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ANALYSIS OF THE EFFECT OF THERMOELASTIC STRESSES OF THE CRYSTALLIZATION OF A SPHERE UNDER WEIGHTLESS CONDITIONS

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In the crystallization of a sphere initially completely molten and then cooled slowly over its entire surface, thermoelastic stresses are created in the solid phase. If the intensity of the shear streasses reaches the critical value – the yield point – a region of plastic deformation appears. A description was given in [1] of experiments involving crystallization of copper and silver specimens in the form of spheres (the amount of impurity was 0.001% in the copper specimen and 0.004% in the silver specimen) under weightless conditions. It was noted that the structure of the specimens obtained indicates a nearly complete lack of convective motion in the melt. It is interesting to study the effect of thermoelastic stresses on the crystallization of specimens under weightless conditions and on the structure of the crystals obtained.

The study [2] indicated that it might be possible to form a shrinkage cavity during the crystallization of a sphere if the solid phase is denser than the liquid phase. The occurrence of thermoelastic stresses is one possible cause of shrinkage cavity formation. In the model in [2], the cavity begins to form at the very beginning of the crystallization process. Thus the stresses in the solid phase are due only to incompatible thermal strains, not to shrinkage of the material, and it can be anticipated that the resulting stresses will not have an appreciable effect on subsequent crystallization.

Here we study the process of crystallization without the formation of a shrinkage cavity.

1. The material is assumed to be incompressible in the liquid state and it is assumed that the crystallization process occurs in the absence of external effects (under weightless conditions and in vacuum).

The crystallization process was studied numerically for metals (copper, aluminum, silver) in [3] and for semiconducting materials (germanium, silicon) in [4]. The problem was formulated in an isotropic approximation for all of the materials.

We introduce a spherical coordinate system r, φ, θ with its origin at the center of the sphere. We have the following relations for the liquid phase:

$$\frac{\partial T_2}{\partial t} = \frac{\lambda_2}{\rho_2 c_2} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T_2}{\partial r} \right); \tag{1.1}$$

$$P = -p(t) I, \tag{1.2}$$

where T_2, ρ_2, c_2, and λ_2 are the temperature, density, specific heat, and thermal conductivity of the liquid phase; P is the stress tensor; I is a unit tensor.

The behavior of the material in the solid phase is described by a system of thermoelastoplasticity equations. Due to spherical symmetry, only the normal components of the stress tensor σ_r, σ_φ, σ_θ, are nontrivial, while $\sigma_\varphi = \sigma_\theta$. The following equilibrium equation holds throughout the region of the solid state

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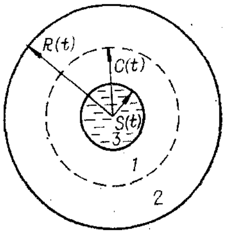

Fig. 1

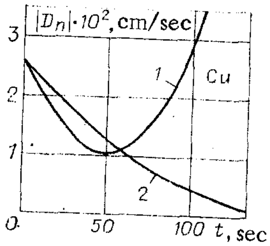

Fig. 2

$$\frac{\partial\sigma_r}{\partial r}+\frac{2}{r}(\sigma_r-\sigma_\varphi)=0. \tag{1.3}$$

The relations of Hooke's law are satisfied in the elastic region

$$\frac{\partial W}{\partial r}=\frac{1}{E}(\sigma_r-2\nu\sigma_\varphi)+\alpha(T_1-T_0); \tag{1.4}$$

$$\frac{W}{r}=\frac{1}{E}((1-\nu)\sigma_\varphi-\nu\sigma_r)+\alpha(T_1-T_0), \tag{1.5}$$

where E is Young's modulus; ν is Poisson's ratio; α is the coefficient of linear expansion; W is the displacement of particles of the solid phase; T_0 is the melting point.

Figure 1 shows the following regions which come into existence during crystallization of the sphere: 1) region of plastic strains; 2) region of elastic strains; 3) liquid phase. The von Mises condition is satisfied in the plastic region

$$|\sigma_\varphi-\sigma_r|=\frac{2}{\sqrt{3}}k, \tag{1.6}$$

where k is the yield point.

The occurrence of thermoelastic stresses is examined only during crystallization of the sphere, without study of its subsequent cooling. Then assuming that the sphere cools sufficiently slowly so that the thermal perturbation during crystallization will be sufficiently small, we can assume that the Young's modulus and yield strength k are independent of temperature. The Poisson ratio ν is also practically independent of temperature.

The temperature distribution in the solid phase is discribed by the heat-conduction equation [6]

$$(1+a)\frac{\partial T_1}{\partial t}=\frac{\lambda_1}{\rho_1 c_1}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T_1}{\partial r}\right), \tag{1.7}$$

where $a=\frac{(1+\nu)E\alpha^2T_0}{(1-2\nu)(1-\nu)c_1\rho_1}$ is the coupling coefficient.

2. The crystallization front is a surface of nonremovable discontinuity. Thus the following relations are valid on the front [7]

$$[\rho(v-D_n)]=0; \tag{2.1}$$

$$[p_n]=\rho(v-D_n)[v-D_n]; \tag{2.2}$$

$$[q]=\rho(v-D_n)\left[\frac{v^2}{2}+U-\frac{1}{\rho}p_n\right], \tag{2.3}$$

where D_n = dS/dt is the velocity of the crystallization front; v_1 and v_2 are the absolute velocities of particles of the medium; p_n is the normal component of the stress tensor; [q] is the heat flow across the sueface S(t):

$$[q]=q_1-q_2=\lambda_1\partial T_1/\partial r|_{r=S(t)}-\lambda_2\partial T_2/\partial r|_{r=S(t)};$$

U is the internal energy, the sudden change of which at the front is equal to γ; the subscript 1 corresponds to the solid phase, while 2 corresponds to the liquid phase.

Considering that ν_2 = 0, we have the following from (2.1):

$$v_1=\frac{\rho_1-\rho_2}{\rho_1}D_n. \tag{2.4}$$

Inserting (2.4) into (2.2) yields

$$|p_n| = -\frac{\rho_2}{\rho_1}(\rho_1-\rho_2)D_n^2. \tag{2.5}$$

Now, allowing for the fact that $p_{n_2} = p(t)$ — the pressure in the liquid phase — we use (2.3)-(2.5) to find the following relation on the front:

$$\frac{dS}{dt}\left(\rho_2\gamma + \frac{\rho_2-\rho_1}{\rho_1}p(t)\right) = \lambda_1\frac{\partial T_1}{\partial r}\Big|_{r=S(t)} - \lambda_2\frac{\partial T_2}{\partial r}\Big|_{r=S(t)} + \left(\frac{dS}{dt}\right)^3\frac{\rho_2(\rho_1^2-\rho_2^2)}{2\rho_1^2}. \tag{2.6}$$

It is necessary to determine components of the stress tensor σ_r and σ_φ, the temperatures T_1 and T_2, and the position of the front $S(t)$ satisfying Eqs. (1.1)-(1.7) and (2.6) and the initial conditions at $t = 0$

$$T_2(r,0) = \varphi(r),\ S(0) = R_0,$$
$$T_2(R_0,0) = \varphi(R_0) = T_0,\ f(0) = 0,\ p(0) = 0,$$

along with the boundary conditions at $r = R$

$$\begin{gathered}\sigma_r(R,t) = 0,\ T_1(R,t) = T_0 - f(t),\\ W(R,t) = R - R_0,\quad R^3 = S^3 + \frac{\rho_2}{\rho_1}(R_0^3 - S^3).\end{gathered} \tag{2.7}$$

Here, $\varphi(r)$ is the initial temperature distribution in the sphere over the radius; $f(t)$ is a function determining the thermal cooling of the sphere.

3. We will solve the elastoplastic part of the problem, assuming the temperature distribution to be known. The system of equations describing the state of the material in the elastic region has the general solution [8]:

$$\sigma_r^y = -\frac{2C_1}{r^3} + C_2 - \frac{2E\alpha}{(1-\nu)r^3}\int_r^R T^0r^2dr; \tag{3.1}$$

$$\sigma_\varphi^y = \frac{C_1}{r^3} + C_2 - \frac{E\alpha}{1-\nu}\left(T^0 - \frac{1}{r^3}\int_r^R T^0r^2dr\right), \tag{3.2}$$

where $T^0 = T_0 - T_1$. Inserting (3.1) and (3.2) into (1.5), from condition (2.7) we obtain

$$C_1 = \frac{ER^3}{3(1-\nu)}\left(\frac{R-R_0}{R}\right),\quad C_2 = \frac{2C_1}{R^3}.$$

Thus,

$$\sigma_r^y = -\frac{2E\alpha}{(1-\nu)r^3}\int_r^R T^0r^2dr - \frac{2E(R^3-r^3)}{3(1-\nu)r^3}\left(\frac{R-R_0}{R}\right). \tag{3.3}$$

Inserting (3.3) into (2.5), we obtain the relation

$$p(t) = \frac{2E\alpha}{(1-\nu)S^3}\int_S^R T^0r^2dr + \frac{2E(R^3-S^3)}{3(1-\nu)S^3}\left(\frac{R-R_0}{R}\right) + B,$$

where

$$B = -\frac{\rho_2}{\rho_1}(\rho_1-\rho_2)D_n^2.$$

At each moment of time, the boundary C between the elastic and plastic regions can be found from the plasticity condition $|\sigma_r^y - \sigma_\varphi^y|_{r=C} = \frac{2}{\sqrt{3}}k$. Having inserted the expressions for σ_r^y and σ_φ^y, we write

$$-\frac{ER^3}{(1-\nu)C^3}\left(\frac{R-R_0}{R}\right) - \frac{3E\alpha}{(1-\nu)C^3}\int_C^R T^0r^2dr + \frac{E\alpha T_C}{1-\nu} = \pm\frac{2}{\sqrt{3}}k. \tag{3.4}$$

Since the temperature distribution is known, C is determined from (3.4).

Using the von Mises condition, we reduce the equilibrium equation for the plastic region to the form $d\sigma_r^n/dr = -4k(\sqrt{3}r)$. From this

$$\sigma_r^n = -\frac{4}{\sqrt{3}} k \ln r + C_3. \tag{3.5}$$

The constant C_3 can be found from the condition of continuity of the normal stresses on the boundary C:

$$\sigma_r^n |_{r=C} = \sigma_\varphi^n |_{r=C}. \tag{3.6}$$

Inserting (3.5) and (3.3) into (3.6), we obtain

$$C_3 = \frac{4}{\sqrt{3}} k \ln C - \frac{4}{3\sqrt{3}} k - \frac{2E}{3(1-\nu)} \left[\frac{R-R_0}{R} - \alpha T_C^0\right].$$

Then the pressure on the front

$$p(t) = -\frac{4}{\sqrt{3}} k \ln \frac{C}{S} + \frac{4}{3\sqrt{3}} k + \frac{2E}{3(1-\nu)} \left(\frac{R-R_0}{R} - \alpha T_C^0\right) + B.$$

At a certain moment of time, the entire region may change over to the plastic state. The plasticity condition for the boundary at r = R has the form

$$\frac{E\alpha T^0}{1-\nu} - \frac{(R-R_0)E}{2R(1-\nu)} = \frac{2}{\sqrt{3}} k.$$

Calculations show that this equality is satisfied when the crystallization front has traveled a distance corresponding to 0.4-0.8% of the initial radius of the sphere. Here, the pressure on the front

$$p(t) = \frac{4}{\sqrt{3}} k \ln \frac{S}{R} + B.$$

4. The characteristic value of the displacements is taken equal to the maximum value reached at S = 0:

$$W^* = R_0 \left(\sqrt[3]{\frac{\rho_2}{\rho_1}} - 1\right).$$

The characteristic value of the stresses $\sigma^* = k/\sqrt{3}$.

For the materials being studied, $k \approx 10^4$ dyn/cm^2 (in the CGS system) near the melting point. The characteristic temperature is the melting point, while the characteristic radius is R_0.

It is assumed that a sphere of radius R_0 = 1 cm is cooled at the rate of 1 deg/min. Then the time of crystallization in the classical problem (without allowance for thermoelastic stresses) is $t^* \approx 10^2$ sec. We take the mean velocity D_n^* to be equal to $R_0/t^* \approx 10^{-2}$ cm/sec. Thus, the square and the cube of the front velocity in the condition on the front can be ignored, since the coefficients in front of them, in dimensionless notation, are of the second and fourth orders of smallness compared to the coefficients in front of the other terms of the equation. Then (2.5) takes the form $[p_n] = 0$, and (2.6) becomes

$$\frac{dS}{dt}\left(\rho_2 \gamma + \frac{\rho_2 - \rho_1}{\rho_1} p(t)\right) = \lambda_1 \frac{\partial T_1}{\partial r}\bigg|_{r=S} - \lambda_2 \frac{\partial T_2}{\partial r}\bigg|_{r=S}.$$

It should be noted that $(\rho_2 - \rho_1)p(t)/\rho_1 \geqslant 0$ for the cases when $\rho_2 > \rho_1$ and $\rho_2 < \rho_1$.

We will change over to dimensionless variables by means of the formulas

$$\bar{T}_1 = \frac{T_1}{T_0}, \quad \bar{T}_2 = \frac{T_2}{T_0}, \quad \bar{f} = \frac{f}{T_0}, \quad \bar{\psi} = \frac{\varphi}{T_0}, \quad \bar{\sigma}_r = \frac{\sigma_r}{\sigma^*}, \quad \bar{\sigma}_\varphi = \frac{\sigma_\varphi}{\sigma^*},$$

$$\bar{p} = \frac{p}{\sigma^*}, \quad \bar{W} = \frac{W}{W^*}, \quad \bar{S} = \frac{S}{R_0}, \quad \bar{R} = \frac{R}{R_0}, \quad \bar{r} = \frac{r}{R_0}, \quad t = \frac{t}{t^*}.$$

The problem has the following form in dimensionless variables (the bar is omitted):

the heat-conduction equations

$$\frac{\partial T_i}{\partial t} = \mathrm{Fo}_i \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T_i}{\partial r}\right), \quad i = 1, 2,$$

TABLE 1

Variant	Cu	Al	Ag	Ge	Si
Classical	95,3	87,5	638,7	426,2	581,1
With allowance for $(S = 0)$	159	198	951	1004	1475
With allowance for $(S = 0{,}33R_0)$	92	127	554	670	919

TABLE 2

Variant	Cu	Al	Ag	Ge	Si
Classical	1,6	1,56	10,7	9,5	9,7
With allowance for $(S = 0)$	2,65	3,3	15,87	16,7	24,6
With allowance for $(S = 0{,}33R_0)$	1,53	2,12	9,23	11,2	15,3

TABLE 3

Pressure	Cu	Al	Ag	Ge	Si
Initial $\times 10^4$	−0,67	−0,47	−0,14	0,08	0,14
Mean	−66	−35	−85	51	16
Final 10^{-8}	−0,12	−0,14	−0,26	0,09	0,17

$$\mathrm{Fo}_1 = \frac{t^*\lambda_1}{R_0^2\left(\rho_1 c_1 + \dfrac{E\alpha(1+\nu)}{1-\nu}\right)} \approx 10^{-1}, \quad \mathrm{Fo}_2 = \frac{t^*\lambda_2}{R_0^2\rho_2 c_2} \approx 10^2,$$

where the Fourier number Fo_i expresses a certain correspondence between the rate of change in conditions in the environment and the rate of restructuring of the temperature field inside the body;

the thermoelastoplastic part

$$\frac{d\sigma_r}{dr} + \frac{2}{r}(\sigma_r - \sigma_\varphi) = 0, \quad \frac{dW}{dr} = b(\sigma_r - 2\nu\sigma_\varphi) + d(T_1 - 1),$$

$$\frac{W}{r} = b((1-\nu)\sigma_\varphi - \nu\sigma_r) + d(T_1 - 1),$$

$$b = \frac{k}{E\left(\sqrt[3]{\rho^0} - 1\right)} \approx 10^{-3}, \quad d = \frac{\alpha T_0}{\sqrt[3]{\rho^0} - 1} \approx 10^{-1}, \quad \rho^0 = \rho_2/\rho_1,$$

where the number b shows the ratio of the plastic stresses to the elastic stresses; the number d expresses the correspondence between the strains caused by cooling of the sphere and the change in density on the crystallization front;

the condition on the front

$$\frac{dS}{dt}(\varkappa_1 + F_1 p) = \frac{\lambda_1}{\lambda_2}\left.\frac{\partial T_1}{\partial r}\right|_{r=S} - \left.\frac{\partial T_2}{\partial r}\right|_{r=S},$$

$$\varkappa_1 = \frac{\rho_2 \gamma R_0^2}{t^*\lambda_2 T_0} \approx 10^{-1}, \quad F_1 = (\rho^0 - 1)\frac{R_0^2 k}{t^*\lambda_2 T_0} \approx 10^1,$$

where the numbers $\varkappa_i$ and F_1, respectively, represent the ratio of the rate of restructuring of the temperature field within the sphere on the crystallization front and the resulting thermoelastoplastic stresses to the rate of change in conditions in the environment.

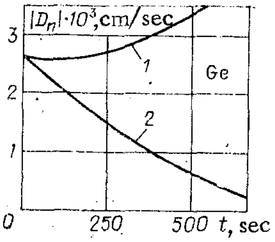

Fig. 3

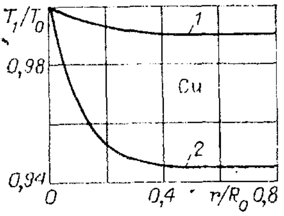

Fig. 4

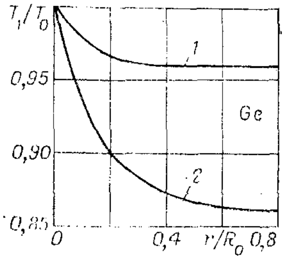

Fig. 5

Numerical results obtained for the materials studied are shown in Tables 1-3 (crystallization time is in seconds; the difference between the initial and final temperatures on the external boundary is in °C; the pressure in the liquid phase is in dyn/cm^2. These three quantities are shown in the respective tables).

Figures 2 and 3 show the dependence of crystallization rate on time, while Figs. 4 and 5 show the radial temperature distribution. Lines 1 and 2 in Figs. 2-5 correspond to the classical problem and the problem with allowance for stresses.

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NUMERICAL STUDY OF THE ACTION OF GAS-EXPLOSIVE TUBE ON THE SURFACE OF A STEEL WALL

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An experimental study was made in [1] of the feasibility of the heat treatment of the inside surface of a steel channel with a gas-explosive discharge. The surface layer of the specimen subjected to such action usually consists of a zone of solidified melt of about 20 µm and a heat-affected zone of about 30 µm, where α–γ–α' structural transformations have taken place. The explosive action of the discharge is accompanied by the removal of a substantial amount of material from the surface of the channel. The depth of the layer removed may reach 100 µm. Such values as these for the depths of the fusion and heat-affected zones and the removed layer are difficult to explain by the thermal effect on the wall of the bunch of shock-compressed gas formed in front of the gas-explosive jet of explosion products (JEP). The convective action of the JEP which follows the shock-compressed gas should be taken as the basis of the removal mechanism, as well as of the appearance of the fusion and heat-affected zones. In fact, the heat flow to the wall of the channel from the plasma bunch and

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