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PROCEDURE FOR CHOOSING MODEL MEDIA FOR MELTED SEMICONDUCTORS UNDER TERRESTRIAL AND OUTER-SPACE CONDITIONS

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Based on the similarity theory, a complete set of dimensionless parameters was found, which would allow one to choose the geometry, temperature, and other conditions leading to similarity between hydrodynamic phenomena in melted semiconductors and model media. Direct calculations performed by the Oberbeck–Boussinesq system of equations validate our theoretical approach to the problem of choosing model media for various liquids and different gravity conditions.

Introduction. The growth of single-crystal materials with desired electrical and other properties is a complex technological problem. Normally, melted semiconductors are low-viscous liquids with high surface tension, which is responsible for their extreme sensitivity to various disturbing factors. The use of shock-mounted platforms and suspensions substantially decreases the level and frequency of external disturbances penetrating into the melt. However, low-frequency modes or small components of mass forces directed along the crystallization front and caused, for instance, by the nonvertical position of the setup may result in appreciable shear flows near the growing surface of the crystal. The presence of a free surface of the melt and the occurrence of temperature gradients in it produce an intense source of disturbances whose detrimental action is very difficult to avoid, especially under the conditions of space environment. Since crystallization normally proceeds at high temperatures in vacuum and the melts are nontransparent for radiation, the diagnostics of processes in melted semiconductors is extremely difficult. One can study the processes in melts solely by studying the grown crystals, which seriously worsens the quality of information. Therefore, the solution of the problem of the proper choice of model media in which hydrodynamic processes are similar to those in melted semiconductors may prove useful for solving the technological problem of obtaining materials with desired properties.

1. Mathematical Model and Dimensional Analysis. The processes in melted semiconductors are usually described by the system of the Oberbeck–Boussinesq equations [1]. A mathematical model for thermogravity flows with allowance for impurity transfer and thermocapillary convection for two-dimensional unsteady problems has been developed and tested on various types of flow [2]. The traditional method of nondimensionalization with respect to a velocity U and the diameter of the flow region (characteristic length) L yields the following similarity parameters [2]:

$$\mathrm{Gr} = \frac{g\beta L^3}{\nu^2}\,\Delta\theta, \qquad \mathrm{Re} = \frac{UL}{\nu}, \quad \mathrm{Fr} = \frac{U^2}{gL}, \qquad \mathrm{We} = \frac{\rho_0 U^2 L}{\sigma_0},$$
$$\mathrm{Mn} = \frac{\sigma_0 k_\sigma L}{\rho_0 \nu^2}\,\Delta\theta, \qquad \mathrm{Pr} = \frac{\nu}{k_\theta}, \qquad \mathrm{Sc} = \frac{\nu}{k_C}, \tag{1}$$

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Here Gr, Re, Fr, We, Mn, Pr, and Sc are the Grashof, Reynolds, Froude, Weber, Marangoni, Prandtl, and Schmidt numbers, respectively, ρ_0 is the density, ν is the kinematic viscosity, σ_0 is the surface tension, β is the thermal expansion, k_θ is the thermal diffusivity, k_C is the diffusivity, k_σ is a constant, g is the free-fall acceleration, and $\Delta\theta$ is the characteristic temperature difference. The surface tension σ is assumed to depend linearly on the temperature θ: $\sigma = \sigma_0(1 + k_\sigma(\theta - \theta_0))$.

A great number of parameters in (1), their nonlinear dependence on input constants, and the nonlinearity of fluid-dynamic equations hinder the effective prediction of crystallization parameters. The problem of a proper choice of similar media for which the numbers in (1) are almost identical is practically insoluble [3]. However, if we use

$$L = (\sigma_0/(g\rho_0))^{1/2} = \delta_\sigma, \quad U = (\sigma_0 g/\rho_0)^{1/4} \quad (t = (L/U)t' = (\delta_\sigma/g)^{1/2}t') \tag{2}$$

as L and U, the equations of motion and the boundary conditions acquire the following form:

$$\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{V}\nabla\boldsymbol{V} = -\nabla(P + z) - \mathrm{Gr}_g\theta\boldsymbol{n}_z + \mathrm{Re}_g^{-1}\Delta\boldsymbol{V}, \quad \operatorname{div}\boldsymbol{V} = 0; \tag{3}$$

$$\frac{\partial \theta}{\partial t} + \boldsymbol{V}\nabla\theta = \frac{1}{\mathrm{Re}_g\mathrm{Pr}}\Delta\theta; \tag{4}$$

$$\frac{\partial C}{\partial t} + \boldsymbol{V}\nabla C = \frac{1}{\mathrm{Re}_g\mathrm{Sc}}\Delta C; \tag{5}$$

$$P - \frac{2}{\mathrm{Re}_g}\boldsymbol{n}\cdot D\cdot\boldsymbol{n} = H + P_a; \tag{6}$$

$$2\boldsymbol{\tau}\cdot D\cdot\boldsymbol{n} = \mathrm{Mn}_g\mathrm{Re}_g\nabla_f\theta. \tag{7}$$

Here t is time, $\boldsymbol{V}$ is the velocity vector, P is the pressure, θ is the temperature, C is the concentration, $\boldsymbol{n}_z$ is the unit vector directed against the gravity force, $\boldsymbol{\tau}$ and $\boldsymbol{n}$ are the vectors normal and tangent to the free surface, D is the deformation rate tensor, H is the curvature of the free surface, P_a = const is the pressure at the free surface, and ∇_f is the gradient along it. All other boundary conditions are assumed to be specified.

From (2), it follows that the Froude and Weber numbers equal unity, and the Prandtl and Schmidt numbers remain unchanged. The other dimensionless parameters are

$$\mathrm{Re}_g = \Big(\frac{\sigma_0^3}{\rho_0^3 g\nu^4}\Big)^{1/4} = \mathrm{M}^{-1/4}, \qquad \mathrm{Gr}_g = \beta\Delta\theta, \qquad \mathrm{Mn}_g = k_\sigma\Delta\theta. \tag{8}$$

Here $\mathrm{M} = \rho_0^3\nu^4 g/\sigma_0^3$ is the Morton number [5].

Involvement of g in characteristic parameters (2) results in the fact that the quantity g enters only Re_g in combination with physical constants of the medium. The parameter Re_g enters Eqs. (3)–(5) in the same manner as the Reynolds number enters the initial equations (it is a coefficient at higher derivatives). This allows one to gain a better insight into the behavior of general solutions of the equations as g varies. The simple structure of other parameters permits easy classification of similar physical phenomena. For two phenomena to be similar, it is necessary and sufficient that the numerical values of all dimensional parameters be equal [3]. From (3)–(7), it follows that it is necessary and sufficient for the above that the Re_g, Gr_g, Mn_g, Pr, and Sc numbers for the two media be equal [with the correspondence between the characteristic flow parameters of each medium given by (2)].

2. Numerical Modeling. The calculations were performed using the COMGA computer code [6]. The equations of motion were solved to yield the stream and vorticity functions in the dimensional form. The nondimensionalization, estimation of the dimensionless parameters, and comparison between the solutions for different media were performed immediately after the numerical solutions were found. The accuracy of the calculations was tested on model problems by calculating on a sequence of meshes with increasingly refined mesh widths. From the experimental data, a mesh with about 8000 nodal points equally spaced over the coordinate axes was chosen. This mesh enabled us to model flows with a Reynolds number as high as 1000. The numerical solutions were compared by matching the flow patterns obtained (stream function and temperature isolines) and the highest and lowest values of the stream function.

TABLE 1

No.	Medium	T, °C	ρ, g/cm^3	ν, cm^2/sec	σ, dyn/cm	Pr	M
1	Water	20	1.00	0.01	72.8	7.1	$2.54 \cdot 10^{-11}$
2	Gallium antimonide (GaSb)	712	6.03	0.0038	454	0.05	$4.80 \cdot 10^{-13}$
3	Water	80	0.97	0.0033	62.6	2.2	$4.32 \cdot 10^{-13}$
4	Germanium	937	5.51	0.001 35	600	0.017	$2.52 \cdot 10^{-15}$

In modeling the initial medium, we used physical parameters of two melted semiconductors, germanium doped with gallium and gallium antimonide doped with tellurium (see Table 1, medium Nos. 2 and 4). These are typical semiconductors widely used in experiments on single-crystal growth. The adopted geometry of the melted region and the boundary conditions were similar to those in the Bridgman method with heating from above. The bottom flat and side cylindrical surfaces were assumed to be rigid, and the attachment conditions for velocity were adopted there. The upper free surface was assumed to be flat. The bottom surface is isothermal, and a linear temperature gradient along the vertical direction was set at the side surface. The temperature difference along the vertical axis of symmetry is 150°C, which is in line with available experimental data on crystal growth [7]. At the free surface, the temperature distribution was assumed to be linear along the radius with a temperature difference of 1°C.

3. Choosing Model Physical Media. Only temperature-related problems are considered below. In this case, for two media to be similar, the equality between Re_g, Gr_g, Mn_g, and Pr in two media is necessary and sufficient. For simplicity, the thermal conductivity of the model medium is set such that the Prandtl numbers of the media are equal to each other. The equality between the Re_g numbers of two similar media can be most easily attained by a proper choice of g in the model medium for given physical constants. Equal values of Gr_g can be obtained by setting the temperature difference for the model medium. Finally, the temperature difference already chosen, the equality between the Mn_g numbers is possible only for a certain value of k_σ of the model medium.

Since two temperature gradients, radial and vertical, are involved in the problem of interest, it is required to decide which of them is of greater importance and, hence, should enter relations (8). The radial temperature gradient depends on the side heating, which gives rise to natural convection in the melt. Upon heating from above, the vertical temperature gradient may affect the flow structure [8]; however, in the absence of a radial temperature gradient, it cannot bring the liquid into motion (steady stratification). Therefore, it is the radial temperature difference that should enter (8), and the equality of the Gr_g numbers implies a certain radial temperature difference to be chosen for the model medium. The vertical difference in temperature can be found from similar reasoning. Thus, an optimal sequence for choosing the external parameters of the problem is established, which results in equal dimensionless parameters (8) of the initial and model media. It remains to find the geometric dimensions of the model medium. We use the Laplace capillary constant as a characteristic length. We find its magnitude for the model medium from the known value of g. From here, with due allowance for the ratio of geometric dimensions of the flow of the initial medium to its capillary constant, the desired characteristic length for the model medium can be easily found.

3.1. *Similarity between Flows at a Large Difference in the Morton Numbers for the Initial and Model Media.* As an example, we consider water as a model medium (see Table 1, medium No. 1). The physical characteristics of the media listed in this table are approximate data and may differ from the values given in reference sources. For $g = 0.097$ cm/sec^2, the M number for water equals the M number for germanium.

We consider a region of radius 1.1 cm and height 1.0 cm, which is filled by a germanium melt. From (2), it follows that $U = 18.07$ cm/sec and $L = 0.333$ cm for germanium. From the found g, with allowance for (2), we obtain $U = 1.63$ cm/sec and $L = 27.39$ cm for water. Then, the height and the radius of the region for water are 82 and 90 cm, respectively.

We determine now the temperature differences for the model medium. Since $\beta = 0.0002$ and 0.0001 for water and germanium, respectively, the temperature differences along the radial and vertical directions are 0.5 and 75°C.

The equality between the Mn_g numbers for the chosen temperature differences is reached at $k_\sigma =$ 0.000333 for the model medium and 0.000166 for the initial medium. Thus, the desired physical, geometric, and temperature parameters for the model medium are found. For the two chosen media and corresponding boundary conditions, two modeling series were performed, which allowed us to establish the steady-state flow patterns. The most intensive flow initiated by thermocapillary convection is observed at the free surface, where the maximum velocity reaches 0.5845 cm/sec. The liquid flow on the free surface is transferred inside the melt and forms a vortex flow under the free surface. Natural convection from a more heated side wall brings the entire melt into motion, with ascent of the melt near the more heated wall and its descent at the axis. These two sources of motion give rise to a three-vortex flow structure with decreasing intensity in the downward direction. The highest and lowest values of the stream function throughout the entire region are 0.003 and -0.01999 cm^3/sec, respectively, and the minimum value of the stream function in the third vortex is -0.00006 cm^3/sec.

The temperature pattern in the melt is stratified into several layers. Normally, melted semiconductors possess high thermal conductivity; therefore, the temperature profiles level off rapidly. In the steady-state pattern, the temperature distribution is practically linear along the vertical axis (the heat here is transferred by diffusion).

In the calculation for the model medium, a similar flow structure and a similar distribution of temperature isolines were obtained. The highest velocity in the melt at the free surface was 0.05166 cm/sec. The highest and lowest values of the stream function in the melt were 1.6137 and -11.1081 cm^3/sec.

The ratio of the minimum and maximum values of the stream function equals 6.66 and 6.88 (absolute values) for germanium and for the model medium, respectively (the difference is within 3%). The access of the minimum values of the stream function nondimensionalized using Eq. (2) yields -0.0099 and -0.0091, respectively (the difference is less than 9%). The Reynolds, Weber, and Froude numbers calculated from the maximum velocity at the free surface and from the characteristic length are 476, 0.0034, and 0.000317, respectively, for the initial medium and 465, 0.0033, and 0.000306, respectively, for the model medium. Taking into account that $Gr = Re^2 Gr_g / Fr$, we establish that the Grashof numbers for the flows under study are identical within 1%. A comparison between the data obtained shows that the dimensionless parameters in this case differ by no more than 3%, the flow structures being identical. Thus, these flows are similar. An analysis of the differences found indicates the necessity to more accurately calculate M for the two media, g, and the characteristic length for the model medium.

The adopted approach allows one to study the behavior of melted semiconductors in terrestrial conditions using a model liquid in the outer space with required values of M and Pr and necessary geometric and temperature parameters. To model the behavior of melts in the outer space by a model liquid on the Earth, one should take a liquid with the Morton number of order 10^{-18} under terrestrial conditions.

3.2. *Similarity between Flows with Close Morton Numbers of the Media.* We consider now medium Nos. 2 and 3 (see Table 1). From the physical viewpoint, these are different media, but the difference in M numbers is only about 10%. Since the Prandtl numbers of the media differ, we set, as we did in Sec. 3.1, the thermal conductivity of medium No. 3 such that the Prandtl numbers of the two media become equal ($Pr = 0.05$). Let medium No. 3 be the initial medium now. The region occupied by the liquid is a cylinder of radius 1.1 cm and height 1.4 cm. Again, the upper surface is assumed to be open and flat. The radial temperature difference across the surface is 1°C, whereas the vertical temperature difference at the axis is 75°C. Thus, under the action of the Marangoni convection and natural convection from the heated wall, a flow develops in the liquid whose steady-state pattern obtained by numerical simulation is shown in Fig. 1. Downward from the free surface, four vortex structures with decreasing intensity are seen. The local extrema of the stream function for them are -0.067, 0.0088, -0.00027, and 0.00015 cm^3/sec, respectively ($Pr = 0.05$). The highest velocity (2.197 cm/sec) is observed at the free surface. Thus, the Reynolds, Weber, and Froude numbers are 732, 0.0823, and 44.77, respectively, and the Grashof number is $8.025 \cdot 10^4$.

The M number for medium No. 2 equals the M number for medium No. 3 at $g = 882$ cm/sec^2. With

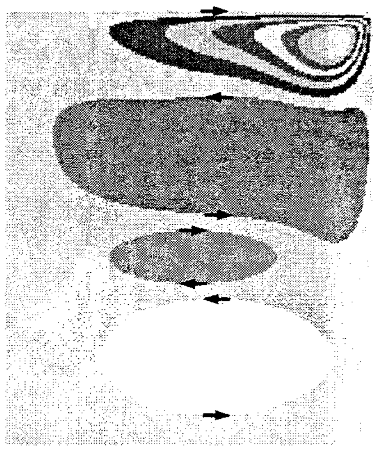

Fig. 1

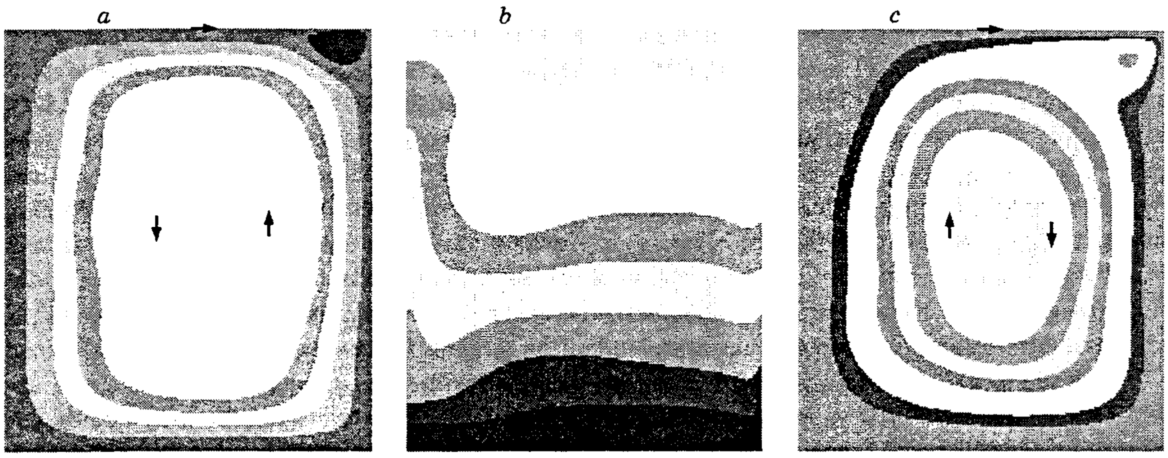

Fig. 2

account of (2), the radius and height of the melted region should be 1.25 and 1.59 cm. The radial temperature difference equals 3.35°C and the vertical one is 251.25°C ($\beta = 0.0002$ for GaSb and 0.00067 for medium No. 3). From the condition of equality of the Mn_g numbers, it follows that $k_\sigma = 0.000906$. Now, all the parameters for flow modeling in the model medium are known. The predicted steady-state flow structure and the field of temperature isolines are the same as in Fig. 1. The highest and lowest values of the stream function are 0.01164 and -0.08798 cm^3/sec. The maximum velocity of the melt equal to 2.225 cm/sec is attained at the free surface. The calculated values of the Reynolds, Weber, and Froude numbers are 731.9, 0.0823, and 44.9, respectively. The minimum dimensionless values of the stream function for the flows of interest were found to be almost coincident: -7.63 and -7.56. Thus, the flows calculated for medium Nos. 2 and 3 are similar to each other.

The above approach permits easy determination of similar flows under terrestrial conditions provided that the Morton (and Prandtl) numbers of the melt and the model medium are equal, by choosing proper geometric and temperature parameters.

3.3. *Similarity by the Prandtl Number.* The Prandtl number exerts a substantial influence both on the flow structure and flow intensity. In the above calculations, the thermal conductivity for the model medium was changed in such a way that the Prandtl number becomes as low as that for the medium under study. Calculations for initial and model media with high Prandtl numbers ($\mathrm{Pr} = 2.2$) yield unsteady oscillatory modes for the velocity and temperature fields (Fig. 2). The flow structure varies passing through several stages: from a two-vortex pattern (Fig. 2a) to a single-vortex one (Fig. 2c). The pair of vortices shows

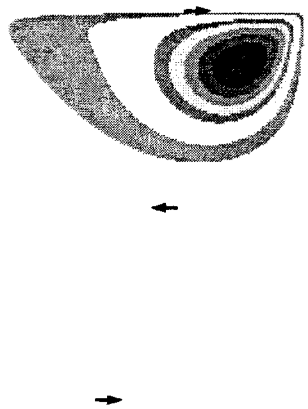

Fig. 3

Fig. 4

local extrema of the stream function equal to 0.16 and -0.0376 cm^3/sec. Initially, under the action of thermocapillary convection, motion beneath the free surface develops, while vortex motion is observed in the remaining part of the flow, which is caused by natural convection from a more heated wall. As a result, a temperature field with an even greater local radial gradient is observed near the axis, the gradient changing its sign near the edge of the flow (Fig. 2b). The latter provides conditions for the development of an oppositely directed vortex motion, which leads to destruction of the main vortex. The new vortex merges with the vortex brought about by the Marangoni convection, and then single-vortex motion of the entire liquid is observed. In the resulting vortex, there are two local extrema of the stream function equal to -0.143 and -0.042 (Fig. 2c). This leads to redistribution of the temperature field in the liquid and gives rise to a flow similar to that shown in Fig. 2a. The process recurs as described above with nearly the same intensity of the flow. The stability of the oscillatory regime is ensured by heating from above.

The Marangoni convection gives rise to much less intensive flow with a local minimum of the stream function roughly equal to -0.036. The maximum velocity in the liquid is 1.5 (Fig. 2c) and 2.5 (Fig. 2a) times greater than the velocity at the free surface.

A comparison between the maximum value of the stream function and the velocity field with the results of flow modeling for low Prandtl numbers (see Sec. 3.2) demonstrates a noticeable increase in the flow intensity in the liquid. This two calculation series show that the Prandtl number of the model medium and that of the melted semiconductor should be as close as possible.

3.4. *Similar Flows in Microgravity Conditions.* Microgravity conditions are modeled by a low value of g in the equations of motion. Therefore, provided that the values of g in the problems of Secs. 3.2 and 3.3 are reduced by an identical factor, the flows remain similar and model the processes under zero-gravity conditions.

Figure 3 shows the flow pattern obtained by numerical simulation for the conditions and media indicated in Sec. 3.2 but for g decreased by a factor of 10^4. The local extrema of the stream function equal -0.1026 and 0.0075 cm^3/sec ($\mathrm{Pr} = 0.05$). An increase in flow intensity compared to the terrestrial conditions was observed: the Reynolds, Weber, and Froude numbers are 797, 0.0976, and 53, respectively, and the Grashof number equals 8.025. Thus, the low values of the Grashof number do not guarantee origination of a flow with low intensity. The temperature distribution is stratified (i.e., it is close to a diffusional flow). However, the temperature is not uniform along the radius in horizontal cross sections to the point at the lower boundary.

The modeling of flows for these media at high Prandtl numbers reveals flow structures similar to those shown in Fig. 3, with the same values of the Reynolds, Weber, Froude, and Grashof numbers. However, the temperature field differs considerably [Fig. 4 (Pr = 2.2); see also Fig. 2b]. Thus, the retarded natural convection leads to steady flow structures for media with high Prandtl numbers.

4. Conclusions. A new form of the equations of motion and heat and mass transfer is proposed, in which natural fluid-dynamic scales of the media under study are used. An increase in the convective heat transfer component is established when passing to microgravity conditions. Convective flows under outer-space conditions are shown to make a greater contribution to the heat redistribution than they do under terrestrial conditions. However, with decreasing g, the development of the flows becomes substantially retarded.

The simple form of the majority of the dimensionless parameters permits a simple classification of similar physical phenomena. Similar steady-state flow patterns for different media and gravity conditions are reached in different periods of physical time. As a rule, the lower g for a flow, the longer the duration of the transition process in it.

The calculations prove the coincidence between the dimensionless hydrodynamic parameters of initial and model media chosen with due regard for their parameters M (or Re_g), Pr, Gr_g, and Mn_g.

The proper choice of similar nonisothermal flows of different media requires, first of all, that the numbers M and Pr of the media be equal. Choosing media with close Pr and M, we can find the required proportion between the characteristic lengths and temperature differences. This, in turn, allows one to find similar flows under terrestrial and outer-space conditions. For the outer-space conditions, it was found possible to obtain flows with similar hydrodynamics for media with different Prandtl numbers. In this case, the only difference is the temperature profiles. This fact can be explained by the predominance of the Marangoni convection. The contribution of natural convection to flow development is vanishingly small. This conclusion clearly demonstrates the importance of making proper allowance for the presence of nongravitational sources of motion, which may prove dominating in new conditions.

Flows caused by impurity-concentration gradients in the melt and at the free surface due to changing gravitational conditions can be studied by analogy with the above-considered nonisothermal problems. The character of the flows for high Schmidt numbers can be estimated from the numerical data obtained for high Prandtl numbers.

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