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Abstract

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PHYSICS

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ON THE CONSTRUCTION OF APPROXIMATE SHOCK ADIABATS OF SOLIDS IN THE HYDRODYNAMIC REGION

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In a number of applied problems connected with the propagation of shock waves in solid media, it is necessary to know the shock adiabats for pressures varying from hundreds of kilobars to hundreds and thousands of megabars. Under such loads the state of solid media is described analogously to that of a liquid and a gas. At present, with the aid of dynamic methods it is possible to obtain shock adiabats up to pressures of the order of 10 megabars. To describe the state of a broad class of solid media at ultrahigh pressures ($10^2 \div 10^5$ Mbar), the Thomas-Fermi statistical model of the atom can be used. In the present note one of the possible methods is considered for interpolating shock adiabats and the thermodynamic state between the regions indicated above.

For constructing shock adiabats, the usual system of dynamic compatibility conditions at the shock-wave front is used, which is closed by the equation of state and by an expression for the internal energy of the form

$$p = p_x + p_t + p_e, \quad \varepsilon = \varepsilon_x + \varepsilon_t + \varepsilon_e,$$

where p_i and ε_i are, respectively, the components of pressure and energy; the index $i = x$ corresponds to the cold part of the state of the medium common to nuclei and electrons; $i = t$ to the thermal nuclear part; $i = e$ to the thermal electronic part.

1. To describe the state of the medium associated with thermal excitation of electrons, the thermal part of the Thomas-Fermi atom model can be used. Calculations for this model were carried out in work ⁽¹⁾. The construction of interpolation formulas on the basis of the data of ⁽¹⁾, satisfying the asymptotics of an incompletely degenerate electron gas in one limiting case ($v \rightarrow 0, T \rightarrow 0$, where v (g/cm³) and T (°K) are specific volume and temperature) and passing into an ideal gas in the other case ($v \rightarrow \infty, T \rightarrow \infty$), leads to the expressions

$$p_e = \frac{452z^{1/3}T^2(vM)^{-1/3}}{1 + 5.45 \cdot 10^{-6}Z^{-2/3}(vM)^{2/3}T} \left[1 + \frac{7.35 \cdot 10^{-2}(Zv \cdot M)^{1/2}}{1 + 4.2 \cdot 10^{-10}Z^{-1}vMT^{3/2}} \right]^{-1} \frac{\text{dyn}}{\text{cm}^2},$$

$$\varepsilon_e = p_e v \left[1.5 + \frac{3.3 \cdot 10^{-5}(ZvM)^{1/3} (T^{3/2}Z^{-32/27} + 3.34 \cdot 10^3)}{1 + 3.43 \cdot 10^{-7}Z^{-2}T^{3/2} + 1.02 \cdot 10^{-8}Z^{-1/3}vMT} \right] \frac{\text{erg}}{\text{g}}, \quad (1)$$

where, as usual, Z is the charge of the atom and M is the weight of 1 gram-atom.

2. In the region of relatively low pressures a solid medium retains its crystalline structure. Therefore the state of the thermal nuclear part is described by the usual thermodynamic relations for solids. In the region of ultrahigh pressures and temperatures the state of the nuclear part approaches that of an ideal gas. To interpolate the state parameters between the indicated regions, one may use

relations analogous to those proposed in work (2):

$$p_t = \frac{3\gamma_1 + \alpha^n}{1 + \alpha^n} \frac{RT}{Mv}, \quad \alpha = - \frac{lRT}{M \left[v^2 \frac{dp_x}{dv} + \frac{2}{3} p_x v \right]},$$

$$\varepsilon_t = \frac{2 + \alpha^n}{1 + \alpha^n} \frac{3}{2} \frac{RT}{M}, \quad \gamma_1 = - \frac{1}{3} - \frac{1}{2} v \frac{\frac{d^2}{dv^2} [p_x v^{2/3}]}{\frac{d}{dv} [p_x v^{2/3}]}, \quad (2)$$

where n is a parameter determined on the basis of experimental data; l is a parameter related to the characteristic Debye temperature:

$$l = \frac{kA^{5/3}h^2}{2\pi(0.715k)^2 e^{2/3} R} \frac{c_0^2}{M^{2/3} v_0^{2/3} \Theta_0^2}, \quad (2')$$

where, in addition to the generally accepted notation: c_0 is the bulk speed of sound; A is Avogadro's number; the index 0 refers to the initial state of the medium. This formula was obtained by M. G. Men'zhulin from the condition of the asymptotic approach, at large α , of the free energy corresponding to expressions (2) to the free energy of an ideal gas.

3. The cold part of the state of a substance in the low-pressure region is associated with the "elasticity" of the crystal lattice, and in the high-pressure region with the repulsive forces of charged particles. In the region of high compressions ($v_0/v > 4$), the cold part of the state is well described by the "cold" Thomas-Fermi atom model (4). In the region of relatively

small compressions, the cold part can be determined from an experimentally constructed shock adiabat (3, 4).

Various methods are possible for interpolating states between the indicated regions (3, 4). The introduction of exchange corrections into the cold Thomas-Fermi model, which somewhat improve the behavior of the cold-compression parameters at not very strong compressions, indicates a possible structure of semiempirical formulas for p_x (5). The dependence for $p_x(v)$ proposed in (5) contains no parameters that correct this quantity on the basis of experimental data, which reduces the possibilities for interpolation accuracy. In the present work an interpolation dependence of the form is used

$$p_x = p_{x\text{T.F.}} \left[1 - (1 - b) \left(\frac{p_{x\text{T.F.}}}{p_{x\text{T.F.}}^0} \right)^{n_1} - b \left(\frac{p_{x\text{T.F.}}^0}{p_{x\text{T.F.}}} \right)^{n_2} \right], \quad (3)$$

where $p_{x\text{T.F.}}$ is the pressure in the cold T.-F. model; the superscript 0 refers to the initial specific volume.

The quantities b , n_1 , and n_2 are determined on the basis of experimental data on the shock adiabat. These parameters are most simply determined from the lower part of the shock adiabat, where

$$p \approx p_x. \quad (4)$$

In expression (3), the function $p_{x\text{T.F.}}(v)$ was approximated on the basis of data (1) by a dependence of the form

$$p_{x\text{T.F.}} = Z^{2/3} \left/ \sum_{i=0}^5 a_i (ZvM)^{(i+5)/3} \right. \quad (5)$$

4. On the basis of the constructed system (1)–(5), using the conditions of dynamic compatibility, shock adiabats were calculated for 19 elements (Fig. 1) and two chemical compounds for the pressure range from the region of applicability of the hydrodynamic description (or from the phase transition) up to high pressures.

To determine the parameters in (3), an approximation of the experimental points on the initial segment of the shock adiabats was used in the form

$$N = C + kU, \quad (6)$$

where N is the front velocity, and U is the mass velocity.

In the work, experimental points published to date in the literature were used. The calculations performed showed that

Fig. 1. Shock adiabats; curves—calculation; points—experimental data

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the interval of possible variation of the parameter b from (3) is associated with the choice of reasonable roots of the quadratic equations obtained when determining the parameters n_1 and n_2 from the quantities C and k in (6) (either $0 < b < 1$, or $1 < b < \infty$). When the values of b are varied within the indicated intervals, the shock adiabat practically does not change. In the calculations, either $b = 0.1$ or $b = 2$ was used.

The quantity l , calculated by formula (2'), is of order 1 for all the materials considered. Therefore, in calculating the shock adiabats in Fig. 1, $l = 1$ was adopted for all materials. In order to obtain the best agreement between the calculated shock adiabats and the experimental data in the high-pressure region, for K, Na, Th, and CsBr, NaCl, and Al it was assumed that $n = 0, 1$, while in all other cases $n = 1$.

In conclusion, we note that the relations presented make it possible to carry out an *a priori* construction of an approximate shock adiabat of a solid medium, if the bulk modulus, the initial density, and the Grüneisen coefficient are known. The latter can be calculated by means of a known thermodynamic relation from the thermal and mechanical characteristics of the unperturbed medium. However, the indicated method of construction (without taking into account experimental data on shock adiabats in the low-pressure region) leads to approximate shock adiabats that, in a number of cases, possess lower accuracy.

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