

EQUATIONS OF STATE OF THE ELASTIC ENERGY
OF METALS IN THE CASE OF A NONSPHERICAL
STRAIN TENSOR

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Interpolation expressions of the equations of state and the coefficient of thermal conductivity are presented for iron (α -phase), aluminum, nickel, lead, and titanium. These expressions constitute a new way of writing the equations of state presented in [1]. The expression for the "cold energy" is interpolated within the compression interval $0.9 \leq \delta \leq 2.0$ in such a way that the cold pressure and the square of the velocity of sound would be polynomials of powers $\delta - 1$.

1. The objective of this work is to reduce the equation of state to a form which is convenient in the study of processes in a transition region, when the pressure is still close to unity, but nonlinear processes are already significant. In this region we cannot confine ourselves to the consideration of the spherical strain tensor. Therefore we must introduce, into the cold energy of the material, a term which takes into account the distortion energy. This term is introduced in such a way that the energy of cold deformation in the case of small strains would coincide with the cold energy used in the linear theory of elasticity. In the case of comparatively small compressions and small deviators of the strain tensor, the expressions being used lead to the ratio of velocities of the longitudinal and transverse waves which according to the theory of Debye arises from the representation of the thermal part of the energy [1] (the velocity of the transverse waves depends on the temperature, but the authors found no information in the literature which would enable to take into account this dependence: also the tensor dependence of thermal conductivity on the direction of deformation of the medium is not taken into account).

The investigation being described here was undertaken to formulate the equation of state in a form which is suitable for the closure of the equations of the nonlinear theory of elasticity proposed in [2]. For the complete closure of these equations it is necessary yet to specify the dependence of the relaxation time τ of shear stresses on the state of the medium.

For the description of a triaxial strain $x_i' = a_i x_i$ we can use the tension coefficients a_i along the principal axes ($i=1, 2, 3$).

Following [2], instead of a_i we introduce the parameters and invariants of the strain tensor

$$\delta = \rho / \rho_0 = (a_1 a_2 a_3)^{-1}, \quad \alpha_i = \ln a_i, \quad d_i = \alpha_i - (\alpha_1 + \alpha_2 + \alpha_3) / 3$$

$$D = 1/2 (d_1^2 + d_2^2 + d_3^2), \quad \Delta = d_1 d_2 d_3 = 1/3 (\bar{d}_1^3 + \bar{d}_2^3 + \bar{d}_3^3)$$

For small strains α_i practically coincide with ε_i , the principal values of the strain tensor, while a_i coincides with the principal values of its deviator. Considering strains that are close to spherical strains we confine ourselves to the linear dependence of the internal energy per unit mass of the matter on D with a coefficient which depends on the density.

The dependence of the energy on the entropy S has been taken from [1]. The coefficient $\gamma(\delta)$, depending on the temperature, in the expression for the Debye temperature $\theta = \theta_0 \gamma(\delta)$ is represented by an

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TABLE 1

	Fe	Al	Cu	Ni	Pb	Tl
c_0 , km/sec	5.694	6.1215	4.651	5.437	2.151	5.853
b_0 , km/sec ²	2.8659	2.9408	2.1409	2.4852	0.81231	2.9633
ρ_0 , g/cm ³	7.840	2.785	8.900	8.860	11.340	4.510
τ_0 , 10 ⁻¹⁰ sec	0.712	0.767	0.950	0.797	3.40	0.787
θ_0 , °K	420	390	315	375	88	380
c_0^* , km/sec	5.718	6.201	4.685	5.616	2.213	5.835

TABLE 2

	Fe	Al	Cu	Ni	Pb	Tl
e_{00}	-0.042677	-0.086910	-0.090295	0.13409	-0.087230	10.9249
e_{01}	0.476118	4.49551	-0.047651	-1.25740	-0.392806	33.0090
e_{02}	0.639602	-0.38037	-0.83229	-1.099112	-0.087247	31.14893
e_{11}	2.6917	3.5769	3.4054	8.0180	4.8950	1.18037
e_{12}	-0.017537	1.0168	0.89094	10.661	6.9338	-2.84806
e_{13}	-0.13352	-0.44743	-0.40499	44.448	1.4611	1.5210
γ_0	0.005786	0.009617	0.005713	0.005351	0.002288	0.005773
γ_1	1.6723	2.1171	2.02934	3.95918	2.7746	1.0762
γ_2	-0.40804	-0.33262	-0.31394	4.0723	1.0464	-1.7366
γ_3	0.11311	0.093944	0.084733	0.70964	-0.11896	0.82778
$10^4 \cdot k_0$	0.9021	3.4845	4.0831	0.1777	0.07468	0.04201
k_1	0.33095	0.14615	0.19683	0.39467	0.68182	0.28947
s_0	0.7143	0.7520	0.9390	0.7820	3.335	0.7710

interpolation polynomial. An interpolation is carried out for the Debye function which in the case being considered is suitable for temperatures which are not too low. In the range of temperatures being studied we can neglect the high-temperature corrections ([1], Chapter 3).

We present below the expressions for the equation of state and the coefficient of thermal conductivity. The required explanations of the method used to obtain them are given below

$$E(\delta, D, s) = \frac{1}{2}(c_0^2 - \frac{4}{3}b_0^2)(\delta - 1)^2 e_0(\delta) + 2b_0^2 e_1(\delta) D + c_0^2 \gamma_0 [\gamma(\delta) g(s) - g(s_0)(1 + \gamma_1(\delta))]$$

$$g(s) = s + 0.05/s, \quad s_0 = 293/\theta_0$$

$$S = \frac{c_0^2 \gamma_0}{\theta_0} [\ln(s/s_0) + 0.025(s^{-2} - s_0^{-2})]$$

$$\kappa = (c_0^4 \rho_0 \tau_c / \theta_0) [k_0 \delta^{3/2} / (1 - k_1 \theta_0 / T)], \quad T = \theta_0 \gamma(\delta) s$$

Here by s we have denoted the entropy variable

$$s = T / (\theta_0 \gamma(\delta))$$

$$e_0(\delta) = 1 + (\delta - 1)[e_{00} + e_{01}/\delta + e_{02} \cdot 3(\ln \delta + 1 - \delta + (\delta - 1)^2/2) / (\delta - 1)^3]$$

$$e_1(\delta) = 1 + e_{11}(\delta - 1) + e_{12}(\delta - 1)^2 + e_{13}(\delta - 1)^3$$

$$\gamma(\delta) = 1 + \gamma_1(\delta - 1) + \gamma_2(\delta - 1)^2 + \gamma_3(\delta - 1)^3$$

The values of the quantities with dimensions c_0 , b_0 , ρ_0 , τ_c , θ_0 and the remaining dimensionless coefficients are presented in Tables 1 and 2. They all have the meaning of interpolation constants.

The equation of state presented above allows us, by means of the relationships ([2])

$$\sigma_i = -\rho^2 E_p + \rho E_{Dd_i}, \quad p = \rho^2 E_e$$

to compute the principal stresses σ_i and the mean pressure

$$p = -(\sigma_1 + \sigma_2 + \sigma_3) / 3$$

As a result, we have

$$\sigma_i = -p + 2\rho_0 b_0^2 \delta e_1(\delta) d_i$$

$$p = \rho_0 [(c_0^2 - \frac{4}{3}b_0^2)(\delta - 1)p_0(\delta) + b_0^2 p_1(\delta) \delta^2 D + c_0^2 \gamma_0 \delta^2 (p_2(\delta) g(s) - p_2(1) g(s_0))]$$

$$p_0(\delta) = 1 + p_{01}(\delta - 1) + p_{02}(\delta - 1)^2 + p_{03}(\delta - 1)^3$$

$$p_1(\delta) = p_{10} + p_{11}(\delta - 1) + p_{12}(\delta - 1)^2$$

$$p_2(\delta) = p_{20} + p_{21}(\delta - 1) + p_{22}(\delta - 1)^2$$

TABLE 3

	Fe	Al	Cu	Ni	Pb	Ti
p_{01}	1.4527	2.1167	1.94175	2.5924	1.86895	4.67294
p_{02}	0.15063	1.14810	0.83013	2.4222	0.67277	3.5558
p_{03}	-0.064015	-0.13037	-0.13544	0.20113	-0.13085	16.3873
p_{10}	2.6917	3.5769	3.4054	8.0180	4.8950	1.18037
p_{11}	-0.035074	2.0336	1.78118	21.322	13.868	-5.6961
p_{12}	-0.40056	-1.34229	-1.2150	133.34	4.3833	4.5630
p_{20}	1.6723	2.1171	2.02934	3.95918	2.7746	1.0762
p_{21}	-0.81608	-0.66524	-0.62788	8.1446	2.0928	-3.4732
p_{22}	0.33933	0.28183	0.25420	0.21289	-0.35679	2.4833
c_1	2.8332	4.0314	3.74843	5.9741	3.95792	6.55516
c_2	0.29332	2.6973	2.0385	8.21226	2.9530	6.048182
c_3	-0.21467	-0.49868	-0.50313	12.9625	0.90073	43.6665
b_1	2.6917	3.5769	3.4054	8.0180	4.8950	1.18037
b_2	-0.017537	1.0168	0.89094	10.661	6.9338	-2.84806
b_3	-0.13352	-0.44743	-0.40499	44.448	1.4611	1.5210

The expressions for the squares of the velocities of the longitudinal and transverse sound waves, c^2 and b^2 , calculated for a spherical strain tensor ($a_1=a_2=a_3=\delta^{-1/3}$), have the form

$$c^2 = c_0^2[1 + c_1(\delta - 1) + c_2(\delta - 1)^2 + c_3(\delta - 1)^3] c_0 \gamma_0 g(s) (\partial/\partial\delta) [\delta^2 p_2(\delta)]$$

$$b^2 = b_0^2[1 + b_1(\delta - 1) + b_2(\delta - 1)^2 + b_3(\delta - 1)^3]$$

The square of the cold velocity of sound c_*^2 is obtained by discarding, from the expression for c^2 , the term proportional to the entropy function $g(s)$

$$c_*^2 = c_0^2[1 + c_1(\delta - 1) + c_2(\delta - 1)^2 + c_3(\delta - 1)^3]$$

[In the interpolation used $b=b(\delta)=b_*(\delta)$ and does not depend on temperatures.] The coefficients p_{ij} , c_i , b_i of the interpolation polynomials for the pressure and the velocity of sound are presented in Table 3. In all the expressions presented under $\delta = \rho/\rho_0$ we understand the compression relative to the state at a zero pressure and $T=293^\circ$. The velocities of sound c_0 and b_0 are referred to the state $\delta=1$, $D=0$, $T=0$. In Table 1 we have presented the velocities of sound c_0^* for $\delta=1$, $D=0$, $T=293^\circ$, calculated from the expression

$$c_0^* = c_0[1 + \gamma_0 g(s_0)(2p_{20} + p_{21})]^{1/2}$$

2. The expression ([1])

$$E_*(\delta) = \frac{3A}{B\rho_0} \exp[B(1 - \delta^{-1/3})] - \frac{3K}{\rho_0} \delta^{1/3}$$

was taken as the initial equation of state of the cold matter.

The representations of the cold pressure and the modulus of cold volume compression that arise from this expression have the form

$$p_*(\delta) = \rho_0 \delta^2 \frac{\partial E_*}{\partial \delta} = A \delta^{2/3} \exp[B(1 - \delta^{-1/3})] - K \delta^{1/3}$$

$$M(\delta) = \frac{1}{\rho_0} \frac{\partial p_*}{\partial \delta} = \frac{2A}{3\rho_0} \delta^{-1/3} \left(1 + \frac{B}{2} \delta^{-1/3}\right) \exp[B(1 - \delta^{-1/3})] - \frac{4K}{3\rho_0} \delta^{1/3}$$

The modulus of volume compression is connected with the velocities of the longitudinal and transverse sound waves $c_*(\delta)$ and $b_*(\delta)$ by the relationship

$$M(\delta) = c_*^2 - 4/3 b_*^2$$

The velocities marked with an asterisk are calculated from the cold equation of state. In [1] three different methods are proposed for the interpolation of the dependence of the Debye temperature on the density ([1], page 43, (2.45)). The variant with $m=0$ is equivalent to the relationship

$$\gamma(\delta) = \theta_0 \delta^{\epsilon+1/3} \sqrt{M(\delta)/M(1)}$$

TABLE 4

	Fe	Al	Cu	Ni	Pb	Ti
A	0.37347	0.22863	0.27797	0.17491	0.28332	0.09161
Γ	1.68	2.13	2.04	1.91	2.78	1.18
B	6.9790	10.578	9.6801	13.603	9.1318	22.8721
ε	-0.102	-0.322	-0.234	1.034	0.580	-3.328
μ , g/mole	55.85	26.98	63.54	58.71	207.21	47.90

TABLE 5

	Fe	Al	Cu	Ni	Pb	Ti
α , 10^{-5} degree $^{-1}$	651	423	433	692	428	546
κ_0 , 10^6 g·cm/ sec 3 ·degree	73.3	226	402	58.6	34.8	21.0

The constants A, B, ρ_0 , θ_0 , ε characterize the material and are presented in [1]. The quantity K has the form

$$K = A + \Gamma \frac{\theta_0}{c_0^2} \frac{3R}{\mu} \left[\frac{293}{\theta_0} + 0.05\theta_0/293 \right]$$

Here Γ is the Grüneisen parameter, R is the universal gas constant and μ is the atomic weight.

To determine the velocity of transverse waves, we postulate a Debye interpolation expression for $\theta(\rho)$ having the form

$$\frac{1}{c_*^2} + \frac{2}{b_*^2} = \left(\frac{h}{k} \right)^3 \frac{18\pi L \rho_0}{\mu} \frac{\delta}{\theta^3(\delta)}$$

where h is the Planck constant, k is the Boltzmann constant and L is the Avogadro number. From this expression, as well as from the equation

$$c_*^2 - 1/b_*^2 = M(\delta)$$

we can determine the values $b_*(\delta)$ for each fixed δ . The authors set up tables of the functions $M(\delta)$, $b_*^2(\delta)$, $\gamma(\delta) = \theta(\delta)/\theta_0$ in the interval $0.9 \leq \delta \leq 2.0$; these were then approximated by cubic polynomials of $(\delta - 1)$. The expressions for $E_*(\delta, D)$, $p_*(\delta)$ are obtained by quadratures of the relationships

$$\frac{dp_*}{d\delta} = \rho_0 M(\delta), \quad \frac{\partial E_*(\delta, D)}{\partial \delta} = \frac{p_*(\delta)}{\rho_0 \delta^2}, \quad \frac{\partial E_*(\delta, D)}{\partial D} = 2b_*^2(\delta)$$

The expression for the total energy is obtained by addition, to $E_*(\delta, D)$, of the thermal energy of Debye

$$E = E_*(\delta, D) + \theta(\delta) g(T/\theta(\delta))$$

Putting $s = T/\theta(\delta)$, we obtain

$$g(s) = \frac{3R}{\mu} \left[\frac{3}{8} + sD \left(\frac{1}{s} \right) \right], \quad D(z) = \frac{3}{z^3} \int_0^z \frac{x^3 dx}{e^x - 1}$$

$$S = \frac{1}{s} g(s) + \int \frac{g(s)}{s^2} ds$$

according to the theory of Debye.

The expressions approximating $D(z)$ for high and low temperatures are known, and are presented in [1]. Having in view application to deformation of metals during explosions, when we can assume that the temperature is higher than or not much less than the Debye temperatures, the approximate expression

$$D(z) = 1 - \frac{3}{8} z + \frac{1}{20} z^2$$

holds, from which

$$g(s) = \frac{3R}{\mu} s \left(1 + \frac{1}{20s^2} \right), \quad S = \frac{3R}{\mu} \left[\ln s + \frac{1}{40s^2} \right] - S_0$$

These expressions have a limited region of applicability; for example, in the case $s = 1/20$ the monotonicity of S is violated. When there is a need to consider low temperatures, we can use more accurate approximations of $D(z)$, making use of the same relationships for $E_*(\delta, D)$, $\theta = \gamma(\delta)\theta_0$. In view of these restrictions the interpolation expressions of Sec. 1 are applicable for intervals of compressions $0.9 \leq \delta \leq 2.0$ and temperatures $100 \leq T \leq \theta_e$, where θ_e is the temperature of electron degeneracy ($T \approx 0.5 \cdot 10^6 Z^{4/3}$,

Ze is the charge of the nucleus, and e is the charge of an electron). The deviation of the interpolated quantities $\gamma(\delta)$, $b_*^2(\delta)$, and $M(\delta)$ from the values of the approximating polynomials on the interval $1.0 \leq \delta \leq 2.0$ is approximately 1%, while on the interval $0.9 \leq \delta \leq 1.0$ it is respectively approximately 5%.

The values of the coefficients A , B , ε , Γ , as well as the atomic weight μ , used in the interpolation expressions of Sec. 1 are presented in Table 4. When carrying out the calculations for the universal physical constants, we took the following values: $h = 6.62 \cdot 10^{-27}$ erg·sec, $k = 1.38 \cdot 10^{-16}$ erg/degree, $L = 6.02 \cdot 10^6$ kmole $^{-1}$, $R = 8.31 \cdot 10^7$ g·cm/sec 2 ·degree·mole.

3. In metals the process of heat conduction takes place in the main as a result of diffusion of free electrons; the time for the establishment of a thermal equilibrium between the electron gas and the lattice is of the order of 10^{-11} sec. In connection with this, when considering processes with characteristic times greater than 10^{-8} sec, we need not take into account the heat exchange between the lattice and the electron gas, taking their temperatures as identical, and can assume that the heat propagation is given by the coefficient of thermal conductivity κ of electrons.

Between the electrical conductivity σ , the thermal conductivity κ and the temperature T ($T > \theta_0$) the relationship (the Wiedemann–Franz law)

$$\kappa/\sigma T = \text{const}$$

holds.

This law is valid in the case $\theta_e < T < \theta_e$ for pure metals (θ_e is the degeneracy temperature of free electrons). For metals contaminated by additions it is valid for $0 < T < \theta_e$ ([3, 4]).

The electrical resistance σ^{-1} linearly depends on the temperature (see [3])

$$\sigma^{-1} = (T - T^*)/A$$

To clarify the dependence of σ on the density ρ , we can use the proportionality between σ and the density of electron gas and the inverse proportionality of σ to the magnitude of the maximum velocity v_μ of electrons in the degenerate Fermi gas ([3])

$$\sigma \sim \frac{N}{V} v_\mu^{-1}, \quad v_\mu = \sqrt{\frac{2\mu_0}{m}}, \quad \mu_0 = \frac{h^2}{8m} \left(\frac{3}{\pi} \frac{N}{V} \right)^{2/3}$$

Here N is the number of free electrons in the volume V , m is the mass of an electron, N/V is proportional to the density of the material $\rho = \rho_0 \delta$. Hence $\sigma \sim \sigma^2/3$. Combining the dependence of σ on the temperature and density with the Wiedemann–Franz law, we have

$$\kappa \sim \delta^{2/3} / (1 - T^*/T)$$

We represent this relationship in the form

$$\kappa(\delta, T) = c_0^4 \tau_c k_0 \delta^{2/3} / (1 - k_1 \theta_0 / T)$$

The multiplier with dimensions is made up from the velocity of longitudinal sound waves c_0 , the Debye temperature θ_0 , and the Debye time $\tau_c = 2\pi h / \theta_0$. The dimensionless constants k_0 and k_1 are chosen with respect to the values of the coefficient of thermal conductivity κ_0 for $T = 293^\circ$, $\delta = 1$, and from the temperature coefficient of resistance $\alpha = (-1/\sigma) (\partial \sigma / \partial T)$, which are tabulated in [5]. The values used are given in Table 5.

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