Shock-wave loading of elconites: Numerical investigation

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Abstract. The results of numerical experiments on modeling shock-wave loading of metal composites – elkonites, which are sintered refractory materials (W, WC or Mo) impregnated with fusible metal (Ag or Cu) using thermodynamically equilibrium model TEC (thermodynamic equilibrium components) are presented. Interest in the research of compressibility of such mixtures is associated with the possibility of creating materials with the necessary properties, and with the properties of the materials themselves. The modelling of materials with such components is carried out to develop the promising direction of obtaining materials with specified properties. The good agreement of the model calculations with the data of different authors, which are determined on the basis of experiment, is obtained.

1. Introduction
The results of numerical experiments on modeling shock-wave loading of metal composites (elkonites) are presented. The materials are sintered from refractory materials—tungsten, tungsten carbide or molybdenum (W, WC, Mo) impregnated with low-melting metals such as silver or copper (Ag, Cu). The thermodynamic equilibrium model TEC (thermodynamic equilibrium components) is used for the investigation. The model allows us to describe reliably both solid and porous alloys and mixtures, including taking into account the possibility of a polymorphic phase transition of components under shock-wave loading. The interest in studying the compressibility of such mixtures is related to the possibility of creating materials with the necessary properties and to the properties of the materials themselves. The dynamic loading of solid and porous alloys of various compositions of W, WC or Mo, in combination with Ag or Cu, such as Cu–W, Ag–W, Cu–WC, Ag–W are described by the model.

It is necessary to change purposefully thermodynamic parameters to implement the necessary conditions for creating materials with the specified properties for development of the shock-wave synthesis method and for other explosive technologies. For this purpose, the compressibility of multicomponent mixtures of various compositions is investigated, and groups of metal compositions whose elements consist mainly of the refractory metals W, WC, Mo combined with Cu are of great interest [1-6]. The combination of these elements allows one to create dense solid metals with excellent wear resistance and strength at high temperatures, combined with good thermal and electrical conductivity. The properties of both metals Cu and W combines in alloy, so the material is heat resistant, resistant to ablation, with high thermal and electrical conductivity, and easy to process. It is
used for the manufacture of engines and electrical devices in aviation and space industries. The mechanical and physical properties of Cu–W alloy are changed in different composition, thermal and electrical conductivity increase with the amount of copper, and the hardness, strength, and mechanical wear resistance increase with the amount of tungsten or tungsten carbide.

The present paper will mainly describe and discuss the modelling shock-wave loading of metal composites based on W, WC by using the model TEC, which combined with experimental results. The paper is structured as follows: the calculation model is stated in section 2; the numerical simulation model for investigated materials is presented in section 3; section 4 presented the conclusions derived from the results of the researching.

2. Calculation model
The model of shock-wave loading with allowance for gas in the pores is used for different materials [7–10] for calculating of thermodynamic parameters for porous mixtures under dynamic loadings. The model is able to describe the parameters in wide range values of pressures under shock wave loading. The model is based on the assumption of thermodynamic equilibrium of all material components at high dynamic loads. For this reason, the model is designated as Model TEC (thermodynamic equilibrium components). In order to describe the behavior of condensed phases, the equations of state (EoS) of Mie-Grüneisen type are used. The equations that determine the state of the condensed component are written as follows:

\[ P(\rho, T) = P_c(\rho) + P_T(T), \quad E(\rho, T) = E_c(\rho) + E_T(T) \]  

(1)

\[ P_T(\rho, T) = \Gamma_0 E_T(T), \quad E_T(T) = c_v(T - T_0) \]  

(2)

Here \( P_c, E_c, P_T, \) and \( E_T, \) are potential and thermal components of pressure and specific energy respectively, \( c_v \) is specific heat capacity; \( T_0 \) is initial temperature. Initial energy \( E_0 \) under normal conditions is considered to be equal to zero by taking into account the pressure region of applicability of this model > 3 GPa. Cold pressure component \( P_c \) is described by a Tait-type equation. Therefore, the thermal and caloric forms of the equation of state for condensed component are as follows:

\[ P(\rho, T) = A \left( \rho / \rho_0 \right)^k - 1 + P_T \]  

(3)

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

(4)

Here current density is \( \rho \) and initial density is \( \rho_0. \) The conditions of conservation of 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 at the wave front are written. The obtained equations, together with the EoS of each component allow to calculate dependencies \( P(U) \) or \( D(U) \) \( (U, D \) are mass and wave velocities); \( A, k \) are coefficients in EoS of condensed component. The following expression can be obtained for a material with \( n \) condensed components \( (\mu_{i0} \text{ is the volume fraction of the } i\text{-th phase of the substance})\):

\[ P = \sum_{i=1}^{n} \frac{A_i \mu_{i0}}{\sigma_i} \left[ \frac{h_i - k_i + 1}{k_i - 1} \sigma_i k_i - h_i - 1 \right] \]  

\[ \sum_{i=1}^{n} \frac{\mu_{i0}}{\sigma_i} h_i + \frac{h_g}{\sigma_g} \left( 1 - \sum_{i=1}^{n} \mu_{i0} \right) - 1 \]  

(5)

Here \( h_i = 2 / \Gamma_i + 1, \quad i = 1 \ldots n; \quad h_g = 2 / (\gamma - 1) + 1, \quad \sigma_i = \rho_i / \rho_{i0}, \quad \sigma_g = \rho_g / \rho_{g0} \) are the degrees of compression ratio of the corresponding component, \( \mu_{i0} \) are the volume fraction, \( \rho_{i0}, \rho_i \) are the density
of the \(i\)-th phase of the substance ahead of the shock wave front and behind it, respectively \((i = 1...n)\); \(\rho_g, \rho_{g0}\) are current and initial gas densities, \(\gamma = 1.41\) (ratio of specific heats for gas). 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 \(P\), which allow us to construct the shock adiabat of investigated material. The function \(\Gamma = \frac{P_fV}{E_T}\) that determines the contribution of the thermal component depends explicitly only on the temperature \(\Gamma(T)\) in the model [7–10].

3. Modeling results and discussion

The results of modeling thermodynamic parameters and data obtained from experiments [11, 12] are shown in figure 1 in the pressure \(P\) and compression ratio variables \(\sigma = \rho/\rho_0\). The reliable description of the available data is obtained, and the parameters defined for pure materials allow one to describe data of experiments for alloys and mixtures of different porosity values with experimental accuracy.

The available experimental data are reliably described without significant errors for all porosity values in the framework of the considered model for the mixtures of copper and tungsten. The value porosity \(m\) is defined as the ratio of the density of the monolithic substance to the initial density of the sample. The adiabates of this mixture of the following compositions, indicating the weight fractions and porosity values \(m\) are shown on figure 1. The modeling is performed for mixtures Elkonite 2125C, W(25)Cu(75) \(m=1.014\); Elkonite 1W3, W(55)Cu(45), \(m=1.0195\); Elkonite 3W3, W(68)Cu(32), \(m=1.022\), Elkonite 10W3, W(76)Cu(24), \(m=1.068\). The calculated curves and data obtained from experiments are shown with a 0.2 shift in the compression value for clarity.

![Figure 1. Shock adiabats in the coordinates of pressure and compression ratio for porous mixture W and Cu: 1 \(m=1.014\), 2 \(m=1.0195\), 3 \(m=1.022\), 4 \(m=1.068\).](image)

Experimental points are from Ref. 11.

The simulation results and available experimental data [11] for the mixture of copper and tungsten carbide (elconite TC10) with mass fractions of WC(56)Cu(44) are shown in figure 2. The additional calculations for the components of the mixture are given for comparison. As noted in [2], the experimental data for TC-10 agree with the calculated data, which are performed using the mixed method worse than for Cu—W elconites. In this case, the value \(m=1.0\) for TC-10, which means that there is no porosity of this sample. The estimation of the temperature values along the shock adiabat
shows significant difference between temperature of TS-10 components in mixture and temperature when the pure material is shown in figure 3. The consideration of the components interaction is necessary for both solid and porous samples for thermodynamic parameters calculating of such components mixtures.

Figure 2. Shock adiabats for mixture TC10 and its components: Calculation: 1 for TC10, 2 for WC, 3 for Cu. Experimental points for mixture 4 are from Ref. 11, for WC points 5, for Cu points 6, 7, 8 are from Ref. 12.

Figure 3. Temperature value along the shock adiabat for mixture TC10 and its components: Calculation: 1 for TC10, 2 for WC, 3 for Cu.
The same calculations were performed for a mixture of silver and tungsten carbide (elconite G-12) WC(40)Ag(60). The results of calculations and available experimental data for G-12 are shown in figure 4.

![Figure 4](image)

**Figure 4.** Shock adiabats for mixture G-12 and its components: Calculation: 1 for G-12, 2 for WC, 3 for Ag. Experimental points for mixture 4 are from Ref. 4, for WC points 5 are from Ref. 12, for Ag points are 6 from Ref. 13, 7 from Ref. 14, 8 are from Ref. 15.

4. Conclusion
The good agreement of the model calculations with the data of different authors, which are determined on the basis of experiment, is obtained. The model allows us to describe the dynamic loading of solid and porous alloys of different compositions consisting of W, WC or Mo, in combination with Ag or Cu, such as Cu-W, Ag-W, Cu-WC, Ag-W. The targeted selection of compositions for mixtures and ratios of their components can be performed using this model for obtaining the specified characteristics of solid and porous materials and mixtures under shock wave loading. The results allow one to create purposefully the necessary conditions for the synthesis of new materials in the future.

Appendices
TEC - thermodynamic equilibrium components
EoS - equation of state

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