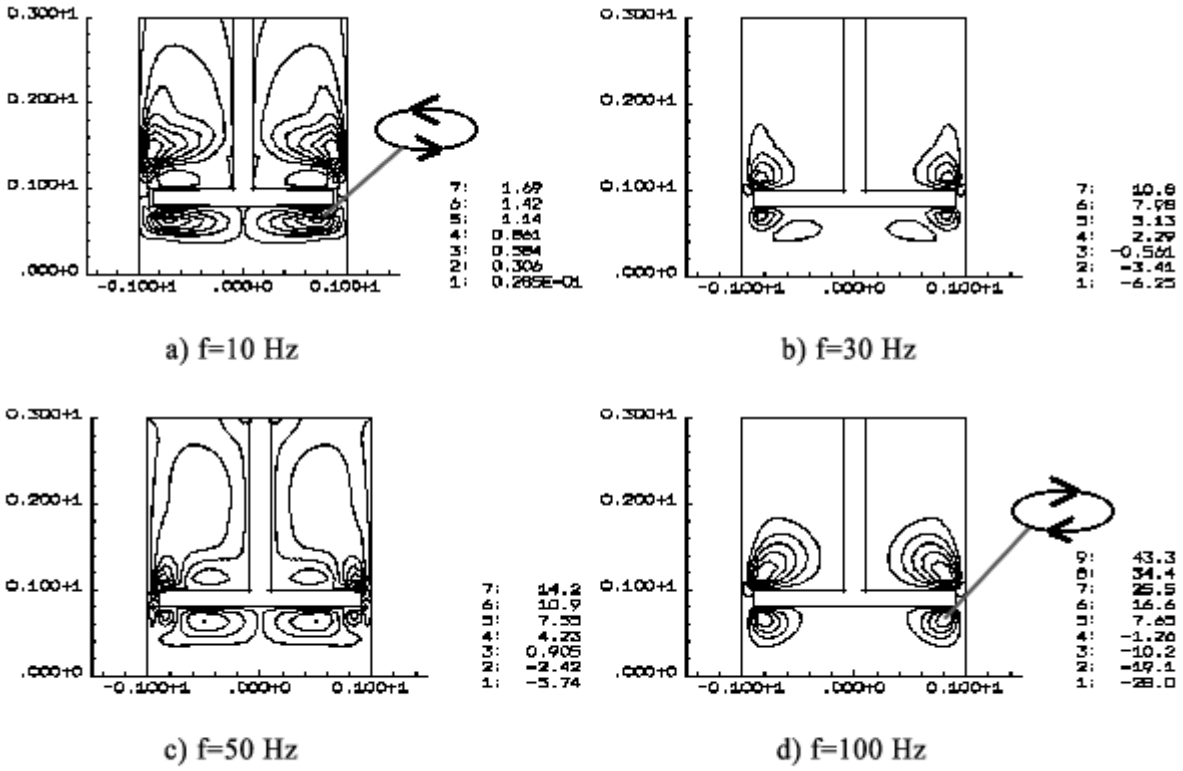


Fig. 2. Influence of frequency of vibrations on average vibrational flow (AVF) (A=100μm, Gr=2 10^6, Pr=5.43)

Some special feature of the influence of the frequency on the AVF was detected in calculations: with increase of frequency the AVF can change its direction. It is shown in Fig. 2, which presents The AVF stream function isolines for four values of the frequency: a) f=10 Hz, b) f=30 Hz, c) f=50Hz and d) f=100 Hz. With increase of the frequency (vibrational Reynolds number Re_{vibr}) from f=10 Hz up to f=100 Hz the intensity of the AVF also grows, while the AVF direction is changing due to exchange of momentum between vortexes. The direction of the AVF is changing from clockwise at f=10 Hz (Fig. 2a) to anticlockwise at f=100 Hz (Fig. 2d) (negative values of the AVF stream function correspond to the clockwise flow). The fight between the convective and vibrational vortexes can be observed. Under the vibrator the thermal convective flow has anticlockwise direction, while the AVF has opposite direction. It can be expected that this fight can essentially effect the dopant distribution and the shape of the solid-liquid interface.

4. Influence of amplitude on shape of solid-liquid interface

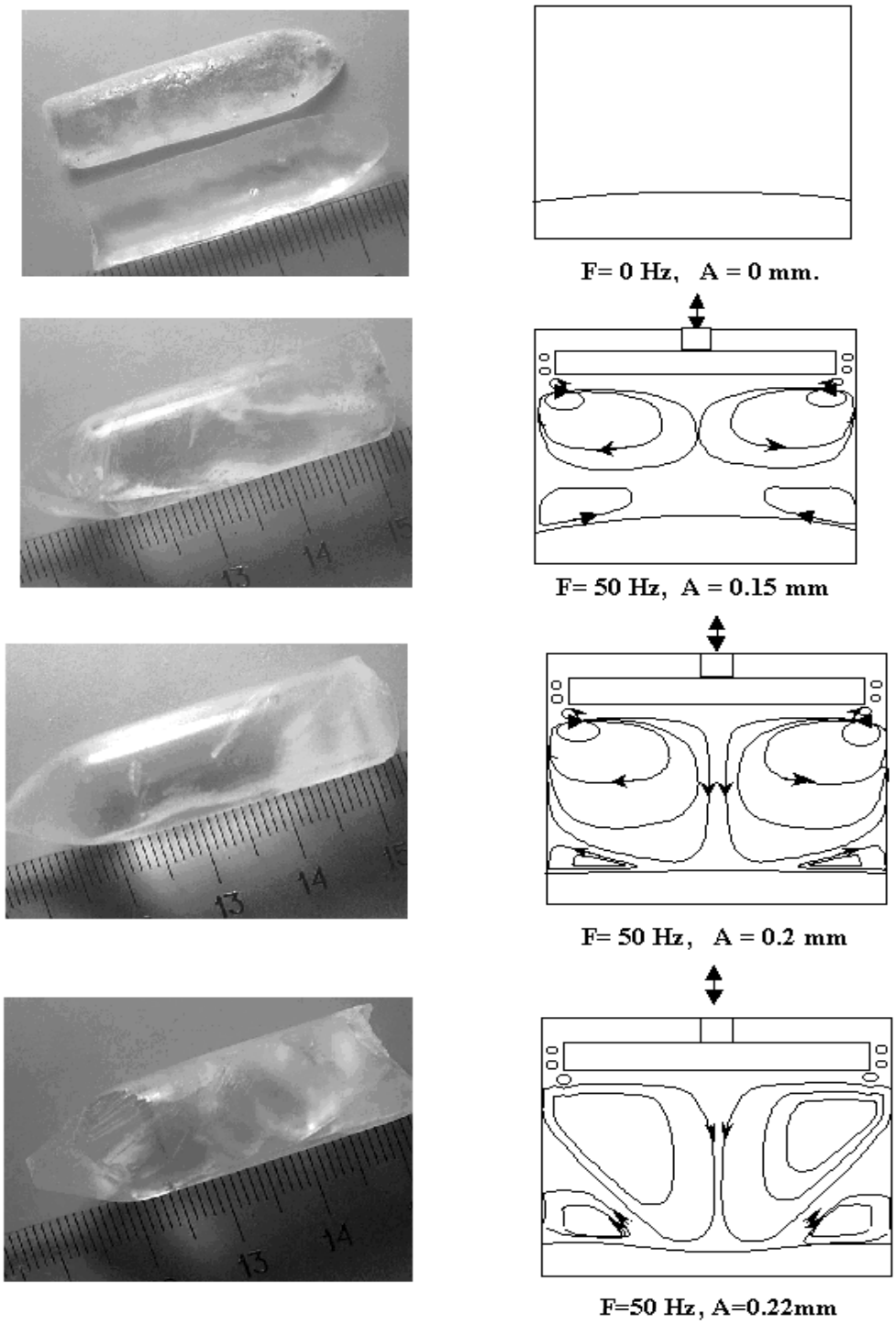


Fig.3 Images of Ag:$NaNO_3$ single crystals grown under vibrattions and corresponding flow patterns in the melt and shape of solid-liquid interface (experemental data)

The influence of the amplitude on the shape of the solid-liquid interface is shown in Fig. 3. These data were obtained experimentally by the group of Prof. E.V.Zharikov. The left-hand side of the

Fig. 3 shows the photographs of the grown crystals, the right hand side shows the melt flow, observed in the experiment. The vertical progressive harmonic vibrations had a frequency 50Hz and amplitudes in the interval of 0.18-0.22 mm. By varying the amplitude it is possible to effect the curvature of the solid-liquid interface. This fact looks quite promising.

5. Influence of vibrator geometry on the AVF

Due to variety of possible arrangements of the crucible and the vibrator it is difficult to provide the systematic study of the influence of the geometry on the AVF, Nevertheless some particular selected cases were calculated. The results can be seen in Fig. 4, 5.

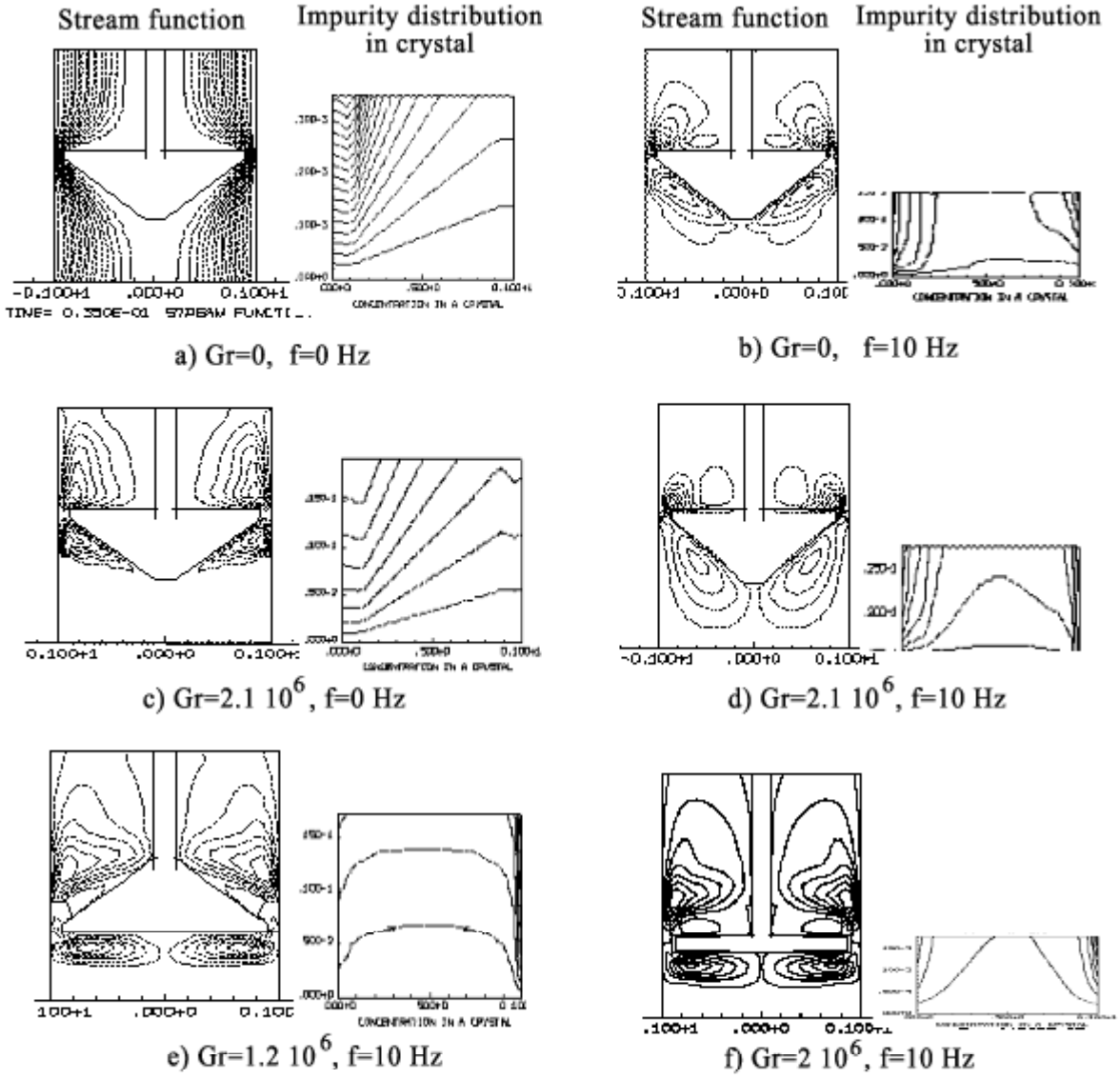
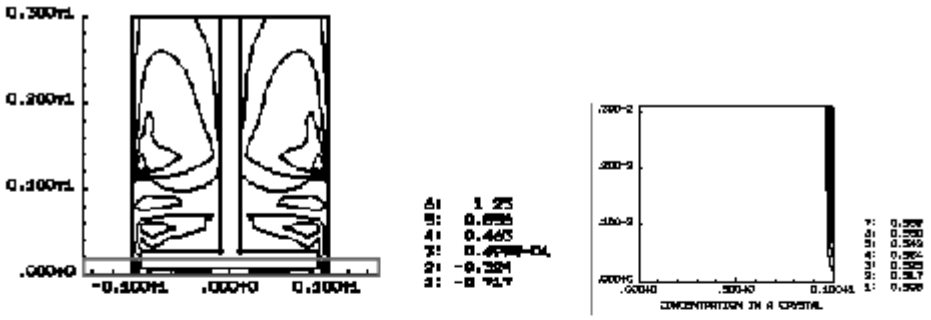


Fig.4 Stream function of AVF and impurity distribution in crystal
(A=100 μm, Pr=5.43, Sc=500)

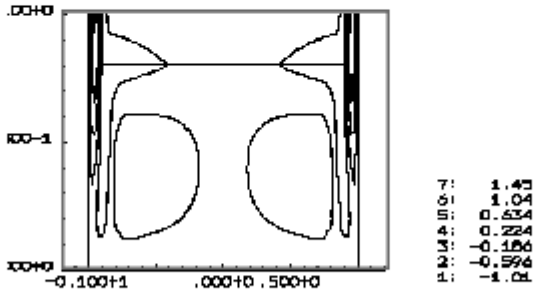
In Fig. 4a-d the isolines of the AVF stream function in the melt and the dopant isolines in the crystal are presented for a nabla-shaped vibrator, in Fig. 4e - for a delta-shaped vibrator and in

Fig. 4e, 5 - for the traditional shape vibrator and various distances between the vibrator and the solid-liquid interface.
It is seen from Fig. 4a-d that in these cases if the vibrations and the thermal convection are absent (i.e. no gravity applied) the dopant distribution in the crystal is inhomogeneous on radial direction. The separated from each other effects of the vibrations (Fig. 4b) and the thermal convection (Fig. 4c) and also their interaction are illustrated in Fig. 4d.
These pictures show also the calculated dopant distributions in the crystal. The conclusion follows that in these cases the thermal convection is weak and its influence on the dopant distribution in presence of the vibrations is negligible. The leading factor, which mainly effects the dopant distribution, is the vibration. Analogical conclusion concerning the role of the vibrations in the temperature distribution was made in [1,2].
The structure of the AVF and the dopant distribution in the crystal for the delta-shaped vibrator are presented in Fig. 4e. In this case the AVF is almost the same as in the case of the nabla - shaped vibrator (see Fig. 4e).



a) Stream function

c) Isolines of concentration in the crystal (Sc=500)

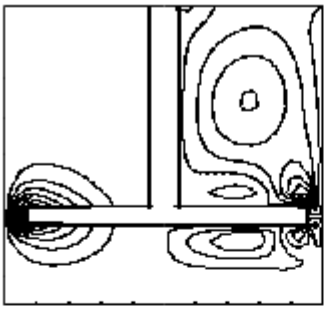


b) Stream function (in the bottom part of area, under the vibrator)

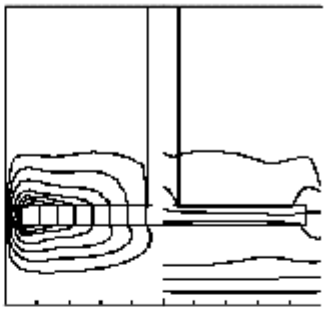
Fig.5 Vibration and natural convection.
Vibrator located close to front of crystallization
(A=100 μm, f=10 Hz Gr=2 10^6 , Pr=5.43)

The Fig. 5 shows the AVF flow structure for the case of small distance between the traditionally shaped vibrator and the melt-crystal interface. It is seen, that in this case the AVF consists of two vortices, situated horizontally (Fig. 5b). Therefore the effectivity of radial dopant spreading goes down in this case (Fig. 5c). The inhomogeneuity concentrates near side walls of the crucible and the most of the crystal becomes homogeneous.

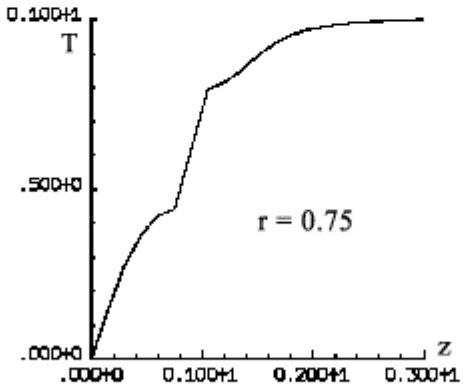
6. Influence of rotation on the AVF



a) On the left - stream function,
on the right - stream function of AVF



b) On the left - azimutal velocity,
on the right - temperature



c) profile of the temperature (r=0.75)

Fig.6 Vibration and rotation
(A=100μm, f=50hz, Ω=9rpm, Gr=2 10^6, Pr=5.43)

Joint action of vibrations and the rotation of the baffle can be seen in Fig. 6. The results are presented for used in practice rotation frequency ω=9rpm and for vibration frequency f = 50 Hz. The following graphs are demonstrated: the stream function (Fig. 6a), azimutal velocity (left part, Fig, 6b), temperature (right part, Fig. 6b) and the vertical temperature profile along the line r=0.75. The influence of the rotation on the AVF is weak in this case (compare with profile in Fig. 1b), because of the difference in time scales for vibration and rotation-induced flows and small values of rotational Reynolds number. But it should be mentioned that the rotation levels the radial temperature distribution.

CONCLUSIONS

The vibrations can decrease the thickness of the boundary layers at the solid-liquid interface and it is of principle importance for the crystal growth. It is shown that by applying the vibrations the temperature gradient near the solid-liquid interface can be changed as well as the crystal growth

rate and the flow direction. It is found that these effects take place in both terrestrial and microgravity environment.

The study shows that the vibrations can be used as a simple and effective governing tool (more simple to apply than microgravity, rotation or magnetic field), to improve the conditions of crystal growth and the quality of the final product.

REFERENCES

1. G.Z.Gershuni and D.V.Lubimov, (1998). Termal vibrational convection. John Willey&Sons Ltd., 357p.
2. A.I. Fedyushkin, N.G. Bourago, (2001) Influence of vibrations on boundary layers in Bridgman crystal growth. Procidings of 2nd Pan Pacific Basin Workshop on Microgravity Sciences 2001, paper CG-1073.
3. A.I. Fedyushkin, N.G. Bourago, (2001) Influence of vibrations on Marangoni convection and melt mixing in Czochralski crystal growth. Procidings of 2nd Pan Pacific Basin Workshop on Microgravity Sciences 2001, paper CG-1072.
4. N. G. Bourago and V. N. Kukudzhanov, (1988) Numerical Simulation of Elastic Plastic Media by Finite Element Method, Pre-print IPMech AS USSR, N.326, 1988, pp. 1-63;
   Second edition in book "Computer Mechanics of Solids", issue 2, Nauka, 1991, pp. 78-122.
5. N.G.Bourago, (1994) Numerical methods for non-linear processes in elastic plastic media. in “Lectures of FEM-94 Seminar”, Chalmers Univ. of Technology,Gothenburg, pp. 1-15.
6. N.G.Bourago, A.I.Fedyushkin, V.I.Polezhaev, (1997) Modelling of unsteady submerged heating crystal growth in ground-based and microgravity environment. Physical sciences in microgravity. Proceedings of joint Xth European and VIth Russian Symposium on Physical sciences in microgravity. St. Peterburg, Russia, 15-21 June 1997 , vol. II, pp.170-173.
7. A.I.Fedyushkin, N.G. Bourago, (1999) Impurity distribution in submerged heater method with and without rotation. Proceedings of the Int.Conf. on Computational Heat and Mass Transfer.April 26-29, 1999, N.Cyprus, Turkey, pp. 207-215.