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DYNAMICS OF THE BEHAVIOR OF A GAS-BUBBLE NUCLEUS IN A HETEROPHASE MEDIUM

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UDC 669.18:532.529

The behavior of the nucleus of a gas bubble in a heterophase medium is an important problem in the investigation of the evolution of gas-shrinkage porosity in alloys crystallized in a certain temperature interval [1-4] and in a study of dynamical and mass-transfer phenomena in gas–liquid systems moving through a porous disperse media [5-8]. The general solution of this type of problem under the conditions of inhomogeneity of the temperature and concentration fields and in the presence of convection motions of the liquid phase poses a complicated mathematical problem. We therefore confine the ensuing discussion to a simplified mathematical model of the growth of the nucleus of a gas bubble in a homogeneous quasiequilibrium zone of a binary alloy [9], generalizing the solution to the case of the growth of a gas bubble in an isothermal liquid-saturated porous disperse medium.

We consider the crystallization of a binary alloy containing dissolved gas. We assume that the volume occupied by the alloys is small enough for the internal thermal resistance of the substance to be neglected in comparison with the external thermal resistance and for the crystallization of the alloy to be regarded as a volume process. We neglect shrinkage effects in crystallization, assuming that the nucleation of a bubble is associated with the displacement of dissolved gaseous component by the growing solid phase, while the motion of the melt is elicited by the variation of the gas-bubble radius due to gas diffusion from the intercrystalline liquid. We also assume that the vapor density in the bubble interior is negligible in comparison with the density of the gas, the distance between the centers of the bubbles is much larger than the characteristic diameter d_1 of the dendritic (structural) cell, and the diameter $2r_p$ of the bubble itself is so small that the convective diffusion of the gas toward the bubble surface as a result of its ascension can be disregarded. The equations of continuity and momentum transfer have the following form in a spherical coordinate system attached to the center of the bubble [9]:

$$\frac{\partial}{\partial r}(r^2 f_l u) = 0; \tag{1}$$

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial r}\right) = -\frac{\partial p}{\partial r} - \frac{\mu f_l u}{K_p(f_l)} + \frac{\mu}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) - 2u\right], \tag{2}$$

where u is the velocity of the liquid, f_ℓ is the cross section of the liquid phase (porosity), p is the pressure in the liquid, $K_p(f_\ell)$ is the permeability of the heterogeneous zone, ρ is the density of the liquid, μ is the dynamic viscosity of the liquid, and r is the radial coordinate. Equations (1) and (2) must be integrated subject to the boundary conditions on the surface of the bubble ($r = r_p$):

Novosibirsk. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 4, pp. 68-76, July-August, 1986. Original article submitted June 17, 1985.

 0021-8944/86/2704-0538$12.50

$$u = \dot{r}_p; \tag{3}$$

$$p = p_g - 2\sigma/r_p - 4\mu\dot{r}_p/r_p. \tag{4}$$

Here $\dot{r}_p$ is the rate of change of the bubble radius, and p_g is the gas pressure in the bubble interior. We assume that the concentrations of the alloying component (C_1) and the gaseous component (C_2) far from the bubble ($r \to \infty$) are related to the cross section f_ℓ of the liquid phase by Scheil's rule [1]:

$$C_i = C_{i0}/f_l^{1-k_i}, \tag{5}$$

where k_i is the distribution coefficient of the i-th component. Neglecting the influence of dissolved gas, we specify the liquidus temperature in the form of a linear function of the concentration C_1: $T_\ell = T_A - \beta_{10}C_1$. It follows from the quasiequilibrium condition [1, 2] that

$$T = T_A - \beta_{10}C_1. \tag{6}$$

We obtain from Eq. (5) with i = 1 and from Eq. (6)

$$f_l = \left(\frac{T_A - T_{l0}}{T_A - T}\right)^{1/(1-k_1)}, \tag{7}$$

where $T_{\ell 0} = T_A - \beta_{10}C_{10}$.

We assume for definiteness that the cooling rate of the melt $v_T = \partial T/\partial t = \text{const}$, so that

$$T = T_{l0} - v_T t. \tag{8}$$

Then from Eq. (7) with allowance for (8) we have

$$f_l(t) = [1 + (v_T/\Delta T_0)\, t]^{-1/(1-k_1)},\ \Delta T_0 = T_A - T_{l0}. \tag{9}$$

Integrating Eqs. (1) and (2) subject to the boundary conditions (3) and (4), we obtain

$$u = r_p^2\dot{r}_p/r^2; \tag{10}$$

$$r_p\ddot{r}_p + \frac{3}{2}\dot{r}_p^2 + \nu\left[\frac{f_l r_p}{K_p(f_l)} + \frac{4}{r_p}\right]\dot{r}_p + \frac{2\sigma}{\rho r_p} = \frac{p_g - p_\infty}{\rho}. \tag{11}$$

Here p_∞ is the pressure far from the bubble, which is equal to the sum of the gas pressure above the surface of the melt and the metallostatic pressure at the level of the bubble, and $\nu = \mu/\rho$.

The distribution of the concentration of the gaseous components in the liquid surrounding the bubble is given by the convective diffusion equation [9], which we write with allowance for Eqs. (9) and (10) in the form

$$\frac{\partial C_2}{\partial t} + \frac{r_p^2\dot{r}_p}{r^2}\frac{\partial C_2}{\partial r} = \frac{D_2}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_2}{\partial r}\right) + \frac{k^* v_T/\Delta T_0}{1 + v_T t/\Delta T_0}C_2,\ k^* = \frac{1-k_2}{1-k_1}. \tag{12}$$

We augment this equation with the initial and boundary conditions

$$C_2|_{t=t_p} = C_{20}/f_{lp}^{(1-k_2)}; \tag{13}$$

$$C_2|_{r\to\infty} = C_{20}(1 + v_T t/\Delta T_0)^{k^*}, \tag{14}$$

where $f_{\ell p}$ is the cross section of the liquid phase at the instant t_p of nucleation of the bubble and is determined from the condition

$$p_{gp}(t_p) = p_\infty + 2\sigma/r_p^* \tag{15}$$

(r_p^* is the critical bubble radius). The gas bubble in the radius is related to the saturated gas concentration on the bubble surface according to Henry's law (j = 1) or Sievert's law (j = 2):

$$C(r_p, t) = K_j p_g^{1/j}, \; t \geqslant t_p. \tag{16}$$

From relations (5), (15), and (16) we find

$$f_{lp} = \left[C_{20}/K_j(p_\infty + 2\sigma/r_p^*)^{1/j}\right]^{1/(1-k_2)},$$

and from Eq. (9) with allowance for the latter expression,

$$t_p = \frac{\Delta T_0}{v_T}\{[C_{20}^{-1}K_j(p_\infty + 2\sigma/r_p^*)^{1/j}]^{k^*} - 1\}. \tag{17}$$

In the derivation of the expressions for $f_{\ell p}$ and t_p we have assumed that if the melt is an undersaturated gas solution in the initial state, the gaseous components are displaced into the surrounding liquid during the crystal growth process as a result of their weak solubility. The concentration C_2 then increases according to the law (5), attaining its saturation value at the time t_p. The nucleation of a gas bubble characterized by the equilibrium (critical) value of the radius r_p^* is possible in this case. The boundary condition on the bubble surface follows from the equation for the conservation of mass M of the gas inside the bubble:

$$\frac{dM}{dt} = FD_2\rho\frac{\partial C_2}{\partial r}\bigg|_{r=r_p}. \tag{18}$$

Since $M = (4\pi/3)r_p^3\rho_g$, $F = 4\pi r_p^2$, and the density ρ of the gas in the bubble is related to the pressure p_g by the ideal-gas equation of state $\rho_g = p_g/R_gT(t)$, after simple transformations we obtain from Eq. (18)

$$\frac{\partial C_2}{\partial r}\bigg|_{r=r_p} = \frac{r_p/3}{D_2\rho R_g T(t)}\left[\dot{p}_g + p_g\left(\frac{3\dot{r}_p}{r_p} + \frac{v_T}{T(t)}\right)\right]. \tag{19}$$

We have thus reduced the problem to the solution of the system (11), (12) subject to the conditions (13), (14), (16), (19).

The presence of the moving unknown boundary $r_p(t)$ complicates considerably the integration of the convective diffusion equation. We therefore transform to the new space variable

$$\xi = (r^3 - r_p^3)/3r_{p0}^3, \; \xi \in [0, \infty),$$

where r_{p0} is the initial bubble radius, the value of which can differ from r_p^* in the general case. Adopting r_{p0}, $t_0 = r_{p0}^2/D_2$, C_{20}, ΔT_0 as the scales for the corresponding physical quantities, we write Eq. (12) subject to the conditions (13), (14), (16), (19) in the dimensionless form

$$\frac{\partial C}{\partial \tau} = \frac{\partial}{\partial \xi}\left[(R^3 + 3\xi)^{4/3}\frac{\partial C}{\partial \xi}\right] + \frac{k^* w}{1 + w\tau}C; \tag{20}$$

$$C(\xi, \tau_p) = (1 + w\tau_p)^{k^*}; \tag{21}$$

$$C(\infty, \tau) = (1 + w\tau)^{k^*}, \; \tau > \tau_p; \tag{22}$$

$$\frac{\partial C}{\partial \xi}\bigg|_{\xi=0} = \frac{1}{R\Theta(\tau)}\left\{\frac{\dot{P}_g}{3} + \left[\frac{\dot{R}}{R} + \frac{w}{3\Theta(\tau)}\right]P_g\right\}; \tag{23}$$

$$C(0, \tau) = \bar{K}_j P_g^{1/j}, \; \Theta(\tau) = \Theta_A - 1 - w\tau, \; \Theta_A = T_A/\Delta T_0, \tag{24}$$

where $C = C_2/C_{20}$; $R = r_p/r_{p0}$; $\tau = t/t_0$; $\bar{K}_j = K_j p_0^{1/j}/C_{20}$; $w = v_T t_0/\Delta T_0$; $P_g = p_g/p_0$; $p_0 = R_g\rho C_{20}\Delta T_0$. The expression for P_g follows from (11):

$$P_g = P_\infty + K_\mu\left[\frac{f_l R}{K_{p1}(f_l)} + \frac{4}{R}\right]\dot{R} + \frac{K_\sigma}{R} + K_D(R\ddot{R} + 3\dot{R}^2/2). \tag{25}$$

Here $P_\infty = p_\infty/p_0$; $K_\mu = \mu/p_0t_0$; $K_D = \rho(D/r_{p0})^2/p_0$; $K_\sigma = 2\sigma/r_{p0}p_0$; $K_{p1} = K_p/r_{p0}^2$.

Influence of an Alternating External Pressure on the Evolution of a Bubble. We consider the dynamics of the behavior of a gas bubble in a heterogeneous region when diffusion processes can be neglected and the pressure p_∞ in the liquid varies with time as

$$p_\infty = p_\infty^0 - p_e \sin\omega(t - t_p). \tag{26}$$

Moreover, we assume that the gas in the bubble interior obeys the adiabatic law

$$p_g = p_{g0}(r_{p0}/r_p)^{3\gamma},\ p_{g0} = p_\infty^0 + 2\sigma/r_{p0}$$

(γ is the adiabatic exponent). In this case the problem reduces to the solution of Eq. (11) in conjunction with (26) under the initial conditions at $t_1 = 0$

$$r_p(0) = r_{p0},\ \dot{r}_p(0) = 0. \tag{27}$$

Here and elsewhere we refer time to the instant t_p ($t_1 = t - t_p$). We note that Eq. (11), in contrast with the familiar Rayleigh equation, contains not only the Stokes resistance ($4\nu\dot{r}_p/r_p$), but also the additional term $\nu f_\ell r_p \dot{r}_p/K_p(f_\ell)$, which characterizes the filtration resistance and depends on K_p and f_ℓ.

Assuming below that the crystals have a spherically symmetrical shape, we determine the permeability of the heterogeneous region according to [10

$$K_p = \zeta_0 f_l^3/(1-f_l)^{4/3},\ \xi_0 = d_1^2/64. \tag{28}$$

We investigate the case of small deviations of the bubble radius from its initial position, assuming that $p_e/p_\infty^0 \ll 1$. Let

$$r_p = r_{p0}(1+\varphi),\ |\varphi| \ll 1.$$

To within first-order terms, Eqs. (11) and (27) in conjunction with (26) and the latter relations acquire the form

$$\ddot{\varphi} + \nu\left[\frac{f_l}{K_p(f_l)} + \frac{4}{r_{p0}^2}\right]\dot{\varphi} + \frac{3\gamma}{\rho r_{p0}^2}\left[p_\infty^0 + \frac{2\sigma(3\gamma-1)}{3\gamma r_{p0}}\right]\varphi = \frac{p_e}{\rho r_{p0}^2}\sin\omega t_1, \tag{29}$$

$$\varphi(0) = 0,\ \dot{\varphi}(0) = 0.$$

Equation (29) describes the forced oscillations of the system with a variable dissipative force $\sim 2\delta = \nu[f_l(t)/K_p(f_l) + 4r_{p0}^2]$. Inasmuch as $\delta > 0$, the oscillations of the bubble are bounded as $t_1 \to \infty$ [11]. For sufficiently small cooling rates ($v_T \ll \Delta T_0\omega/2\pi$) the variation of the quantities f_ℓ, $K_p(f_\ell)$ during a time $t \le 2\pi\omega^{-1}$ can be neglected, and we can set $f_l = f_{lp} = (1 + w\tau_p)^{-1/(1-k_1)}$, $K_p(f_{lp}) = K_{p0} = \text{const}$. The damping factor is readily estimated in this case:

$$\delta_0 = 2^{-1}\nu\left[f_{lp}/K_{p0} + 4/r_{p0}^2\right], \tag{30}$$

along with the natural frequency of the bubble:

$$\omega_0 = \left\{\frac{3\gamma}{\rho r_{p0}^2}\left[p_\infty^0 + \frac{2\sigma(3\gamma-1)}{3\gamma r_{p0}}\right] - \delta_0^2\right\}^{1/2}. \tag{31}$$

The efficiency of the external action on the gas bubble depends on the nearness of the oscillation frequency of the pressure field to the natural frequency of the bubble. Using relations (30) and (31), we give numerical estimates of δ_0 and ω_0 for the alloy Fe + C, specifying $r_{p0} = 10^{-5}$ m, $f_{\ell p} = 0.5$, $K_{p0} = 10^{-11}$ m², $\gamma = 1.4$, and $p_\infty^0 = 1.1\cdot10$ N/m². The physical parameters of the alloys are taken equal to $\nu = 10^{-6}$ m²/sec, $\rho = 7\cdot10^3$ kg/m³, and $\sigma = 1.8$ N/m. Carrying out appropriate computations, we find $\delta_0 \cong 4.5\cdot10^4$ sec⁻¹ and $\omega_0 = 1.4\cdot10^6$ sec⁻¹. It is evident from this result that the natural frequencies decay rapidly ($t_1 \cong 10^{-5}$ sec) and the bubble then oscillates at the frequency of the external field and with the dimensionless amplitude

$$A_\varphi = (p_B/\rho r_{p0}^2)\left[(\omega_1^2 - \omega^2)^2 + 4\omega^2\delta_0^2\right]^{-1/2},$$

where $\omega_1^2 = 3\gamma\left[p_\infty^0 + 2\sigma(3\gamma - 1)/3\gamma r_{p0}\right]/\rho r_{p0}^2$. With an increase in the filtration resistance [decrease in $K_p(f_\ell)$] the damping factor increases, and the natural frequency decreases, tending to zero as $\delta_0 \to \omega_1$. With an increase in the amplitude of the external pressure p_e the amplitude of the oscillations increases. Its maximum value corresponds to $\omega = \omega_0$. In the case of sufficiently high values of p_e, bubble collapse (implosion) is possible. The cavitation of a gas bubble in a liquid is known [12] to be accompanied by high stresses, the values of which can exceed the tensile strength of the dendrite branches and cause them to fracture. An effect of this kind can be utilized to enhance the dispersity of the primary dendritic structure, which has a positive influence on the physical and mechanical properties of a solidifying metal. However, if the permeability of the zone in the given cross section is small and does not allow impregnation of the substance due to filtration of the melt, the resulting stresses can disrupt the integrity of the solidfying melt and lead to the formation of hot cracks.

Initial Stage of Bubble Growth with Gas Diffusion. We first consider the behavior of a gaseous inclusion in a constant pressure field ($\omega = 0$) at small times ($t \ll r_p^2/D$), when the perturbation of the concentration C_2 is restricted to a thin boundary layer satisfying the condition $r^3 - r_p^3 \ll r_p^3$. It is evident from the preceding analysis that the inertial forces in the case of slow processes (small ω) and large dissipation in the system exert a weak influence on the behavior of the bubble in the zone, and so we write Eq. (11) in an approximate form, discarding the first two terms $\sim\ddot{r}_p$ and $\dot{r}_p^2$:

$$\nu(f_l r_p/K_p + 4/r_p)\dot{r}_p + 2\sigma/\rho r_p = (p_g - p_\infty)/\rho \quad (p_\infty = p_\infty^0), \tag{32}$$

which is equivalent to neglecting the inertial terms on the left-hand side of Eq. (2). We set

$$R = r_p/r_{p0} = 1 + \varphi, \ |\varphi| \ll 1. \tag{33}$$

Substituting the latter in Eq. (32) and retaining only up to first-order terms, we obtain the following after conversion to dimensionless form:

$$P_g = K_\mu[4 + f_{lp}/K_p(f_{lp})]\dot{\varphi} - K_\sigma\varphi + P_\infty + K_\sigma. \tag{34}$$

We take $\tau_p = t_p/t_0$ as the origin of the dimensionless time τ, and we adopt the saturation gas concentration C_{2s} at the time τ_p as the new scale for the concentration C_2:

$$C_{2s} = \overline{K}_j P_{gp}^{1/j} = (1 + w\tau_p)^{k^*}.$$

Here τ_p is given by Eq. (17).

Linearizing Eqs. (20)-(24) as $\tau \to 0$, $\xi \to 0$ and taking Eqs. (33) and (34) into account, we obtain

$$\frac{\partial\overline{C}}{\partial\tau} = \frac{\partial^2\overline{C}}{\partial\xi^2} + w_1\overline{C}; \tag{35}$$

$$\overline{C}|_{\tau=0} = 1, \ \overline{C}|_{\xi=0} = P_{g0}^{*1/j}(1 + P_{g1}/jP_{g0}); \tag{36}$$

$$\overline{C}|_{\xi\to\infty} \to 1 + w_1\tau, \ [\partial\overline{C}/\partial\xi]_{\xi=0} = \Theta_p^{-1}d\chi(\tau)/d\tau, \tag{37}$$

where

$$\chi = P_{g0}(1 + w_2\tau) + (3P_{g0} - K_\sigma)\varphi + K_\mu^*\dot{\varphi}; \tag{38}$$

$$P_{g1} = K_\mu^*\dot{\varphi} - K_\sigma\varphi; \ K_\mu^* = K_\mu[4 + f_{lp}/K_p(f_{lp})], \tag{39}$$

$$P_{g0}^* = (P_\infty + K_\sigma)/(P_\infty + K_\sigma/R^*), \ R^* = r_p^*/r_{p0},$$

$$\overline{C} = C_2/C_{2s}, \ w_1 = k^*w/(1 + w\tau_p), \ w_2 = w/\Theta_p, \ \Theta_p = \Theta_A - 1 - w\tau_p.$$

To solve Eq. (35) subject to the conditions (36) and (37), we invoke the one-sided Laplace transform, with the result

$$\bar{C}(\xi,\tau)=(1+w_1\tau)\left[1-\frac{\Theta_p}{\sqrt{\pi}}\int_0^\tau \frac{(d\chi/d\zeta)(1-w_1\tau)\,e^{-\xi^2/4\sqrt{\tau-\zeta}}}{\sqrt{\tau-\zeta}}\,d\zeta\right]. \tag{40}$$

The solution (40) is written with allowance for the assumption $w_1\tau \ll 1$, in correspondence with which $\exp(\pm w_1\tau)$ is approximated by a linear function $\exp(\pm w_1\tau) \approx 1 \pm w_1\tau$. Setting $\xi = 0$ in Eq. (40), we write the relation in the form of an Abel integral equation

$$F(\tau)=\int_0^\tau \frac{\Phi(\zeta)}{\sqrt{\tau-\zeta}}\,d\zeta, \tag{41}$$

where $\Phi(\zeta) = (d\chi/d\zeta)(1 - w_1\zeta)$; $F(\tau) = \sqrt{\pi}[1 - \bar{C}(0, \tau)/(1 + w_1\tau)]/\Theta_p$. If we consider $F(\tau)$ to be a known function, we have the solution of Eq. (41)

$$\Phi(\tau)=\frac{1}{\pi}\left[\frac{F(0)}{\sqrt{\tau}}+\int_0^\tau \frac{F'(\zeta)}{\sqrt{\tau-\zeta}}\,d\zeta\right],$$

where the prime denotes differentiation with respect to ζ. We write this result with allowance for the expression for $\Phi(\tau)$ and the assumption $w_1\tau \ll 1$ in the form

$$\frac{d\chi}{d\tau}=\frac{1}{\pi}\left[\frac{1+w_1\tau}{\sqrt{\tau}}F(0)+\int_0^\tau \frac{F'(\zeta)(1+w_1\tau)}{\sqrt{\tau-\zeta}}\,d\zeta\right]. \tag{42}$$

Integrating Eq. (42) with respect to τ for $\chi(0) = P_{g0}$, $\varphi = \dot{\varphi} = 0$ and making use of expressions (38) and (39), we find

$$K_\mu^*\dot{\varphi}+(3P_{g0}-K_\sigma)\varphi=-w_2P_{g0}\tau-$$
$$-\frac{1}{\pi}\left[(1+w_1\tau)\int_0^\tau \frac{F(\zeta)\,d\zeta}{\sqrt{\tau-\zeta}}-2w_1\int_0^\tau F(\zeta)\sqrt{\tau-\zeta}\,d\zeta\right]. \tag{43}$$

Here $F(\tau) \simeq (\sqrt{\pi}/\Theta_p)[\Delta C_0^* - P_{g0}^{*1/j}w_1\tau - (P_{g0}^{*1/j}/jP_{g0})(K_\mu^*\dot{\varphi} - K_\sigma\varphi)]$; $\Delta C_0^* = 1 - P_{g0}^{*1/j}$; $F(0) = \sqrt{\pi}\Delta C_0^*/\Theta_p$.

Regarding the right-hand side of Eq. (43) as a known function of the variable τ, we integrate it with respect to τ for $\varepsilon(0) = 0$, neglecting small terms $\leq\tau^3$ and setting $(a_0\tau)^2 \ll 1$:

$$\varphi=(1-a_0\tau)\left[\frac{2a_1}{3}\tau^{3/2}-\frac{a_2}{2}\tau^2-a_3\int_0^\tau \frac{\varphi(\zeta)\,d\zeta}{\sqrt{\tau-\zeta}}+O(\tau^3)\right], \tag{44}$$

where $a_0 = (3P_{g0} - K_\sigma)/K_\mu^*$; $a_1 = 2\Delta C_0^*/(\sqrt{\pi}\Theta_p K_\mu^*)$; $a_2 = w_2 P_{g0}/K_\mu^*$; $a_3 = P_{g0}^{*1/j}/(j\sqrt{\pi}\Theta_p P_{g0})$.

We seek a solution of Eq. (44) by the method of successive approximations, taking $\phi = 0$ as the zeroth approximation. Stopping with the second approximation, we have

$$\varphi(\tau)=(1-a_0\tau)\left[\frac{2a_1}{3}\tau^{3/2}-\frac{1}{2}\left(a_2+\frac{\pi a_1 a_3}{2}\right)\tau^2+O(\tau^3)\right].$$

It is evident that in the isothermal case ($w = a_2 = 0$), when $\Delta C^* = a_1 = 0$ (the initial radius r_{p0} is equal to the critical r_p^*), the bubble is in an unstable equilibrium state. If $r_{p0} > r_p^*$ and it is dissolved if $r_{p0} < r_p^*$, consistent with [13]. Under nonisothermal conditions ($x \neq 0$, $a_2 \neq 0$) for $\Delta C_0^* = 0$ ($r_{p0} = r_p^*$) the bubble is dissolved, i.e., an equilibrium state does not exist. Bubble growth is possible when $r_{p0} > r^*$.

Numerical Solution. We use a numerical procedure to solve the problem of bubble growth with allowance for diffusion transfer of the dissolved gas. Neglecting the inertial terms in Eq. (25), as before, we write the basic system (20)-(25) in the dimensionless form

$$\frac{\partial C}{\partial\tau}=\frac{\partial}{\partial\xi}\left[(3\xi+R^3)^{4/3}\frac{\partial C}{\partial\xi}\right]+\frac{k^*w}{1+w(\tau_p+\tau)}C,\quad \tau\to\tau-\tau_p; \tag{45}$$

$$\dot{R} = (P_g - P_\infty - K_\sigma/R)/[K_\mu(f_l R/K_{p1} + 4/R)]; \quad (46)$$

$$\dot{P}_g = P_g\left[\frac{3(\Theta_A-\Theta)}{P_g} R \frac{\partial C}{\partial \xi}\bigg|_{\xi=0} - \frac{w}{\Theta_A - \Theta} - \frac{3\dot{R}}{R}\right]; \quad (47)$$

$$R|_{\tau=0} = 1, \ P_g|_{\tau=0} = P_\infty + K_\sigma, \ C|_{\tau=0} = 1; \quad (48)$$

$$C|_{\xi=0} = \bar{K}_j P_g^{1/j}, \ C|_{\xi\to\infty} = [1 + w\tau/(1+w\tau_p)]^{k^*}. \quad (49)$$

We determine an additional relation governing the value of $(\partial C/\partial\xi)_{\xi=0}$ from Eq. (45). Bearing in mind that C is bounded and has continuous first and second derivatives with respect to ξ in the domain $\xi \in [0, \infty)$, we multiply the left- and right-hand sides of Eq. (45) by $e^{-\lambda\xi}$ and integrate the result with respect to ξ from 0 to ∞:

$$\frac{\partial C}{\partial \xi}\bigg|_{\xi=0} = -\lambda C|_{\xi=0} - \frac{1}{R^4}\int_0^\infty e^{-\lambda\xi}\left\{\frac{\partial}{\partial\xi}\left[(3\xi + R^3)^{4/3}\frac{\partial C}{\partial \xi}\right] + \lambda C(R^3+3\xi)^{1/3}[4 - \lambda(R^3+3\xi)]\right\}d\xi \quad (50)$$

(λ is a positive constant). We replace the semiinfinite interval of integration in relation (5) by a finite interval ($0 \le \xi \le \xi^*$), and we write the integrand as

$$f_0 = \frac{1}{h}\left[(R^3+3h)^{4/3}\frac{C_2 - C_1}{h} - R^4\frac{\partial C}{\partial\xi}\bigg|_{\xi=0}\right] + \lambda C|_{\xi=0} R(4-\lambda R^3) \quad (\xi=0),$$
$$f_k = e^{-\lambda\xi_k}\left\{\frac{1}{h^2}\left[(R^3+3\xi_{k+1})^{4/3}(C_{k+2}-C_{k+1}) - (R^3+3\xi_k)^{4/3}(C_{k+1}-C_k)\right] + \lambda C_k(3\xi_k + R^3)^{1/3}[4 - \lambda(3\xi_k + R^3)]\right\} \quad (0 < \xi \le \xi^*), \quad (51)$$

where $h = \xi^*/N$; $k = 1, 2, \ldots, N$; $\xi_k = hk$; C_k is the value of C at the point ξ_k; and C_{N+1}, C_{N+2} are determined by linear interpolation. Replacing the integration operation in Eq. (50) by summation according to Waddell's rule and carrying out a transformation with allowance for the expression for the integrand from (51) and the value of $C|_{\xi=0}$ from (49), we obtain

$$\frac{\partial C}{\partial\xi}\bigg|_{\xi=0} = -\frac{10}{7}\lambda C|_{\xi=0} - \frac{3h}{7R^4}\left[(R^3+3h)^{4/3}\frac{C_2-C_1}{h^2} + \lambda C_0|_{\xi=0}(4-\lambda R^3) + 5f_1 + f_2 + 6f_3 + f_4 + 5f_5 + f_6 + \sum_{k=1}^{N/6-1}(f_{6k} + 5f_{6k+1} + f_{6k+2} + 6f_{6k+3} + f_{6k+4} + 5f_{6k+5} + f_{6k+6})\right]. \quad (52)$$

The system (45)-(47) subject to the conditions (48), (49), (52) is solved by the method of lines [14]. Accordingly, we approximate the derivatives in Eq. (45) by the corresponding finite differences:

$$\dot{C}_1 = \frac{1}{h}\left[(R^3+3h)^{4/3}\frac{C_2-C_1}{h} - R^4\frac{\partial C}{\partial\xi}\bigg|_{\xi=0}\right] + \frac{k^* w}{1+w(\tau_p+\tau)}C_k,$$
$$\dot{C}_k = \frac{1}{h^2}\left[(R^3+3\xi_k)^{4/3}(C_{k+1}-C_k) - (R^3+3\xi_{k+1})^{4/3}(C_k - C_{k-1})\right] + \frac{k^* w}{1+w(\tau_p+\tau)}C_k, \quad k = 2, 3, \ldots, N.$$

These equations in conjunction with (46), (47), and (52) represent a system of ordinary differential equations, which we have solved numerically on a BÉSM-6 computer by the Runge–Kutta method.

As an example, we consider the behavior of a gas bubble in a heterogeneous zone of the alloy Fe + 0.5% C + $2\cdot10^{-3}$ H_2. The initial data are $k^* = 1.276$, $p_\infty = 1.1\cdot10$ N/m², $\sigma = 1.85$ N/m, $\nu = 10^{-6}$ m²/sec, $D_2 = 1.2\cdot10^{-7}$ m²/sec, $r_{p0} = 10^{-5}$ m, $v_T = 10^3$ °C/sec. Some results of

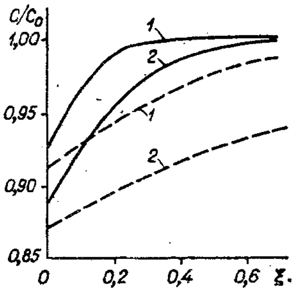

Fig. 1

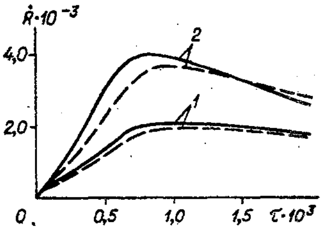

Fig. 2

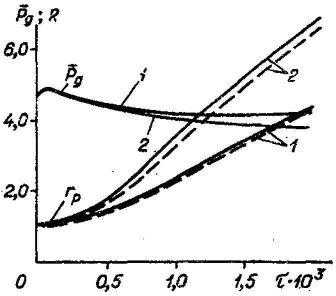

Fig. 3

the computations are given in Figs. 1-3. Figure 1 shows the distribution of the relative concentration along the coordinate ξ for $\tau = 10^{-3}$ and $2\cdot10^{-3}$ (solid and dashed curves) at $f_{\ell p} = 0.2$ and 0.3 (curves 1 and 2), Fig. 2 shows the variation of the dimensionless bubble growth rate $\dot{R}$, and Fig. 3 shows the time variation of the dimensionless values of the bubble radius R and the gas pressure $\bar{p}_g = p_g/p_a$ in the bubble interior for $r_{p0}/r_p^* = 1.025$, $f_{\ell p} =$ 0.2 and 0.3 [curves 1 and 2; the solid lines correspond to the inclusion of inertial terms in Eq. (11)]. It is evident from Fig. 2 that the growth rate $\dot{R}$ increases in the initial stage according to a law close to $\sqrt{\tau}$ and then diminished quite rapidly after attaining a certain maximum, tending to zero as $\tau \to \infty$. The characteristic period of the evolution of this process is $\sim 3\cdot10^{-6}$ sec. The bubble radius increases by a factor of ~ 6 during this time. The influence of the cooling rate for values of $v_T \lesssim 10^3$ °C/sec is only slightly manifested in the behavior of the bubble, because f_ℓ and $K_p(f_\ell)$ vary insignificantly during the time $\sim 10^{-6}$ sec. The inclusion of inertial terms in the generalized Rayleigh equation (11) has a significant effect on the bubble-growth dynamics for $f_{\ell p} \gtrsim 0.2$, when the filtration resistance becomes sufficiently small (see Figs. 2 and 3).

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FLOW OF MATTER ONTO THE SURFACE OF A CRYSTAL UNDER CONDITIONS OF TURBULENT NATURAL CONVECTION

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UDC 532.526

In this work, the rate of growth of crystals from the gas phase under conditions of turbulent natural convection is determined.

The flow of matter onto the surface of a growing crystal is caused by a gradient, created by a corresponding temperature gradient in the medium, of the concentration of the active component in the gas phase. This could result in natural convection, whose effect on the rate of growth of the crystal also depends on the orientation of the system. The growth of crystals in vertical cylindrical ampuls is studied below. In this case, unstable stratification must exist in the gas phase in order for natural convection to arise, and this happens, for example, when the source ("hot" surface) is situated near the substrate ("cold" surface). It is assumed below that the natural convection is turbulent. We note that the conditions necessary for this are partially realized in practice. Like in [1], it is assumed that the gas phase is a binary mixture of active and inert components.

In the presence of turbulent pulsations the time-averaged rate of growth of the crystals, i.e., the velocity of the gas–solid interface, is given by the expression

$$\zeta = -\frac{\rho}{\rho^*}\left(v_n + \frac{1}{\rho}\langle \rho' v_n' \rangle\right), \quad \rho^* \gg \rho. \tag{1}$$

Here ρ and v_n are the average density and the component of the velocity of the gas phase normal to the front; ρ^* is the density of the crystal (ρ^* = const); and the prime indicates pulsation. Thus in order to find ζ it is necessary to know the velocity distribution in the gas phase and the correlation $\langle \rho' v_n' \rangle$. We shall confine our attention to the case when the gas density is a linear function of the temperature T, $\rho'/\rho = -\beta T'$ (β is the coefficient of volume expansion).

As the crystals grow the radial variation of the average temperature T is negligible compared with the variation along the axis. In addition, the Reynolds numbers, constructed based on the average velocity of the directed flow, are low (Re $\sim$ 1). Thus in this case the turbulence is determined by the effect of thermogravitational forces only. Under these conditions the balances of the second moments of the pulsations of the velocity and temperature [2, 3], written in the Boussinesq approximation, have the form

$$\frac{k}{l} E^{1/2}\langle v_x' v_r' \rangle + \beta g \langle v_r' T' \rangle = 0, \tag{2}$$

$$\frac{k}{l} E^{1/2}\langle v_x' v_\varphi' \rangle + \beta g \langle v_\varphi' T' \rangle = 0, \quad \frac{k}{l} E^{1/2}\langle v_r' v_\varphi' \rangle = 0,$$

Moscow. Translated from Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, No. 4, pp. 76-78, 1986. Original article submitted May 30, 1985.

 0021-8944/86/2704-0546$12.50