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Stability of the elastoplastic equilibrium of the solid phase during crystallization of a sphere in zero gravity

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Models have been developed[1-3] for the phase transition in a system which consists of an elastic solid phase transition in a system which consists of an elastic solid phase and a melt. In Refs. 1 and 2 the conditions for heterogeneous phase equilibrium were studied under isothermal conditions. In Ref. 2 the problem of the stability of isothermal equilibrium was studied for a nonlinear elastic material with a liquid melt.

In Ref. 3 a nonisothermal, spherically symmetric problem was studied for the solidification of a melted sphere, cooled from the outside under conditions of zero gravity. It was shown that the stresses which arise due to the change in density of the material on solidification have a significant impact on the heat transfer and on the movement of the boundary of the solid shell. A mathematical model was formulated there. In it the behavior of the material in the solid phase was described by the equations for isotropic quasistatic thermoelastoplasticity. Convective motion in the liquid core was not considered. The heat transport equations for the liquid and solid phase were united using the Stefan condition, obtained[3] from the general conditions at a strong discontinuity. This condition takes into account the surface forces in the energy balance at the crystallization front. It was shown that when the crystallization front moves toward the center of the sphere, the pressure in the liquid phase rises in absolute value, which leads to a significant slowing of its rate of motion in comparison with the purely thermal problem of Stefan.

At some point in time in the process, the intensity of the tangential stresses on the crystallization front reach the flow limit, and a region of plastic deformation arises at the front. With time, the boundary $r = C_0(t)$ between the elastic and plastic region shifts away from the crystallization front, $r = S_0(t)$, toward the outer boundary of the sphere, $R = R_0(t)$. Therefore, the crystallization process proceeds through three stages as time progresses. In the first stage, all of the solid phase is in the elastic state. In the second stage, the region $S_0(t) < r < C_0(t)$ is in the plastic state, while the region $C_0(t) < r < R_0(t)$ is elastic. In the third stage, all of the solid shell resides in the plastic state.

In the present work we have analyzed the problem of small perturbations in the spherically symmetric solution for all three of these stages. the main result is the demonstration of a bifurcation of this solution, which is treated as an instability of the quasiequilibrium state of the solid phase. It is shown that for the first two stages just the thermoplastic stresses lead to the bifurcation of the fundamental, spherically symmetric solution.

We shall consider a perturbation of the spherically symmetric solution for the crystallization of a liquid sphere. We assume that the outer surface of the sphere is cooled in spherically symmetric fashion. Then, as the solid phase begins to form, the spherical symmetry of the outer surface is not destroyed because of capillary forces. The behavior of the material in the solid phase is described by the equations for uncoupled quasistatic thermoelastoplasticity. When $S(\vartheta, \varphi, t) < r < R(\vartheta, \varphi, t)$, we have

$$\frac{\partial T_1}{\partial t} = \chi_1 \Delta T_1, \quad \sum_j \nabla_j P_1^{ji} = 0. \tag{1}$$

In the liquid phase $0 < r < S(\vartheta, \varphi, t)$ we have the relations

$$\frac{\partial T_2}{\partial t} = \chi_2 \Delta T_2, \quad P_2 = -p(t)I. \tag{2}$$

Here T_1, T_2, χ_1, and χ_2 are the temperatures and thermal diffusivities of the solid and liquid phases; I is the unit tensor; Δ is the Laplacian operator; P_i is the stress tensor with the physical components σ_{kl} in the solid phase; P_1^{ij} are the contravariant components of the tensor P_1; and $p(t)$ is the pressure in the liquid phase, determined from the solution itself. In the elastic region $C(\vartheta, \varphi, t) < r < R(\vartheta, \varphi, t)$ the Jamail–Neumann law is valid.

In the plastic region $S(\vartheta, \varphi, t) < r < C(\vartheta, \varphi, t)$ the plasticity condition of Tresk applies:

$$(\sigma_{kk} - \sigma - 2/3K)(\sigma_{ll} - \sigma - 2/3K) = \sigma_{kl}^2, \quad k \neq l. \tag{3}$$

where $\sigma = (\sigma_{rr} + \sigma_{\vartheta\vartheta} + \sigma_{\varphi\varphi})/3$. We assume that the flow limit K is independent of temperature.

At the crystallization front $r = S(\vartheta, \varphi, t)$ we impose a continuity condition on the tangential and normal components of the stress vector, a condition for local thermodynamic phase equilibrium, and condition of the Stefan type[3]:

$$\begin{aligned} &\mathbf{n}_S P_1 \mathbf{n}_S = -p(t), \quad \mathbf{n}_S P_1 - (\mathbf{n}_S P_1 \mathbf{n}_S)\mathbf{n}_S = 0, \quad T_1 = T_2 = T_0, \\ &\left(\rho_2 \Lambda - \frac{\rho_2 - \rho_1}{\rho_1}\sigma_r\right)\mathbf{D}\cdot\mathbf{n}_S = (\lambda_1 \nabla T_1 - \lambda_2 \nabla T_2)\cdot \mathbf{n}_S, \\ &\nabla = \left[\frac{\partial}{\partial r}, \frac{1}{r}\frac{\partial}{\partial \vartheta}, \frac{\partial}{r \sin\vartheta \partial\varphi}\right]. \end{aligned} \tag{4}$$

At the outer surface $r = R(\vartheta, \varphi, t)$ we impose the conditions

$$\begin{aligned} &\mathbf{u} = \mathbf{R} - \mathbf{R}_{(0)}, \quad \mathbf{n}_R P_1 \mathbf{n}_R = 0, \\ &\mathbf{n}_R P_1 - (\mathbf{n}_R P_1 \mathbf{n}_R)\mathbf{n}_R = 0, \quad T_1 = (1 - F(t))T_0. \end{aligned} \tag{5}$$

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In the expressions (4) and (5), Λ is the latent heat of crystallization; ρ_1, λ_1, ρ_2, and λ_2 are the densities and thermal conductivities of the solid and liquid phases; $\mathbf{D}$ is the velocity vector for the crystallization front; $F(t) > 0$ is a function of time determined by the cooling law; and T_0 is the crystallization temperature. The vectors $\mathbf{n}_S$ and $\mathbf{n}_R$ are, respectively, the unit vectors normal to the surfaces $r = S$ and $r = R$, and $R_{(0)}$ is the initial radius of the liquid sphere.

In (5) the equality of the displacement vector $\mathbf{u}$ to the difference of the vectors $\mathbf{r} = \mathbf{R}(\vartheta, \varphi, t)$ and $\mathbf{R}_{(0)} = (R_{(0)}, 0, 0)$ follows from the assumption that in the distorted phase the particles which lie on the outer surface $r = R(\vartheta, \varphi, t)$ remain on that surface. The second and third conditions in (5) indicate that the surface $r = R(\vartheta, \varphi, t)$ is free of stress and is isothermal at all times.

If an elastoplastic transition arises, then at this boundary we consider only continuity conditions for the components of the stress tensor, since the problem of plasticity under condition (3) is solvable in terms of the stress. In addition to Eqs. (1)-(5), we add the condition for conservation of the total mass of the material and the initial conditions, as presented in Ref. 3. Numerical calculations were performed, beginning with a small thickness for the solid shell, determined from the initial asymptote for the main solution. The initial temperature distribution in the liquid sphere is assumed to be known.

STABILITY OF THE SPHERICAL SOLID PHASE

We shall seek a solution of the problem (1)-(5) in the form

$$\mathbf{u} = \mathbf{u}^0(r, t) + \alpha \mathbf{u}^1(r, \vartheta, \varphi, t), \quad \sigma_{ij} = \sigma_{ij}^0 + \alpha \sigma_{ij}^1(r, \vartheta, \varphi, t),$$
$$R = R_0(t) + \alpha R^1(\vartheta, \varphi, t), \quad S = S_0(t) + \alpha S^1(\vartheta, \varphi, t),$$
$$T_i = T_i^0(r, t) + \alpha T_i^1(r, \vartheta, \varphi, t),$$

where the functions with zero indices are those constructed in Ref. 3 as solutions of the problem (1)-(5) one-dimensional in the spatial coordinate, and α is a small quantity. Linearizing the equations of equilibrium and thermal conductivity (1) and (2), the conditions (3)-(5), and the mass conservation condition with respect to the main solution u_r^0, T_1^0, T_2^0, R_0, S_0, and p_0, we obtain equations for the small perturbations.

We shall consider quasistationary perturbation, with a time dependence which is parametric. We impose the quasistationarity condition because we are not studying the evolution of the perturbations but rather the possibility of loss of stability of the solid phase, in a state of quasistatic equilibrium.

From the linearized boundary conditions at the outer surface $r = R_0(t)$, we obtain

$$u_r^1 + \frac{du_r^0}{dr} R^1 = R^1, \tag{6}$$

$$\sigma_r^1 + \frac{d\sigma_r^0}{dr} R_1 = 0; \quad \sigma_{r\vartheta}^1 - \frac{\sigma_\vartheta^0}{R_0} \frac{\partial R_1}{\partial \vartheta} = 0; \tag{7}$$

$$\sigma_{r\varphi}^1 - \frac{\sigma_\vartheta^0}{R_0 \sin \vartheta} \frac{\partial R_1}{\partial \varphi} = 0,$$

$$T_1^1 + \frac{dT_1^0}{dr} R_1 = 0, \tag{8}$$

and at the crystallization front $r = S_0(t)$:

$$\sigma_r^1 + \frac{d\sigma_r^0}{dr} S_1 = 0, \quad \sigma_{r\vartheta}^1 - \frac{\sigma_\vartheta^0 - \sigma_r^0}{S_0} \frac{\partial S_1}{\partial \vartheta} = 0, \tag{9}$$

$$T_1^1 + \frac{dT_1^0}{dr} S_1 = 0, \quad T_2^0 + \frac{dT_2^0}{dr} S_1 = 0, \tag{10}$$

$$\lambda_1 \frac{\partial T_1^1}{dr} - \lambda_2 \frac{\partial T_2^1}{dr} = \left(\lambda_2 \frac{d^2 T_2^0}{dr^2} - \lambda_1 \frac{d^2 T_1^0}{dr^2} \right) S_1. \tag{11}$$

Clearly, the presence of the phase boundary significantly differentiates this problem from that of the thermal stability of a body under the influence of a load, which is studied in elasticity theory.

For perturbations of the main equilibrium state of the elastic solid phase the temperature at the perturbed front must remain equal to the temperature of crystallization. If there is no perturbation of the temperature profile, then the boundary conditions (8) and (10) imply directly that $R_1 = S_1 \equiv 0$. Consequently, no elastic instability can arise: The problem of small perturbations for the displacement field has only a trivial solution. Therefore, the problem we are considering does not have any analogy with that studied in Ref. 4, which had to do with the stability of an elastic spherical shell, under various uniform pressures on its inner and outer surfaces.

If at some moment of time there appear branching solution, then the perturbation of the displacements may grow with time, since the pressure drop at the surface of the solid phase increases during the solidification process.[3] In this sense, it is legitimate to speak of the loss of stability of the growing solid phase.

In the problem of the small perturbations we shall represent the temperature profile as a series of spherical harmonics of degree n:

$$Y_n = \sum_{m=0}^{n} P_n^m(\cos \vartheta) (\alpha_n^m \cos \varphi + \beta_n^m \sin \varphi),$$

where $P_n^m(\cos \vartheta)$ is the associated Legendre polynomial of order m. The solution of the displacements in the elastic region of the solid phase is also obtained, using the ideas of Pankovich and Neiber,[5] as a series in Y_n, $\partial Y_n/\partial \vartheta$, and $(\sin \vartheta)^{-1} \cdot \partial Y_n/\partial \varphi$, whose coefficients are determined from the boundary conditions.

The coefficients of the series depend parametrically on time are independent of m. A perturbation with $n = 1$ corresponds to a displacement of the crystallizing sphere which does not distort the spherical surface. Therefore, we shall not consider such a perturbation. A perturbation for $n \geq 2$ automatically satisfies the mass conservation law, and in order to find the series coefficients with $n \geq 2$, it is sufficient to require that Eqs. (6)-(11) be satisfied. For a given main solution, when the determinant Δ of this system is set to zero, we find a critical thickness for the growing shell, at which a family of $(2n + 1)$ parametric solutions of order n emerge from the main solution. These solutions depend on the arbitrary parameters α_n^m, β_n^m, for $m = 0, \ldots, n$.

A numerical study of the determinant Δ was performed for $n \leq 20$, and $0 < \gamma < 1$, where γ is the ratio of S_0 to R_0. The material parameters correspond to those of silicon and copper. The initial radius $R_{(0)}$ was varied between 1 and 10 cm. The rate of cooling at the outer surface was varied between 1°C/min and 1°C/s. It was shown that in all cases the determinant Δ may take on null values in the range $0 < \gamma < 1$ only for $n = 3, 5$. For $n = 5$ the critical point γ_{cr} is close

to the right side of the segment (0, 1). Consequently, the bifurcation for $n = 5$ occurs earlier. The value is $\gamma_{cr} \approx 0.8$ for the two materials, and is virtually independent of the rate of cooling of the sample.

Since as stability is lost (when $\gamma > \gamma_{cr}$) the spherically symmetric solution in the solid phase exhibits development of a plastic zone $C_0 < r < S_0$, in order to determine the small perturbation using the plasticity condition of Tresk (3), we obtain an equation which has a solution in the form of a series in spherical harmonics Y_n. At the boundary $r = S_0$ the conditions for the stress (9) remain unchanged, while at the boundary $r = C_0$ there is an additional condition for the stress. Substituting the elastoplastic solution into the corresponding boundary conditions, we obtain for each n a system of twelve homogeneous linear equation for twelve unknowns. Numerical calculations for the "elastoplastic" determinant ($n \geq 2$) showed that for $n \neq 3.5$ it does not go to zero for $0 < \gamma < 1$. For $n = 3.5$ its behavior is analogous to that of the determinant for the elastic solution, and $\gamma_{cr} \approx 0.8$.

We shall ow consider the solidification process, beginning at the time t_*, at which the entire solid phase enters the plastic state. The four boundary conditions on the stresses (7) and (9) enable us to separate the problem for finding σ_r^1, σ_ϑ^1, σ_φ^1, $\sigma_{r\vartheta}^1$, $\sigma_{r\varphi}^1$, and $\sigma_{\vartheta\varphi}^1$ from the temperature-dependence problem. For a flow limit K which is constant the temperature regime does not influence the elastic stability of the quasiequilibrium state of the solid phase. Substituting the plastic solution into the boundary conditions, we obtain four homogeneous algebraic equations relative to four unknowns. Analysis of the determinant for this system showed that the earlier the entire solid phase enters the plastic state, the larger n_{cr} is the order of the spherical harmonics which enter the solution). In experiments on the crystallization of spherical samples,[6] apparently, this situation has been realized. Close to the crystallization point the flow limit is $\sim 10^{-6}E$, where E is the Young's modulus.[7] Therefore, even at small thickness the solid phase becomes entirely plastic.[3] Estimates show that the branching solution will be of very high order, with $n_{cr} \sim$ 100-150. Such a perturbation leaves the sample surface nearly spherical, creating a multicellular structure in the bulk. This result agrees with the experimental data reported in Ref. 6.

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Cavity formation in nonlinearly elastic bodies with dislocations and disclinations

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Cavity formation in a nonlinearly elastic cylinder of incompressible material containing a line defect (a wedge disclination or a screw dislocation) was studied by Lur'e[1] using the methods of nonlinear elasticity theory. The dependence of the cavity radius on the defect parameter was determined. An analysis was made of the behavior of the cylinder energy in the case of cavity formation and in the absence of a cavity. The influence of surface energy was considered.

The discontinuous solutions of nonlinear elasticity theory, accompanied by cavity formation, for the example of radially symmetric deformation of an elastic sphere were studied in Refs. 2-4. The possibility of cavity formation on the axis of a wedge disclination was shown by the methods of molecular dynamics in Ref. 5. The possibility of the existence of a continuous solution in the problem of the equilibrium of a cylinder with a screw dislocation was established in Ref. 6 for the particular case of a compressible elastic body.

1. Dislocations and disclinations in nonlinearly elastic bodies were studied in Refs. 7-8. Following these works, we shall examine the following transformation of the reference (undeformed) configuration to the actual (deformed) configuration:

$$R = R(r), \quad \Phi = \kappa\varphi, \quad Z = \lambda z, \tag{1}$$

where r, φ, z and R, Φ, Z are the cylindrical coordinates in the reference configuration and the actual configuration, respectively.

The transformation (1) describes the deformed state of a cylinder with a wedge dislocation. The case $\kappa < 1$ corre-

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