Thermodynamic parameters of heterogeneous materials under shock-wave loading in presentation of equilibrium model

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Abstract. The results of numerical experiments on modeling of shock wave loading of solid and porous heterogeneous materials on the example of molybdenum and some alloys included molybdenum as a component are presented. A thermodynamically equilibrium model is applied to describe the behavior of solid and porous materials. This model ensures good compliance with the experiment in a wide range of pressures. The gas in pores, which is a component of the medium, is taken into account in this model. The equation of state of the Mie–Gr"uneisen type with allowance for the dependence of the Gr"uneisen coefficient on temperature is used for condensed phases. The applied model allows the behavior of the molybdenum with porosity from 1 to 3 to be calculated under shock-wave loading at pressures above 5 GPa in the one-velocity and one-temperature approximations, as well as on the assumption of equal pressures for all the phases. Computational results are compared with the well-known experimental results obtained by different authors. The model permits the shock-wave loading of solid and porous alloys with molybdenum in their composition to be described reliably solely by using species parameters.

1. Introduction
Investigations of the behavior of porous materials (mixtures and alloys) under shock-wave loading are of interest in many problems of modern science; in this regard new models appear for the description of the behavior of such materials (for example, [1, 2]). These investigations are important in solving the applied problems of dynamic compaction, shock-wave synthesis, and other explosive technologies. Owing to a large variety of materials by compositions of components and by porosities, in order to describe the behavior of powder materials it is desirable to use the equations of state of the materials components alone; in this instance it is necessary to have a sufficiently simple model that complies well with the experiment in a wide range of pressures for both solid and porous materials.

Despite the large number of approaches to the choice of the equation of state of a solid body under dynamic loadings [3–7], the problem of calculation of the equation of state in its exact mathematical formulation is scarcely solvable, because the initial equations are extraordinarily difficult. Therefore, numerous simplifications are performed in practice that would capture the main features of real phenomena. It is possible to consider that the compliance of a model equation of state with the experiment is the main criterion of its applicability.
2. Calculation and discussion

In order to describe the behavior of porous media, alloys and mixtures under dynamic loadings, a model of shock-wave loading with allowance for gas in the pores is used [8, 9]. The model is based on the assumption of thermodynamic equilibrium of all the components of a material under shock-wave loading (model TEC—thermodynamic equilibrium components). Thermodynamic equilibrium means the equality between the velocities, pressures, and temperatures. In order to describe the behavior of condensed phases, the equations of state of the Mie–Grüneisen type are used. The equations that determine the state of the condensed component are written as follows:

\[ P(\rho, T) = P_X(\rho) + P_T(\rho, T), \quad E(\rho, T) = E_X(\rho) + E_T(T), \]

\[ P_T(\rho, T) = \Gamma \rho E_T(T), \quad E_T(T) = c_V(T - T_0). \]

Here \( P_X, E_X, P_T, \) and \( E_T \) are the potential and thermal components of pressure and specific energy, respectively; \( c_V \) is the specific heat capacity; \( T_0 \) is the initial temperature; and \( \Gamma \) is the Grüneisen coefficient. By taking into account the pressure region of applicability of this model \( \geq 5 \) GPa that is of interest to us, initial energy of a substance under normal conditions is considered to be equal to zero. Cold pressure component \( P_X \) is described by a Tait-type equation. Therefore, the thermal and caloric forms of the equation of state for a condensed component with current density \( \rho \) and initial density \( \rho_0 \) are as follows:

\[ P(\rho, T) = A \left( \frac{\rho}{\rho_0} \right)^k - 1 + \Gamma c_V(T - T_0), \]

\[ E(\rho, T) = A \left( \frac{1}{k - 1} \left( \frac{\rho}{\rho_0} \right)^{k-1} + \frac{\rho_0}{\rho} - \frac{k}{k - 1} \right) + E_T. \]

The ideal gas equation of state is taken for a gas. The conditions of dynamic compatibility at the wave front are written, namely, the conditions of conservation of the mass flux for each component of the material and the conditions of conservation of momentum and energy fluxes for the media considered as a whole [8]. The obtained equations, together with the equations of state of each component, are sufficient to find dependences \( P(U) \) or \( D(U) \) (\( P, U, \) and \( D \) are the pressure, mass velocity, and wave velocity, respectively; \( A, k, \Gamma \) the coefficients in the equations of state of condensed component). These dependences can be treated as a shock adiabat of a multicomponent material. The following expression can be obtained for a material with \( n \) condensed components (\( \mu_{i0} \) is the volume fraction of the \( i \)-th phase of the substance):

\[ P = \frac{\sum_{i=1}^{n} \frac{\mu_i}{\sigma_i} A_i \left( h_i - \frac{k_i + 1}{k_i - 1} \sigma_i^{n_i} + \frac{2k_i\sigma_i}{k_i - 1} - h_i - 1 \right)}{\sum_{i=1}^{n} \frac{\mu_i}{\sigma_i} h_i + \frac{n}{\sigma_0} (1 - \sum_{i=1}^{n} \mu_{i0}) - 1} \]

Here \( h_i = 2/\Gamma_i + 1, \quad i = 1, n, \quad h_g = 2/(\gamma - 1) + 1. \sigma_i = \rho_i/\rho_{i0} \) are the degrees of compression of the corresponding component, \( \mu_{i0} \) are the volume fraction, \( \rho_{i0} = \rho_{i1} \) are the density of the \( i \)-th phase of the substance ahead of the shock wave front and behind it, respectively (\( i = 1, \ldots, n, \) and \( g \)); \( \gamma = 1.41 \) (ratio of specific heats). By adding to equation (5) \( n \) relationships that follow from the equations of state of \( n + 1 \) components and expressing the equality in the temperatures of all the components, we finally have \( n + 1 \) equations for \( n + 2 \) unknowns \( P, \sigma_i (i = 1, \ldots, n \) and \( g \), which allow us to construct the shock adiabat of the material. In the case of calculation of the behavior of a solid material, we assume that \( \sum_{i=1}^{n} \mu_{i0} = 1 \).

Porous materials are characterized by a considerable increase in temperature upon dynamic loading. In order to describe the behavior of powder materials, a model was tested, in which
the Grüneisen coefficient depended explicitly on temperature alone $\Gamma (T)$. Application of this dependence turned out to be promising for the description of the behavior of both solid and porous materials, as well as powders and mixtures on their basis upon shock compression for pressures above 5 GPa. The analysis of the experimental data of solid and porous materials resulted in the empirical dependence of the Grüneisen coefficient on temperature in the following form [8, 9]:

$$\Gamma(T) = \left[ \left( \Gamma (T_0) - \Gamma (T_{\infty}) \right)^{-1} + C (T - T_0) \right]^{-1} + \Gamma (T_{\infty}).$$

(6)

Coefficient $C$, which allows describing the experimental points upon moderate compression, is determined by intermediate value $\Gamma (T^*)$ at temperature $T = T^*$, as follows:

$$C = \left[ \left( \Gamma (T^*) - \Gamma (T_{\infty}) \right)^{-1} - \left( \Gamma (T_0) - \Gamma (T_{\infty}) \right)^{-1} \right]^{-1} (T^* - T_0).$$

(7)

These parameters were determined for the best correspondence of calculated data to the data that were collected on the experiment basis. Asymptotic value $\Gamma_{\infty}$ corresponds to the maximum temperatures.

Based on the experimental data for molybdenum with a density of $\rho_0 = 10.206$ g/sm$^3$ the following parameters were determined for the equations (3–7): $A = 95$ GPa, $n=3.0$, $\Gamma (T_0) = 1.58$, $\Gamma (T_{\infty}) = 0.5$, $\Gamma (T^*) = 1.15$, $T^* = 23000$ K, $C = 2.663 \times 10^{-5}$. The experimental data on the properties of the solid and porous molybdenum under dynamic loads in the range of pressure values from 5 to 2000 GPa [10–15] was used to assess the accuracy of the model descriptions of shock-wave loading of molybdenum. Data obtained on the basis of the experiment for solid molybdenum with a density of $\rho_0 = 10.206$ g/sm$^3$ and the calculations of shock adiabat on the model TEC in the coordinates pressure compression is shown in figure 1.

The simulation results of shock wave loading of molybdenum of different values of porosity is shown in figure 2 solid lines indicating the values of porosity corresponding calculation. The subsequent calculations showed that the parameters defined for solid molybdenum, allow us to describe data in the range of porosity $m$ (the ratio of the density of solid substance to the density of the sample) from 1 to 3 with the accuracy of the experiment for pressures above 5 GPa.

The model TEC allows adequate calculations isentropic unloading of the shock-compressed material [16]. The condition in the unloading wave is described by the Riemann integral. The index H refers to the initial condition on the shock adiabatic, index S meets the corresponding
Figure 2. The shock adiabats of porous samples of molybdenum: 1—results of model TEC; 2—experimental data for \( m = 3.1 \) [14], 1.8 and 1.3 [15].

conditions on isentrope, \( V \) is the relative volume:

\[
V_S = V_N - \int_{P_N}^{P_S} \left( \frac{dU}{dT} \right)^2 dP.
\]  

(8)

The calculations shown in figure 3 describe well the data obtained on the basis of the experiment during unloading for continuous (\( m = 1 \)) and for porous molybdenum (\( m = 2.304 \)), the experimental data on the properties of porous molybdenum under dynamic loads [17, 18].

These parameters, which were obtained for pure molybdenum, were used for accurate modeling of shock-wave loading of solid and porous alloys based on molybdenum. Alloys in this case are treated as mixture with zero fraction of air. The experimental results are present in [19] for the alloy of molybdenum and rhenium with a density of mixture \( \rho_0 = 14.71 \text{ g/cm}^3 \). This alloy can be considered as monolithic on the basis of data on mass fractions of components (\( m = 1 \)) [9]. The calculation shows that for this alloy the value of porosity: \( m = 1.004 \), which corresponds to the measurement accuracy. The same article data are present also for an alloy of molybdenum and titanium with the initial density \( \rho_0 = 5.24 \text{ g/cm}^3 \), the value of porosity determined for this alloy based on mass fractions of components: \( m = 1.04 \). As noted in [19], an additive approximation, which is often used in calculations, works well for a number of alloys, however in some cases the deviation of calculated data and data obtained on the basis of the experiments available. In [8] it was shown that at values of porosity greater than 1.02 accounting of porosity allows to solve the problem of systematic deviations of the calculated and experimental data for alloys of copper and tungsten. As can be seen in figure 4 the model TEC can reliably simulate the thermodynamic parameters of shock-wave loading as monolithic alloy Mo-Re and porous alloy Mo-Ti.
The shock adiabats and unloading isentropes of solid and porous molybdenum. Model TEC: solid line—the shock adiabats $1—m = 1, 2—m = 2.304$, the dotted line—adiabatic unloading. Data: 3–5 [17]; 6, 7 [18].

**Figure 3.** The shock adiabats and unloading isentropes of solid and porous molybdenum. Model TEC: solid line—the shock adiabats $1—m = 1, 2—m = 2.304$, the dotted line—adiabatic unloading. Data: 3–5 [17]; 6, 7 [18].

**Figure 4.** Shock adiabats of molybdenum alloys with rhenium and titanium. Calculation: $1—$alloy Mo–Re $m = 1.04, 2—$alloy Mo–Ti $m = 1$. Data: 3—alloy Mo–Re $m = 1.04; 4—$alloy Mo–Ti $m = 1$ [19].

The calculated and experimental data for these alloys are shown in figure 4. As for the description of dynamic loading, we need to know the composition and density of the alloy, which allows determining its porosity and the volume fraction of the components. The component settings are taken the same as in the description of pure substances. As we can see from the calculations, the proposed scheme describe the behavior of the mixture under dynamic loads allows to describe the behavior of both solid and porous alloys.

The data for the alloys of molybdenum with uranium was taken from [12]. The simulation is performed for the following three compositions: alloy uranium–molybdenum (2.0), weight fraction U(98.0)–Mo(2.0) with an initial density of the alloy $\rho_0 = 18.58$ g/cm$^3$, alloy uranium–
molybdenum (3.0), U(97.0)—Mo(3.0) $\rho_0 = 18.447 \text{ g/cm}^3$, alloy uranium–molybdenum (8.3), U(91.7)—Mo(8.3) $\rho_0 = 17.312 \text{ g/cm}^3$. For the first and second composition, the porosity value differs from 1 by less than 1%, so they can be considered monolithic, for the third alloy the value of the porosity is defined as $m = 1.025$. The calculated and experimental data for these alloys are shown in figure 5. Good agreement is shown between the calculation and data from experiments for all of the alloys Mo–U. The deviation of the predicted points for the first alloy at pressure value of 264 GPa, likely due to the accuracy of the experiment, as a comparison under these conditions, values of wave speeds for this alloy are lower than for the grades two and three, having a lower density.

3. Summary
The equation of state of the Mie–Grüneisen type together with the condition of thermodynamic equilibrium of the mixture components (alloys in this case can be considered as mixture with zero fraction of air) gives a closed system of equations that defines the parameters under dynamic loading. The assumption on the thermodynamic equilibrium implicitly takes into account the interaction between the components, which becomes especially significant in the case of porous media. Dependence $\Gamma(T)$, proposed for the description of porous media, makes it possible to describe the available experimental data for porous materials in wide ranges of porosities and pressures under dynamic loading within the accuracy of the experiment [20]. The chosen parameters of the model ensured the reliable description of behavior of molybdenum within porosity range from 1 to 3 and for pressures above 5 GPa and the shock-wave loading of molybdenum based alloys. The parameters of the model for other components of the alloy were determined separately. As a result, in order to describe the behavior of a mixture under dynamic loadings, it is necessary to know only the volume fractions of its components. The present model made it possible to choose the ratios between the mixture components in order to obtain the prescribed characteristics under the shock-wave loading of solid and porous heterogeneous materials.

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