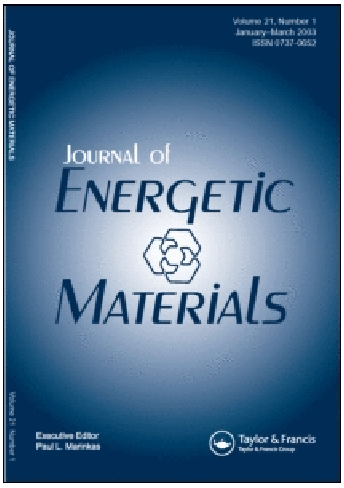

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A Multicomponent Medium Model for Reacting Porous Mixtures Under Shock Wave Loading

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A multicomponent medium model for numerical simulation of reacting mixture behavior under shock wave loading is proposed. In the model, every component of a mixture simultaneously occupies the same volume as the mixture. An equality of components pressure is chosen as a condition for joint deformation of components. Components interact with each other, exchanging momentum, energy, and mass in the presence of chemical reactions. Parameters of explosive loading are determined experimentally and theoretically. The interaction of a steel impactor accelerated by an explosion with a cylinder ampoule that contains a porous reacting mixture of aluminum and sulfur powders is modeled by using the finite element method.

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Introduction

At present the branches of physics and the mechanics connected with studying mechanical and physical–chemical processes taking place during the action of strong shock waves on metals, minerals, polymers, and other solids are intensively developing. It is connected with the development of both traditional directions of human activity, where explosion and high-speed impact are used, and the development of new production methods and is caused by the necessity to decrease costs in the manufactories of space and aerotechnics in power engineering, chemistry, and minerals industries and modern machine building. An explosive representing a compact lightweight and cheap energy source of high density and capacity gives the opportunity of doing such huge and useful work [1–3]. Most explosive technologies are used in metalworking during shaping, welding, cutting, hardening, and compression. Many of these operations have already been applied in industry and the influence of shock wave loading on the proceeding solid-phase reactions has not been investigated enough to reach a technological stage due to lack of experimental data as well as numerical techniques that correctly describe the process.

Synthesis of new materials under equilibrium conditions is completely studied. Prospects are connected with producing metastable compounds in nonequilibrium conditions by means of dynamic loading. High pressures and speeds of a substance causing an initiation of chemical reactions create extreme conditions for production of new materials. In addition, shock waves cause mechanochemical activation of a mixture, high rate of fragmentation, and mixing of particles, which creates favorable conditions for initiation and proceeding superfast chemical reactions [2].

Consequences of shock wave loading of substances are sure to be too diverse and complicated to be predictable. However, systematic fundamental investigations in physics and chemistry of shock waves with the use of specific systems open vast possibilities to manage the processes of structural chemical and phase transformations and allow improving essential properties of materials and even producing new materials with unique properties. In addition, a detailed description of interphase interactions in multicomponent media is rather complicated but also extremely important for the estimation of medium parameters depending on the macroscopic structure and component properties of the medium.

For numerical simulation of such media, it is necessary to take into account all the components and compressibility of a mixture, variability of process parameters, and presence of chemical reactions. These additional effects do not allow using the results received within the framework of traditional description of the multicomponent medium as a homogeneous one, where a mixture is described by the single-phase medium equation and average properties do not correspond to the properties of a separate phase [4].

The aim of this article is to develop a model of a multicomponent medium for numerical prediction of porous reacting mixture behavior under shock wave loading.

Formulation of the Problem

The system of equations governing the nonstationary adiabatic motion of every component in a space-fixed volume of a compressible solid mixture V bounded by a surface S with allowance for the exchange of momentum, energy, and mass between components as well as the evolution of microdamage and chemical transformations comprises the continuity equation, the equation of motion, and the energy equation [1,3]:

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla \alpha_i \rho_i \mathbf{v}_i = \sum_{j=1}^{N} J_{ji}, \quad (i = 1, 2, \ldots, N), \tag{1}$$

$$\alpha_{\imath} \rho_i \frac{d_i \mathbf{v}_i}{dt} = \nabla \alpha_i \sigma_i + \alpha_i \sum_{j=1}^{N} \alpha_j \mathbf{R}_{ji}, \quad (i = 1, 2, \ldots, N), \tag{2}$$

$$\alpha_i\rho_i\frac{d_iE_i}{dt} = \alpha_i\sigma_i\varepsilon_i + \alpha_i\sum_{j=1}^{N}\alpha_j\Phi_{ji}, \quad (i = 1, 2, \ldots, N), \tag{3}$$

$$\frac{d_i}{dt} \equiv \frac{\partial}{\partial t} + v_i^k\frac{\partial}{\partial x^k}.$$

Here t is the time, ρ_i is the real density (mass of component per unit volume of component), $\boldsymbol{v}_i$ is the velocity vector, v_i are the velocity components, E_i is the specific internal energy, $\sigma_{i_{kj}} = -P_i\delta_{i_{kj}} + S_{i_{kj}}$ are the stress-tensor components, P_i is the pressure, $\varepsilon_{i_{kj}}$ are the components of the strain rate tensor, $S_{i_{kj}}$ are the components of the stress deviator, $\boldsymbol{R}_{ji}$ is the exchange of momentum between i and j components, Φ_{ji} is the exchange of energy between i and j components, J_{ii} is the mass transfer, and N is the number of components.

In contrast to homogeneous mixtures, where every component occupies the whole volume of a mixture ($V_1 = V_2 = \ldots = V_N = V$), in heterogeneous mixtures every component occupies only a part of volume ($V_1 + V_2 + \ldots + V_N = V$). In this connection, in the theory of multicomponent mixtures the variable α_i ($i = 1, 2, \ldots, N$) is used to determine volume fractions occupied by every component [1]:

$$\alpha_1 + \alpha_2 + \cdots + \alpha_N = 1, \quad (\alpha_i \geq 0), \tag{4}$$

$$\alpha_i = \rho_i^*/\rho_i, \tag{5}$$

here ρ_i^* is the reduced density (mass of component per unit volume of medium).

To solve the shock wave loading problems of porous reacting mixtures, the finite element method is used [5–7]. On the basis of this method every component of a mixture simultaneously occupies the same volume as the mixture and consists of a set of the final elements connected with the node points. Inside every element, components interact with each other, exchanging momentum, energy, and mass (in the presence of chemical reactions) within the framework of the multicomponent medium model. After interaction of components and their summary contribution to node forces of an element, the components in a mixture obtain the velocity of the corresponding element.

In modeling chemical reactions under shock wave loading, we use the zeroth-order kinetic relation [4,8] characterized by a constant rate of chemical transformations:

$$J_{ji} = \frac{d\eta}{dt} = \begin{cases} 0, & \text{if } \eta = 1 \text{ or } (\,T_i < T_{\eta_i} \text{ and } P < P_\eta\,) \\ (P_\eta), & \text{if } \eta < 1 \text{ and } (T_i \geq T_{\eta_i} \text{ or } P \geq P_\eta) \end{cases}, \quad (6)$$

$$f(P_\eta) = \begin{cases} K_0, & \text{if } P < P_\eta \\ K_p\, K_0, & \text{if } P \geq P_\eta, \end{cases}$$

here T_i is the temperature; P is is the matched pressure of components; T_{η_i}, P_η, K_p, and K_0 are the constants; and η is the conversion degree.

Under these conditions the chemical reaction is forced, initiated, and proceeds due to performance of the criterion on pressure or temperature. The reaction stops if both critical conditions are not satisfied. The constant of the reacting mixture K_0 is a structurally dependent quantity and is determined primarily by the component particle size. The value K_0 increases with the increase in dispersity of mixture components [9].

The exchange of momentum between i and j components may be represented by [1,10]:

$$R_{ji} = a_{ji}(v_j - v_i) + J_{ji} v_{ji}, \quad (i = 1, 2, \ldots, N; i \neq j), \qquad (7)$$

$$\sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j R_{ji} = 0.$$

One of the possible relationships for the calculation of a_{ji} is as follows [10]:

$$a_{ji} = a \rho_j \rho_i$$

here a is the constant.

The exchange of energy between i and j components may be represented by [1,10]:

$$\Phi_{ji} = \varphi_{ji}(P_j - P_i) + \psi_{ji}(T_j - T_i) + J_{ji}E_{ji}, \quad (i = 1, 2, \dots, N; i \neq j), \tag{8}$$

$$\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j \Phi_{ji} = 0.$$

Functions a_{ji} in (7) and φ_{ji} and ψ_{ji} in (8) depend on the aggregative and phase state of i and j components, size, shape, and roughness of particles and mechanical and thermal properties of components.

The equation describing the change in the specific volume of pores is as follows [11]:

$$\frac{dW_{f_i}}{dt} = \begin{cases} 0, \quad \text{if } |P_{s_i}| \leq P_i^* \text{ or } (P_{s_i} > P_i^* \text{ and } W_{f_i} = 0) \\ -\text{sign}(P_{s_i})K_{f_i}(|P_{s_i}| - P_i^*)(V_{2_i} + W_{f_i}), \\ \text{if } P_{s_i} < -P_i^* \text{ or } (P_{s_i} > P_i^* \text{ and } W_{f_i} > 0), \end{cases} \tag{9}$$

here P_{s_i} is the pressure in a solid component of the mixture, and $V_{1_i}, V_{2_i}, P_{k_i}, K_{f_i}$ are experimental material constants.

Pressure in the undamaged component of the mixture is a function of specific volume and internal energy, and over the entire range of loading conditions it is determined by the Mie-Grüneisen equation of state according to the formula [12]:

$$\begin{aligned} P_i = {} & \rho_{0_i} u_{c_i}^2 \mu_i + \rho_{0_i} u_{c_i}^2 [1 - \gamma_{0_i}/2 + 2(b_i - 1)] \mu_i^2 \\ & + \rho_{0_i} u_{c_i}^2 [2(1 - \gamma_{0_i}/2)(b_i - 1) + 3(b_i - 1)^2] \mu_i^3 + \gamma_{0_i} \rho_{0_i} E_i, \end{aligned} \tag{10}$$

Here $\mu_i = V_{0_i}/(V_i - V_{f_i}) - 1$; γ_{0_i} is the Grüneisen coefficient; V_{0_i} and V_i are the initial and current specific volumes, respectively; and u_{c_i} and b_i are the constants of the Hugoniot shock adiabat described by the relation [3]

$$u_{s_i} = u_{c_i} + b_i u_{p_i},$$

here u_{s_i} is the shock wave velocity and u_{p_i} is the particle velocity of a component behind the shock wave front.

The equality of components pressure is used as a condition for joint deformation of components in the mixture [1]

$$P = P_i(V_i, E_i) = P_j(V_j, E_j). \tag{11}$$

The change in porosity is assumed to be influenced only by the spherical stress component or pressure, whereas the components of the stress deviator are bounded by the independent deviatoric yield function [12]:

$$2G_i\left(\varepsilon_{i_{kj}} - \frac{1}{3}\varepsilon_{i_{qq}}\delta_{i_{kj}}\right) = \frac{dS^0_{i_{kj}}}{dt} + \lambda_i S_{i_{kj}},$$

where $dS^0_{i_{kj}}/dt$ is the Jaumann derivative given by:

$$\frac{dS^0_{i_{kj}}}{dt} = \frac{dS_{i_{kj}}}{dt} - S_{i_{kq}}W_{i_{jq}} - S_{i_{jq}}W_{i_{kq}},$$

and $2W_{i_{kj}} = \partial\upsilon_{i_i}/\partial x_j - \partial\upsilon_{i_j}/\partial x_i$. The parameter λ_i is zero for elastic deformation, and for plastic deformation it is determined from the von Mises yield criterion [12]:

$$S_{i_{kj}}S_{i_{kj}} = \frac{2}{3}\sigma_i^2.$$

Here G_i is the shear modulus and σ_i is the dynamic yield point [11]:

$$G_i = G_{0_i}K_{T_i}\left(1 + \frac{c_iP_i}{(1+\mu_i)^{1/3}}\right)\frac{V_{3_i}}{(V_{f_i} + V_{3_i})},$$

$$\sigma_i = \begin{cases} \sigma_{0_i}K_{T_i}\left(1 + \frac{c_iP_i}{(1+\mu_i)^{1/3}}\right)\left(1 - \frac{V_{f_i}}{V_{4_i}}\right), & \text{if } V_{f_i} \le V_{4_i} \\ 0, & \text{if } V_{f_i} > V_{4_i} \end{cases}, \tag{12}$$

$$K_{T_i} = \begin{cases} 1, & \text{if } T_{0_i} \le T_i \le T_{1_i} \\ \frac{T_{m_i} - T_i}{T_{im} - T_{i_1}}, & \text{if } T_{1_i} < T_i < T_{m_i} \\ 0, & \text{if } T_i \ge T_{m_i} \end{cases}$$

Here T_{m_i} is the melting point of components and c_i, V_{3_i}, V_{4_i}, and T_{1_i} are the constants of components. In the computations, the function $K_{T_i}(T_i)$ was chosen to model the nonthermal character of plastic deformation and dynamic strength of solids at high strain rates ($10^4\,\mathrm{s}^{-1}$ or higher).

To calculate the temperature, the following relationships are used [3]:

$$dT_i = \begin{cases} d(E_i - E_{i_{0x}})/c_{p_i}, & \text{if } T_i < T_{i_m} \\ 0, & \text{if } T_i = T_{i_m} \\ d(E_i - E_{i_{0x}} - \delta H_{i_m})/c_{p_i}, & \text{if } T_i > T_{i_m} \end{cases},$$

where the specific heat c_{p_i} increases linearly as the temperature increases to the melting point of the substance [4,5]:

$$c_{p_i} = \begin{cases} c^0_{p_i} + \frac{c^L_{p_i} - c^0_{p_i}}{T_{i_m} - T_{i_0}}(T_i - T_{i_0}), & \text{if } T_{i_0} \le T_i < T_{i_m} \\ c^L_{p_i}, & \text{if } T_i \ge T_{i_m} \end{cases}.$$

Experimental and Numerical Results

To determine the parameters for explosive loading, the aluminum (Al, size of particles <100 µm) and sulfur (S, size of particles 100–300 µm) powders were used. The mass fractions of components are as follows: Al, 35; S, 65. Components were mixed in an AGO-2U planetary mill. The mixture was pressed into eight tablets with a diameter of 14.2 mm and thickness of 7.5 mm. The porosity was 0.15 (15% of total volume). The tablets were placed into a steel cylindrical ampoule with an external diameter of 20 mm. The ampoule was closed with a lid. The mixture in the ampoule was loaded by a steel impactor with an external diameter of 37 mm and wall thickness of 3 mm accelerated by explosion products. The mixture of ammonium/nitrate of ammonium in a proportion 1/1 with a density of 1.07 g/cm^3 was used as an explosive. The external diameter of the explosive was 64 mm. The assembly was located in the field of two X-ray tubes (Orion 600), which photographed the ampoule loading.

The X-ray photographs of the assembly are given in Fig. 1a before and during explosive loading. The exposure time was 1.5 ns. The analysis of X-ray photographs showed that the detonation velocity of explosive was 3.3 km/s, calculated Chapman-Jouguet pressure was 3.3–3.6 GPa depending on the assumed polytropic coefficient of detonation products 2.2–2.5. The distance passed by a detonation wave with a velocity of 3.3 km/s from the top of the impactor (ignoring the conic part of the ampoule lid) was 63.6 mm, and the angular deflection of accelerated impactor was 4.7 degrees (Fig. 1b). Melted sulfur trickled from the ampoule after loading and there was a hydrogen sulfide smell as well that testified to the reaction of aluminum sulfide synthesis. The external diameter of the ampoule after explosive loading was 19.2 ± 0.2 mm in the top part and 20 ± 0.2 mm in the bottom part.

To determine the parameters of explosive loading numerically, the axially symmetric problem of interaction between a steel cylindrical impactor accelerated by explosion products in the mode of sliding detonation and a cylindrical ampoule containing the porous mixture of aluminum and sulfur was

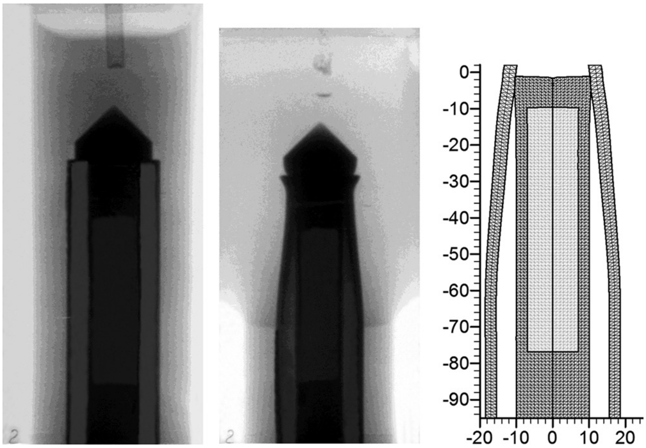


Figure 1. X-ray photographs of the assembly before (a) and during (b) explosive loading; the calculated configuration of an assembly section at 19 μs (c).

considered. For numerical simulation of the porous mixture behavior under explosive loading the multicomponent medium model (1)–(11) considered above is used.

Within the framework of the multicomponent medium model, every component is supposed to occupy simultaneously the same volume as a mixture. Every component is characterized by the volume and mass concentration. Components interact with each other, exchanging momentum, energy, and mass in the presence of chemical reactions. An equality of the components' pressures is chosen as a condition for joint deformation of the components.

For the mathematical description of explosive loading it is necessary to know the pressure of explosion products acting on a cylindrical impactor versus time. In this work, the detonation process is supposed to be stationary, and the velocity of the pressure change (drop) of explosion products in time is constant. Under such assumptions the pressure change can be described by the equation

$$P = P_0 - kt, \quad (t = 0 \ldots \Delta t),$$

which is the equation of a straight line with a coefficient k and initial ordinate P_0. The coefficient k is determined from the formula

$$k = \frac{P_0}{\Delta t}.$$

Then the final equations for calculation of explosion product pressure on the lateral wall of a cylindrical impactor are as follows:

$$P = P_0 - \frac{P_0}{\Delta t}t, \quad 0 \le t \le \Delta t,$$

$$P = 0, \quad t > \Delta t,$$

$$\Delta t = \frac{\Delta}{c}, \quad c = \frac{D}{2},$$

where Δ is the thickness of the explosive layer, c is the overall velocity of unloading wave (estimation), and D is the detonation velocity. For $\Delta = 13.5\,\mathrm{mm}$ and $D = 3.3\,\mathrm{km/s}$, the time length of the pressure pulse is $\Delta t \approx 8.2\ \mu\mathrm{s}$. P_0 is varied in calculations to obtain agreement between numerical and experimental results.

In Fig. 1c the calculated configuration of an assembly section characterizing the simulation results of explosive loading at $19\,\mu\mathrm{s}$ at the specified $P_0 = 4\,\mathrm{GPa}$ are illustrated. The calculation results showed that by this moment the distance passed by the detonation wave with a velocity of 3.3 km/s was 63 mm, and the angular deflection of the accelerated impactor was 4.76 degrees. The obtained numerical results for simulation of explosive loading and dynamics of the explosion product's influence on an impactor are in a good qualitative and quantitative agreement with experiments with an accuracy of 1.3%.

Based on the obtained parameters for explosive loading, the interaction of a steel impactor (D_3, Fig. 2) accelerated by an explosion with a cylinder ampoule (D_1), which contains a porous reacting mixture of aluminum and sulfur powders (D_2), is modeled. The height of the ampoule is 30 mm, the thickness of the lateral wall is 2 mm, and the bottom and cover are 2 mm. The diameter of the impactor is 36 mm, and the thickness of the impactor wall δ_0 is 4 mm. The composition of the mixture is 0.65 mass fraction of sulfur

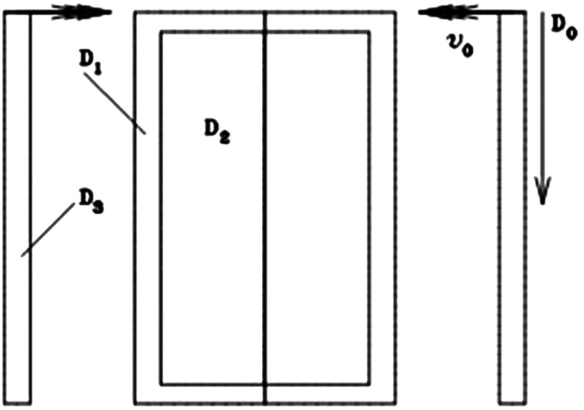


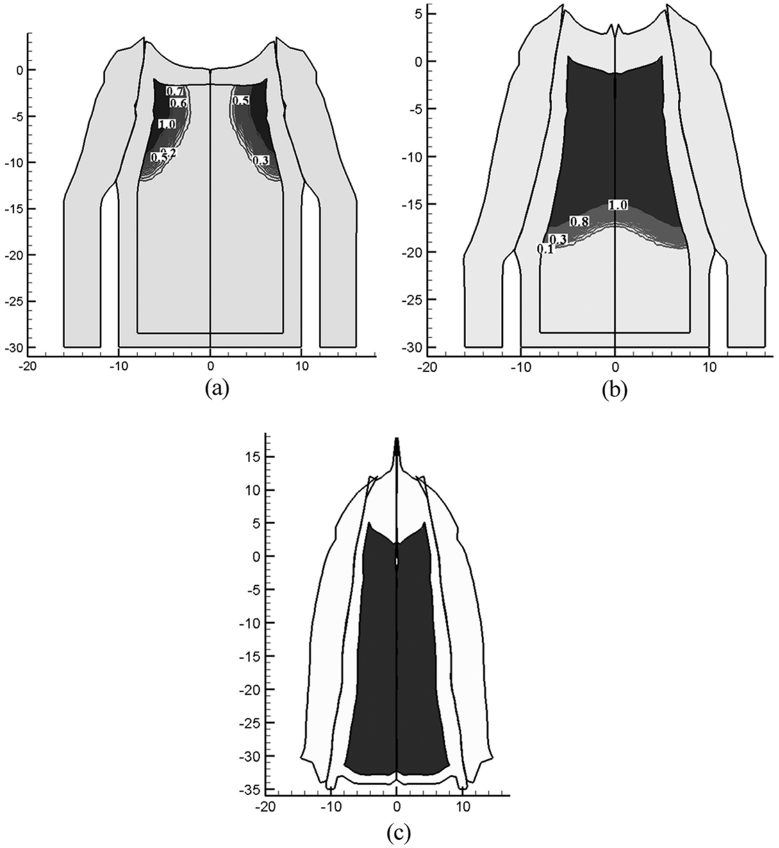
Figure 2. Statement of the problem for shock wave loading of the Al-S reacting porous mixture.

and 0.35 mass fraction of aluminum, which corresponds to the stoichiometric reaction with the synthesis of aluminum sulfide (Al_2S_3). The investigated specimen (D_2) of the pressed porous mixture is 26 mm in height and 16 mm in diameter. The initial porosity of the specimen is of 40%. The detonation velocity (D_0) is 3,300 m/s.

A superfast chemical reaction in the specimen occurs when the critical value $T_\eta = 392.5\,K$ or $p_\eta = 2\,GPa$ is exceeded [4]. In the range of the initial conditions considered, the chemical reaction is initiated due to the performance of criterion on temperature (melting point of sulfur) and proceeds up to completion of aluminum sulfide synthesis (Al_2S_3). The rate of chemical transformations K_0 is 4,816 GJ/(kg*s). The enthalpy of chemical reaction ΔH is 4,816 kJ/kg.

Figure 3 illustrates shock wave synthesis of aluminum sulfide and isolines distribution of chemical transformations in an axial section of the ampoule. At the initial stage of Al_2S_3 synthesis, the chemical reaction is initiated in lateral layers of the mixture as the shock wave front primarily presses the mixture layers adjoining to the lateral walls of the ampoule. At 4 μs (Fig. 3a) the formation of Al_2S_3 is observed in the lateral layers of the specimen. At 6 μs (Fig. 3b) the chemical reaction continues to proceed with the formation of Al_2S_3. By 10 μs (Fig. 3c), the chemical reaction proceeded completely in the whole specimen with the formation of Al_2S_3. It should be noted that the highest pressures develop in an axial area of the cylinder and can lead to melting, intensive mixing, and the formation of cavities in the center of the specimen. By 10 μs (Fig. 3c) the formation of a small cavity is clearly observed in the top axial part of reacted specimen. Figure 3 illustrates that chemical transformations between Al and S are initiated in a transmitted shock wave and proceeded completely with the formation of Al_2S_3 and the increase in velocity of the impactor and detonation can lead to the formation of cavities in materials.

Figure 4 shows the change of aluminum sulfide (Al_2S_3) densities during a chemical reaction for various initial impact velocities and initial component's porosity of 0.4. Peaks of the Al_2S_3 densities practically coincide for different impact velocities



(a) (b) (c)

Figure 3. Distribution of isolines for conversion degree in axial section of the ampoule for $V_0 = 2{,}000$ m/s and $T =$ (a) 4, (b) 6, and (c) 10 µs.

under consideration. After completion of the chemical reaction and shock wave synthesis the higher Al_2S_3 densities are observed for the lower impact velocity $v_0 = 1{,}000$ km/s (line 3) and close enough to the density of nonporous Al_2S_3 (line 4, Fig. 4).

The results testify that the increase in impact velocity and accordingly in pressure and temperature during shock wave loading of reacting components can lead to production of materials with low density.

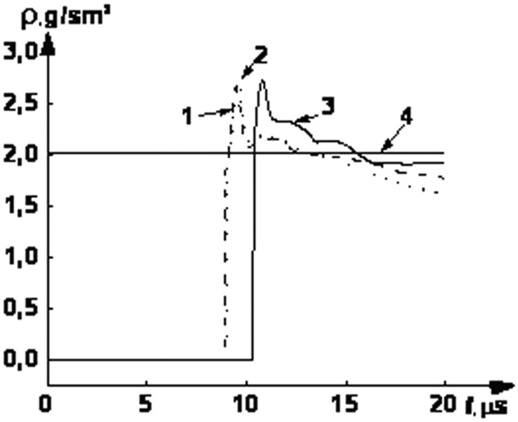


Figure 4. Density of aluminum sulfide versus time in the center of the ampoule for different initial impact velocities: 1, $\upsilon_0 = 2{,}000\,\text{m/s}$; 2, $\upsilon_0 = 1{,}800\,\text{m/s}$; 3, $\upsilon_0 = 1{,}000\,\text{m/s}$; 4, density of nonporous AL_2S_3 ($2.02\,\text{g/cm}^3$).

Conclusions

The analysis shows that shock wave synthesis of aluminum sulfide can be divided into several stages. At the first stage, there is a process of dynamic compaction and then synthesis of aluminum sulfide takes place when the critical value (S) on temperature is exceeded.

It has been established that in the range of the initial conditions considered, the chemical reaction is initiated due to the performance of criterion on temperature and proceeds up to completion of aluminum sulfide synthesis.

The results of computations have shown that there are optimal parameters of shock wave loading that provide the maximal density of a final reaction product.

The increase in velocity of the impactor during shock wave loading of reacting components can lead to the formation of cavities in materials and production of materials with low density.

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