EQUATION OF STATE AND HUGONIOT OF MATTER WITH DISTANCE INTERACTING MOLECULES

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Qualitatively from physical considerations, as well as on the basis of experimental data, as well as computer modeling received fundamental relation $\boldsymbol{p_H = p_p \times (V_0/V)}$, *connecting pressure behind the shock wave front throw potential component. Advanced drawing concept of co-volume and free volume for thermal movement of particles, allows to build two parts equation of state with potential and thermal components of pressure, which allows to calculate parameters of condensed matter, the sound speed at high densities of energy. For the proposed equation of state, you need knowledge of only the shock Hugoniot of matter. As an example, it is considered the characteristics of iron as a major component of the Earth's core, at high pressures and temperatures.*

Introduction. For calculations are commonly used semi-empirical equations of state, based on shock wave and static experimental data at high temperatures and pressures [1-6]. A number of challenges, in particular in the analysis of the Earth's interior, achieved temperatures are below evaporation and ionization temperatures. Consequently, such tasks are not advisable to use wide-ranging multiphase equation of state, which can substantially complicate the modeling processes studied.

In addition, the known approaches when building the equations of state require measurement or calculation of additional parameters, fitting coefficients for each substance. Therefore, building appropriate to the practical needs of equation of state for calculation of thermodynamic characteristics of condensed matter in the range of moderate and high pressure and temperature remains an important objective is the aim of the present work.

Two parts equation of state of condensed matter. In constructing of equation of state at high temperatures and pressures, particularly in explosive processes, well proven simple model based on the concept of compressed co-volume, in which the thermal pressure of an ideal gas particles is created in "free" of elastic particles volume [2, 3]. Co-volume compressible model equation of state, you can give the appearance of:

$$V(p, T) - V_C(p) = RT/p \equiv V_i(p, T) \tag{1}$$

where V -volume, p -pressure, T - temperature, V_C - co-volume (own volume of elastic particles, pressure-dependent). The right part of the formula expresses the amount of V_i that ranked the system of point particles of an ideal gas under p and T.

Equation of state of condensed matter can also be represented as the sum of the potential p_p and thermal “hot” p_h components of the whole pressure [5]:

$$p(V, T) = p_p(V) + p_h(V, T). \tag{2}$$

Equations of state in the form of (1) and (2) are simple and physically "transparent", but beside of shock-wave data, require a number of additional parameters are defined to adequately describe the behavior of condensed matter at high energy densities.

Comparing (1) and (2), consider the equation of state as follows:

$$p(V, T) = p_p(V) + p_h(V_i, T), \tag{3}$$

where $V_i = V - V_C$.

In equation (3), as in (1), (2), you must know the dependence of potential pressure component p_p from density ρ.

Equation of sate of matter, including shock adiabat, is completely determined by the potential interaction of particles of matter, their weight and their mutual arrangement [7, 8], or the equivalent, of the potential compression curve of substances. Submission of equation of state in the form (3) with potential and thermal components of pressure allows to take advantage of direct dependence of full pressure behind the front shock waves from potential component pressure. So, consider how obtained in [9, 10] from comparisons of experimental shock adiabat and low-temperature isotherms of several substances, the universal connection of full pressure p_H and potential component pressure p_p behind the front for not a very high shock waves:

$$p_H = p_p \frac{\rho}{\rho_1} \quad . \tag{4}$$

Ratio (4) is valid when the initial values of the potential p_{p1} and heat p_{h1} pressures before the shock wave front can be neglected, and the initial density ρ_1 close to the density of solid matter under normal conditions, that usually happens in shock-wave experiments with condensed matter. At very high pressures, the ratio of (4) may be restricted to limit the compression shock wave $\rho/\rho_1 \approx 4$ [5].

Consider the physical sense (4), in terms of the model under consideration, in the case of sufficiently strong shock wave, where pressure and temperature before shock wave front can be neglected with comparison to the shock wave pressure $p_H = \rho_1 DU$, where ρ_1 - the initial density, D is the velocity of the shock wave, U - mass speed of matter behind the front. Given that $\rho_1/\rho = (D - U)/D$ ratio (4) rewrite as:

$$p_p = \rho_1 (D - U)\, U,$$

then the hot component of pressure behind the front shock wave:

$$p_h = \rho_1 U^2. \tag{5}$$

For the case $p_H >> p_1$ to compare (5) with the final ratios for front shock wave in an ideal gas, given, for example, in [5]:

$$p_H = \frac{2\rho_1 D^2}{\gamma + 1} \quad , \tag{6}$$

$$\frac{D-U}{D} = \frac{\gamma - 1}{\gamma + 1} \quad , \tag{7}$$

where is the adiabatic index γ. Since in an ideal gas $p_H \equiv p_h$ then get that the models of relationships between (5) and (6, 7) can agree on, if the thermal pressure of condensed matter to simulate point particles with an ideal gas $\gamma = 1$, i.e. gas with the number of atoms in a molecule $n >> 1$. In such a case, the model would also be more in line with real matter rather than with gas monoatomic here's why. In the dense condensed matter atoms does not move freely and commit thermal fluctuations among equilibria, like atoms in polyatomic molecules.

Relation (5) in terms of the model considered can also be justified as follows: with the passage of the shock front point particles of ideal polyatomic gas, simulating the thermal properties of matter, collided with the "plunger" is not elastic, unlike the monatomic gas, but stop at "piston", gaining mass speed equal to U as a result, providing thermal pressure on the piston to $\rho_1 U^2$ regardless of the speed of the shock wave.

Shock compression of a pre-heated and porous matter. Initial temperature before shock usually above 0K. Also in shock-wave compaction, sintering of powders achieved temperatures higher than in the case of continuous samples. On the other hand, shock compression is not in one but in a series of shock waves with the same final pressure results in less heat matter and, consequently, to another character transformations of substances. So, consider within this model of shock compression of matter when initial pressures p_{p1} and p_{h1} cannot be neglected.

Go back to the equation of state in the form of equation (3). Pressure of an ideal gas with $\gamma = 1$, filling, on the model the whole volume, under shock compression changes proportionally ρ/ρ_1 [5]. The dependence of full pressure behind the shock wave front from potential component is expressed by the ratio (4). Therefore, shock adiabat pre-heated condensed matter with an initial pressure $p_1 > 0$ and density ρ_1 greater then density ρ_0 ($p = 0$, $T = 0$), for example, before the front of the reflected shock wave, we get the following:

$$p_H = (p_p + p_{h1}) \frac{\rho}{\rho_1} \quad . \tag{8}$$

Substances of the same elemental composition may have identical initial conditions but different density ρ_{11} and ρ_{12} and, therefore, different Hugoniot (e.g. porous and solid phases carbon graphite or diamond phase). We assume that after the shock wave compression, or phase transition (e.g. of graphite in diamond) substances have equal potential components of pressure at equal densities behind shock wave. If we neglect the initial components of the pressure before the shock wave front, then according to (8):

$$p_{H1}=p_p\frac{\rho}{\rho_{11}}\ ,\qquad p_{H2}=p_p\frac{\rho}{\rho_{12}}\ .$$

Then get that Hugoniots of one substance, but with different initial densities should be bound by the ratio:

$$\frac{p_{H1}(\rho)}{p_{H2}(\rho)}=\frac{\rho_{12}}{\rho_{11}}\ , \tag{9}$$

and shock adiabat cold ($T_1 = 0$) "porous" matter ($\rho_1 < \rho_0$):

$$p_H=p_p\frac{\rho}{\rho_1}\frac{\rho_0}{\rho_1}\ . \tag{10}$$

In the case of weak shock wave pressure p_H may be comparative with initial values p_{h1} and p_{p1} . This condition can be met given (8) and, at the same time, (10), if a shock adiabat pre-heated matter to take the next (for $\rho > \rho_0 > \rho_1$):

$$p_H=(p_p+p_{h1})\frac{\rho}{\rho_1}\frac{\rho_0}{\rho_1}\ . \tag{11}$$

Then:

$$p_p=p_H\frac{\rho_1}{\rho}\frac{\rho_1}{\rho_0}-p_{h1}\ . \tag{12}$$

Thus, the ratio of (11) allows to calculate parameters of matter when shock wave processes in hot and porous solids and processes with an abrupt density caused by phase transitions or chemical reactions, which is important for the tasks.

Temperature of condensed matter. To calculate the temperature will take the value of V_C as in the model of compressible co-volume [2], equals to the value on the curve of potential compression calculated according to (12), for p_p equal to the total pressure p_H behind the front shock wave. Then the volume available for thermal movement of particles of an ideal gas:

$$V_i = V(p, T) - V_C(p), \tag{13}$$

where $V(p, T)$ volume of matter behind the shock wave front as well as the pressure of an ideal gas equals RT/V_i, the equation of state (3) takes the form:

$$p(V,T)=p_p(V)+\frac{RT}{V_i}\ . \tag{14}$$

Temperature of matter, therefore:

$$T=\frac{p_h V_i}{R}\ . \tag{15}$$

Because the values are included in the equation (15) are known (3), (12), (13), if you know the shock adiabat of matter p_H (V) so equation (15) allows to calculate the temperature of matter, for example, behind the shock wave front. (It should be noted that according to the model of compressible co-volume [2] it is obtained considerably higher temperature:

$$T=\frac{pV_i}{R}$$

Thus, to calculate the temperature, as in [2], the notion of "free volume" V_i used. The model under consideration differed from this in [2] that the potential pressure and thermal pressure ideal gas particles, accepted equal total pressure p and his elastic p_p and thermal p_h. I.e. in the discussed model elastic particles, and ideal gas particles fill the whole volume *V*, but in calculating the temperature, point particles with the mass for thermal motion is available only part of the total volume.

This can be interpreted as follows. Moving in its "free" volume having mass particle collides with an elastic, does not have mass, but with the dimensions of the particle, which instantly transmits the pulse particle in a nearby free volume and further along the chain. Emerging so quasi-particles impetus from wall to wall receptacle is transmitted with higher speed than with the free motion of the particles. In the solid state physics this corresponds to the term “gas” of phonons, filled with elastic particles volume. The notion of phonons as quasi-particles helps describe many, including thermal properties of solids by using the kinetic theory of gases. When this phonon gas behaves like an ideal gas, which gives grounds to simulate the thermal properties of condensed matter by the particles of an ideal gas and in the interim between gas and solid state.

(For further, it should be emphasized that, as in the solid state physics of phonons, gas and ideal gas in the models fill the entire volume together with atoms or elastic particles.)

Temperature calculation of shock compression of porous and pre-heated matter. Bearing in mind that $p_h = p_H - p_p$ with the obtained expressions (11) and (12) (15), after transformation you can get the temperature behind the front shock wave at a pressure p_H :

$$T = \frac{p_H \left(1 - \frac{\rho_1 \rho_1}{\rho \rho_0}\right) V_i}{R} + T_1 \frac{V_i}{V_{i1}} \tag{16}$$

If you accept that:

$$\frac{p_{h1} V_{i1}}{R} = T_1 \quad .$$

Thus, to calculate the temperature shock-compressed condensed enough to know shock adiabat of matter when $p_0 \approx 0$, $T_0 \approx 0$, or shock when adiabat $p_1 \approx 0$, $T_1 > 0$ and density ρ_0 (when $p_0 \approx 0$, $T_0 \approx 0$). If there are no experimental data, then it can be assumed from the percussion adiabat condensed substances summarized [9, 10]:

$$D = U + 3.4 \left(\frac{\rho_1}{\mu_e}\right)^{1/3} U^{1/2} + 9.1 \left(\frac{\rho_1}{\mu_e}\right)^{2/3} \tag{17}$$

where *D* and *U* in km/s, ρ and μ in g (cm^3 and mol, respectively), and ρ_1 is not much different from ρ_0. μ_e - effective atomic (molecular) mass of matter, which for most simple substances close to the atomic mass, for mixtures to the mean value for chemical compounds depends on the composition and the nature of the relationships of atoms [9, 10].

Comparison of calculations with known data. To compare the results of the calculations on the proposed equation of state is the most complete and from different sources of data to measure the temperature of Matter when shock compression. These include, in particular, experiments with matter, more "appropriate" for temperature measuremments, for example, transparent [11].

Argon. In [12] the obtained experimental data on shock-wave compression liquid argon approximates by two lines:

$$D = 0.971 + 1.912U - 0.11U^2 \qquad U \leq 3.84 \text{ km/s} \tag{18}$$

$$D = 2.82 + 1.137U \qquad U > 3.84 \text{ km/s.} \tag{19}$$

Shock adiabat (18), (19) in ρ, *p* coordinate is shown in fig. 1 (line *1*). But there are also other data on shock compression of liquid argon [13] and [14]. Therefore, in the calculation for the basic shock adiabat of liquid argon to conveniently take generalized dependence (17), which is consistent with both experimental data [12] and [13, 14] and is a fairly good smooth averaging. Taking in (17) $\rho_1 = 0.9$ g/cm^3 and atomic mass of argon $\mu_e = 39.95$ g receive:

$$D = U + 1.11 \times U^{1/2} + 0.974 \quad . \tag{20}$$

Heat and potential pressure components before front shock wave in liquid argon when $\rho_1 = 0.9$ g/cm^3 and $p_1 \approx 0$ are not zero and are related by $p_{h1} \approx -p_{p1}$. Density of argon ρ_0 with $T = 4$K is about 1.77 g/cm^3 [15]. Consequently, a potential component of the pressure needed for the equation of state

(14), we find using the ratio (12). Then under $\rho_1 = 0.9$ g/cm^3 ($T = 86$K), $\rho_0 = 1.77$ g/cm^3 ($T = 4$K) we get:

$$p_p = p_H \frac{1.4}{\rho} \times \frac{1.4}{1.77} - p_{h1} \quad . \tag{21}$$

When the density $\rho = 1.77$ g/cm^3 potential pressure component p_p behind the front shock wave in liquid argon, expressed by the ratio (21), take zero. When the initial density $\rho_1 = 1.4$ g/cm^3 the initial value of the thermal pressure component p_{h1} from the equation (21) is about 0.87 GPa for the shock adiabat (20). Calculated for such a value p_{h1} according to the formula (21) potential pressure curve p_p shown in fig. 1 (line *2*), together with experimental data on argon compression with $T = 298$K [16].

In [12] are measured reflected shock wave parameters for initial values $p_1 = 144$ GPa, $\rho_1 = 4.37$ g/cm^3 and $p_1 = 268.7$ GPa, $\rho_1 = 5.12$ g/cm^3. In fig. 1 are compared calculated from shock adiabat (18) and (19) using the ratios (11), (12) reflected shock adiabat argon (lines *3* and *4*) and experimental data [12].

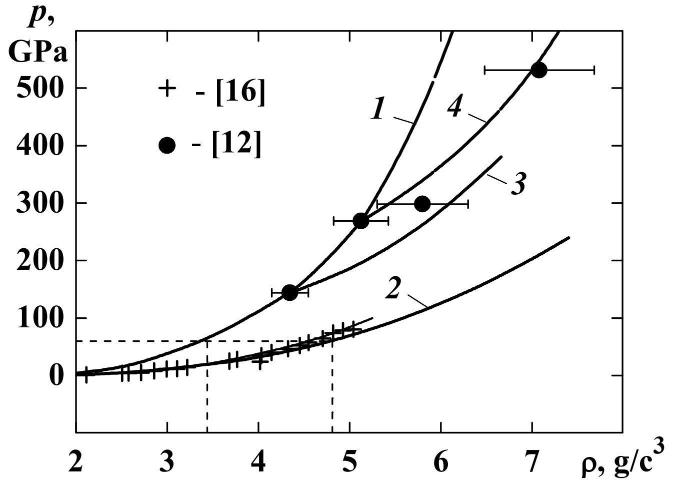

Fig. 1. Shock-wave data and potential pressure of argon. Calculation, comparison with experiment [12], [16]. *1* -shock adiabat of liquid argon (18), (19). *2* - calculation of p_p by Hugoniot (20). *3* and *4* -calculation of reflected shock adiabat.

In fig. 2 are the results of the measurement of brightness temperature behind the shock wave front in liquid argon [12, 14, 17]. Shown in fig. 2 temperature calculation is made using the formula (16) with a potential component of pressure (21) on shock adiabat (20) (line *1*) and shock adiabat [14] with extrapolation (line *2*). It should be noted that the estimated temperature shock-compressed argon provided in [12, 14], in the area of high pressure is also significantly higher than the experimental values. The authors of [12, 14] explain this discrepancy by electronic excitation and reflection of radiation in optical measurements.

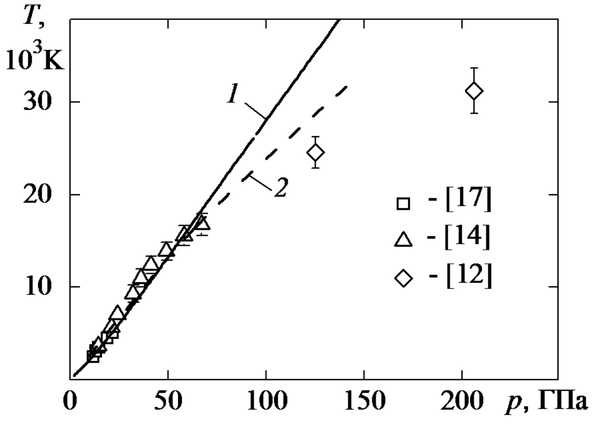

Fig. 2. Temperature behind the shock wave front in liquid argon. Calculation, comparison with experiment [12] [14], [17]. ***1*** -calculation on shock adiabat (20), ***2*** -calculation on shock adiabat [14].

The above calculation temperature of shock-compressed Argon is made according to the following pattern (dashed line in Fig. 1). On shock adiabate (20), for example, when U = 6.35 km/s, we obtain: D = 10.13 km/s. $p = \rho_1 DU =$ **90** GPa, $\rho = \rho_1 D/(D - U)$ = **3.75** g/cm^3 (V = 10.65 cm^3/mol.) these settings under (21) p_p = 24.88 GPa, $p_h = p - p_p$ = **64.31** GPa.

According to the model, at pressure p the own volume of elastic particles V_C - part of a full volume V and equals volume on the curve of potential compression under pressure $p_p = p$. When potential pressure. p_p = 90 GPa argon density calculated by (21), equals to 5.43 g/cm^3, as can be seen from fig. 1, i.e. V_C = 7.35 cm^3/mol. $V_i = V - V_C$ = **3.3** cm^3/mol.

When pressure $p_1 \approx 0$ GPa argon density **0.9** g/cm^3, i.e. V_1 = 28.54 cm^3/mol. When the same potential pressure p_p = 0 GPa density of argon, as above, about **1.77** g/cm^3, therefore, V_C = 2.36 cm^3/mol. $V_{i1} = V_1 - V_C$ = **6.49** cm^3/mol.

Substituting the above selected numerical values in bold values in the expression for the temperature of (16), get (omitting for brevity):

$$T=\frac{90\times\left(1-\frac{1.4}{3.75}\times\frac{1.4}{1.77}\right)\times 3.3}{8.314}+0.086\times\frac{3.3}{5.97}=25.2\times10^{3}K \; .$$

In the case of strong shock waves can be neglected with initial values and calculate the temperature from a simpler equation (15) for example, *(p)* = 90 GPa:

$$T=\frac{64.31\times3.3}{8.314}=25$$

Iron. Iron and its alloys are basic materials used in constructions exposed to external shock, liquid Earth's core and inner solid consist primarily of iron. Iron and its alloys can experience a number of phase transitions with temperature and pressure rise. It is therefore important the knowledge of the characteristics of iron at high temperatures and pressures.

Assume the basic iron shock adiabat curve (17), which brings the known experimental data, including shown in [6]:

$$D = U + 1.82U^{1/2} + 2.59 \qquad 1.40 \le U \le 26.3 \text{ km/s.} \tag{22}$$

When the shock compression iron goes into hexagonal close packed (hcp) phase of this phase at a with density 8.27 g/cm^3 [18] at $p \approx 0$, $T \approx 0$, whereas the density of iron before shock wave front ρ_1 = 7.85 g/cm^3. So, necessary for calculations of potential component of pressure and, consequently, co-volume $V_C(p)$, will count with the help of equation (12):

$$p_p=p_H\frac{7.85}{\rho}\times\frac{7.85}{8.27} \tag{23}$$

When the density ρ = 8.27 g/cm^3 potential part of pressure p_p for close packed (hcp) phase, expressed by the ratio (23), take zero. When iron density ρ_1 = 7.85 g/cm^3 the initial value of the thermal pressure component p_{h1} from the equation (23) is about 4.50 GPa for the shock adiabat (22).

In fig. 3 calculation of temperature shock-compressed iron made by the formula (16) with a potential component of pressure (23) on the shock adiabat (22), compared with data [19-21].

Temperature calculation was performed according to the following scheme. The shock adiabat (22), for example, when U = 4.6 km/s, we obtain: D = 11.09 km/s. $p = \rho_1 DU$ = **400** GPa, $\rho = \rho_1 D\,/\,(D - U)$ = **13.41** g/cm^3 (V = 4.17 cm^3/mol.) these settings under (23) p_p = 217.8 GPa, $p_h = p - p_p$ = **182.2** GPa.

According to the model, at a pressure p the own volume of elastic particles V_C is part of a whole volume V and that is the volume on the curve of potential compression pressure $p_p = p$. When potential pressure p_p = 400 GPa iron density calculated by (23), equals to 15 g/cm^3, i.e. V_C = 3.64 cm^3/mol, $V_i = V - V_C$ = **0.55** cm^3/mol.

When pressure $p_1 \approx 0$ GPa iron density **7.85** g/cm^3, i.e. $V_1 = 7.11$ cm^3/mol. With this potential pressure $p_p = 0$ GPa close packed density phases of iron is about **8.27** g/cm^3, therefore, $V_C = 6.75$ cm^3/mol, $V_{i1} = V_1 - V_C =$ **0.36** cm^3/mol.

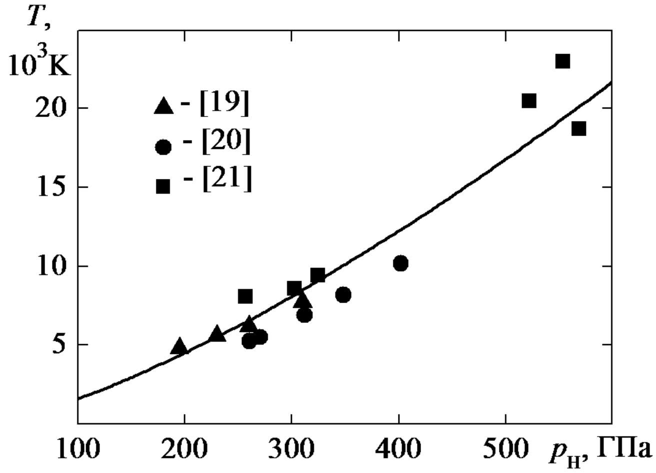

Fig. 3. Temperature behind the shock wave front in the iron. Calculation, comparison with experiment [19], [20] [21]. Line - calculation by use of shock adiabat (22).

Substituting the above selected numerical values in bold values in the expression for the temperature of (16), get (omitting for brevity):

$$T=\frac{400\times\left(1-\frac{7.85}{13.41}\times\frac{7.85}{8.27}\right)\times 0.55}{8.314}+0.293\times\frac{0.55}{0.36}=12.2\times10^3 K$$
.

In the case of strong shock waves can be neglected with initial values and calculate the temperature from a simpler equation (15) for example, $p = 400$ GPa:

$$T=\frac{182.2\times 0.55}{8.314}=12.0\times10^3 K$$
.

Adiabatic processes in compressed and preheated matter. Speed of sound. Consider the adiabatic compression matter when initial pressures p_{p1} and p_{h1} not negligible. Back to the equation in the form of (3, 14) potential compression or expansion along the $p_p(\rho)$ is reversible, pressure of ideal gas with $\gamma = 1$, distributed throughout the volume V, changes proportionally V_1/V [5]. So, in the model isentrope get the following:

$$p_S=p_p+p_{h1}\frac{\rho}{\rho_1} \quad . \qquad (24)$$

Thus, to calculate the adiabatic changes of state of matter it's enough to know its shock adiabat at $p_0 \approx 0$, $T_0 \approx 0$, or shock adiabat at $p_1 \approx 0$, $T_1 > 0$ and density ρ_0 (when $p_0 \approx 0$, $T_0 \approx 0$). If no such data exists, then one can proceed from the adiabat condensed substances in aggregated form (17). Using the ratio (24), you can calculate the speed of sound in matter with density ρ and pressure p_h :

$$c_S^2=\frac{dp_S}{d\rho}$$

$$c_S^2=\frac{dp_p}{d\rho}+\frac{p_h}{\rho} \qquad (25)$$

It should be noted that the ratio (25) rightly for slow compression of matter, and applicable to very low frequency sound waves, such as seismic, frequency of which some Hertz. Due to the phenomenon of high-frequency sound dispersion fluctuations, wave rarefaction can spread faster.

Lowering the conversion, for substances with shock adiabat, presented in the form of line segments (or tangent to the shock adiabat) $D = A + BU$ get a volume sound velocity in matter:

$$c_{s^2}=(D-U)^2\left[\frac{2(D-U)}{A}-1\right]\frac{\rho_1}{\rho_0}+\frac{p_h}{\rho} \tag{26}$$

where the value of D , U , and A are for the shock adiabat p_{H} when the density ρ behind the front.

Comparison of iron parameters with the Earth's core. For the Earth is known change with depth velocities of seismic waves, pressure and density, temperature is calculated approximately, but in different variants of calculation may vary on thousands of degrees. It is believed that the core is mostly iron. While the inner core solid, due to high pressure, external liquid.

Compressing iron to densities of the Earth’s core, then, without changing the density, warming up, you can get the required geophysical values as density and pressure. The temperature and speed of sound will be single-valued functions of the density and pressure, and can be calculated in the case of iron by ratios (22), (16) and (26). In fig. 4 and fig. 5 shows the results of the calculations of temperature and velocity of sound in iron, which are compared with the corresponding geophysical values for liquid core [22, 23]. You can see that design temperature are above possible values, and estimated speed of sound are low. Therefore, iron cannot be the only component of the Earth's core.

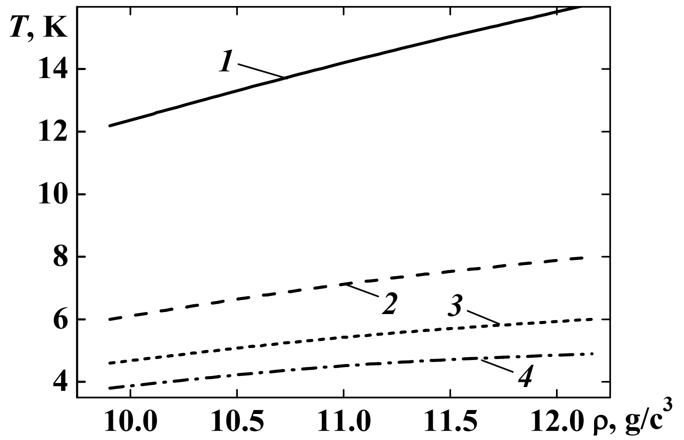

Fig. 4. ***1*** -liquid Iron temperature calculated by (16) with the density and pressure of liquid outer core of the Earth. ***2***, ***3*** and ***4*** - the Earth's core temperature calculation, listed in [22].

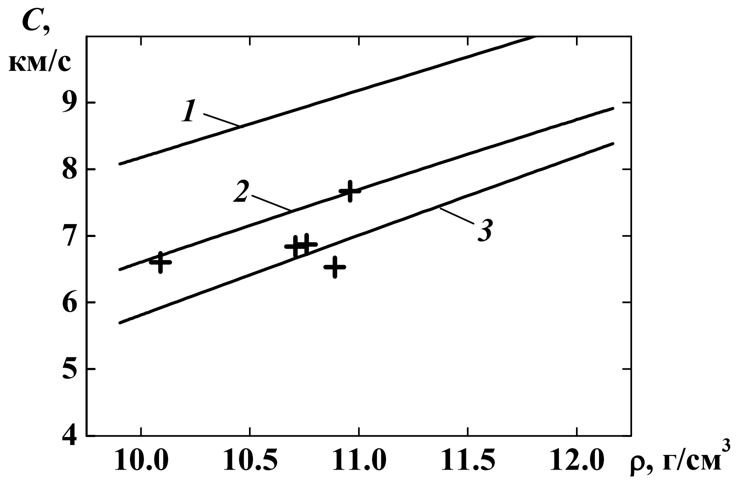

Fig. 5. ***1*** - the speed of sound in the core of the Earth [23]. Calculation of velocity of sound in liquid iron by formula (26): ***2*** - if the density and pressure as in the outer core of the Earth; ***3*** - along the shock adiabat. + - experimental speed of sound for shock wave [24, 25] (improved).

Iron-nickel the additive in the Earth's core can be carbon in the diamond phase, which reduces the density, but increases the speed of sound to the required values [24]. Other light supplements, reducing density, not enough increase the speed of sound in Matter.

Modeling of equations of state of matter by methods of molecular dynamics. The proposed equation of state based on the simple, but fundamental ratio (4):

$$p_H = p_p \frac{\rho}{\rho_1},$$

to be universal and applicable to condensed matter at not very high pressure behind the shock wave front. It is therefore interesting to his independent verification that can be performed by the methods of molecular dynamics.

Modeling of shock compression was solved by means of the Monte Carlo method. Interaction of particles matter set pair potential of Lennard-Jones:

$$U(r) = 4\varepsilon\left[\left(\frac{b}{r}\right)^{12} - \left(\frac{b}{r}\right)^{6}\right] \qquad (27)$$

and potential exp -6:

$$U(r) = \frac{\varepsilon}{1-6/\alpha}\left[\left(\frac{6}{\alpha}\right)\exp\left[\alpha\left(1-\frac{r}{b}\right)\right] - \left(\frac{b}{r}\right)^{6}\right]. \qquad (28)$$

Thermodynamic parameters of matter when the shock compression was computed as in [26]. In the calculations, the system checks the conservation laws: energy, momentum and angular momentum. When calculating, the forces going paralleling at multiple cores using Protocol OMP.

In fig. 6 shows an example of a completed calculations for liquid argon. However, in the case of argon shock adiabat built by the ratio (11) by the isotherms at 0 (K) [16].

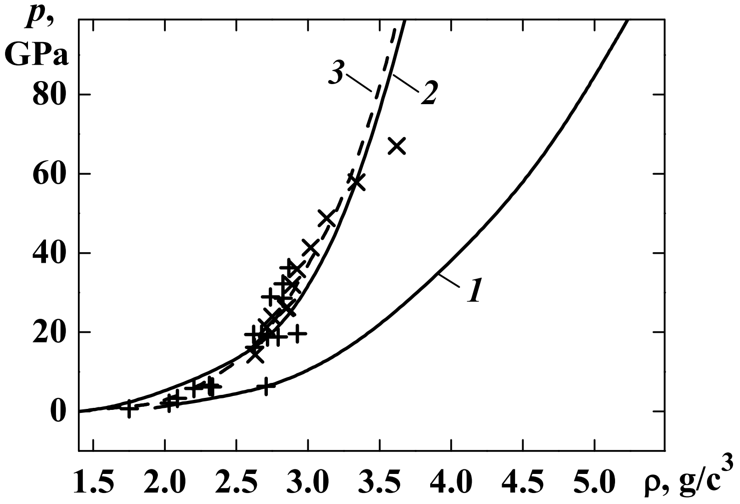

Fig. 6. Comparison of the results of calculation of the shock adiabat of argon and experimental data. ***1*** - isotherm at T = 0K [16]; ***2*** -calculation of the shock pressure by ***1*** due ratio (12); ***3*** -calculation of shock simulation with potential (27). The point is to experiment: × - [6]; + [13].

You can see that the results are consistent within error when measuring shock adiabat as well as proximity given in [16] zero isotherm and simplifications in simulation. Satisfactory results were obtained when comparing calculations with experimental data in the case of iron and other chemical elements.

Conclusion. Qualitatively from physical considerations and quantify molecular dynamics techniques is justified by the fundamental ratio $\boldsymbol{p_p = p_H\times(\rho_0/\rho)}$ linking the potential component of pressure and total pressure behind the front shock waves in condensed matter at not very high pressures, but it is necessary to note the following: When shock compression due to high temperatures and specific shock compression substance may undergo phase transitions, induce, ionization of atoms at high temperatures the atoms displaced of equilibria, in contrast to the state at a temperature of 0 K. Therefore the potential pressure behind the shock wave p_p may differ significantly from the curve of a cold compress at $T = 0$K.

Additionally attracted the well-known idea that thermal movement of dense matter can be modeled by ideal gas particles, in this work, modified to build thermal equations of state of condensed matter.

The resulting equation of state allows you to simply and clearly expect the temperature, speed of sound, the adiabatic state changes of matter when high energy densities. Therefore, the equation of state may be useful when planning experiments and evaluation of substances under shock-wave processing, physics of the Earth and other planets without complicated calculations.

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