A MULTICOMPONENT MEDIUM MODEL FOR POROUS MIXTURES UNDER EXPLOSIVE LOADING

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Synthesis of new materials under equilibrium conditions is completely studied. Prospects are connected with producing metastable compounds in nonequilibrium conditions by means of explosive 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 [1]. Consequences of explosive 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.

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

The system of equations governing the nonstationary adiabatic motion of every component in a space-fixed volume of a compressible solid mixture 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. An equality of components pressure is chosen as a condition for joint deformation of components.

To solve the explosive loading problems of porous mixtures, the finite element method is used. 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.

We consider the axisymmetric problem of explosive loading of multicomponent mixtures (Al-S and Al-S-C) placed into a cylindrical steel ampoule. The porosity of the mixture was 0.4 (ratio between the volume of pores and total volume). The height of the cylindrical sample was 64 mm, the diameter was 14 mm. The thickness of the lateral wall of the ampoule was 3 mm, the thickness of top and bottom lids was 10 mm. The height of the ampoule was 84 mm, the external diameter was 20 mm. In the computations the actions of the detonation products surrounding the ampoule was simulated by the action of pressure on the upper part of the ampoule in a vertical (axial) direction and on the lateral surface of the ampoule in a horizontal (radial) direction. In the axial direction the action started at the initial moment of the process, and in the radial direction the action stated during propagation of the detonation wave from top to bottom [2]. The detonation velocity was $D = 2.8$ km/s on the basis of experimental data. The $P_0 = 3.2$ GPa value was chosen on the basis of numerical and experimental evaluations.

The results of computations have shown that there are optimal parameters of explosive loading that provide the obtaining of materials with desired properties. For an example, the thickness of the explosive layer essentially influences on the positive results of explosive loading. Insufficient thickness of explosives, as well as the excessive thickness may be a reason for an incompletely compacted final product or lead to the formation of cracks or damage. Explosive synthesis was also found to depend on dispersity and duration of explosive loading. A decrease in the particle size of reagents simplifies and accelerates reactions.

REFERENCES

1] *D.E. Eakins, N.N. Thadhani.* Shock compression of reactive powder mixtures, Int. Mater. Rev.- 2009. -V.54 (4).-P. 181–213.

2] *S.A. Zelepugin, O.V. Ivanova, A.S. Yunoshev, V.V. Sil'vestrov.* The development of the aluminum sulfide synthesis reaction on explosive loading of a cylindrical ampoule, Doklady Physical Chemistry.-2010.-V. 434(2).-P.172–176.