Model of Shock Wave Action on Porous Materials
and Mixtures

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Introduction

Methods based on shock wave impact on the substance are widely used to create innovative materials throughout the world. The production of composite materials, in particular, materials that based on multicomponent mixtures of metallic and nonmetallic powders are of great interest. Shock wave loading (SWL) of such mixtures can activate the chemical and phase transformations of the substances and contribute to the creation of entirely new materials with unique properties.

Results

Efficiency of SWL studies of the multicomponent mixtures with the aim of creating new materials mostly depends on the possibility of predicting the behavior of the components based on the properties of each component in the mixture and its contribution to the process with different intensities of dynamic effects. Today it seems impossible to construct a model, which will describe all the factors associated with the given process. Therefore the question of creating models that allows you to calculate at least the thermodynamic parameters (pressure, density, mass velocity, and temperature) for each component of the mixture. There are a lot of models, but they all are adapted to the occasion of maximum two condensed components in the mixture and work in limited ranges of possible pressures. The calculation methods based on the use of wide-range equations of state (EOS) of substances should be mentioned separately. They may be used to calculate SWL parameters of multicomponent mixtures, but these EOS for each component of the mixture contain dozens of free parameters and experimentally determined constants. In this regard, the calculations become very cumbersome and time consuming.

The thermodynamic equilibrium components (TEC) model developed to describe the behavior of porous mixtures is based on the assumption that all of the components of the mixture, including gas in pores, are in thermal equilibrium under the shock wave loading. EOS of the Mie–Grüneisen type are used to describe the behavior of the condensed phases. The initial internal energy and pressure of the substances are zero under normal conditions, taking into account the field of use of this model for pressures over 5 GPa. Hence, the equation of state for condensed component with the current and initial densities \( \rho \) and \( \rho_0 \), pressure \( P \), specific heat \( c_v \) and Grüneisen coefficient \( \Gamma \) has the form

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

where \( T \) and \( T_0 \) are the current and initial temperatures. For gas, we use the equation of the state of ideal gas. We write the conditions of dynamic compatibility on the shock wave front, which are laws of conservation of the mass flux for each component of the mixture and laws of conservation of momentum and energy fluxes for the mixture as a whole \([1, 2]\). The resultant equations combined with the equation of state for each component are sufficient to find dependences of the type \( P(U) \) or \( D(U) \) (\( U \) and \( D \) are the mass and wave velocity, respectively), which can be treated as the shock adiabats (SA) of the multicomponent mixture. We suppose that the Grüneisen coefficient depends explicitly only on the temperature \([1, 2]\). For the mixture of two condensed components with the initial volume percentage \( \mu_{10} \) and \( \mu_{20} \) we can obtain the expressions
\[ P = \left( Z_1 + Z_2 \frac{\mu_{20}}{\mu_{10}} \sigma_1 \right) \left( h_1 + \frac{\mu_{10}}{\mu_{20}} \sigma_1 h_2 + \frac{(1 - \mu_{20}/\mu_{10}) \mu_{10}}{\mu_{20}} h_g - \frac{\sigma_1}{\mu_{10}} \right)^{-1}, \]

\[ Z_i = A_i \left[ \left( h_i - n_i \sigma_i + 2 n_i \sigma_i \right) \frac{n_i}{n_i - 1} - h_i - 1 \right], \]

where \( A_i \) and \( n_i \) are the constants, \( \sigma_i = \rho / \rho_0 \) are the degrees of compression of the corresponding components, \( i = 1, 2, g \). Here \( \rho_g \) is the gas density and \( \gamma \) is the ratio of specific heats. We obtain three equations for four unknown variables \( P, \sigma_1, \sigma_2, \) and \( \sigma_g \), which allow us to construct the shock adiabat of the mixture on the supposition of the equality of the temperatures of the components. If we assume that \( \mu_{20} = 0 \) in Eq. (2), which means the absence of the second component, we obtain the equations for a porous medium. If we additionally assume that \( \mu_{10} = 1 \), then we obtain the system of equations for a solid material. We can easily construct SA for the greater number of components of the mixture generalizing the corresponding equations. Some of the results of the comparison calculations [1, 2] for the TEC method with known experimental and calculated results of the different authors are listed below (SA, dual compression shock waves, evaluation of the temperature).

The calculations for TEC method are shown in Fig. 1 for aluminum when the porosity values \( m \) from 1.4 to 8, where \( m \) is the ratio of the densities of the solid and porous substances. The calculated data correspond well to the data obtained on the basis of experiment.

![Fig. 1](image1.png)

**Fig. 1** Pressure-density diagram of porous aluminum. All calculations lines of this work are performed for TEC Method. Data [3] from different sources: 1—2—\( m = 1.4 \); 3—\( m = 1.7 \); 4—7—\( m = 2 \); 8, 9—\( m = 3 \); 10—\( m = 8 \)

In order to obtain information about the thermodynamic properties of substances within the range of densities that exceed the density of a single compression, the states under repeated shock compression are recorded. As is seen from the results shown in Fig. 2, the model under consideration enables the experimental data on the double compression of aluminum to be described with an accuracy of the experiment within the available range of data.

The calculation-experimental estimation [5] of temperature is shown in Fig. 3 along the shock adiabat of solid

![Fig. 2](image2.png)

**Fig. 2** Shock adiabat and adiabats of double compression of aluminum. TEC model calculations: solid line denotes the shock adiabat, and dashed line denotes the double compression. Experiment: 1, 6—[3], 2—5—[4]

![Fig. 3](image3.png)

**Fig. 3** Comparison of temperatures along the shock adiabat of bismuth. The ten model calculations: 1. Experiment: 2 [7]
bismuth, as well as the TEC model calculations. The estimation of temperature for bismuth is within the region of the scatter of experimental data. It indicates on the reasonable estimates of temperature by the TEC model.

The TEC model allows us to calculate adequately isentropic unloading of the shock-compressed material. The results of the calculations, shown in Fig. 4 describe well the data obtained on the basis of the experiment when unloading for solid \((m = 1)\) and porous bismuth \((m = 2.459)\). Note that temperature values 24,500 K and 43,300 K obtained in the calculation for the points began unloading of porous bismuth at pressures 43 GPa and 73 GPa, respectively.

The calculations of the mixtures with two solid phases on the TEC method shows that the model describes well the data of SWL of the mixtures with the components having similar parameters, and for the mixtures with significantly different parameters of the components. The calculations for the mixture of tungsten and paraffin that have the large difference values of density were given in [6] for the three models, with varying degrees of accuracy describing the data obtained on the basis of the experiment. The calculations are shown for the SC-Criterion (single component), the KEA method (kinetic energy averaging). These two methods operate on the principle of additivity, which is widely used, giving a satisfactory description of the experiments at relatively low pressures for alloys. The third model is the Turbulent Entropy Method; the attempt is made to consider the interaction of the components. Adding to the figure from [6] the curve calculated on the TEC method, it can be seen that only the model made it possible to adequately describe all the available data of SWL of the tungsten-paraffin mixture, Fig. 5.

TEC method allows us to describe, in particular, the region of the polymorphic phase transition, considering the material in the region of phase transition as a mixture of phase of low-pressure and phase of high-pressure in SWL. The calculation of SA mixture of quartz \(\text{SiO}_2\) and aluminum \(\text{Al}\) is shown in Fig. 6, when SWL, taking into account the phase transition in quartz. TEC method makes it possible to describe the behavior of the mixture with two components undergoing phase transition at SWL [7]. This calculation is shown in Fig. 7 for nonporous mixture of aluminum nitride \(\text{AlN}\) and silicon nitride \(\text{Si}_3\text{N}_4\) with an equal volume fraction, taking into account the phase transition in the nitrides.

![Fig. 4 Shock adiabat (solid curve) and unloading isentropes (dotted curves) for solid bismuth: 1—unloading from the SA point with pressure of 96, 240, 314, 430, 670 GPa \((m = 1)\); unloading from the SA points with pressures of 43 and 73 ITla \((m = 2.459)\). Experiment: [3]](image1)

![Fig. 5 Pressure-density diagram of mixture tungsten-paraffin](image2)

![Fig. 6 Shock adiabat of Al, \(\text{SiO}_2\), and their mixtures. The calculations lines: 1—mixture, 2—\(\text{SiO}_2\), 3—Al. Experiment: [3]](image3)
The SWL of carbides with different porosity is described by the TEC method, treating them as the mixture of the corresponding chemical composition. The significant description is obtained for the carbides with equal volume fractions and for boron carbide B₄C having, respectively, a ratio of 1:4 (Fig. 8). Such calculations have not been previously held for boron carbide. Similar results are shown in Fig. 9 for porous carbides.

Adding the appropriate equations, you can write a function similar to Eq. (2) and build SA to materials with lots of components. As an example, the experimental data and the model calculation of the TEC are shown in Fig. 10 for Wood’s alloy (density of $p_0 = 10.14 \text{ g/cm}^3$) consisting of four components: bismuth, cadmium, selenium, and lead. The data obtained on the basis of experiments on shock wave loading of this alloy is given in [8, 9], weight composition wt% at % Bi(40), Cd(9.5), Sn(9.5), and Pb(41).

**Conclusions**

Thus, the presented TEC method allows to describe adequately the known results (shock adiabat, double compression shock waves, adiabatic expansion of shocked substance, and temperature evaluation) in the whole range of possible pressures for virtually all solid and porous materials and mixtures for which experimental data are available. It should be noted that the proposed method of constructing the SA of
the mixture allows you to monitor the compression not only of the mixture as a whole, but also the compression of each component separately.

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References