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INTERACTION OF LASER RADIATIOBN WITH MATTER. LASER PLASMA

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Equation of matter state in the average-ion model for a laser-produced plasma

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Abstract. A thermodynamically consistent model for calculating the equation of plasma state in the average-ion approximation is proposed. The model takes into account the chemical bonds in a solid, the pressure of electron shells of an ion, which arises upon the ion compression, and also the degeneracy of the electron gas at high densities and low temperatures. The calculations of shock compression of different materials, such as liquid deuterium, Al, Be, Fe and Au, carried out using this model showed that it provides a satisfactory description both of the existing experimental results and of the results of calculations involving the Thomas – Fermi model over a broad range of pressure behind the shock front. The isotherms of the above materials calculated in the average-ion approximation and using the Thomas – Fermi model are compared for different temperatures.

1. Introduction

Upon absorption of high-power laser radiation, the states of a condensed matter with an extremely high energy density can be produced. In particular, such states are currently attained in the experiments on inertial plasma confinement at the major laser facilities (NOVA in the USA, ISKRA-5 in Russia, Gekko-12 in Japan, etc.). This allows one to use these facilities for experimental studies of the equations of state under extreme conditions. In particular, experiments on the compression of liquid deuterium were recently performed at the NOVA laser facility in the USA [1]. Similar conditions are also realised in ion beam–matter interaction experiments, in experiments with liners, pinches, and in explosion experiments, including those with shock tubes.

Such experiments are analysed employing numerical gas-dynamic simulations, which requires a knowledge of the equations of matter state. The equations of state are usually written in the form of the dependence of pressure p and the energy E of the matter on the density ρ and temperature T. The precision attained in the numerical simulations depends substantially on the accuracy of the equation of state in use (in particular, typical applications require that the data calculated from the equation of state should be accurate to about 15 – 20% or better). In addition, gas-dynamic simulations involve significant difficulties unless the data calculated from the equations of state are represented as relatively smooth functions of the density and temperature. It is also required that the specific heat $c_V = (\partial E/\partial T)_{\rho=\text{const}}$ and the sound velocity $c_s^2 = (\partial p/\partial \rho)_{S=\text{const}}$ (where S is the entropy) would be positive throughout the parameter range of interest (i. e., the density and temperature ranges involved in the simulation) while the energy and the pressure would be thermodynamically consistent.

Many experimental (see the review [1] and references therein) and theoretical (see, e. g., Ref. [2]) papers have been devoted to the study of the equations of state. Among the models widely used to calculate the equation of state of any material is the model based on the Thomas – Fermi approximation [2]. Alhough this model is a universal one, it nevertheless has several limitations. First, this model can be applied only in the case of a local thermodynamic equilibrium. Second, numerical calculations of the solution of the nonlinear differential equation for the self-consistent potential and electron density distributions are time-consuming. For this reason, this model can be used in gas-dynamic codes only in the form of pre-calculated tables.

The range of density and temperature variations which characterises the state of matter in a laser-produced plasma, is extremely broad: from densities that are higher than and equal to the solid-state density and temperatures close to zero (strongly compressed material behind the shock wave front) to extremely low densities and high temperatures ~ 1 keV (nonequilibrium hot coronal plasmas). Therefore, there is demand for a universal technique capable of describing the equation of matter state in broad temperature and density ranges.

The development of multilevel kinetic models in the average-ion approximation permits constructing a model of the equation of state, which is valid under the conditions remote from the state of local thermodynamic equilibrium (which is impossible within the framework of the Thomas – Fermi model). Such conditions are realised, for instance, in the corona of a laser-produced plasma. The term corona is used in reference to the region of a hot and tenuous ($T \sim 1$ keV, $\rho \sim 1$ mg cm^{-3}) plasma, which strongly absorbs intense laser radiation. The average-ion model permits us to take into account the states of matter whereby the effect of pressure of the cold material proves to be significant (for instance, the material behind the shock wave front). This allows us to extend the range of the model validity to a broad

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temperature and density range to describe the states of matter which include, on the one hand, the states of a strongly compressed material with densities exceeding those of solids and, on the other, the states of a hot and tenuous plasma.

2. Energy of the electron component of a nonideal plasma

Consider a plasma consisting of ions of a different sort with nuclear charges Z_j, atomic numbers A_j, and densities C_j. As is accepted in the average-ion approximation we will describe the distribution of the occupation numbers of ions over the degree of ionisation of the jth element by a single ion. For this ion, the distribution of the occupation numbers or the populations P_{jk} (which now are treated as continuous functions of the plasma parameters) over the atomic levels with quantum numbers k is such that the degree of ionisation of this average ion $Z_j^* = Z_j - \sum_k P_{jk}$ is equal to the average degree of ionisation of the jth element.

Let ρ, T_e, and T_i are the plasma density and the electron and ion temperatures, respectively. The average degree of ionisation and the average atomic weight of the plasma are calculated from the expressions

$$\langle Z\rangle = \sum_j C_j Z_j^*, \quad \langle A\rangle = \sum_j C_j A_j.$$

The electron and ion densities are defined in terms of the plasma density, the average atomic weight, and the average charge as follows: $N_i = N_A\rho/\langle A\rangle$, $n_e = \langle Z\rangle n_i$, where N_A is the Avogadro number.

The electron and ion plasma components can be treated as two weakly interacting components each of which makes an additive contribution to the complete equation of state. For ions, the ideal Boltzmann gas approximation is adequate for the calculation of the equation of state virtually over the entire pressure and temperature ranges of interest to us, which are typical of laser–matter interactions. This means that the ion energy E_i per unit plasma mass and their pressure can be calculated from the expressions

$$E_i = c_{Vi}T_i, \quad p_i = \frac{c_{Vi}T_i\rho}{\gamma - 1}, \quad c_{Vi} = \frac{N_A}{\langle A\rangle}, \quad \gamma = \frac{5}{3}. \tag{1}$$

The electron state can be described by the equation of state of the type (1), only at very high temperatures and low densities, when the plasma ions are fully ionised and, on the one hand, the energy expenditures for the ionisation are small compared to the energy of thermal motion of free electrons and, on the other hand, the degeneracy of the electron gas can already be neglected, i. e., the electron energy is much higher than the Fermi energy. For a low-density plasma ($\rho \leqslant 10^{-2}$ g cm^{-3}) at a temperature of about 1 keV (typical parameters for the corona of a laser-produced plasma), such conditions are realised for a relatively small (below 20) charge of the ion nucleus, i. e., for relatively light elements. For heavy elements or lower temperatures that are characteristic of the X-ray corona ($T_e \sim 0.09 - 0.3$ keV, $\rho \sim 0.2 - 1$ g cm^{-3}), the plasma is no longer fully ionised and, even if the degeneracy can still be neglected (i. e., the electron temperature is still higher than the Fermi energy), the ionisation losses of the thermal energy should be included in the equation of state. For still lower temperatures and higher densities, the contribution of the electron-gas degeneracy becomes the crucial one.

Nevertheless, in this case of a strongly nonideal plasma, all the electrons may also be considered as being distributed between two subsystems with a discrete (bound electrons) or a continuous (free electrons) energy spectrum. The bound electrons are described by the occupation numbers P_{jk} as before, whereas free electrons can be characterised by a temperature T_e. If the exchange interaction energy for these two systems can be neglected, the total energy of the electron plasma component can be calculated as the sum of energies of its different subsystems:

$$E_e = E_{fe} + E_{be} + E_{ci} + E_{cb}, \tag{2}$$

Apart from the above-mentioned free- (E_{fe}) and bound-electron (E_{be}) energies, expression (2) also takes into account the correlation energy E_{ci} of the Coulomb interaction between ions and the chemical binding energy E_{cb} in a solid. We consider each term in expression (2) separately.

2.1. Energy of free electrons

If it is assumed that free electrons do not interact with ions, the Fermi statistics can be applied to them and we can use the known formula for the energy of a Fermi gas [3]

$$E_{fe} = \frac{\sqrt{2}m_e^{3/2}T_e^{5/2}}{\pi^2\hbar^3\rho} I_{3/2}\left(\frac{\mu}{T_e}\right). \tag{3}$$

Here, $I_{3/2}(\mu/T_e)$ is the Fermi integral of degree $v = 3/2$ (by definition, $I_v(x) = \int_0^\infty y^v[\exp(y-x)+1]^{-1}\mathrm{d}y$) and μ is the chemical potential of free electrons. For $I_{3/2}(x)$, the approximation

$$I_{3/2}(x) = \frac{3}{2}I_{1/2}(x)\Big\{1 + 1.031\big[I_{1/2}(x)\big]^{2/3} + 0.144\big[I_{1/2}(x)\big]^2\Big\}^{1/3}. \tag{4}$$

can be used.

This approximation ensures proper (correct to second-order terms of the Taylor expansion) passages of E_{fe} (3) to the limit of E_{fe} in the equation of state of an ideal Boltzmann gas at high temperatures of free electrons and to the limit of E_{fe} in the equation of a degenerate Fermi gas at low temperatures.

The Fermi integral of degree 1/2 is in turn related to the free-electron density n_e by the normalisation condition [3]

$$n_e = \frac{\sqrt{2}(m_eT_e)^{3/2}}{\pi^2\hbar^3} I_{1/2}\left(\frac{\mu}{T_e}\right). \tag{5}$$

Therefore,

$$E_{fe} = \frac{3}{2}\frac{T_en_e}{\rho}\left[1 + 1.031I_{1/2}^2\left(\frac{\mu}{T_e}\right) + 0.144I_{1/2}^2\left(\frac{\mu}{T_e}\right)\right]^{1/3}. \tag{6}$$

Indeed, in the limit of very high temperatures and low densities, we obtain from (6) the expression for the energy of an ideal Boltzmann gas

$$E_{fe} = \frac{3}{2}\frac{n_eT_e}{\rho}.$$

In the opposite limit of low temperatures and high densities, we obtain the expression for the energy of a degenerate Fermi gas:

$$E_{\rm fe} = E_{\rm fe}^{(0)} + \frac{c_{Ve}^{(0)}}{2} T_{\rm e}^2, \quad E_{\rm fe}^{(0)} = \frac{3\left(3\pi^2\right)^{2/3} \hbar^2 n_{\rm e}^{5/3}}{10 m_{\rm e} \rho},$$

$$c_{Ve}^{(0)} = \left(\frac{\pi}{3}\right)^{2/3} \frac{m_{\rm e}}{\hbar^2} \frac{n_{\rm e}^{1/3}}{\rho}.$$

2.2. Energy of bound electrons

For known level populations P_{jk} of the jth ion, the energy of bound electrons is defined as in the standard model of hydrogen-like average ion [4, 5]:

$$E_{\rm be} = \beta \sum_j C_j E_j, \quad E_j = -\sum_{k=1}^{N_j^{\max}} P_{jk} (Q_{jk}/k)^2, \tag{7}$$

where E_j is the energy of bound electrons of the jth ion; Q_{jk} is the screened-nucleus charge in the kth level of the jth ion; $\beta = I_{\rm H} N_{\rm A} / \langle A \rangle$; $I_{\rm H} = e^2/2a_0$ is the ionisation potential of hydrogen; $a_0 = \hbar^2/m_{\rm e}e^2$ is the Bohr radius of an electron; and $N_j^{\max}$ is the maximum number of levels for the jth ion.

In the general case of arbitrary temperatures, the population of each ion is found by solving a system of kinetic equations [5]. However, in the limit when the electron temperature tends to zero, the solution of this system of equations is only slightly different from the population density distribution in accordance with the statistical weights (zero-temperature populations) g_k of each level. For an isolated hydrogen-like atom, $g_k = 2k^2$ and electrons occupy the lowest-energy levels up to some level with the principal quantum number $k_{\max}$ determined from the atom neutrality condition. Taking into account that in the general case, each level of the jth ion is also characterised, in addition to the principal quantum number k, by the orbital quantum number l, we can write

$$g_{lk} = \sum_{l=0}^{k-1} g_{jkl}, \quad g_{jkl} = 2(l+1), \quad l = 0, 1, ..., k-1.$$

Let $P_{jkl}^{(0)}$ be the population of the kth level (with an orbital quantum number l) of the jth neutral isolated atom; then,

$$P_{jk}^{(0)} = \sum_{l=0}^{k-1} P_{jkl}^{(0)}, \quad P_{jkl}^{(0)} = g_{jkl}, \quad Z_j = \sum_{k=1}^{k_{\max}} P_{jk}^{(0)}.$$

When atoms are compressed, the degeneration is lifted and some electrons become free. In addition, the interaction of atoms or ions with each other also changes the bound-state energies. This effect is automatically taken into account both in the simple Thomas–Fermi model [6] and in the more sophisticated models of self-consistent field of the Hartree–Fock model type [7].

Generally speaking, the effect of surrounding ions on the electron distribution in the average-ion model can be taken into account only phenomenologically. Thus, it was proposed in Ref. [8] to introduce such a dependence of the statistical weight of the state ξ on the material density, which is characterised by two quantum numbers k and l, that the statistical weight of the isolated ion state would be obtained at low densities, while at high densities the statistical weight would tend to zero. Such a dependence models the lift of the degeneration of the state ξ caused by the interaction with the surrounding ions (e. g., due to the Stark level splitting), with the result that a part of the bound states transfer to the continuous spectrum.

The simplest function possessing these properties is the function of the form

$$g_{j\xi} = \frac{P_{j\xi}^{(0)}}{1 + \alpha_{j1} (R_{j\xi}^{(0)}/R_0)^{\alpha_{j2}}}, \tag{8}$$

where $R_0 = (\langle A \rangle / \frac{4}{3} \pi N_{\rm A} \rho)^{4/3}$ is the radius of the ion sphere and $R_{j\xi}^{(2)}$ is the effective radius of the orbit of the level ξ of an isolated jth ion. It has been proposed [5] that the average dipole interaction radius $R_{jkl} \sim \langle 1/r^2 \rangle^{-1/2}$ be used as the effective shell radius in the average-ion model with inclusion of the l splitting. For given quantum numbers k and l and with hydrogen-like electron wave functions, this radius is calculated by the formula

$$R_{jkl} = \frac{a_0 k^{3/2}}{Q_{jk}} \left(l + \frac{1}{2}\right)^{1/2}. \tag{9}$$

Therefore, the average degree of ionisation $\langle Z \rangle$ of a cold material with the density ρ can be calculated from expressions (8) and (9) as

$$\langle Z \rangle = \sum_j C_j \sum_\xi \left(P_{j\xi}^{(0)} - g_{j\xi}\right). \tag{10}$$

Following Refs [5, 8], we found the coefficients α_{j1} and α_{j2} in (8) at which the density dependence of the degree of ionisation of a cold (for $T = 0$) material determined by expressions (8)–(10) was most close to a similar dependence derived using the Thomas–Fermi model [6]. Fig. 1 shows the constants α_{j1} and α_{j2} for elements with different nuclear charges (different atomic numbers) Z_j from 1 to 100. One can see that coefficients α_{j1} and α_{j2} are quasi-periodic, slowly increasing (in the sense of the average value) functions of the atomic number of the element with the period corresponding to the structure of electron shell filling in different elements. As Z_j increases, the average values of the coefficients vary from 8.5 to 11 for α_{j1} and from 2 to ~ 3 for α_{j2}. Fig. 2 compares the density dependences of the average degree of ionisation calculated by the Thomas–Fermi model and by formulas (8)–(10) for a number of chemical elements with different nuclear charges Z_j and constants α_{j1} and α_{j2} corresponding to these elements.

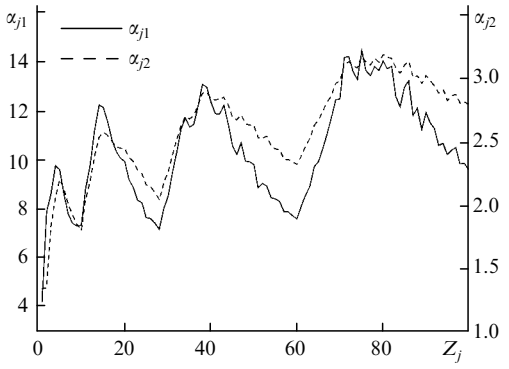

Figure 1. Constants α_{j1} and α_{j2} as functions of the atomic number of an element.

By returning to the case of arbitrary temperatures, we can separate from the general expression for the energy of bound electrons (7) the term related to the pressure-induced ionisation and the term caused by the temperature increase, i. e., to represent $E_{\rm be}$ in the form:

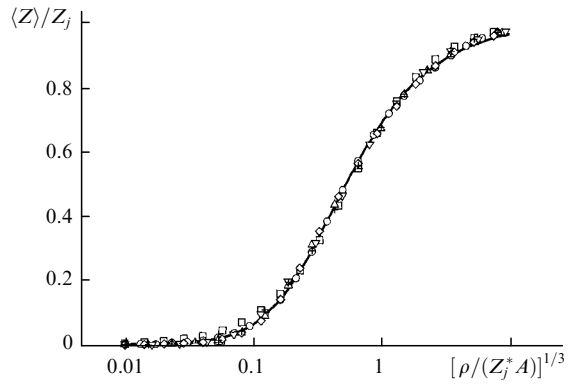

Figure 2. Dependence of the 'cold' degree of ionisation on the density calculated using the Thomas – Fermi model (the solid curve) and the average-ion model for a nuclear charge $Z_j = 1$ (□), 10 (○), 20 (△), 40 (▽), 60 (◇), and 80 (+).

$$E_{\rm be} = E_{\rm be}^{p} + E_{\rm be}^{T}. \tag{11}$$

In this case, $E_{\rm be}$ is calculated by formula (7) with the populations determined from the solution of the system of kinetic equations for a given plasma density and temperature; $E_{\rm be}^{\rm p}$ is calculated from formula (7) but with the populations corresponding to a given density for a zero temperature, i. e., equal to the statistical weights calculated by formulas (8) and (9). The second term in expression (11) accounts for the thermal energy losses by ionisation. (The losses by ionisation defined in precisely this way are taken into account in the conventional equation of state for the average-ion model in the SNDP code [9]). This term only weakly depends on the density and therefore makes no contribution to the electron pressure, whereas the first term depends only on the density and determines the contribution of electron shells to the 'cold' pressure, which will be discussed below.

2.3. Correlation energy of the Coulomb interaction between ions

Another density effect, which was mentioned above, results from a reduction in the bound-state energies of the ion of the jth element located in the Coulomb field of its neighbours. The correlation energy of plasma particles in the zero-temperature limit can be calculated as in Ref. [3] for the case of an ideal Boltzmann plasma:

$$E_{\rm ci} = -0.5\beta a_0 \frac{\langle Z\rangle^2}{R_0}\left[1 - \exp\left(-\frac{R_0}{R_{\rm D}}\right)\right], \tag{12}$$

where

$$R_{\rm D} = \frac{V_{\rm F}}{\sqrt{3}\omega_{\rm pe}} = \frac{(3\pi^2)^{1/3}\hbar}{2e\sqrt{3\pi m_{\rm e}}}\left(\frac{\langle A\rangle}{\langle Z\rangle \rho N_{\rm A}}\right)^{1/6}$$

is the Debye radius for a degenerate plasma; $\omega_{\rm pe}$ is the electron plasma frequency; and the Fermi velocity $V_{\rm F}$ [10] is used instead of the electron thermal velocity. The lowering of the ionisation potential of the level ξ is determined from the expression

$$\Delta E_{\xi} = -\frac{\partial E_{\rm ci}}{\partial\langle Z\rangle}. \tag{13}$$

2.4. Chemical binding energy

The free-electron pressure of the plasma of a metal calculated in the degenerate Fermi gas approximation at solid-state densities and a zero temperature amounts to tens and even hundreds of kilobars. In real materials, so high a pressure is balanced by chemical binding forces. In order to obtain a correct equation of state that is valid at densities close to the solid-state density, corrections should therefore be introduced to take into account the chemical bond of atoms and molecules in a material.

Following Refs [2, 11], we define the chemical binding energy by the semiempirical formula:

$$E_{\rm cb} = \varepsilon_0\left[1 - \exp\left\{b\left[1 - \left(\frac{\rho_{\rm s}}{\rho}\right)^{1/3}\right]\right\}\right], \tag{14}$$

where $\rho_{\rm s}$ is the density of a solid. The constants ε_0 and b in formula (14) are found from the condition that the total pressure of the electron component $p_{\rm e}^{\rm tot}$ for the initial density equal to the solid-state density $\rho_{\rm s}$ under normal conditions and at a zero material temperature is equal to zero [$p_{\rm e}^{\rm tot}(\rho_{\rm s},0) = 0$] and that the compressibility B is equal to the experimental compressibility of the material measured under normal conditions [$B(\rho_{\rm s},0) = B_{\rm exp}$]. Then, the total electron energy is written as

$$E_{\rm e}^{\rm tot}(\rho, T_{\rm e}) = E_{\rm fe} + E_{\rm be} + E_{\rm ci} + E_{\rm cb} + E_0, \tag{15}$$

where

$$E_0 = -(E_{\rm fe} + E_{\rm be} + E_{\rm ci} + E_{\rm cb})|_{\rho=\rho_{\rm s},T_{\rm e}=0}$$

$$\equiv -E_{\rm e}(\rho = \rho_{\rm s}, T_{\rm e} = 0).$$

3. Pressure of the electron component

In accordance with thermodynamic equalities, the electron pressure is defined in terms of the derivative of the total electron energy $E_{\rm e}^{\rm tot}$ with respect to the density for a constant entropy or in terms of the derivative of the total free energy $E_{\rm e}^{\rm tot}$ with respect to the density for a constant temperature:

$$p_{\rm e}^{\rm tot}(\rho, T_{\rm e}) = \rho^2 \left.\frac{\partial E_{\rm e}^{\rm tot}}{\partial\rho}\right|_{S=\rm const} = \rho^2 \left.\frac{\partial F_{\rm e}^{\rm tot}}{\partial\rho}\right|_{T_{\rm e}=\rm const}.$$

In this case, the total free energy can also be represented as the sum of the corresponding free energies [$F_{\rm e}^{\rm tot}(\rho,T_{\rm e}) = F_{\rm fe} + F_{\rm be} + F_{\rm ci} + F_{\rm cb}$] and the total pressure is equal to the sum of partial pressures [$p_{\rm e}^{\rm tot}(\rho,T_{\rm e}) = p_{\rm fe} + p_{\rm be} + p_{\rm ci} + p_{\rm cb}$].

Because $E_{\rm ci}$ and $E_{\rm cb}$ depend only on the density, the corresponding free energies are merely equal to the correlation energy and the chemical binding energy. We represented the bound electron energy as the sum of two terms (11), the first of which depends only on the density and the second one only on the temperature. Hence, the bound-electron pressure will be determined only by the first term in formula (11). For free electrons, we obtain a conventional pressure–energy relationship [3], but with a correction arising from the fact that the average plasma charge $\langle Z\rangle$ depends on the density ρ when the material is compressed at a zero temperature.

Eventually we arrive at the following expressions for the calculation of partial pressures:

$$p_{\rm fe} = \frac{2}{3}\rho E_{\rm fe} + \langle Z\rangle f_Z \frac{\partial E_{\rm fe}}{\partial\langle Z\rangle}\bigg|_{T_{\rm e}=0} = \frac{2}{3}\rho E_{\rm fe} + \frac{5}{3} f_Z \rho E_{\rm fe}^{(0)},$$

$$f_Z = \frac{\rho}{\langle Z\rangle}\frac{\partial\langle Z\rangle}{\partial\rho}\bigg|_{T_{\rm e}=0}, \quad p_{\rm be} = \rho^2 \frac{\partial E_{\rm be}^p}{\partial\rho},$$

$$p_{\rm ci} = \frac{2}{3}\rho E_{\rm ci}\left[0.5 + 3f_Z + 0.25(f_Z - 1)\frac{(R_0/R_{\rm D})\exp(-R_0/R_{\rm D})}{1-\exp(-R_0/R_{\rm D})}\right], \tag{16}$$

$$p_{\rm cb} = -\frac{E_0 b\rho_{\rm s}}{3}\left(\frac{\rho}{\rho_{\rm s}}\right)^{3/2}\exp\left\{b\left[1-\left(\frac{\rho_{\rm s}}{\rho}\right)^{1/3}\right]\right\}.$$

Accordingly, knowing the total pressure and having calculated the density derivative of the pressure, one can find the sound velocity $c_{\rm s}$ and the compressibility B:

$$c_{\rm s} = \left(\frac{\partial p_{\rm e}^{\rm tot}}{\partial\rho}\right)^{1/2}, \qquad B = \rho\frac{\partial p_{\rm e}^{\rm tot}}{\partial\rho}.$$

Therefore, formulas (3) – (5), (7), (11), (12), and (14) – (16) completely describe the thermodynamically self-consistent equation of electron state for the ionisation model in the average-ion approximation.

4. Results of calculations

The approach outlined above was realised in the SNDP and MIMOZA-ND gas dynamic codes. The results of calculations of the shock compression of a material in our model were compared with experimental data and also with the results of calculations employing the Thomas–Fermi model. The calculations were performed for liquid D_2, Be, Al, Fe, and Au for pressures behind the shock wave front varied from 0.01 to 1000 Mbar.

Our calculations showed that using in expression (8) the constants α_{j1} and α_{j2} determined from the fit to the 'cold' ionisation curve (see Fig. 1) proved to be a relatively crude approximation when the results of calculations made by the SNDP code were compared with experiments and with the Hugoniot adiabat using the equation of state according to the Thomas – Fermi model. This is illustrated in the $p-\rho$ diagram of iron (Fig. 3). Generally speaking, the degree of ionisation in the Thomas – Fermi model is not a well-defined quantity, being conventional in character. A physically well-posed, uniquely determined characteristic is the total electron energy.

In the average-ion model for $T = 0$, the total electron energy (neglecting the chemical binding energy) is uniquely determined by formulas (3), (7), and (12). These formulas ensure qualitatively correct density dependences both in the high- ($E \propto \rho^{3/2}$ as $\rho \to \infty$) and low-density ($E \to$ const as $\rho \to 0$) limits. Therefore, constants α_{j1} and α_{j2} determined from the fit to the 'cold' pressure dependence of the total electron density should be the best approximation. Fig. 4 depicts the calculated 'cold' plasma-density dependences of the total electron energy (counted from the energy of the electrons $E^{(0)}$ of an isolated, completely neutral atom) for the Thomas – Fermi model and the energies of the ions of several elements for the average-ion model with the optimised constants α_{j1} and α_{j2}. One can see that it is possible to select the constants α_{j1} and α_{j2} so that the electron energy calculated using the average-ion model agrees satisfactorily with the results of calculations within the framework of the Thomas – Fermi model over a broad range of plasma density.

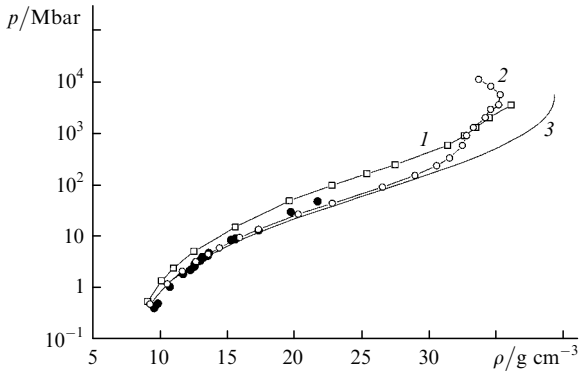

Figure 3. Shock adiabat of iron calculated using the equation of matter state in the average-ion model (*1*, *2*) for the constants $\alpha_1 = 7.64$ (*1*) and 3.72 (*2*), $\alpha_2 = 2.14$ (*1*) and 3.03 (*2*) and the results of experiments [1, 12, 13] (●) and calculations employing the equation of matter state in the Thomas – Fermi model (*3*).

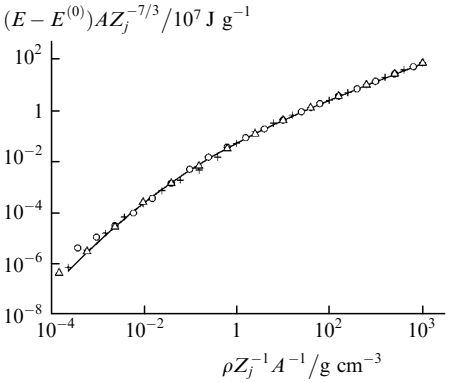

Figure 4. Density dependences of the electron energy at zero temperature for the Thomas – Fermi model (the curve) and of the energies of Al (+), Fe (○), and Au (△) ions for the average-ion model for optimal α_{j1} and α_{j2} constants.

The SNDP calculations of shock compression performed for iron with the new constants α_{j1} and α_{j2} are also illustrated in Fig. 3. In this case, it has been possible to obtain a better agreement between the results of calculations and experimental data throughout the pressure range up to 30 Mbar. The largest deviation from the calculations employing the Thomas–Fermi model arises at high pressures (above 100 Mbar) where, unfortunately, we failed to find experimental data. This disagreement is caused by shell effects, which should, broadly speaking, manifest themselves at high plasma pressure and temperature and which are disregarded in the Thomas – Fermi model.

Considering the aforesaid, we optimised the constants α_{j1} and α_{j2} and then calculated the shock adiabats of the remaining materials (liquid D_2, Be, Al, and Au) employing the SNDP code and the constants obtained. The results of calculations as presented in the form of $p-\rho$ diagrams in Figs 5 – 8. As a whole, our model is in satisfactory agreement both

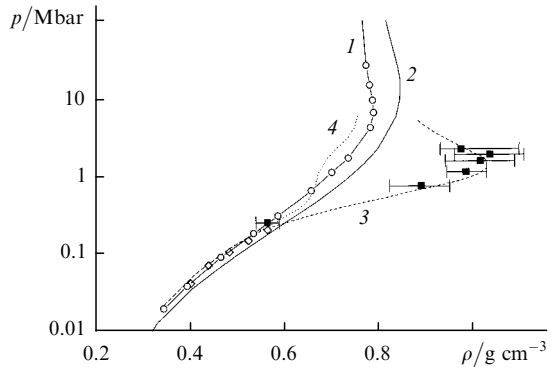

Figure 5. Shock adiabat of liquid deuterium calculated using the equation of matter state in the average-ion model (*1*) as well as the results of experiments of Refs [14] (◇) and [15] (■), of the calculations using the equation of matter state in the Thomas – Fermi model (*2*), and of Refs [16] (*3*) and [17] (*4*).

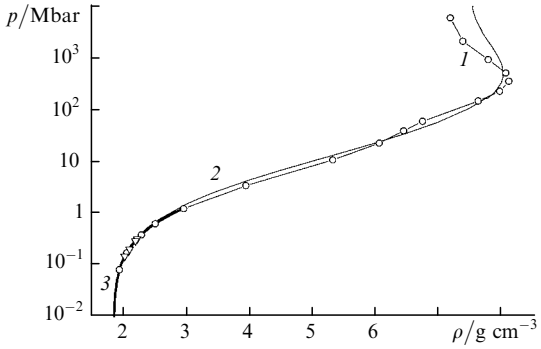

Figure 6. Shock adiabat of beryllium calculated employing the equation of matter state in the average-ion model (1) and results of the experiments of Ref. [18] (▽), of the calculations employing the equation of matter state in the Thomas – Fermi model, and of Ref. [1] (*3*).

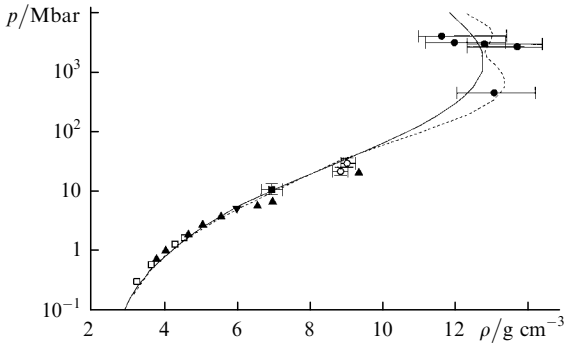

Figure 7. Shock adiabat of aluminium calculated employing the equation of matter state in the average-ion model (the dashed line) and also the results of experiments of Vladimirov et al. (●), Ragan (□), Al'tshuler et al. (▲), Volkov et al. (■), Kormer et al. (▼), and Mitchell et al. (○) (see Ref. [2]) and of calculations employing the equation of matter state in the Thomas – Fermi model (the solid line).

with experiments and the calculations performed using the Thomas – Fermi model. As for iron, the deviation for the selected elements is largest in the high-pressure domain (over 10 Mbar), where experimental data are scarce (with the exception of aluminium, Fig. 7). In this case, the calculations based on the average-ion model reveal the atomic shell structure, which is, naturally, absent in the Thomas – Fermi approximation.

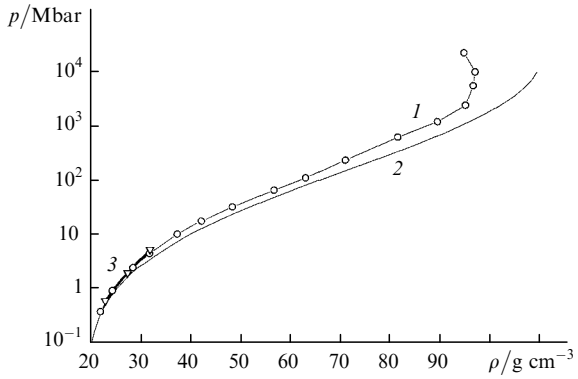

Figure 8. Shock adiabat of gold calculated employing the equation of matter state in the average-ion model (1) and also the results of experiments of Ref. [1] (▽, *3*) and of calculations employing the equation of matter state in the Thomas – Fermi model (*2*).

One can see from Fig. 5 that the average-ion model cannot describe the latest data on the shock compression of liquid deuterium obtained in the experiments on the NOVA laser facility [15]. This is primarily explained by the fact that the average-ion model does not take into account the structure of deuterium molecules and therefore cannot describe the molecule dissociation upon the shock compression of liquid deuterium. Meanwhile, it is the dissociation that causes a sharp increase in the compressibility of deuterium in the 1 – 3 Mbar pressure range (see, e. g., Ref. [16]).

Figs 9 and 10 depict the isotherms of aluminium and gold for $T = 0.01$, 0.1, 0.5, and 1 keV obtained using the average-ion model and also the corresponding dependences calculated

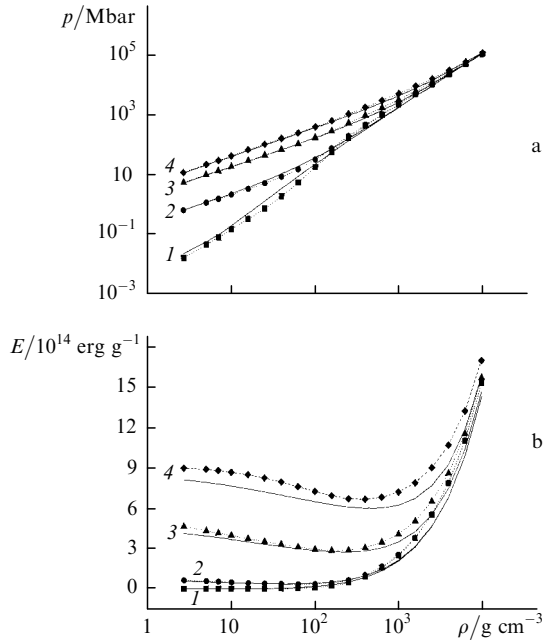

Figure 9. Dependences $p(\rho)$ (a) and $E(\rho)$ (b) for aluminium calculated in the average-ion model (the dotted lines) and in the Thomas – Fermi model (the solid lines) for $T = 10$ (■, *1*), 100 (●, *2*), 500 (▲, *3*), and 1000 eV (◆, *4*).

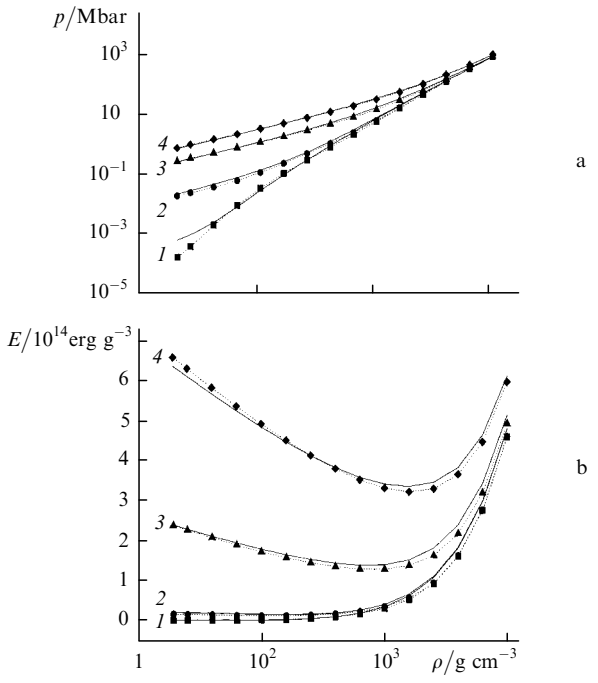

Figure 10. Dependences $p(\rho)$ (a) and $E(\rho)$ (b) for gold calculated in the average-ion model (dots) and in the Thomas – Fermi model (the solid curves) for $T = 10$ (■, *1*), 100 (●, *2*), 500 (▲, *3*), and 1000 eV (◆, *4*).

in the Thomas – Fermi model. The dependences $p(\rho)$ are in close agreement in both these cases. As for the dependences $E(\rho)$ (in Figs 9b and 10b, the energy is counted from the energy of the material for a solid-state density and $T = 0$), the agreement is satisfactory for gold, while a somewhat larger discordance is seen in the case of aluminium. In particular, a nonmonotonic behaviour of the $E(\rho)$ dependence is supposedly due to the shell effects in the average-ion model.

It should be noted that as a whole the proposed model of the equation of state for the ionisation kinetics in the average-ion approximation describes adequately the behaviour of a broad spectrum of materials (from the lightest to heavy ones) over a broad temperature and density range, provided the constants α_{j1} and α_{j2} for the calculation of the statistical weight of the levels at high plasma densities are selected from the 'cold' electron energy curve rather than from the 'cold' ionisation curve, as was done previously.

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