Numerical investigations of oxides and silicates under shock-wave loading

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Abstract. By using thermodynamic equilibrium model TEC (thermodynamic equilibrium components) results of numerical experiments of modeling of shock wave loading of oxides, silicates and mixtures are presented. The model allows to consider the presence of a polymorphic phase transition under shock wave loading of the materials, which is important for accurate modeling of thermodynamic parameters of pure substances and mixtures. The significant change of volume of the region of phase transition components included in the mixtures allows us to expand the range of variation of thermodynamic parameters of the mixtures under shock wave loading. The results allow us to create purposefully the necessary conditions for the synthesis of new materials in future. Interest in the research of compressibility of such mixtures is associated with the possibility of creating materials with desired properties and with the properties of the materials themselves. The good agreement of these model calculations with the experimental data of different authors is obtained. The model allows to describe dynamic loading of solid and porous mixtures comprising oxides, silicates as components quartz SiO2, Periclase MgO, Corundum Al2O3, Spinel MgAl2O4, Enstatite Mg2[Si2O6].

1. Introduction
It is necessary to change deliberately thermodynamic parameters for the implementation of the necessary conditions for the creation of materials with desired properties during the development of the method of shock-wave synthesis. The researches of compressibility of multicomponent mixtures are performed for this. Oxides and silicates, and also mixtures based on them are of great interest.
Quartz SiO2, zirconium dioxide ZrO2, periclase MgO, corundum Al2O3, and others are of great interest in themselves and in mixes [1–4]. For example, quartz SiO2 is widely used in optical and electronic devices, in the manufacture of silica refractories and quartz glass. Periclase MgO is an important component of magnesite and dolomite refractory. Additional interest from the point of view of the researches of oxides is associated in particular with MgO, for which the phase transition at high pressure was determined [3]. Such researches parameters of the oxides at high dynamic loads not only allow to purposefully change the parameters of shock-wave loading of samples, but more plausible to describe the structure of the earth’s crust.

Abrasive materials are produce from corundum Al2O3. Spinel MgAl2O4 is rare mineral of cubic crystal structure. It is mixed oxide of magnesium and aluminum (volumetric fraction MgO 28.2%; Al2O3 — 71.8%). The name of mineral Enstatite Mg2[Si2O6] is derived from the Greek words ἐνστάτης (estates) "the enemy", "the resistance", which is associated with resistance to the melting of enstatite. Modeling the thermodynamic parameters for mixtures with such components is performed for the development of promising areas to obtain materials with desired properties.
2. Calculation model
In order to calculate thermodynamic parameters of porous mixtures under dynamic loadings, a model of shock-wave loading with allowance for gas in the pores is used [5–7]. The model was able to describe the parameters in a wide range of pressures under shock wave loading, with the possibility of taking into account polymorphic phase transition of the components of the mixtures. The model is based on the assumption of thermodynamic equilibrium of all the components of a material under shock-wave loading, which implies the equality of the velocities, pressures and temperatures. In order to describe the thermodynamic parameters 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:

\[ P(\rho, T) = P_C(\rho) + P_T(T), \quad \text{and} \quad E(\rho, T) = E_C(\rho) + E_T(T) \]  
\[ P_T(T) = \Gamma \cdot \rho \cdot E_T(T), \quad E_T(T) = c_v \cdot (T - T_0) \]  

Here \( P_C, E_C, P_T, \) 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. By taking into account the pressure region of applicability of this model \( > 5 \text{GPa} \) that is of interest to us, initial energy \( E_0 \) of a substance under normal conditions is considered to be equal to zero. Cold pressure component \( P_C \) is described by a Tait-type equation. Therefore, the equation of state for a condensed component with current density \( \rho \) and initial density \( \rho_0 \) are as follows:

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

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. 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):

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

Here \( h_i = 2 \Gamma_i + 1, \quad i = 1 \cdots n, \quad h_g = 2/(\gamma - 1) + 1. \quad \sigma_i = \rho_i/\rho_0, \quad \sigma_g = \rho_g/\rho_0 \) is the compression ratio of components, \( \rho_0, \rho_{i0} \) current and initial gas densities, \( \gamma = 1.41 \) is the ratio of specific heat. 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; \( A, k \) the coefficients in the equations of state of condensed component. These dependences can be treated as shock adiabat of multicomponent material.

The function \( \Gamma = \frac{P V}{E_C} \) that determines the contribution of the thermal component depends explicitly only on the temperature \( \Gamma(T) \) in the model [5–7].

The model TEC may describe the thermodynamic parameters of the materials including the phase transition region [8]. The material is considered as the mixture of low-pressure phase and high-
pressure phase in this area. The simulation results allow us to describe the thermodynamic parameters of the mixture including the components experiencing a phase transition at high dynamic loads. The parameters of the equation of state only their components are used to calculate the shock-wave effects in such mixtures.

3. Numerical results
Calculations of thermodynamic parameters of Corundum Al₂O₃, Spinel MgAl₂O₄, Enstatite Mg₂Si₂O₆ and data obtaining on the basis of the experiments of [9, 10] are shown in Figure 1. The accurate descriptions of the available data are obtained. The model parameters allowing reliable description of the thermodynamic parameters of pure oxides and silicates under shock wave loading are used to simulate the parameters of the mixture of them as components [6].

Model TEC allows us to describe the shock adiabats in the region of phase transition. The reliable description of thermodynamic parameters of quartz SiO₂ taking into account polymorphic phase transition for samples of different porosity is obtained [8]. The similar modeling is performed for periclase MgO with a density of ρ₀=3.584 g/cm³. The data for shock-wave loading of MgO is given in [3] up to value of pressure of 1000 GPa. In addition to the new field of dynamic parameters, the region of phase transition high pressure was discovered. The modeling results of thermodynamic parameters and the data from [3, 10] are shown in Figure 2. Thermodynamic parameters successfully modeling for MgO in the whole range of available experimental data are shown in Figure 2. The presence of a phase transition high pressure oxides, if they exist for other oxides, holds great promise for the analysis of the internal structure of the Earth given the large content of oxides in its composition [2].

Figure 1. Shock adiabata in variable – pressure compression. Calculation – line: 1 – corundum Al₂O₃, 2 – spinel MgAl₂O₄, 3 – forsterite ceramic, Mg₂[SiO₄], 4 – enstatite ceramic Mg₂[Si₂O₆]. The data of experiments 1–4 [9, 10].

Figure 2. Shock adiabats of MgO in the coordinates pressure – compression. Line – calculation for MgO with phase transition, dotted line represents shock adiabata for low-pressure phase, dash-dotted line represents the calculation for the phase of high-pressure. Experimental data – 1 [10], 2 [3].
The accuracy of the description of thermodynamic parameters of the mixtures, taking into account phase transitions of the components under shock wave loading, was determined by calculations of shock wave loading of mixture with quartz. In Figure 3 the results are shown obtained for the mixtures of epoxy and quartz mixture, volume fraction vol% Epoxy(60)SiO₂(40) $\rho_0=1.66$ g/cm$^3$ consequently. The calculation corresponds well to the data of the experiments until the value of pressure 50 GPa. It is assumed that the phase transition of the components of the mixture starts under the same conditions as for the pure substances. Due to the fact that the calculation was carried out for the mixtures with low porosity, the estimated the pressure value to the beginning of the phase transition can be considered justified. This assumption has been confirmed by the calculations of the mixtures with two components undergo phase transition [11].

The parameters that gave the opportunity to reliably describe the thermodynamic parameters of epoxy resins in a wide range of dynamic parameters, has allowed to describe with the precision of the experiment the thermodynamic parameters of the mixtures with other materials, which are characterized by high strength and heat resistance. The calculated and experimental data for these mixtures in the coordinates (pressure – compression) are shown in Figures 4–7. It is necessary to know the composition and density of the mixture for the description of thermodynamic parameters for shock wave loading. The component parameters are taken the same as in the description of pure substances. Thermodynamic parameters for the mixture of epoxy resin with Corundum, volume fraction, vol% Epoxy (60) Al₂O₃ (40), respectively, $\rho_0=2.307$ g/cm$^3$, the porosity, determined on the basis of data [10] $m=0.93$ are shown in Figure 4. The porosity $m$ is defined as the ratio of the density of monolithic material to the density of the sample.
The modeling results of the thermodynamic parameters for the mixture of epoxy resin with Spinel, volume fraction, vol % Epoxy (60) MgAl$_2$O$_4$ (40), $\rho_0 = 2.171$ g/cm$^3$, $m=0.97$ are shown here. The experiments data from [10] and modeling results of thermodynamic parameters, which are defined by the model TEC for mixture of epoxy resin with Enstatite, volume fraction, vol% Epoxy (60) Mg$_2$Si$_2$O$_6$ (40), $\rho_0 = 2.017$ g/cm$^3$, $m=0.93$ are shown too.

The good correspondence of the calculations to data obtained on the basis of experiments for mixtures with epoxy resin are shown. The deviation of the calculated points for the mixture of quartz at pressure above 60 GPa and for the other mixtures above 80 GPa are probably due, in part, to the possible existence of polymorphic phase transition including for epoxy resin. In the presence of experimental data that allow to accurately, determining the region of phase transition, the model TEC can be used in this case. The possibility of calculating the thermodynamic parameters of a mixture with multiple components that are experiencing a phase transition under shock wave loading was shown in [11].

4. Conclusion

The data of the model TEC calculations correspond well to the experimental data by various authors. The model parameters, that allow us to reliably describe the behavior of pure materials under shock wave loading, were used to simulate thermodynamic parameters of oxides, silicates and mixtures based on them mixtures including components experiencing a phase transition under shock wave loading. A significant change in volume in the region of the polymorphic phase transition components included in the mixtures allows expanding the range of changes of thermodynamic parameters of the mixtures under shock wave loading. The results obtained allow creating purposefully the necessary conditions for the synthesis of new materials. This model allows for specific selection of compositions of mixtures and the ratios of their components with the aim of obtaining the specified characteristics under shock-wave loading of solid and porous materials and mixtures.

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