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Simple equation of state to describe behavior of solid and porous aluminum samples under impact compression and isentropic unloading

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A small-parameter equation of state of aluminum has been constructed, whose Gruneisen coefficient is specified as a logarithmic dependence on the density. The parameters of the equation of state of aluminum have been defined for the density range from 1.4 to 7 g/cm^3. The porous material has been regarded as a simple thermodynamically equilibrium mixture of aluminum and air. The model uses only parameters of the equations of state and mass fractions of the mixture components. Shock adiabats for the aluminum samples with different initial porosities, curves of repeated compression and unloading isentropies, as calculated using this model, turn out to be close to respective experimental data. This indicates applicability of the proposed approach to constructing the equation of state of aluminum in order to describe properties of this metal (both in a pure form and in mixtures) both in the region of multiple compression and in the region of depression.

Keywords: shock adiabat, unloading isentropy, single-continuum approximation, heterogeneous mixture, thermodynamic equilibrium, single-temperature approximation, single-speed approximation, Gruneisen coefficient

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Introduction

Active use of aluminum is based on such properties thereof as lightness, plasticity, conductivity, corrosion resistance, whereas its low cost as compared to other metal plays a significant role. Aluminum alloys have diverse properties and this diversity is obtained by introducing various alloying additives into the alloys. For example, in aircraft construction and shipbuilding great significance is paid to reduction of weight and high strength of the aluminum alloys as compared to steel. Construction of seaplanes includes welding of magnalium (aluminum-magnesium) corrosion-resistant alloys. The aluminum-magnesium alloys are actively used in oil and chemical industries, since they have high corrosion resistance. Due to high conductivity and temperature-gradient resistance aluminum is widely used in electrical engineering. The alloying additives make it possible to produce materials with desired properties, whose basic component is aluminum. In a compressed form, full information about production, processing, application of aluminum and its physical, chemical and thermodynamic properties is contained in [1]. The same article of the encyclopedia shows that the properties of the alloys and the compounds containing aluminum depend on a nature of the alloying component. Prior to describing various mixtures, it is necessary to obtain a model reliably representing behavior of the mixtures as well as parameters of the equation of state of each component in these mixtures. The new models for describing the behavior of the solid and porous samples of the mixtures [2–5] appear as it is caused by tasks of modern science: these are problems of dynamic compacting, shock-wave synthesis and other explosion technologies. Based on the fact that the mixtures differ by a large variety of the compositions, it is necessary to provide for them the simplest model which uses only the parameters of the equations of state of the very compositions and their mass fractions in the mixture. In this regard, the present study is performed to obtain the parameters of the simple equation of state for aluminum at high pressures and temperatures.

The review [6] considers the problems and methods of constructing the equations of state of substances, describes principles of constructing semi-empirical models and lists main requirements to the equations of state. Many studies are dedicated to constructing the equation of state of aluminum (see, for example, the papers [6–13] and references therein). In particular, the paper [7] proposes a rather complex equation of state of this metal taking into account phase transformations (melting and evaporation) in the wide range of the densities and the temperatures. The paper [13] has developed the more simple equation of state of aluminum in the form of dependence of pressure on a specific volume and internal energy, which also well agrees with the data of shock-wave experiments with the solid and porous samples. The present paper has constructed the equation of state of aluminum based on the previously proposed simple model [4] (in variables the specific volume and temperature) that is conveniently used in the calculations of thermodynamic characteristics of the mixtures (alloys) which include this metal.

1. Mathematical model and calculation procedure

It is mentioned in the paper [14] that the task of obtaining the equation of state of a condensed body can not be solved by methods of statistical thermodynamics in an accurate mathematical representation. The literature contains a large number of approaches to selecting the equation of state when describing the shock-wave processes [5–18]. Construction of the semi-empirical equations of state includes defining a form of the functional dependence, while the parameters of this equation are chosen to best correspond to the experimental data [6,14].

It is noted in the paper [16] that during mathematical modelling of the shock-wave phenomena it is possible to used the equation of state in the form of the Mie-Gruneisen equation in order to describe the behavior of the condensed substances

$$P = P_X + \rho\gamma E_T, \tag{1}$$

where P_X — the elastic component of the pressure; the second summand on the right-hand side (P_T) — the thermal component of the pressure, $P_T = \gamma\rho E_T$; ρ — the medium density; γ — the Gruneisen coefficient; E_T — the thermal component of the internal energy. In order to describe the thermal part of the pressure, the paper [4] proposes the logarithmic dependence of the Gruneisen coefficient on the density.

$$\gamma = \gamma_0 r^{-\ln r}. \tag{2}$$

Here $r = \rho/\rho_0$ — the compression ratio; ρ_0 — the parameter of the equation of state (in case of the condensed substance it is its density at the normal conditions); γ_0 — the constant, the parameter of the equation of state. The dependence (2) makes it possible to adequately represent the behavior of the Gruneisen coefficient both for the solid and the highly-porous materials as well. It is noted in [5,14,16] that in the studies dedicated to shock-wave loading the Gruneisen coefficient can be described by the formula

$$\gamma = \gamma_0 r^{-l}, \tag{3}$$

where $l > 0$, $l = \text{const}$. When calculating the shock adiabats for the highly-porous materials, use of the expression (3) for description of the Gruneisen coefficient results in increase of the Gruneisen coefficient with growth of intensity of the shock wave. This is due to the fact that in anomalous behavior of the shock adiabats, at which the final density of the shock-compressed substance turns out to be less than the normal density, the ratio r becomes less than unity ($r^{-1} > 1$). The paper [19] has shown on the example of copper that use of the Gruneisen coefficient in the form of (3) with the exponent $l > 0$ for description of the porous material does not agree with the experimental data. The paper [4] discusses shortcomings of the equation of state with the Gruneisen coefficient (3) when describing the behavior of the porous materials and gives references to studies which attempt to use another form of the dependence for the Gruneisen coefficient (of those published after [4] it is worth mentioning the studies [13,20–29]). Even the paper [4] has already demonstrated a capability of the equation of state with the Gruneisen coefficient (2) to adequately describe the behavior of copper under shock compression and made a comparison with calculated adiabats of other authors, who use the equation of state of copper with a large number of the parameters. The present paper demonstrates applicability of the equation of state model as proposed in the paper [4] for describing the behavior of aluminum under pulse loading and subsequent unloading.

The use of the logarithm in the exponent of the relationship (2) results in that the Gruneisen coefficient decreases with any behavior of the adiabats, since a logarithm sign depends on the argument value and when $r^{-1} > 1$ the exponent becomes negative. When describing the elastic part of the pressure by means of the Tait equation, the equation of state (1) takes the form

$$P = P_X + \gamma_0\rho_0 r^{1-\ln r} c_{V0} T,$$
$$P_X = A[r^n - 1] - \gamma_0\rho_0 r^{1-\ln r} c_{V0} T_0, \tag{4}$$

where c_{V0} — the specific heat capacity with the constant volume (herein, it is assumed to be a constant value); T — the temperature; T_0 — the normal temperature, $T_0 = 293\,\text{K}$; A and n — the constants characterizing cold (when $T = 0$) compression of the substance. The parameter A can be found by the formula $A = c_0^2\rho_0/n$, where c_0 — the volume speed of sound under the normal conditions. Simplicity and convenience of use of these equations are due to the fact that the properties of an individual substance are described by using a set of the small number of the parameters ($\rho_0, c_0, n, c_{V0}, \gamma_0$).

The internal energy is also represented as a sum of two summands:

$$E = E_X + c_{V0} T. \tag{5}$$

Here E_X — the elastic part of the compression energy, which associated with the pressure elastic component by the relationship $P_X = \rho^2 dE_X/d\rho$. After integration, the expression for the elastic part of the energy takes the following form:

$$E_X = \frac{A}{(n-1)\rho_0}[r^{n-1} - 1] + \frac{A}{\rho_0}[r^{-1} - 1]$$
$$- \gamma_0 c_{V0} T_0 \frac{\sqrt{\pi}}{2}\operatorname{erf}(\ln r) - c_{V0} T_0,$$

where $\operatorname{erf}(x)$ — the error function,

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int\limits_0^x \exp(-t^2)dt,$$

for which the recent study [26] provides an approximation expression of quite high accuracy; and it is this expression that was used in the calculations below. The thermal part of the internal energy (5) is defined by the relationship $E_T = c_{V0}T$.

The paper [30] has proposed a method of constructing the equation of state of the equilibrium N-component mixture, wherein the equation of state of each component is defined in the same form. The paper [31] has substantiated application of the equation of state of the form (4) for air.

In the present study the porous N-component mixture is considered as a heterogeneous medium, whose pores are filled with air. The pores are considered to be closed and isolated, so the gaseous component does not leak out of a solid substance-air system and it does not take into account evaporation of the solid substance and increase of the mass fraction of the gaseous substance under the shock wave. The porosity m is understood as a ratio of the normal density of a monolith (ρ_{T0}) to the initial density of the porous sample (ρ_{00}). The present study excludes consideration of effects of phase transitions (melting and evaporation). As shown by the calculations by means of more complex models of the equations of state [7,32,33], in which the phase transitions are taken into account, the effect of substance melting in the shock wave is slightly noticeable at the shock adiabats in variables of the Hugoniot equations for samples of the different initial porosity. The results of calculations [33] by the equation of state of aluminum with taking into account melting and evaporation indicate that under shock compression of the solid and porous samples with an initial state in the solid phase of metal there are pressures which are noticeably higher than on an evaporation curve at the same temperatures. Therefore, a below boundary of the applicability region in terms of pressure (with the densities less than the density of liquid aluminum in the melting point under the atmospheric pressure) for the represented model of the equation of state can be an isobar passing through the critical point of liquid-vapor transition.

By various estimates, the pressure in the critical point (P_{cr}) for aluminum is 0.197 [7], 0.329 [34], 0.3988 [35], 0.45 [36], 0.597 GPa [37]. It should be noted that in all the said estimates P_{cr} does not exceed 1 GPa. The density of liquid aluminum in the melting point under the atmospheric pressure, in accordance with the equation of state [7], is approximately equal to $2.4\,\mathrm{g/cm^3}$. It means that at the densities less than $2.4\,\mathrm{g/cm^3}$ and under the pressures below 1 GPa the represented model only qualitatively describes the metastable states of aluminum (including a region of tensile stresses [37]).

Describing multi-component mixtures shall take into account interaction and mutual influence of the components, thereby highly complicating the mathematical models, since it has to describe both processes in separate components and effects of interaction between these components as well. But in some cases, the multi-component mixture may be considered as one continuum, thereby significantly simplifying the task. For example, in case of propagation of strong shock waves whose pressures are essentially higher than strength-related stresses, conditions of equality of phase pressures are used as conditions of joint motion. At this, when the effects of relative motion of the components are insignificant and the mixture is in the thermodynamic equilibrium, the following conditions are met $P_i = P$, $T_i = T$, $u_i = u$ (P_i, T_i, u_i — pressure, temperature and mass speed of the i component; P, T, u — the same for the mixture). Then, the medium motion can be described as motion of a single continuum with a special equation of state which takes into account properties of the mixture components and their mass fractions. It results in significant reduction of the number of the equations. Within a framework of such a method of mixture description, it is assumed that the equations of state of the components in the mixture are the same as in a free state. For simple mixtures which do not form bonds in an atomic scale, the paper [38] describes the principles of constructing the model of interacting and interpenetrating continuums. The method of describing the mixture by a single continuum is considered in the studies [19,39,40] et al. Within the framework of this method of describing the mixture of the continuums in the thermodynamic equilibrium, the paper [19,30] has proposed a method of constructing the equation of state of the equilibrium N-component mixture, in which the equation of state of each component is defined in the same form.

When describing the heterogeneous mixtures (mixtures with macroscopic nonuniformities), it is customary to use a hypothesis of additivity of the mixture volume by components volumes [38]:

$$V = \sum_{i=1}^{N} V_i,$$

where V — the specific volume of the mixture; V_i — the volume of the i component in a unit mass of the mixture. From this relationship, the expression is obtained for the density of the multi-component mixture as

$$\frac{1}{\rho} = \sum_{i=1}^{N} \frac{x_i}{\rho_i}, \tag{6}$$

where x_i and ρ_i — the mass fraction and the density of the i component. The density of the i component is a mass of the i-th component in a unit volume of the i-th component ($\rho_i = x_i/V_i$). After identical transformations from the equations of state (4) written for each component and for the mixture, the densities of the mixture and the components are expressed via relationships of the following type

$$\rho = \rho_0\left(\frac{P + kA_{\max}}{A}\right)^{1/n} \times \left[1 - \frac{kA_{\max} - A + \gamma_0\rho_0 r^{1-\ln r} c_{V0}(T - T_0)}{P + kA_{\max}}\right]^{1/n},$$

where k is a positive number; $A_{\max} = \max\{A_1, \ldots, A_N\}$; A_i — the compression ratio of the i component. It is easy to substitute such expressions for the component densities into (6) and to equate respective coefficients of P and $(T-T_0)$ in Taylor expansions for the right and left parts of the obtained equality to each other [19]. Then, it is possible to obtain the expressions for the parameters of the equation of state of the mixture A, ρ_0, n, γ_0 through respective parameters and the mass fractions of the components [19]:

$$n=\frac{R_1R_3}{R_2^2}-1,\ A=kA_{\max}-\frac{nR_2}{R_1},$$

$$\rho_0=\frac{1}{R_1}\left(\frac{A}{P+kA_{\max}}\right)^{1/n},\ \gamma_0\frac{nR_4}{c_{V0}}\left(\rho_0R_1\right)^{\ln(\rho_0R_1)}, \qquad (7)$$

where

$$R_1=\sum_{i=1}^{N}\frac{x_i}{\rho_{i0}}R_{5i},\ R_2=\sum_{i=1}^{N}\frac{x_i}{\rho_{i0}}R_{5i}\frac{kA_{\max}-A_i}{n_i},$$

$$R_3=\sum_{i=1}^{N}\frac{x_i}{\rho_{i0}}R_{5i}(n_i+1)\left(\frac{kA_{\max}-A_i}{n_i}\right)^2,$$

$$R_4=\sum_{i=1}^{N}\frac{x_i\gamma_{i0}c_{V0i}}{n_i}R_{5i}^{-\ln R_{5i}},\ R_{5i}=\left(\frac{A_i}{P+kA_{\max}}\right)^{1/n_i}.$$

The specific heat capacity with the constant volume for the mixture is defined by the relationship

$$c_{V0}=\sum_{i=1}^{N}x_ic_{V0i}.$$

Here, ρ_{i0}, γ_{i0}, n_i, c_{V0i} are the normal density, the constant parameter of the Gruneisen coefficient, the compression index, the specific heat capacity with the constant volume of the i component. The value $k=2$ guarantees the converging condition is met [19]. The paper [19] shows how to calculate the mass fraction of the gaseous component when knowing the values of the mixture porosity and the mass fractions of the solid components. The paper [41] shows that it is possible to neglect the presence of the gas in the pores. It is clear from the relationships (7) that „contribution" of the gaseous component to the mixture parameters can be neglected due to smallness of the mass fraction of this component. However, the present study uses general formulation of the model [19,30] which can also be applied for calculations of the characteristics of the mixtures of several condensed components (which corresponds to the aim of this study). Thus, the simple (small-parameter) model of the equation of state of the thermodynamically equilibrium N-component mixture is obtained. This model is checked by comparing the calculated shock adiabats and unloading isentropies with the experimental data.

Previously, it was shown in the paper [27] that with variation of the pressure value in the formulas (7) the values of the parameters of the equation of state of the mixture A, ρ_0, n and γ_0 vary insignificantly. Therefore, the subsequent calculations use the constants A, ρ_0, n and γ_0 found by the formulas (7) when $P=0$ for the mixture of aluminum and air with the mass fractions that correspond to the considered porosity of the samples.

The Hugoniot equations for the initially still medium when the pressure in the undisturbed medium is zero are as follows

$$\rho_{00}D=\rho(D-u),\ P=\rho_{00}Du,\ E-E_0=\frac{P}{2}\left(\frac{1}{\rho_{00}}-\frac{1}{\rho}\right), \qquad (8)$$

where ρ_{00} $(\rho_{00}=\rho_{T0}/m)$, E_0 are the density and the internal energy of the mixture upstream a shock wave front; u, P, ρ, E — the mass speed, the pressure, the density and the internal energy of the medium downstream the shock wave front; D — the shock wave front speed. When the relationships (8) are supplemented with the equations of state of the medium (4), (5) with parameters defined by the relationships (7) and the Gruneisen coefficient in the form of (2), it results in the system of equations for the unknown u, D, E, P, ρ. By defining the value of the mass speed of the medium downstream the shock wave front, it is possible to determine values of all the desired magnitudes.

2. Modeling results and comparison with the experiment

With all the values of the sample porosities, all the calculations of the shock adiabats and the unloading isentropies for the solid and porous samples of aluminum have used the same parameters of the equation of state of the components as specified in the table.

Parameters of the equations of state of air and aluminum

Substance	ρ_{i0}, kg/m^3	c_{i0}, km/s	n_i	c_{V0i}, kJ/(kg·K)	γ_{i0}
Air	1.3	0.343	2.20	0.718	0.16
Aluminum	$2.712\cdot10^3$	5.33	3.46	0.8975	1.65

The Figures 1 and 2 show the calculated shock adiabats for aluminum in the coordinates "the mass speed downstream the shock wave front-the shock wave front speed" and "the density-the pressure downstream the shock wave front", respectively, and the data obtained based on the experiments [42–46] as well as the results of the calculations [7,10,11,13,47]. Good qualitative and quantitative compliance of the calculated results and the experimental data in the wide range of the pressures shows that the mathematical model of the equation of state in the present study very well describes the behavior of aluminum in the shock wave.

For comparison, the Figures 1 and 2 show the results of calculations by means of other equations of state of aluminum [7,10,13]. It also shows the dependences [11,47] for the shock adiabat of the solid samples of this metal, which are obtained by generalizing the shock-wave data (including those of [42–46]) and the results of the calculation as per quantum-statistics models by Thomas-Fermi with

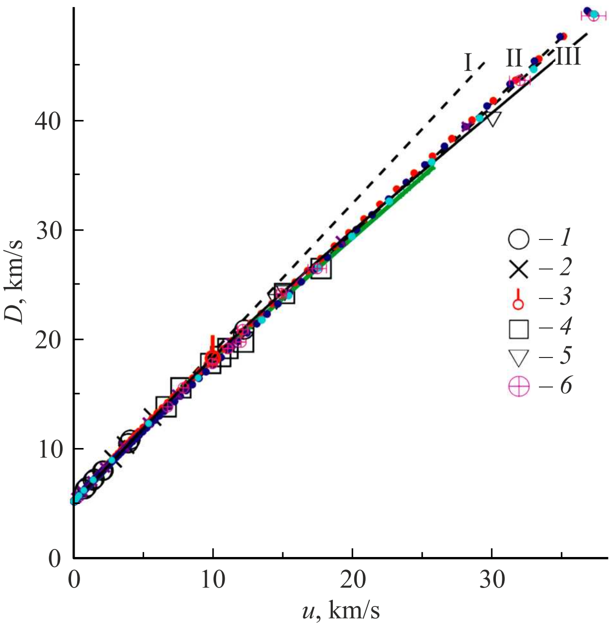

Figure 1. Shock adiabats of the solid aluminum samples in the coordinates $u{-}D$. The calculation results: the black solid line — the equation of state provided in the present study; the red dots — [13]; the blue dots — [47]; the light-blue dots — [11]; the violet crosses — [7]; the green solid line — [10]. Experimental data: *1* — [42]; *2* — [43]; *3* — [44]; *4* — [45]; *5* — [46]; *6* — interpretation [11]; the dashed lines I, II, III — the shock adiabats calculated using the experimentally determined dependences (10), (11) and (12), respectively.

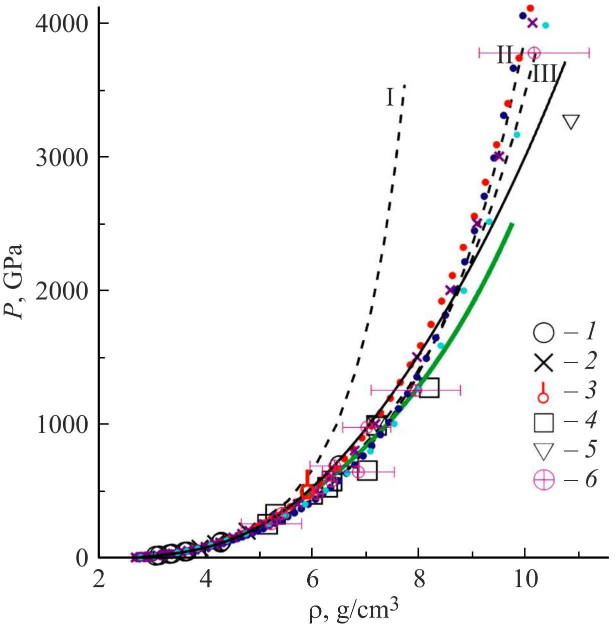

Figure 2. Shock adiabats of the solid aluminum samples in the coordinates $\rho{-}P$. Designations as in Fig. 1.

corrections [47] and by Hartree-Fock-Slater [11]. It is clear that all the provided approaches produce close results with the pressures of at most 1 TPa and the densities of at most 7 g/cm^3, which may be regarded as the upper boundary of the applicability region for the equation of state of aluminum given herein.

During the shock-wave experiments, the most accurate and reliable measurements are measurements of the shock wave speed (which can be measured in the easiest way) and of the mass speed of the substance downstream the shock wave front. The other shock wave parameters are found by substituting the mass speed and the shock wave speed into the Hugoniot equations (8). The fuller representation has been provided by comparing the sound speed values obtained by means of this model and given in the experimental papers. The sound speed squared $C_s^2 = (\partial P/\partial\rho)_S$ defines isentropic compressibility of the substance and a slope of tangent of the Poisson adiabat in the point (ρ, P). The unloading starts in the point (ρ_H, P_H) on the Hugoniot shock adiabat and the isentropic (adiabatic) sound speed characterizes a speed of propagation of unloading waves throughout the compressed substance. For this model of the equation of state with the Gruneisen coefficient in the form of (2), an expression connecting the temperature and the density on the unloading isentropy is as follows

$$\frac{T}{T_H} = \exp\left(-\gamma_0 \sum_{j=0}^{\infty} \frac{(-1)^j}{j!(2j+1)} \left[(\ln r)^{2j+1} + (\ln r_H)^{2j+1}\right]\right). \tag{9}$$

The index H refers to the initial state in which the entropy $S = S_H$. Using the relationship (9) for the temperature-density relation on the Poisson adiabat there is the expression for the sound speed squared

$$C_s^2 = V_0 r^{-1}\Big[n(P_X + A) + (\gamma + 1 - 2\ln r)P_T\Big] + \gamma c_{V_0} T_0 (n - 1 + 2\ln r).$$

There is also good match shown by the results of comparing the calculated and experimental [48–50] sound speeds in the coordinates the mass speed — the sound speed on the shock adiabat, as shown on Fig. 3.

The shock compression of the samples by two subsequently passing waves provides information about the thermodynamic properties of the substance within a range of the densities exceeding the density of single-time shock-wave compression. The comparison of the calculated results and the experimental data [51–53] in Fig. 4 allows concluding that the proposed model can be taken to adequately represent the experimental data for compression of the aluminum samples in the two shock waves.

Fig. 5 compares the calculated curves as per the proposed model of the equation of state and the calculation results [7,43]. It should be noted that on the shock adiabat as per the results of [7] Fig. 5 clearly exhibits breaks of the dependence of temperature on the compression ratio, which are related to aluminum melting under shock loading at the pressures of 113 and 178 GPa. This effect is neglected both

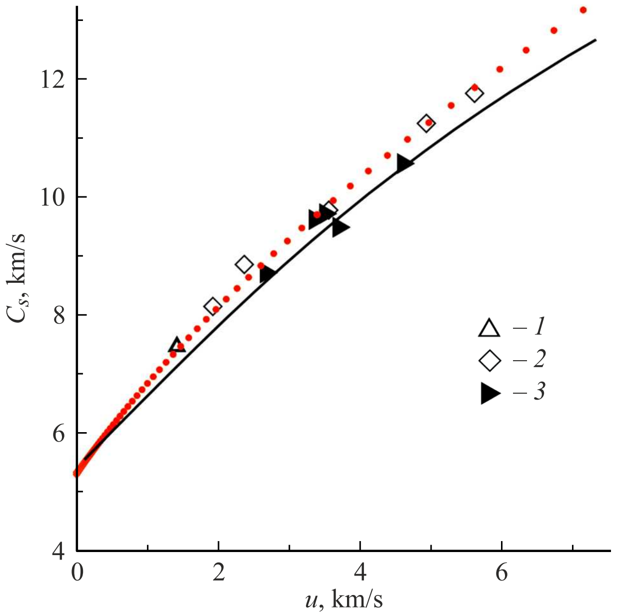

Figure 3. Sound speed on the shock adiabat in the solid aluminum samples in the coordinates $u{-}C_s$. The results of the calculations: the solid line — the equation of state given herein; the red dots — [13]. The experimental data: *1* — [48]; *2* — [49]; *3* — [50].

in the proposed model of the equation of state and in the model [43]. Under the pressures below 113 GPa (i.e. at the compression ratios ρ/ρ_{T0} from 1 approximately to 1.6) all the results of Fig. 5 are close to each other.

In order to obtain more complete information about the thermodynamic properties of the substance at the high pressures and temperatures, the same substance is experimentally studied at the different initial densities. The shock compression of the porous bodies is performed to the high pressures in order to neglect effects related to the material strength, and on the adiabat portions at which the substance is compacted to the normal density, the pressure is accepted to be zero. During the calculations of the shock adiabats, with all the values of porosity the same values of the parameters of the equation of state have been used.

The Figures 6 and 7 show the calculated shock adiabats for the initially porous aluminum samples in the coordinates "the mass speed downstream the shock wave front-the shock wave front speed" and "the density-the pressure downstream the shock wave front", respectively, and the data obtained based on the experiments [44,54–56]. The Figures 6 and 7 also include the results of the calculations of [10,13] for comparison. Good qualitative and quantitative compliance of the calculated adiabats as per the proposed model, the results of [10,13] and the experimental data of [44,54–56] within a wide range of the pressures and the porosities shows that the mathematical model of the equation of state given in the paper quite well describes the behavior of the porous material in the shock wave. Hence, a lower boundary of the applicability region of the equation of state of aluminum given herein in terms of the density may be indicated by the value of 1.4 g/cm^3 (at the high pressures).

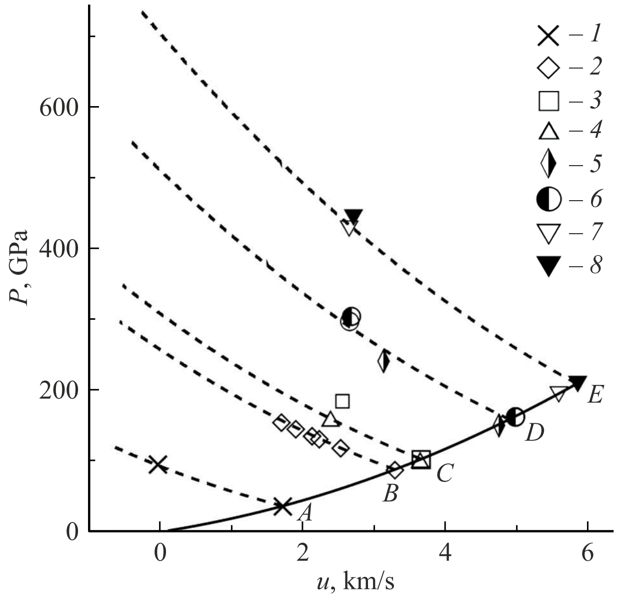

Figure 4. The shock adiabat (the solid line) and the adiabats of repeated loading (the dashed lines) for the initially solid aluminum samples in the coordinates $u{-}P$, which are calculated as per the equation of state provided in the present study, and the respective experimental data (*1* — [51]; *2* — [52]; *3–8* — [53]). The letters A, B, C, D, E mark the initial points of the adiabats of repeated shock compression with the coordinates A (1.72, 36), B (3.29, 87.3), C (3.657, 102), D (4.978, 162), E (5.849, 208.8).

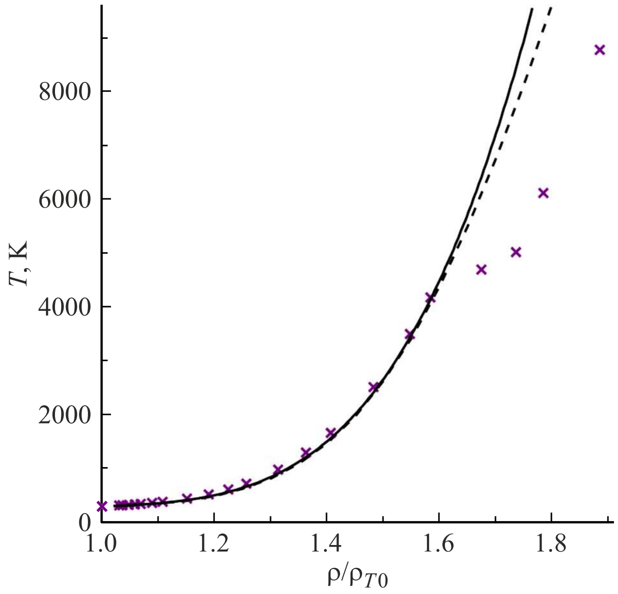

Figure 5. Dependences of temperature on the compression ratio on the shock adiabat of the solid aluminum samples as per the proposed equation of state (the solid line) and the other models (the dashed line — [43]; the violet crosses — [7]); $\rho_{T0} = 2.712\,\text{g/cm}^3$.

The unloading isentropies represent the behavior of the medium within a region of the reduced densities under adiabatic expansion. The model of the equation of state has been checked by calculations for a case of isentropic unloading of the material subjected to the shock-wave compression. Fig. 8 compares the calculated curves and the experimental data [57–59] for isentropic expansion out of the state of the shock-compressed solid aluminum samples. The increase of the mass speed in a depression wave on the portion from a certain point on the Hugoniot adiabat to a point, wherein the pressure is zero, is determined by the Riemann integral along the isentropy

$$u_r = \int_{v_H}^{v} \left[-\left(\frac{\partial p}{\partial v}\right)_S\right]^{1/2} dv,$$

where v_H, v are, respectively, specific volumes on the Hugoniot adiabat when the pressure $P = P_H$ and on the unloading isentropy when the pressure $P = 0$. The speed of a free surface is described by the relationship $u_{fs} = u_H + u_r$, u_H is a mass speed downstream the shock wave front. Good match of the results (except for the two points [58,59] at the densities below 2.4 g/cm^3 and under the pressures below 1 GPa) confirms reliability of description of the aluminum behavior under shock compression and subsequent isentropic unloading as per the proposed equation of state within the region of its applicability.

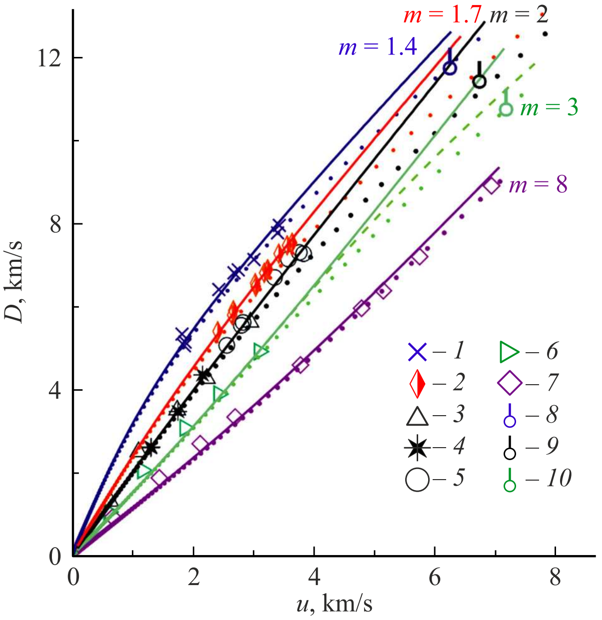

Figure 6. Shock adiabats of the initially porous aluminum samples in the coordinates $u{-}D$. The results of the calculations: the solid lines — the equation of state given herein; the dots — [13], the dashed line — [10]. The experimental data: *1, 2* — [54]; *3* — [55] ($m = 2.009$); *4* — [56] ($m = 2.012$); *5* — [57] ($m = 2.009$); *6* — [58]; *7* — [56]; *8–10* — [44].

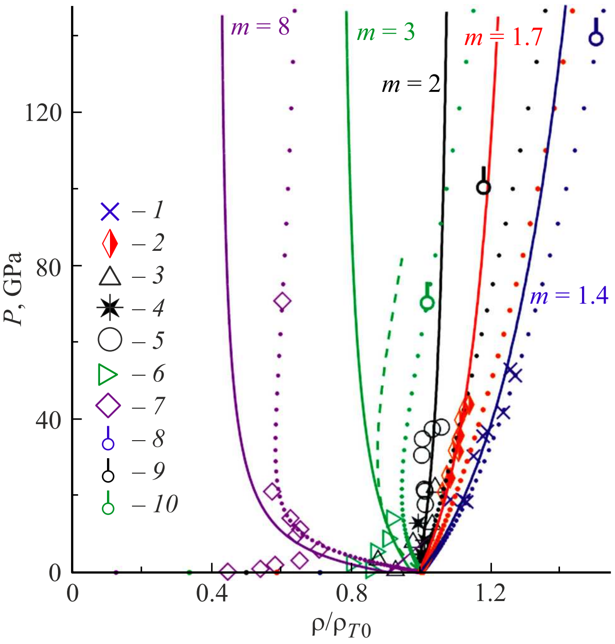

Figure 7. Shock adiabats of the initially porous aluminum samples in the coordinates $\rho/\rho_{T0} - P$. Designations as in Fig. 6.

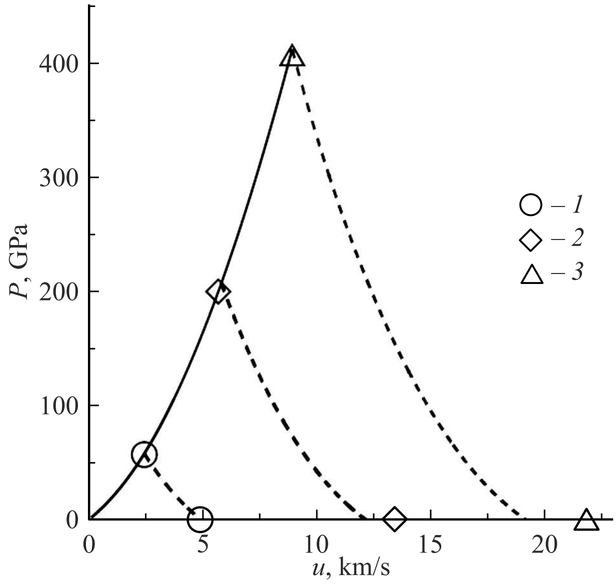

Figure 8. The Hugoniot adiabat (the solid line) and the Poisson adiabats (the solid lines) of the initially solid aluminum samples in the coordinates $u{-}P$. Experimental data: *1* — [57]; *2* — [58]; *3* — [59].

3. Region of model applicability

When describing the thermodynamic properties of metal at high pressures and temperatures, it is customary to take into account effects of reduction of isochoric heat capacity of an ion subsystem with increase of the temperature and increase of isochoric heat capacity of an electron subsystem (in proportion to the temperature) [44]. It can be expected that within a certain region of the densities and the temperatures these effect compensate each other. As shown in the recent studies [60,61], at the temperatures of dozes of thousand of Kelvins, a value of thermal pressure (a sum of contributions of the ion and electron subsystems) can be assumed to be proportional to the temperature $P_T = g(V)T$, where g is a certain volume function. In this case, the form of thermal pressure $P_T = \gamma\rho E_T$ (γ — the Gruneisen coefficient depending on the volume; $E_T = c_{v0}T$), which is used herein, does not require separately taking into account the contributions of the ion and electron subsystems (which, however, narrows the region of model applicability).

The values of γ_0 under the normal conditions for aluminum, which are obtained by the different methods in [21,62], lie within the range from 1.7 to 2.14. When calculating these magnitudes, various assumptions and constants have been used. Herein, the value $\gamma_0 = 1.65$ is assumed. The limit value of the Gruneisen coefficient — Γ_∞ — at the temperatures tending to infinity, is assumed to be 2/3 [6,13,14]. For the Gruneisen coefficient defined by the dependence (2), the values of the compression ratio r, at which the inequality $\gamma \geq 2/3$ is met, lie within the range $r \in (0.3856; 2.59)$. For the value $r = 2.59$ for the solid aluminum samples ($m = 1$), in the performed calculations, the mass speed, the pressure and the temperature downstream the shock wave front take the following values, respectively $u = 14.57$ km/s; $P = 940$ GPa; $T = 78850$ K. The test and calculated data for the solid aluminum samples have been compared to show (Fig. 1 and 2) that the model well describes the behavior of the samples both for the compression ratios within the found range and outside it as well. The paper [43] says that neither model for the Gruneisen coefficient is advantageous for describing the experimental data in the calculations of pulsed loading and isentropic unloading of the materials. In some cases, the calculation accuracy is improved by using $\Gamma_\infty \neq 2/3$, $C_{VP} \neq 3R$ (C_{VP} — heat capacity of an lattice with the constant volume, R — the gas constant). Fig. 1 demonstrates qualitative and quantitative match of the calculated adiabats and the test data up to the values of the mass speed $u \approx 15$ km/s, so does Fig. 2 up to the values of the compression ratio $r \approx 2.6$. Unfortunately, the author could not make comparison for shock-wave loading of the highly-porous aluminum samples with the values $r < 0.5$ due to absence of experimental data.

For the shock adiabat of the solid aluminum samples, the paper [63] provides the following relationships:

$$D = 5.333 + 1.356u; \quad 0 \leq u \leq 6.1, \tag{10}$$

$$D = 5.9 + 1.19u; \quad 4.28 < u < 62.3, \tag{11}$$

$$D = 6.541 + 1.158u; \quad 6.1 \leq u \leq 22. \tag{12}$$

Using the linear dependence $D = a + bu$ makes it possible to represent the pressure on the shock adiabat (using the break relationships (8)) in the following form

$$P = \frac{a^2\rho_{00}(1 - \rho_{00}/\rho)}{1 + b\rho_{00}/\rho - d)^2}.$$

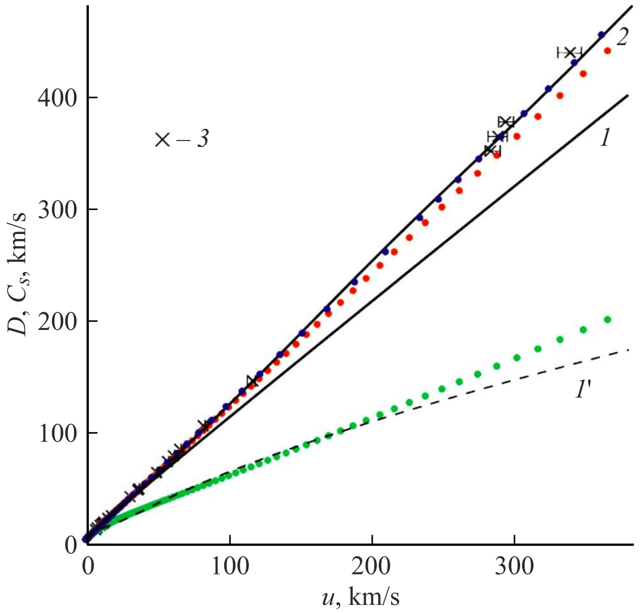

Figure 9. Dependences of the shock wave speed (the solid lines, the red and blue dots) and the sound speed in the shock-compressed substance (the dashed line and the green dots) on the mass speed. The results of the calculations: the lines *1* and *1'* — the equation of state given herein; the line *2* — [11]; the red and green dots — [13]; the blue dots — [47]. The experimental data: *3* — interpretation [11].

The shock adiabats calculated by these formulas are shown in Fig. 1 and 2. In the relationships (10)–(12) the slope of the shock adiabat is defined by a value of the coefficient b, that is found based on results of analysis of the experimental data. It is not fixed for each material. Description of the shock adiabat using the relationships of the type $D = a + bu$ within a large interval of the mass speeds requires defining several such relationships with different values of a and b within subintervals. The dependence proposed in [4] for the Gruneisen coefficient well describes variation of the adiabat slope by applying a variable exponent ($-\ln r$), whose values depend on the compression ratio.

The Figures 9 and 10 have compared the shock adiabats for the solid aluminum samples calculates as per the proposed model with the data of [11], in the coordinates "the mass speed — the wave speed" and "the compression ratio — the pressure", respectively. The Figures 9 and 10 also include results of calculations of the shock adiabat of aluminum as per the equation of state [13] and the quantum-statistics models by Thomas-Fermi with corrections [47] and by Hartree-Fock-Slater [11].

The comparison indicates that the shock adiabats within the pressure range below 1 TPa calculated as per the proposed model well agree both with results of the other model and with the experimental data of [11] as well. Fig. 9 also shows the dependences of the sound speed in the shock-compressed substance on the mass speed

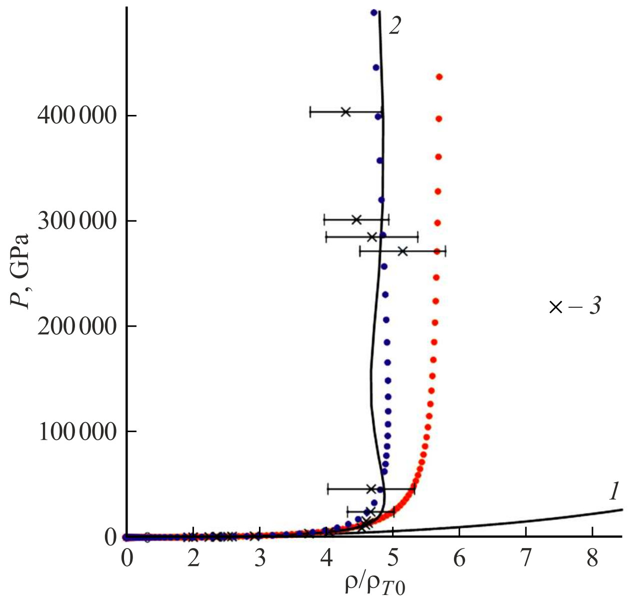

Figure 10. Shock adiabats of the solid aluminum samples in the coordinates $\rho/\rho_{T0} - P$. Designations as in Fig. 9.

downstream the shock wave front as per the proposed model and the equation of state [13].

The logarithmic dependence (2) has been applied to describe the adiabats of loading and unloading by means of the two-term Mie-Gruneisen equation of state (without involving a term with temperature squared) for the shock-wave data within the pressure range of at most 1 TPa at the densities from 1.4 to 7 g/cm^3. It should be noted that the experimental points [56] of Fig. 7 at the pressures up to 6 GPa refer to an area of influence of the strength effects hindering full closure of the pores under shock compression; in order to describe these points [56], it is required to involve additional models except for the equation of state (see, for example, [64]).

Conclusions

It has been shown that the equation of state for aluminum in the Mie-Gruneisen form with the elastic part for the pressure like the Tait equation with two selected parameters n and γ_0 with good reliability describes the behavior of the solid (in one and two shock waves) and porous aluminum samples under shock compression and isentropic unloading. The provided model of the Gruneisen coefficient as defined by the formula (2) makes it possible to widen the range of applicability of the equation of state to the high values of porosity ($m \approx 8$). Detailed comparison with the shock-wave data confirms adequacy of the proposed model of the equation of state for describing the aluminum behavior within the region of its applicability of at most 1 TPa at the densities from 1.4 to 7 g/cm^3 (except for the pressure region below 1 GPa at the densities below 2.4 g/cm^3).

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Conflict of interest

The author declares that he has no conflict of interest.

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