EXPERIMENTAL AND NUMERICAL INVESTIGATION OF SHOCK WAVE SYNTHESIS OF SOLID-STATE MIXTURES

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Explosive loading of an aluminum–sulfur mixture and explosive compaction of an aluminum–sulfur–carbon mixture in cylindrical steel recovery ampoules are explored experimentally and numerically. Behavior of the mixture is described by a mathematical model of a multicomponent medium. An appreciable influence of the explosive layer thickness on the final result of explosive compaction has been found. It is shown that the bottom part of the ampoule is damaged due to gas phase formation and a pressure buildup.

Modern technical equipment increasingly requires high-density materials, but some of the materials cannot be processed by traditional methods due to high melting temperatures or rigidity [1]. The use of explosive technologies eliminates these restrictions. The main advantage of explosive loading is a high density of final materials. The advantages of explosive loading ensure its wide application, and although the first experiments were conducted long time ago, the opportunities offered by the method are not exhausted [2, 3]. Experimental research and numerical simulation of such processes allow one to control the structure formation and to produce new materials with a fine-grained structure, as well as gradient, layered, and other materials with unique properties.

The purpose of this paper is to experimentally and numerically study response of aluminum–sulfur and aluminum–sulfur–carbon mixtures to explosive loading.

To determine experimentally the parameters of a cylindrical ampoule that contains a two-component mixture to be used in explosive loading tests, aluminum (Al, size of particles < 100 μm) and sulfur (S, size of particles 100–300 μm) powders have been used. The mass fractions of the components were as follows: Al 35 and S 65. The components were mixed in an AGO-2U planetary mill. The mixture was pressed into 8 tablets 14.2 mm in diameter and 7.5 mm thick. The porosity was 0.15 (15% of the total volume). The tablets were placed into a steel cylindrical ampoule of an external diameter of 20 mm. The ampoule was closed with a top and bottom lids. The mixture in the ampoule was loaded by a steel impactor of an external diameter of 37 mm and wall thickness of 3 mm accelerated by explosion products. A 1/1 ammonite / ammonium nitrate mixture of 1.07 g/cm^3 density was used as an explosive. The external diameter of the explosive charge was 64 mm. The assembly was located in the field of two X-ray "Arion 600" instruments which photographed the ampoule loading.

The X-ray photographs of the assembly are displayed in Figs. 1*a* and 1*b* before and during explosive loading. The exposure time was 1.5 ns. Analysis of the X-ray photographs showed that the detonation velocity of explosive was 3.3 km/s, the calculated Chapman–Jouguet (CJ) pressure was 3.3–3.6 GPa depending on the assumed polytropic coefficient of the detonation products ranging from 2.2 to 2.5. The distance the detonation wave travels at 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 the accelerated impactor was 4.7° (see Fig. 1*b*). 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 mathematically describe explosive loading, one needs to know not only the detonation velocity, but the pressure of explosion products acting on the cylindrical ampoule vs. time as well. In this work, it is assumed that the detonation process is stationary; the pressure of the explosion products varies (drops) linearly in time. Under these assumptions, the equation for calculating the pressure of the explosion products takes the form [2, 3]:

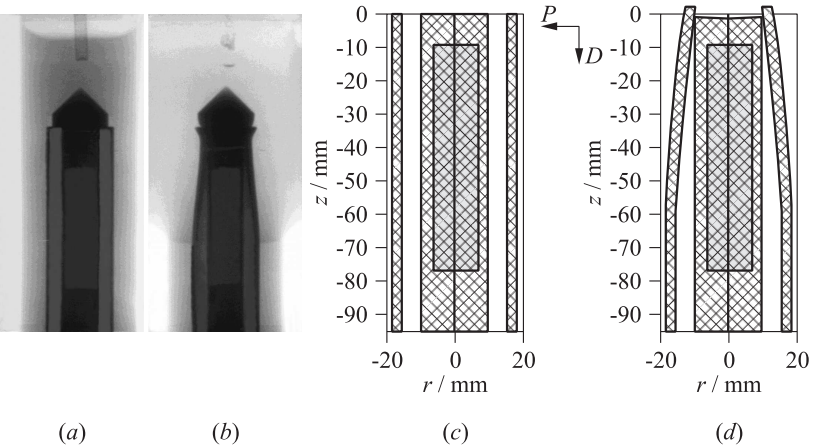

Figure 1 X-ray photographs of the assembly with an external tube before (a) and during (b) explosive loading and computer images of the axial section of the assembly at the 0 (c) and 19 μs (d) instants (P is the pressure and D is the velocity of a detonation wave)

$$P = \begin{cases} P_0 - \dfrac{P_0}{\Delta t}\, t\,, & 0 \le t < \Delta t\,; \\ 0\,, & t \ge \Delta t\,, \end{cases} \qquad \Delta t = \frac{\Delta}{c}\,; \qquad c = \frac{D}{2}$$

where Δ is the explosive layer thickness; c is the average velocity of the unloading wave (estimation); and D is the detonation velocity of explosives. Pressure P_0 is varied in computations to obtain good agreement between numerical and experimental results.

Figures 1c and 1d illustrate the computed configurations of an assembly section that exhibit the results of explosive loading at 0 and 19 μs for $P_0 = 4$ GPa. The numerical results show that by 19 μs, the distance the detonation wave traveled at a velocity of 3.3 km/s was 63 mm and the angular deflection of the accelerated impactor was 4.76°. The numerical results of explosive loading simulation and calculated data on the influence of the explosion products on the impactor are in good qualitative and quantitative agreement with experiments to within 1.3%.

The present authors investigated explosive loading of a cylindrical ampoule that contains a three-component mixture of aluminum, sulfur,

and graphite. To conduct explosive compaction, the inert component (graphite) was added to the mixture of aluminum and sulfur, the overall mixture contained two mass fractions of graphite and tone mass fraction of the Al–S mixture to avoid the reaction between aluminum and sulfur. The mass fractions of the components in the sample (mixture) were as follows: Al — 11.5, S — 21.5, and C — 67; and volume fractions: Al — 9.55, S — 23.35, and C — 67.1. The components were mixed in an AGO-2U planetary mill and then the mixture was compressed into 8 tablets 14 mm in diameter and 8 mm thick. The measured porosity was 0.393 ± 0.005. The tablets were placed into a 84-millimeter long steel ampoule 14 mm in inner diameter and 20 mm in external diameter. The ampoule was closed with lids.

The ampoule was loaded by detonation of an explosive charge which was a 1 : 1 mixture of ammonite 21/79 (TNT / ammonium nitrate) and NaCl. The measured explosive density was 1.2 g/cm^3. The external explosive charge diameter was 50 mm. The measured detonation velocity was 2.8 km/s. The ampoule after explosive loading was uniformly compressed from top to bottom after the experiment. As follows from comparison of the ampoule diameter before and after explosive loading, the compaction degree of the sample is about 97% (residual porosity is 0.03).

To simulate the experimental results of explosive compaction of the mixture, the authors numerically considered an axisymmetric problem of explosive loading of a cylindrical ampoule that contains a three-component inert mixture of aluminum, sulfur, and graphite with the same mass and volume fractions as in the experiment. Behavior of the mixture is described by a mathematical model of a multicomponent medium [2–5]. In the model, every mixture component simultaneously occupies the same volume as the mixture itself. Every component is characterized by its volume and mass concentration. Components interact with each other, exchanging momentum and energy. An equality of components' pressure is chosen as a condition for joint deformation of components.

In the computations, the thickness of the explosive charge layer Δ_z was varied in the axial direction, detonation of which acts on the upper part of the ampoule, in order to study the influence of this parameter on the final shape and size of the ampoule. The value Δ_r for the explosive acting radially on the lateral wall of the ampoule was constant and

equal to 18 mm. Attention was paid to the action of explosive layers on the lateral surface of the ampoule, and the possible influence of the axial explosive layer on the upper part of the ampoule was disregarded. The P_0 value was chosen on the basis of numerical and experimental evaluations and was 3.2 GPa.

Figures 2*b*–2*d* show the evolution process for explosive compaction of a cylindrical ampoule with an inert mixture for different thicknesses of an axial layer of the explosive. The results of computations show a significant influence of the axial explosive layer on the final results of explosive loading. When the thickness Δ_z is low, the influence of lateral load prevails, which leads to elongation of the ampoule in the axial direction (see Fig. 2*b*). When the thickness Δ_z is large, there is an additional load on the upper part of the ampoule, which causes deformation of the top lid of the ampoule (compaction in the axial direction and elongation in the radial direction) and the mixture. The

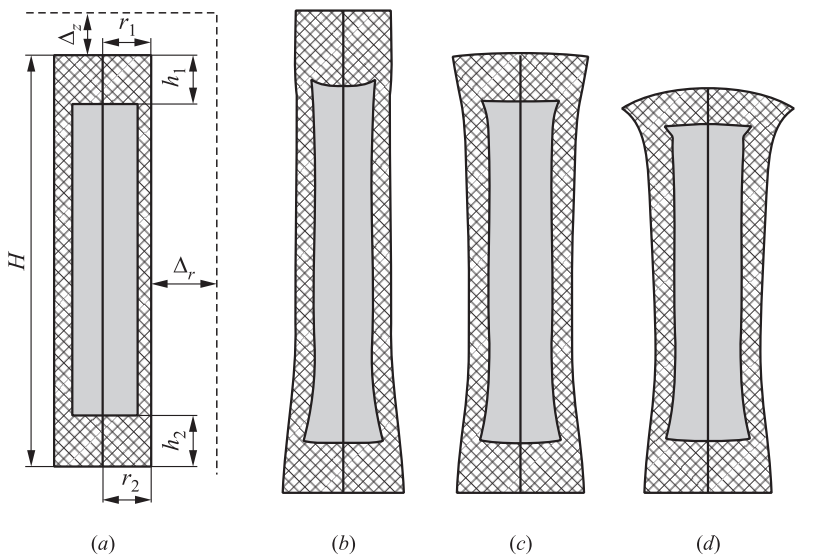

Figure 2 Ampoule at the initial moment of time (*a*) and at 80 μs after explosive compaction for different thicknesses of the axial explosive layer of Δ_z: (*b*) 5 mm; (*c*) 30; and (*d*) 40 mm

parameters of the ampoule, obtained for a thickness of the explosive layer Δ_z = 30 mm, are in good agreement with experimental data.

During explosive loading without external tube, the ampoule was damaged (Fig. 3). The ampoule opened initially in the bottom part and then along the entire length. After the experiment, a lot of drops of up to 4 mm in diameter were detected on the inner surface of the ampoule. X-ray diffraction analysis of the material from the ampoule showed the presence of aluminum sulfide (α and ω phases).

Figure 3 The view of the ampoule after explosive loading of the assembly without external tube

After the analysis of the theoretical and experimental results, the following dynamics was suggested for development of the chemical transformations in the Al–S mixture in a cylindrical ampoule. In the top and central parts of the ampoule, the reaction is initiated in the shock wave by a shock-assisted mechanism and should continue until completed behind the shock wave front. In the case considered, the amplitude and duration of the shock wave are insufficient for full completion of the chemical transformation within the shock wave action time. In the bottom part of the ampoule, none of the reaction initiation criteria are met within the time of the shock wave action. The process radically changes after reflection of the shock wave from the bottom cap of the ampoule. A shock-induced mechanism of forced chemical transformations comes into play, which is responsible for initiation of the chemical reaction, its continuation, and full completion within the shock wave at high pressure.

Acknowledgments

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