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CALCULATION OF STRESSES AND STRAINS DEVELOPING IN FREEZING OF WATER IN CLOSED VESSELS

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The pressures in the liquid core and the breaking stresses in vessel walls developing in symmetric freezing of water in spherically and cylindrically shaped bottles are calculated. It is shown that at surface temperatures of the bottle above -20^{o}C the water in it freezes only partially; at lower temperatures, the pressure in the liquid core attains a maximum value of about 2000 atm, which is preserved until the water freezes completely.

One simple and convenient means of creating high pressures is the ice-bomb method, in which use is made of the effect of abnormal expansion of water in crystallization and its attendant increase in the pressure accompanying the freezing of water in closed vessels. The method was proposed for the first time in 1944 by B. G. Lazarev and A. S. Kan for obtaining high pressures at low temperatures and investigating the influence of such pressures on the transition of certain substances to a superconducting state; a detailed description of a modified version of this method is given [1]. Subsequently, the ice-bomb method has been applied by different authors to the study of galvanomagnetic effects in nonsuperconducting materials at low temperatures. It is believed that this method is convenient for obtaining pressures up to 2000 atm at low temperatures without using standard high-pressure equipment [2]. However, as far as we know, its possibilities for obtaining higher pressures have not yet been investigated.

This work seeks to calculate strains and stresses developing in the case of symmetric freezing of water in tightly plugged bottles of spherical and cylindrical shapes and to evaluate the maximum pressures which can be obtained in a liquid core using the ice-bomb method.

Freezing of Water in Spherically Shaped Bottles. Let us assume that a bottle having a spherical shape is filled with water and is solidly plugged; at the instant of time $t = 0$, symmetric freezing of water begins and the crystallization front moves to the center of the sphere. The process of freezing of water is accompanied by an increase in the volume occupied with water and ice, which leads to a continuous increase in the pressure in the liquid core and to the development of stresses and strains in vessel walls which are due to the phase transformations of the water into ice. The problem is reduced to the calculation of them as functions of the radius of the crystallization front of water, which is determined by solution of the Stefan problem. In the particular case of practical importance where the temperature of the surface of the bottle in which water freezing occurs is maintained constant all the time, one can obtain an approximate solution of this problem using the quasistationary method. Since the process of crystallization of water in the bottle is slow, nearly equilibrium temperature fields are established in the bulk of its walls and in the ice shell:

$$T_1 = \frac{C_1}{r} + C_2 , \quad T_2 = \frac{C_3}{r} + C_4 ,$$

where C_1–C_4 are the arbitrary constants which must be found from the following boundary conditions: the temperature on the bottle surface is T_s = const, i.e., $T_2(R_2) = T_s$; on the interior bottle surface, the conditions of continuity of the temperature and the heat flux

$$T_1 (R_1) = T_2 (R_1) , \quad \lambda_1 \frac{dT_1 (R_1)}{dr} = \lambda_2 \frac{dT_2 (R_1)}{dr} .$$

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must be fulfilled. From these conditions we obtain

$$C_1 = \frac{T_0(\xi) - T_s}{\dfrac{1}{\xi} - \dfrac{1}{R_1} + \dfrac{\lambda_1}{\lambda_2}\left(\dfrac{1}{R_1} - \dfrac{1}{R_2}\right)}, \quad C_2 = T_0(\xi) - C_1 .$$

On the crystallization front of the liquid, the temperature $T_1(\xi) = T_0$, where T_0 is the temperature of stable equilibrium of the ice–water phases. Furthermore, the Stefan condition must be fulfilled, which, at comparatively low pressures (of the order of tens of atmospheres), is written in the form

$$\lambda_1 \frac{dT_1}{dr}\bigg|_{r=\xi} = \rho L \frac{d\xi}{dt} .$$

In the spherical coordinate system with the origin at the center of the sphere, the strain **u** is directed along the radius and is a function of only r and ξ. The components of the strain tensor ε_r, ε_θ, and ε_φ are related to the displacement $u(r)$ by the formulas

$$\varepsilon_r = \frac{du}{dr}, \quad \varepsilon_\theta = \varepsilon_\varphi = \frac{u}{r} . \tag{1}$$

In what follows, we will consider only the case where the stresses and strains in solid shells are related by the Hooke law. Then the radial and tangential components of the stress tensor are expressed in terms of the displacement $u(r)$ by the relations [3]

$$\sigma_r = \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)\frac{du}{dr} + 2\nu\frac{u}{r}\right], \tag{2}$$

$$\sigma_\theta = \frac{E}{(1+\nu)(1-2\nu)}\left[\nu\frac{du}{dr} + \frac{u}{r}\right]. \tag{3}$$

The equilibrium equation is written in the form

$$\frac{d\sigma_r}{dr} + \frac{2}{r}(\sigma_r + \sigma_\theta) = 0 ,$$

and with account for (2) and (3) we obtain

$$u = ar + \frac{b}{r^2} . \tag{4}$$

The components of the stress tensor σ_r and σ_θ are expressed in terms of a and b by the formulas

$$\sigma_r = \frac{E}{(1+\nu)(1-2\nu)}\left[(1+\nu)\,a - 2\,(1-2\nu)\frac{b}{r^3}\right], \tag{5}$$

$$\sigma_\theta = \frac{E}{(1+\nu)(1-2\nu)}\left[(1+\nu)\,a + (1-2\nu)\frac{b}{r^3}\right]. \tag{6}$$

We now apply relations (2)–(6) to a system consisting of a liquid core and a two-layer solid shell, one of which is formed by ice, while the other is formed by the vessel walls.

Let, at a certain instant of time, the crystallization front of the liquid determined by the coordinate $r = \xi$ move to an infinitely small distance $d\xi$. Additional small displacements due to the increase in the volume of an infinitely thin crystallized ice layer occur in both the liquid core and the solid compound shell. Equality (4) for each medium is

$$\delta u\,(r) = \delta a r + \delta b\,\frac{1}{r}\,, \quad 0 \le r < \xi\,; \tag{7}$$

$$\delta u_1\,(r) = \delta a_1 r + \delta b_1\,\frac{1}{r}\,, \quad \xi < r < R_1\,; \tag{8}$$

$$\delta u_2\,(r) = \delta a_2 r + \delta b_2\,\frac{1}{r}\,, \quad R_1 < r < R_2\,. \tag{9}$$

We note that condition (8) loses its meaning when $\xi \to 0$, since ξ and $d\xi$ become quantities of the same order of smallness. Therefore, all the solutions which will be obtained below lose their meaning at the instant of disappearance of the liquid phase. To determine arbitrary constants one must formulate the boundary conditions.

When $r = 0$, the displacement in the liquid core must remain finite; hence, we must set $\delta b = 0$ in equality (7). On the bottle surface, the radial component of the stress is equal to zero, i.e., $\sigma_{r2}(R_2) = 0$. By virtue of this solution, equality (5) takes the form

$$(1 + \nu_2)\,\delta a_2 - 2\,(1 - 2\nu_2)\,\frac{\delta b_2}{R_2^3} = 0\,. \tag{10}$$

We now formulate the conjugation conditions at contact boundaries.

In crystallization of a water layer of thickness $d\xi$, the volume of the system increases by $4\pi\xi^2\beta d\xi$. Thus, an additional volume is rammed as it were between the liquid layer and the ice layer, as a result of which the liquid particles near the phase boundary produce radial displacements into the liquid core while the ice particles produce displacements in the opposite direction. This means that the displacements of the liquid and the ice undergo a discontinuity on the crystallization front. They are related by the relation

$$\delta u_1\,(\xi) - \delta u_2\,(\xi) = \beta d\xi\,;$$

with account for (7) and (8), it can be written in the form

$$\delta a_1 + \frac{\delta b_1}{\xi^3} - \delta a = -\,\beta\,\frac{d\xi}{\xi}\,. \tag{11}$$

The second condition which must be fulfilled at the water–ice phase boundary follows from the equality of the pressures on both sides of this boundary:

$$\delta p = -\,\delta\sigma_r\,(\xi)\,.$$

Taking account of the fact that the change in the pressure δp in the liquid core is related to the relative change in the volume div ($\delta\mathbf{u}$) by the relation

$$\delta p = -\,\frac{1}{K}\,\mathrm{div}\,(\delta\,\mathbf{u}) = -\,\frac{3\delta a}{K}\,,$$

we can write this condition as

$$(1+\nu_1)\,\delta a_1 - 2\,(1-2\nu_1)\,\frac{\delta b_1}{\xi^3} = \frac{3\,(1+\nu_1)\,(1-2\nu_1)}{KE_1}\,\delta a_1\,. \tag{12}$$

At the contact boundary between the ice and the interior bottle wall, the displacements and the pressures are continuous: $\delta u_1(R_1) = \delta u_2(R_1)$ and $\delta\sigma_1(R_1) = \delta\sigma_2(R_1)$, which leads to the following relations:

$$\delta a_1 + \frac{1}{R_1^3}\,\delta b_1 - \delta a_2\,\frac{1}{R_1^3}\,\delta b_3 = 0\,, \tag{13}$$

$$\delta a_1 - 2\,\frac{1-2\nu_1}{1+\nu_2}\,\frac{\delta b_1}{R_1^3} - \frac{E_2}{E_1}\,\frac{1-2\nu_1}{1-2\nu_2}\,\delta a_2 + \frac{2E_1}{E_2}\,\frac{1-2\nu_1}{1+\nu_2}\,\frac{\delta b_2}{R_1^3} = 0\,. \tag{14}$$

Thus, to determine six arbitrary constants we have the linear algebraic system of equations (10)–(14) in which only one equation (11) is inhomogeneous. Solving this system according to the Cramer formula, we obtain

$$\delta u = \frac{\beta}{3}\,\frac{n-mz}{A_1 n + B_1 mz}\,\frac{dz}{z}\,r\,,\quad 0 \le r \le \xi\,;$$

$$\delta u_1 = -\beta\,\frac{m}{KE_1}\left[(1-2\nu_1)\,r + (1+\nu_1)\,\frac{R_1^3}{2r^2}\right]\frac{dz}{A_1 n - B_1 mz}\,,\quad \xi \le r \le R_1\,;$$

$$\delta u_2 = -\beta\,\frac{3\,(1-\nu_1)}{KE_1\,(1+\nu_2)}\,\frac{R_1^3}{R_2^3}\left[(1-2\nu_2)\,r + (1+\nu_2)\,\frac{R_2^3}{2r^2}\right]\frac{dz}{A_1 n - B_1 mz}\,,\quad R_1 \le r \le R_2\,;$$

where

$$A_1 = 1 + \frac{3\,(1+\nu_1)}{2KE_1}\,;\quad B_1 = 1 - \frac{3\,(1-2\nu_1)}{KE_1}\,;\quad z = \frac{\xi^3}{R_1^3}\,;\quad m = 1 + \frac{1+\nu_1}{1+\nu_2}\,\frac{E_2}{E_1}\,\frac{R_1^3}{R_2^3} + \frac{2\,(1-2\nu_2)}{1+\nu_2}\,\frac{R_1^3}{R_2^3} - \frac{E_2}{E_1}\,\frac{1+\nu_1}{1+\nu_2}\,;$$

$$n = 1 + 2\,\frac{1-2\nu_1}{1+\nu_2}\,\frac{E_2}{E_1}\left(1 - \frac{R_1^3}{R_2^3}\right) + 2\,\frac{1-2\nu_2}{1+\nu_2}\,\frac{R_1^3}{R_2^3}\,.$$

Integrating these expressions from $z = 1$ to $z = \xi^3/R_1^2$, we find the total displacements produced by all the points of the system over the entire period of motion of the crystallization front from the interior bottle wall to $r = \xi$:

$$u\,(r) = \frac{\beta}{3A_1}\left[\ln\frac{\xi^3}{R_1^3} + \frac{9\,(1-\nu_1)\,\dfrac{KE_1}{KE_1 - 3\,(1-2\nu_1)}\ln M}{2KE_1 + 3\,(1+\nu_1)}\right] r\,,\quad 0 \le r \le \xi\,; \tag{15}$$

$$u_1\,(r) = \frac{\beta M}{KE_1 - 3\,(1-2\nu_1)}\left[(1-2\nu_1)\,r + (1+\nu_1)\,\frac{R_1^3}{2r^2}\right],\quad \xi \le r \le R_1\,; \tag{16}$$

$$u_2\,(r) = \frac{3\beta\,(1-\nu_1)\,M}{m\,(1+\nu_2)\,[KE_1 - 3\,(1-2\nu_1)]}\,\frac{R_1^3}{R_2^3}\left[(1-2\nu_1)\,r + (1+\nu_2)\,\frac{R_2^3}{2r^2}\right],\quad R_1 \le r \le R_2\,; \tag{17}$$

where

$$M = \ln \frac{A_1 n - B_1 m z}{A_1 n - B_1 m} . \tag{18}$$

For the pressure in the liquid core we have the formula

$$p = -\frac{\beta}{3KA_1}\left[\ln z + \frac{9\,(1-\nu_1)}{2KE_1 + 3\,(1+\nu_1)}\,\frac{KE_1}{KE_1 - 3\,(1-2\nu_1)}\ln M\right]. \tag{19}$$

From equalities (5) and (6) with account for (16) and (17) we obtain the components of the stress tensors:

$$\begin{gathered}
\sigma_{r1} = \frac{\beta M}{KE_1 - 3\,(1-2\nu_1)}\left[1 - 2\nu_1 - (1+\nu_1)\,\frac{R_1^3}{r^3}\right], \quad \xi \le r \le R_1 ; \\
\sigma_{\theta 1} = \frac{\beta M}{KE_1 - 3\,(1-2\nu_1)}\left[1 - 2\nu_1 + (1+\nu_1)\,\frac{R_1^3}{2r^3}\right], \quad \xi \le r \le R_1 ;
\end{gathered} \tag{20}$$

$$\begin{gathered}
\sigma_{r2} = \frac{3\beta M\,(1-\nu_1)}{m\,(1+\nu_2)\,[KE_1 - 3\,(1-2\nu_1)]}\,\frac{R_1^3}{R_2^3}\left[1 - 2\nu_2 - (1+\nu_2)\,\frac{R_2^3}{r^3}\right], \quad R_1 \le r \le R_2 ; \\
\sigma_{\theta 2} = \frac{3\beta M\,(1-\nu_1)}{m\,(1+\nu_2)\,[KE_1 - 3\,(1-2\nu_1)]}\,\frac{R_1^3}{R_2^3}\left[1 - 2\nu_2 + (1+\nu_2)\,\frac{R_2^3}{2r^3}\right], \quad R_1 \le r \le R_2 .
\end{gathered} \tag{21}$$

Formulas (16)–(21) solve the problem posed. They enable one to calculate the pressure in the liquid core and the stresses and strains developing in the walls of a spherically shaped bottle in the process of freezing of water in it.

Upon substitution of the corresponding values of the parameters into (18), it acquires a cumbersome form; however it can be substantially simplified when $\xi / R_1 > 0.5$.

The evaluations show that the expression under the logarithm in (18) differs little from unity; therefore, we can use the expansion

$$\ln x = x - 1 - \frac{(x-1)^2}{2} - \frac{(x-1)^3}{3} - \dots ,$$

which is observed when $0 < x \le 2$. Having restricted ourselves to the first term, we obtain

$$M \approx -\frac{B_1 m}{A_1 n - B_1 m}\left(1 - \frac{\xi^3}{R_1^3}\right).$$

In the same approximation, we can write

$$\ln \frac{\xi^3}{R^3} \approx -1 + \frac{\xi^3}{R_1^3} .$$

Then (15)–(17) in the first approximation take the form

$$u(r) = -\frac{\beta}{3} r \left\{ \frac{\left(1 - \frac{R_1^3}{R_2^3}\right)\left(1 - \frac{\xi^3}{R_1^3}\right)}{A_2 - B_2 \frac{R_1^3}{R_2^3}} + \frac{1}{2A_1} \left[1 + \frac{E_1}{E_2} \frac{m^2 B_1 (1 + \nu_2)^2}{K E_2 (1 - \nu_1) \left(A_2 - B_2 \frac{R_1^3}{R_2^3}\right)} \left(1 - \frac{\xi^3}{R_1^3}\right) \right] \right\}, \quad 0 \le r \le \xi ;$$

$$u_1(r) = \frac{\beta m (1 + \nu_2)}{3 K E_2 (1 - \nu_1) \left(A_2 - B_2 \frac{R_1^3}{R_2^3}\right)} \left[(1 - 2\nu_1) r + (1 + \nu_1) \frac{R_1^3}{2 r^2} \right] \left(1 - \frac{\xi^3}{R_1^3}\right), \quad \xi \le r \le R_1 ;$$

$$u_2(r) = \frac{\beta}{K E_2 \left(A_2 - B_2 \frac{R_1^3}{R_2^3}\right)} \frac{R_1^3}{R_2^3} \left[(1 - 2\nu_2) r + (1 + \nu_2) \frac{R_2^3}{2 r^2} \right] \left(1 - \frac{\xi^3}{R_1^3}\right), \quad R_1 \le r \le R_2 ;$$

where

$$A_2 = 1 + \frac{3(1 + \nu_2)}{2 K E_2} ; \quad B_2 = 1 - \frac{3(1 - 2\nu_2)}{K E_2} .$$

For the corresponding components of the stress tensor we obtain the following expressions:

$$\sigma_{r1} = \frac{\beta E_1 (1 + \nu_2)}{3 K E_2 (1 - \nu_1) \left(A_2 - B_2 \frac{R_1^3}{R_2^3}\right)} \left(1 - \frac{\xi^3}{R_1^3}\right) \left(1 - \frac{R_1^3}{r^3}\right), \quad \xi \le r \le R_1 ;$$

$$\sigma_{\theta 1} = \frac{\beta E_1 (1 + \nu_2)}{3 K E_2 (1 - \nu_1) \left(A_2 - B_2 \frac{R_1^3}{R_2^3}\right)} \left(1 - \frac{\xi^3}{R_1^3}\right) \left(1 + \frac{R_1^3}{2 r^3}\right), \quad \xi \le r \le R_1 ;$$

$$\sigma_{r2} = \frac{\beta}{K \left(A_2 - B_2 \frac{R_1^3}{R_2^3}\right)} \frac{R_1^3}{R_2^3} \left(1 - \frac{\xi^3}{R_1^3}\right) \left(1 - \frac{R_2^3}{r^3}\right), \quad R_1 \le r \le R_2 ; \tag{22}$$

$$\sigma_{\theta 2} = \frac{\beta}{K \left(A_2 - B_2 \frac{R_1^3}{R_2^3}\right)} \frac{R_1^3}{R_2^3} \left(1 - \frac{\xi^3}{R_1^3}\right) \left(1 + \frac{R_2^3}{2 r^3}\right), \quad R_1 \le r \le R_2 .$$

The breaking stresses $\sigma_{\theta 2}$ on the bottle surface increase in the process of freezing of water. If the ultimate tensile strength of the material from which the bottle is manufactured is attained, the material fails. We find the threshold value of the radius of the crystallization front of the liquid ξ_t at which the exterior surface of the bottle will be broken from the last formula of equalities (22), having set $r = R_2$ and $\sigma_{\theta 2} = \sigma_{cr}$ in it. We will have

$$\xi_t = R_1 \sqrt[3]{1 - \frac{2K\sigma_{cr}}{3\beta}\left(\frac{R_2^3}{R_1^3} A_2 - B_2\right)} \, . \tag{23}$$

The exterior bottle surface will be broken only when the radicand in (23) is positive. If it is less than zero, this will mean that the process of freezing of water in the bottle will be completed without its breaking.

Thus, the condition under which the freezing of water in a spherically shaped bottle cannot lead to its breaking can be written in the form

$$\frac{R_2}{R_1} \geq \sqrt[3]{\frac{1}{A_2}\left(B_2 + \frac{3\beta}{2K\sigma_{cr}}\right)} \, . \tag{24}$$

Freezing of Water in Cylindrically Shaped Bottles. In this case, just as above, the radial displacements are determined by formula (4) while the normal and tangential stresses are expressed in terms of the coefficients a and b as

$$\sigma_r = \frac{E}{1-\nu^2}\left[(1+\nu)\, a - (1-\nu)\, \frac{b}{r^2}\right], \quad \sigma_\theta = \frac{E}{1-\nu^2}\left[(1+\nu)\, a - (1-\nu)\, \frac{b}{r^2}\right].$$

The strains which develop in the bottle in symmetric displacement of the crystallization front of water to the cylinder axis are computed in just the same manner as in the case of the freezing of water in a spherically shaped bottle. The radial displacements are related to ξ in the following manner:

$$u(r) = \frac{\beta}{A'}\left[\ln \frac{\xi^2}{R_1^2} + \frac{4(1-\nu_1)}{KE_1 - 2(1-\nu_1)} M'\right] r, \quad 0 \leq r \leq \xi ;$$

$$u_1(r) = \frac{\beta M'}{KE_1 B' m'}\left[(1-\nu_1)\, r + (1+\nu_1)\, \frac{m' R_1^2}{r}\right], \quad \xi \leq r \leq R_1 ;$$

$$u_2(r) = \frac{2\beta(1-\nu_2)\, M'}{KE_1 B' m'} \frac{R_1^2}{R_2^2}\left[(1-\nu_2) r + (1+\nu_2)\, \frac{R_2^2}{r}\right], \quad R_1 \leq r \leq R_2 ;$$

$$M' = \ln \frac{A' n' - B' m' \dfrac{\xi^2}{R_1^2}}{A' n' - B' m'} , \quad A' = 1 + \frac{2(1+\nu_1)}{KE_1} , \quad B' = 1 - \frac{2(1-\nu_1)}{KE_1} ,$$

$$m' = 1 + \frac{1-\nu_2}{1+\nu_2} \frac{R_1^2}{R_2^2} - \frac{1+\nu_1}{1+\nu_2} \frac{E_2}{E_1}\left(1 - \frac{R_1^2}{R_2^2}\right), \qquad n' = 1 + \frac{1-\nu_2}{1+\nu_2} \frac{R_1^2}{R_2^2} + \frac{1+\nu_1}{1+\nu_2} \frac{E_2}{E_1}\left(1 - \frac{R_1^2}{R_2^2}\right).$$

For the pressure in the liquid core we obtain

$$p = -\frac{\beta}{KA'}\left[\ln \frac{\xi^2}{R_1^2} + \left(\frac{A'}{B'} - 1\right) M'\right]; \tag{25}$$

and for the components of the stress tensor we have

TABLE 1. Phase Diagram Water–Ice I

Solid phase	Pressure, atm	Equilibrium temperature, °C	$\Delta V = V_w - V_{ice}$, cm^3/mole
Ice I	1	0	–1.62
	610	–5	–1.83
	1130	–10	–2.02
	1590	–15	–2.195
	1970	–20	–2.195

$$\sigma_{r1} = \frac{\beta M'}{KB'm'}\left(1 - \frac{R_1^2}{r^2}\right), \quad \sigma_{\theta 1} = \frac{\beta M'}{KB'm'}\left(1 + \frac{R_1^2}{r^2}\right), \quad \xi \le r \le R_1 ,$$

$$\sigma_{r2} = \frac{2\beta E_2 M'}{KB'm'E_1(1+\nu_2)}\left(\frac{R_1^2}{R_2^2} - \frac{R_1^2}{r^2}\right), \qquad \sigma_{\theta 2} = \frac{2\beta E_2 M'}{KB'm'E_1(1+\nu_2)}\left(\frac{R_1^2}{R_2^2} + \frac{R_1^2}{r^2}\right), \quad R_1 \le r \le R_2 .$$

The radius of the crystallization front of the liquid ξ_t at which the exterior bottle surface will be broken is determined from the transcendental equation

$$\frac{KE_1\sigma_{cr}B'm'(1+\nu_2)}{4\beta E_2}\frac{R_2^2}{R_1^2} = \ln \frac{A'n' - B'm'\dfrac{\xi_t^2}{R_1^2}}{A'n' - B'm'} . \tag{26}$$

Hence, restricting ourselves to the first term in the expansion of the logarithm on the right-hand side of the equality, we obtain the approximate formula

$$\xi_t \approx R_1\left[1 - \frac{E_1}{4\beta E_2}\frac{R_2^2}{R_1^2}K\sigma_{cr}(1+\nu_2)(A'n' - B'm')\right]^{1/2} . \tag{27}$$

Just as above, the condition that the bottle will explode for none of the values of ξ_t in the process of crystallization of water can be written in the form

$$\frac{R_2}{R_1} \ge 2\sqrt{\frac{\beta E_2}{KE_1\sigma_{cr}(1+\nu_2)(A'n' - B'm')}} .$$

Substituting here the values of A', B', m', and n', we find

$$\frac{R_2}{R_1} > \left\{\frac{1 + \dfrac{2\beta}{K\sigma_{cr}} - \dfrac{2(1-\nu_1)(1-\nu_2)}{KE_2}}{1 + \dfrac{2(1-\nu_1)(1+\nu_2)}{KE_2}}\right\}^{1/2} . \tag{28}$$

Expression (28) can be employed, in particular, to evaluate the thickness of sewer pipes for which the freezing of water in them will not lead to their breaking.

From formulas (19) and (25) it is clear that the pressure in the liquid core increases infinitely when ξ/R_1 => 0, which is a consequence of the assumption of the constancy and positiveness of the coefficient β at all pressures. However, such an assumption is contradictory to the water–ice phase diagram.

TABLE 2. Elastic and Strength Characteristics of Materials from Which the Bottles Are Manufactured and the Limiting Values of the R_1/R_2 Ratio Keeping the Bottles from Exploding in Complete Freezing of the Water Filling Them

Material	$E \cdot 10^{-10}$, Pa	ν	$\sigma_{cr} \cdot 10^{-7}$, Pa	R_2/R_1	
				spherical bottle	cylindrical bottle
12Kh2N4A steel	19.5	0.23	125.6	1.11	1.248
2Kh13 steel	19.5–20.6	0.23–0.31	68.6	1.208	1.439
Copper alloy: Br. OTsS 6-6-3 (permanent-mold casting) Cu: 5.0–6.0 % Sn 5.0–7.0 % Zn 4.0–6.0 % Pb	9.18	0.23	18.4–25.5	1.56	1.95
STÉR-1-30 glass-cloth-based laminate	2.45	0.3	29.4	1.262	1.723
PTFE-3	9.8–12.7	0.3	2.9–3.9	2.78	4.616
Cast iron	1	0.3	1.5	3.43	5.58
Annealed aluminum	6.85	0.35–0.36	8.96–10.75	1.878	2.74
Ice	1	0.3			

As is well known, depending on the pressure, the liquid core can be in stable equilibrium only with certain polymorphic modifications of ice, denoted by I, III, IV, and VI in order of decrease in the pressure. Table 1 gives the relationship between the pressure, the melting temperature, and the change in the water volume in the case of equilibrium of water and ice I [4].

Further increase in the pressure leads to the appearance of successively ice III, IV, and VI. In all of these three modifications of ice, $\Delta V > 0$, i.e., at $p > 1970$ atm, the crystallization of water is accompanied by a decrease in the volume. It follows that, when the pressure in the liquid core attains its critical value p_{cr} = 1970 atm, which corresponds to the critical radius of the crystallization front ξ_{cr}, further decrease in ξ cannot lead to an increase in the pressure in the liquid core: as soon as a certain portion of water is crystallized, the pressure in the bottle decreases; the equilibrium temperature turns back to its critical value θ_{cr} = –20^{o}C, and the pressure turns back to p_{cr}. Thus, once the radius of the crystallization front attains its critical value, further freezing of water occurs at constant pressure in the liquid core and at a constant negative temperature of the ice–water equilibrium of –29^{o}C. This fact introduced substantial corrections into the formulas (19) and (25) obtained above, which hold only as long as the crystallization-front radius is larger than ξ_{cr}; with further freezing of water, the pressure p in the liquid core remains equal to p_{cr} all the time.

Setting $\sigma_{r1} = -p_{cr}$ in the first formula of (22), we find the critical value of the radius of the crystallization front:

$$\xi_{cr} = R_1 \left[1 + \frac{p_{cr}}{2\gamma} - \sqrt{\left(1 + \frac{p_{cr}}{2\gamma}\right)^2 - 1} \right], \tag{29}$$

where

$$\gamma = \frac{\beta E_1 (1 + \nu_1)}{3KE_2 (1 - \nu_1) \left(A_2 - B_2 \dfrac{R_1^3}{R_2^3} \right)}.$$

The crystallization of water in a spherically shaped bottle can lead to its breaking only when the value of ξ_t determined by formula (23) is higher than ξ_{cr}.

In the case of crystallization of water in cylindrically shaped bottles, instead of formula (29) we obtain

$$\xi_{cr} = R_1 \sqrt{1 - \frac{p_{cr} K A'}{\beta} \frac{A' n' - B' m'}{A' n' - B' m' - \gamma' B' m'}},$$

TABLE 3. Pressure in the Liquid Core for Different Radii of the Crystallization Front of Water (bottles made of 12Kh2N24 high-strength steel)

No.	ξ/R_1	p, MPa			
		spherical bottle		cylindrical bottle	
		$R_2/R_1 = 1.2$	$R_2/R_1 = 1.28$	$R_2/R_1 = 1.289$	$R_2/R_1 = 1.4$
1	0.9	93	81	68	68
2	0.85	124	123	104	105
3	0.8	169	168	141	143
4	0.77	197	197	164	167
5	0.76	207	206	172	175
6	0.75	–	–	180	183
7	0.73	–	–	196	200
8	0.72	–	–	201	–

where

$$\gamma' = \frac{4(1-\nu_1)}{KE_1 - 2(1-\nu_1)} .$$

Table 2 gives the elastic and strength characteristics of a number of materials taken from [5] and the limiting ratios of the radii R_2/R_1 calculated from formulas (23) and (28), beginning with which the complete freezing of water in spherically and cylindrically shaped bottles (manufactured from the above materials) will occur without breaking of the bottles.

It is clear from the table that in freezing of water in bottles with the same wall thickness and manufactured from the same materials, the bottles having a cylindrical shape are broken earlier.

Table 3 gives the pressures (calculated from formulas (19) and (25)) in the liquid core for different radii of the crystallization front of the liquid in the cases of the freezing of water in spherically and cylindrically shaped bottles manufactured from 12Kh2N4A high-strength steel. The calculations were carried out for two different thicknesses of the bottle walls.

When the dependence of the temperature of the ice–water phase equilibrium on the pressure is taken into account the equation of heat balance on the crystallization front, i.e., the Stefan condition, changes substantially. In the case of the crystallization of water in the spherically shaped bottle it takes the form

$$\frac{dQ}{dt} - 4\pi\xi^2\lambda_1 \left.\frac{dT}{dr}\right|_{r-\xi} = 4\pi\xi^2\rho L_1 \frac{d\xi}{dt} ,$$

where $Q = \frac{4}{3}\pi\rho c[273 - T_0(\xi)]\,\xi^3$ is the quantity of heat in the liquid core.

From the data of Table 1 it is clear that the relationship between the pressure and the temperature in ice–water phase equilibrium in the region of pressures to $p_{\rm cr} \approx 2000$ atm can be approximated by the linear function

$$T_0(\xi) = 273 - \alpha p , \tag{30}$$

where $\alpha = 0.01$ deg/atm and p is measured in atmospheres.

Thus, the quantity $Q(\xi)$ can be represented in the form

$$Q = \frac{4}{3}\pi\rho c\alpha p\xi^3 ;$$

then we obtain

$$\frac{dQ}{dt} = 4\pi\rho c\alpha\xi^2 \left(p + \frac{1}{3}\,\xi\,\frac{dp}{d\xi}\right)\frac{d\xi}{dt}\,. \tag{31}$$

Having substituted the value of $\left.\frac{dT}{dr}\right|_{r=\xi}$ and (31) into Eq. (3), we will have

$$\frac{d\xi}{dt} = \frac{\lambda_1 R_1\,[T_0(\xi) - T_\mathrm{s}]}{\rho L_1 \xi^2 \left[1 - \frac{R_1}{\xi} - \frac{\lambda_1}{\lambda_2}\left(1 - \frac{R_1}{R_2}\right)\right]\left[1 - \frac{c\alpha}{L}\left(p + \frac{1}{3}\,\xi\,\frac{dp}{d\xi}\right)\right]}\,, \tag{32}$$

where $p(\xi)$ is found from formula (19). The equation obtained determines the motion of the crystallization front of water only as long as the pressure in the liquid core is lower than the critical pressure.

The thickness of the ice layer h formed is found from the condition of vanishing of the crystallization-front velocity:

$$T_0(\xi) - T_\mathrm{s} = 0\,,$$

which can be written in the form

$$|\theta_\mathrm{s}| = \alpha p(\xi)\,,$$

where θ_s is the surface temperature of the bottle in $^\mathrm{o}$C. Hence we obtain

$$h(\theta_\mathrm{s}) = R_1\left[\frac{|\theta_\mathrm{s}|}{\alpha D} - \sqrt{\left(1 + \frac{|\theta_\mathrm{s}|}{\alpha D}\right)^2 - 1}\,\right],$$

where

$$D = \frac{2\beta E_1\,(1 + \nu_2)}{3KE_2\,(1 - \nu_1)\left(A_2 - B_2\,\frac{R_1^3}{R_2^3}\right)}\,.$$

When $\theta_\mathrm{s} < -20^\mathrm{o}$C, the water in the bottle freezes completely. The law of displacement of the crystallization front upon reaching the critical radius is also determined by Eq. (32), in which the pressure is now considered to be constant and equal to p_cr while the initial condition is specified in the form $\xi|_{t=0} = \xi_\mathrm{cr}$. The equation is easily integrated.

Analogously we solve the problem on freezing of water in cylindrically shaped bottles.

Thus, in the case of the freezing of water in closed thick-walled metallic bottles, a number of features arise which are related to the polymorphic modifications of ice with increase in the pressure. One of the most important features is the constancy of the pressure in the liquid core upon reaching of the critical radius ξ_cr by the crystallization front, which results in the disappearance of the known acoustic effect of crystallization of water related to the density change in phase transformations of substances [6].

The above calculations also yield that the maximum pressures which can be obtained in freezing of water in thick-walled bottles manufactured from high-strength steels are about 2000 atm irrespective of the bottle shape, which is in complete agreement with the data of [1].

NOTATION

T_1, T_2, and T_s, temperature of the ice shell of the walls of the bottle and its surface respectively, $^\mathrm{o}$C; t, time, sec; R_1 and R_2, internal and external radii of the bottle, cm; ξ, radius of the crystallization front of water, cm; λ_1 and λ_2, thermal conductivities of ice and the material of the bottle walls, J/(m·sec·deg); ρ, density of water, kg/m^3; L, specific heat of freezing of water, J/kg; τ, time of complete freezing of water in the bottle, min; r, θ, φ, spherical coordinates; **u**, displacement vector, cm; ε_r, ε_θ, and ε_φ, components of the strain tensor; σ_r, σ_θ, and σ_φ, components of the stress tensor; K, compressibility coefficient of water; E, Young modulus of the materials, Pa; E_1, Young modulus of ice, Pa; E_2, Young modulus of the material of the bottle walls, Pa; ν, Poisson coefficient; ν_1 and ν_2, Poisson coefficients of ice and of the bottle-wall material respectively; a and b, arbitrary constants; $u_1(r)$ and $u_2(r)$, displacements of the points of ice and the bottle, cm; δa, δa_1, δa_2, δb, δb_1, and δb_2, infinitely small arbitrary constants; β, coefficient of volumetric expansion of water in its freezing; K, compressibility coefficient of water, Pa^{-1}; p, pressure in the liquid core, Pa; ξ_t, value of the radius of the crystallization front of water for which the bottle is broken; δ_{cr}, breaking (tensile) strength of the wall material, Pa; p_{cr}, critical pressure, Pa; ξ_{cr}, critical radius of the crystallization front of water; c, heat capacity of water, J/(kg·K); T_s, surface temperature of the bottle, K; T_0, temperature of the ice–water phase equilibrium, K; h, thickness of the ice layer. Subscripts: t, break; cr, critical; s, surface; r, θ, φ, spherical coordinates; w, water; ice, ice.

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