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DETERMINATION OF CERTAIN PHYSICAL PROPERTIES OF A SOLID ON THE BASIS OF THE INTERATOMIC INTERACTION POTENTIAL

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UDC 539.2

The method of computing the dependence of the specific volume of a solid on the pressure and temperature on the basis of the interatomic interaction potential, which is a function of the internal atom energy, is considered. The results obtained are compared with experimental data.

The interaction potential of atoms of a condensed body, which is a function of the atom internal energy, is obtained in [1, 2]. In conformity with this potential, the force f with which a given atom acts on another atom at a remote distance r can be represented as follows

$$f = a\left[(h_0/r)^{\alpha+2} - (h_0/r)^{\beta+2}\right] + bE\,(h_0/r)^{\gamma+2}. \tag{1}$$

Here h_0 is the spacing between two isolated atoms in the equilibrium state ($f = 0$) at an absolute zero temperature ($E = 0$), and α, β, γ, a, b are positive constants.

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The potential mentioned follows from the linear dependence between the mean atom energy E of a condensed body measured from the zero level in a coupled coordinate system, and the energy q emitted by the atom per unit time:

$$q = \varepsilon E. \tag{2}$$

The equation of state of condensed bodies is obtained [1] on the basis of (1), from which the Hooke's, Grüneisen, and linear expansion laws under heating follow. Relationship (2) permits obtaining a heat-conduction integrodifferential equation [2, 3], from which the Fourier heat-conduction equation and a hyperbolic equation used to describe highly intense heat-transport processes [4] follow, in the limit, for an increase in the atom density and the thermal carrier velocities.

It can be shown that dependence (2) is a corollary of the spectral law of atom radiation according to which atoms at the i-th energy level in the frequency ν in the coupled coordinate system, radiate the energy quantas $h\nu$ per unit time [2, 3]

$$q_{i\nu} = \varepsilon_\nu N_{i\nu} ih\nu, \tag{3}$$

where N_{i_ν} is the number of particles at the i-th energy level, and $\varepsilon_\nu \neq \varepsilon_\nu(i)$. Let us note that relationship (3) permits obtaining the Planck formula for the emissivity of a blackbody and the fundamental statistical distribution laws [2, 3].

In statistical thermodynamics a quantum oscillator whose energy, measured from the zero level, can take on the values $E_{i_\nu} = ih\nu$, $i = 0, 1, \ldots$, is set in correspondence to each of the three degrees of freedom of the atom, where the mean oscillator energy is

$$E_\nu = h\nu/[\exp(h\nu/kt) - 1]. \tag{4}$$

In conformity with (3), the radiation energy per unit oscillator with frequency ν is

$$q_\nu = \varepsilon_\nu E_\nu. \tag{5}$$

The exact frequency distribution of the atom vibrations of a solid is not known [5]. Following Debye, we assume that the oscillations with frequency less than ν_D are distributed by a formula known from classical physics, according to which the possible number of electromagnetic waves per unit volume with frequencies in the range from ν to $\nu + d\nu$ is $8\pi\nu^2 d\nu/c^3$, where c is the velocity of light. Oscillations with frequencies greater than ν_D do not exist. The frequency ν_D is selected so that the total number of oscillations would equal the number of degrees of freedom of the atoms per unit volume, i.e., thrice the density of the atoms:

$$3n = \int_0^{\nu_D} \frac{8\pi\nu^2 d\nu}{c^3} = \frac{8\pi}{3c^3}\nu_D^3. \tag{6}$$

Taking (4) into account, the specific internal energy U is determined by the integral

$$U = \int_0^{\nu_D} E_\nu \frac{8\pi\nu^3 d\nu}{c^3} = \frac{8\pi k t^4}{c^3 h^3} \int_0^{h\nu_D/kt} \frac{x^3 dx}{e^x - 1} = 9n \frac{kt^4}{\Theta} \int_0^{\Theta/T} \frac{x^3 dx}{e^x - 1}. \tag{7}$$

The expression obtained, in which $\Theta = h\nu_D/kt$ (the Debye temperature) and $x = h\nu/kt$ are used, agrees with the Debye formula [5].

The radiation energy of n atoms is

$$Q = \int_0^{\nu_D} \varepsilon_\nu E_\nu \frac{8\pi\nu^2 d\nu}{c^3} = \varepsilon U, \tag{8}$$

where the mean coefficient of radiation is

$$\varepsilon = \int_0^{\Theta/t} \frac{\varepsilon_\nu x^3 dx}{e^x - 1} \Bigg/ \int_0^{\Theta/t} \frac{x^3 dx}{e^x - 1}.$$

Dividing (8) by n, we arrive at (2). For $t > \Theta$, the expression $q = \varepsilon_1 t$, $\varepsilon_1 \approx \text{const}$, follows from (2), which was found in studying the heat-conduction mechanism [6]. Relationship (2) is valid for atoms within a solid which release practically all the energy being absorbed because of radiation. The atoms located on the body boundary possess a substantially greater freedom of motion, and in some respects their state approaches the state of the gas. A significant part of the energy they absorbed goes over into kinetic energy and is transferred to adjacent atoms because of collisions.

To set up a relationship between the atom interaction force f and the thermodynamic parameters we use the following model. The solid is a right circular cylinder which is placed in a yoke preventing the possibility of movement of the body atoms in a radial direction. As the normal stress σ changes on the cylinder endfaces, or as its temperature changes, the atoms move along the cylinder axis z. The atoms with density n_0 move uniformly on the planes z_j $(j = 0, 1, \ldots)$ parallel to the endface surface of the cylinder $z = z_0 = 0$, whose area is sufficiently large.

Let us find the interaction force R_{gj} of an atom in the plane z_g with all the atoms in the layer z_j. The resultant interaction force dR_{gj} between an atom with the coordinates $z = z_g$, $y = 0$, $y \perp z$, and the atoms in the area element $2\pi y dy$ in the z_j plane is

$$dR_{gj} = 2\pi y dy n_0 \frac{z_{gj} f \sqrt{z_{gj}^2 + y^2}}{\sqrt{z_{gj}^2 + y^2}}, \quad z_{gj} = z_j - z_g.$$

Integrating dR_{gj} over the whole z_j plane, we obtain

$$R_{gj} = \int\limits_{y=0}^{\infty} dR_{gj} = 2\pi n_0 h_0^2 \left\{ a \left[\frac{1}{\alpha+1} \left(\frac{h_0}{\zeta_{gj}} \right)^{\alpha} - \frac{1}{\beta+1} \left(\frac{h_0}{\zeta_{gj}} \right)^{\beta} \right] + \frac{bE}{\gamma+1} \left(\frac{h_0}{\zeta_{gj}} \right)^{\gamma} \right\} \frac{z_{gj}}{\zeta_{gj}}, \quad \zeta_{gj} = |z_{gj}| = |z_j - z_g|. \tag{9}$$

For convenience in the calculations it is expedient to represent (9) in the form

$$R_{gj} = A \left[\left(\frac{h_1}{\zeta_{gj}} \right)^{\alpha} - \left(\frac{h_1}{\zeta_{gj}} \right)^{\beta} \right] + BE \left(\frac{h_1}{\zeta_{gj}} \right)^{\gamma}, \tag{10}$$

where

$$h_1 = h_0 \left(\frac{\beta+1}{\alpha+1} \right)^{\frac{1}{\alpha-\beta}}, \quad A = 2\pi n_0 h_0^2 a \frac{1}{\alpha+1} \left(\frac{\alpha+1}{\beta+1} \right)^{\frac{\alpha}{\alpha-\beta}},$$
$$B = 2\pi n_0 h_0^2 b \frac{1}{\gamma+1} \left(\frac{\alpha+1}{\beta+1} \right)^{\frac{\gamma}{\alpha-\beta}}.$$

Besides the interatomic interaction forces, surface Φ and mass F forces can act on the body particles in the z axis direction. If a stress σ acts on the cylinder endface, then the mean value of the surface force Φ_0 per unit atom of the outer layer $z = z_0 = 0$ is $\Phi_0 = \sigma/n_0$. The equilibrium equation for an arbitrary body particle projected on the z axis can be written as follows:

$$\sum_j R_{gj} + \Phi_g + F_g = 0, \tag{11}$$

where

$$\Phi_g = \begin{cases} \dfrac{\sigma}{n_0} & \text{for} \quad g = 0, \\ 0 & \text{for} \quad g \neq 0. \end{cases}$$

For simplicity we henceforth neglect the mass force F_g.

The summation in (11) should be over all possible values j. However, function R_{gj} should diminish rapidly as ζ_{gj} grows, hence, the spacing $H_j = z_{j+1} - z_j$ between adjacent atoms is practically independent of j for sufficiently large z_j (when $j \geq J$)

$$H_j = H_J = \text{const} \quad \text{for} \quad j \geqslant J. \tag{12}$$

Condition (12) is confirmed both by the results of computations for different values of J $(30 < J < 150)$ and by the known experimental fact about the independence of the macroscopic body density from their size for invariant external pressure and temperature.

By virtue of (12), it is sufficient to retain terms for which $\zeta_{gj} \leq JH_j$ in (11) for the g-th layer when calculating the sum $\sum_j R_{gj}$. Solution of system (11), (12) permits determination of H_g, $g = 0, 1, \ldots, J$, and

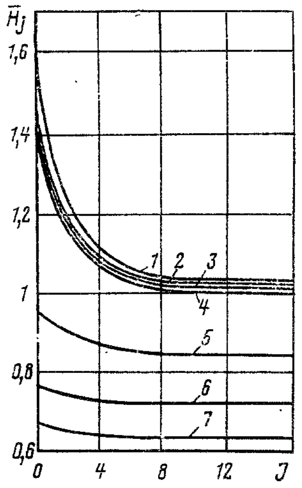

Fig. 1. Dependence of the relative spacing H_j between iron atom layers on the ordinal number of the layer j along the z axis for different stresses σ and temperatures t: 1) t = 0, $\sigma = 0.05 \cdot 10^{11}$ N/m^2; 2) 873°K and 0; 3) 573 and 0; 4) 0 and 0; 5) 0 and $-0.5 \cdot 10$; 6) 0 and $-1.5 \cdot 10^{11}$; 7) -0 and $-3 \cdot 10^{11}$.

$z_g = \sum_{j=0}^{g-1} H_j$, if the A, B, h_1, α, β, γ, Φ_g, and F_g are known.

The method of successive approximations, which can be used to determine the macroproperties of bodies on the basis of an interatomic interaction potential of any kind, is proposed for the solution of the system of nonlinear equations (11) and (12). The method consists of the successive determination of H_g^m for g = 0, 1, . . . , J in the approximations m = 2, 3, ... The first approximation H_g^1 for spacings between atom layers along the z axis can be selected arbitrarily. The determination of H_g^m in the approximation m on the basis of the value H_g^{m-1} is the m-th major cycle of iteration. Each major cycle of iteration consists of J + 1 minor cycles of iteration. This latter is related to determination of the spacing H_g^m, g = 0, 1, . . . , J, on the basis of (11) written for the layer g.

All the spacings except H_g in the minor iteration cycle are considered invariant: $H_j = H_j^m$ for j = 0, 1, . . . , g − 1 and $H_j = H_j^{m-1}$ for j = g + 1, g + 2, . . . , J. In a first approximation, the spacing $H^m_{g(1)}$ is assumed to equal H_g^{m-1}. To determine $H^m_{g(s)}$ in the approximation s, the value $w_{g(s-1)}$ in the left side of [11] is calculated for $H_g^m = H^m_{g(s-1)}$. The deviation of the value $w_{g(s-1)}$ from zero is used as the mismatch signal between $H_{g(s-1)}$ and the desired value of the spacing in this cycle H_g^m which assures satisfaction of [11]. The spacing $H_{g(s)}$ is determined from the relationship

$$H^m_{g(s)} = H^m_{g(s-1)} + \frac{w_{g(s-1)}}{V^m_{g(s-1)}}. \tag{13}$$

The rate of change V_g of the function w_g in H_g is determined by the difference relationship

$$V^m_{g(s)} = \left| \frac{H^m_{g(s)} - H^m_{g(s-1)}}{w_{g(s)} - w_{g(s-1)}} \right|, \quad s \geqslant 2,$$

where $V^m_{g(s)} = V^{m-1}_{g(s-1)}$ for s = 1.

The process of evaluating H_g^m ceases and it becomes

$$H^m_g = H^m_{g(s)} \quad \text{for} \quad \left| \frac{H^m_{g(s)} - H^m_{g(s-1)}}{H^m_{g(s)}} \right| < \delta, \tag{14}$$

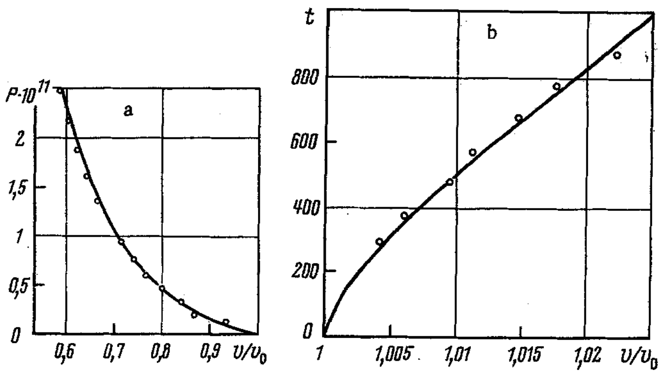

Fig. 2. Change in the relative volume v/v_0 of an iron cylinder in a rigid yoke due to the pressure p, N/m (a) and due to the temperature t, °K (b).

where δ is a certain small positive number. The number M of major iteration cycles is determined by a condition which is analogous to (14):

$$\left| \frac{(z_J^M - z_J^{M-1})}{z_J^M} \right| < \delta.$$

Results of solving system (11)-(12) for iron are represented in Figs. 1 and 2 for different values of the stress σ and the temperature t, °K. The following values are taken for the parameters characterizing iron atom interaction: $A = 1.604 \cdot 10^{-10}$ N; $B = 0.3146 \cdot 10^9$ 1/m; $\alpha = 4.1$; $\beta = 1.01$; $\gamma = 0.92$; $h_1 = 4.51 \cdot 10^{-10}$. Let us note that the dimensionless magnitude of the spacing H_j/h_i was determined during the calculation. The numerical value of h_1 is obtained by starting from the fact that the mean spacing H_J^0 between adjacent iron atom layers is

$$H_J^0 = n^{-3} = \sqrt[3]{\mu/\rho_0 N \cdot 10^3} = 2.27 \cdot 10^{-10} \text{ m}$$

for a pressure $p = 0$ and temperature $t = 0$, where $\mu = 55.85$ is the atomic weight of iron, N is Avogadro's number, $N = 6.0228 \cdot 10^{-23}$, ρ_0 is the density of iron at $p = 0$ and $t = 0$. In conformity with tabulated data, the Debye temperature Θ is taken equal to 453 °K.

Values of the exponents [1, 2] α, β, and γ are determined on the basis of the equation of state of condensed bodies because of comparing theoretical and experimental values of the parameters on the boundary curve for twelve different fluids (including water, mercury, ammonia, and sodium). The exponent α for these fluids varies within the limits $3 < \alpha < 6$, while the quantity β is almost one, and the difference $\beta - \gamma$ turns out to be practically constant and equal to 0.09 [1]. Although the values of α, β and γ for solid iron are obtained by a different means, they are nevertheless in conformity with their values for fluids.

It is seen from Fig. 1 that the relative magnitude of the spacing $\bar{H}_j = H_j/H_i^0$ along the z axis stabilizes sufficiently rapidly for different stresses and temperatures, and remains practically constant for $J > 15$.

The solution of system (11)-(12) permits the determination of a dependence between the stress σ on the cylinder endface and its relative volume v/v_0, where v is the specific volume of iron and v_0 is the specific volume of iron at $\sigma = 0$ and $t = 0$. Experimental data [6] available in the literature set up a relationship between the uniform external pressure p and the relative volume v/v_0. To compare the computed and experimental data we use the relationship, known from elasticity theory, between the quantities σ and p (to which identical changes in the specific volume correspond)

$$\sigma = p \cdot 3 \frac{1 - \mu}{1 + \mu},$$

where the Poisson's ratio μ is a function of temperature.

Results of computing the relative volume v/v_0 of the iron cylinder under consideration are represented by solid lines in Figs. 2a and b as a function of the pressure p and temperature t, respectively. The points are the superposed experimental results: obtained in [7] in Fig. 2a, and presented in tables which characterize the dependence of the density of the free iron body ρ on the temperature in Fig. 2b. Here we use the relationship

$$\frac{v}{v_0} = 1 + \left(\frac{\rho_0}{\rho} - 1 \right) \frac{1+\mu}{3(1-\mu)},$$

which governs the relation between the relative volume v/v_0 of the cylinder in a rigid yoke, on the one hand, and the relative density ρ/ρ_0 ($\rho_0 = 1/v_0$) of the free body from the same material, on the other, for a given temperature t when there are no external forces ($p = 0, \sigma = 0$).

It follows from Fig. 2 that the computed and experimental results are in good agreement. These data can be used to determine the dependence of the elastic moduli, the coefficient of thermal expansion, and some other physical characteristics as a function of the pressure and temperature.

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ANALYSIS OF THERMAL MODEL OF THE CONTACT HEAT TRANSFER OF ROUGH SURFACES

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A thermal model of the contact heat transfer between rough surfaces is considered, taking into account curvature of the current lines in the gaps. Theoretical relations determining the contact thermal resistance at small pressures are obtained.

Formulation of the Problem

One of the parameters which has a significant effect on the thermal conditions in apparatus is the contact thermal resistance (CTR) due to imperfections of the mechanical connection between the contacting surfaces.

In [1-4] a detailed analysis was made of the results of investigations of CTR by Soviet and non-Soviet authors, the mechanism of contact was explained, the physical basis of the heat transfer through the contact zone was discovered, and practical recommendations for the intensification of heat transfer were given. However, as the forms of real mechanical connections are so different and so complex, it is often a laborious task to use the results of [1-4] for the calculation of CTR. There are several reasons for this:

a) the theoretical relations are only adequately reliable for the simplest case of contacting-object geometry — tangency of plane surfaces;

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