Modeling of SHS systems under impact and electro thermal explosion

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1 Modeling of Ti-B and Ti-C systems under high velocity oblique impact

Shock-wave treatment of powder mixture is very promising for producing modified materials. Particular interest attaches to chemical reactions (synthesis) accompanied by shock-wave processing. The products may have improved properties as a result of high-pressure treatment. Chemical reactions in mixtures of elemental powders are often accompanied by rapid release of large amount of energy. The energy release, unlike that in detonation of explosives, is generally manifested by the generation of high temperature, often exceeding the melting temperature of reaction products. Chemical changes in shock-wave loaded inorganic powder mixtures have been investigated by variety of modern analytical techniques [1]. The results of these analytical observations have revealed not only complexity of shock effects on chemical reactions in powder mixture, but also the possibility that only a few of the many possible parameters and mechanisms that could effect the process control the final outcome of chemical reactions. Fracture simulation is performed by means of the kinetic model of destruction of active type, which defines the growth of micro cracks that continuously change the material properties and cause the stress relaxation. The pressure in an undamaged substance is a function of the specific volume, internal energy, and the specific volume of cracks; and in the whole range of loading conditions; it is defined by the equation of state of the Mie-Gruneisen type The finite-element method is used for solving the problem[2]. The steel capsule with the outer diameters of 7.62 mm and length of 22.86 mm with stoichiometric powder mixture (80% Ti + 20% C and 68.9% Ti + 31.1% B) impacts rigid wall. The angle of impact was varied in range from 0o up to 150. Impact velocity was varied up to 1500 m/s. The stoichiometric mixture was formed into cylinder 5.08 mm in diameter and 16.33 mm long. A cylinder was inserted into the capsule. The high-velocity reaction starts if the mixture temperature attained 1944 K or the pressure exceeded 7 GPa. Under favourable conditions the maximum rate of heat deposit from chemical reactions was equal to 313 GJ/(kg*s) up to complete conversion of the reactants. The initial porosity of the powder mixture was 0, 50 and 70 %. Computation results are given in the pressure and temperature histories. They show that heat of reaction is not large enough to cause observable changes in pressure curve. The temperature of the mixture is observed to rise slowly after the initial jump resulting from the shock heating. The temperature rising are much greater when the reaction near impact interface is observed. The calculations show that the chemical reaction takes place for the velocity 1000 m/s and higher; the reaction goes in already compacted area only; an initiation of the chemical process occurs due to the pressure criterion. It is interesting to mark the moment of time \sim 15 µs: the rear part of the steel capsule approaches to the rigid wall.

2 Modeling of electro thermal explosion in layered Ni-Al system

A study of kinetics and macro kinetics of rapid and high-temperature reactions in heterogeneous condensed systems enabling gasless combustion is interesting not only theoretically but also important from practical point of view. It is obviously that the laws of such processes govern not only velocity and limits of combustion of corresponding mixtures, but they influence on depth of reactions and thus on the quality of the SHS products obtained. It is known that the study of mechanisms of gasless combustion of a range of condensed systems including gasless SHS mixtures has been restrained for a long time due to absence of corresponding methods. In the last few years the method of electro thermal explosion (ETE) is widely used for these purposes. The essence of the ETE-method consists of the rapid Joule heating of the green mixture followed by switching off the electrical current and continuous registration of increase of the sample temperature. Due to high rate of self-heating this temperature increase occurs in condition close to adiabatic one. Computations of kinetic parameters are correct if the part of a sample where the temperature is measured is heated without considerable non-homogeneity of temperature field, i.e. there is so called "homogeneous heating". Meanwhile the authors of the ETE-method have noted that depending on conditions of Joule heating (perfection of the contact between the electrodes and surface of the sample, the ratio of the sample length and diameter and so on) ETE may occurs as spatially inhomogeneous process and even as a combustion wave. A model of heating of a cylindrical sample, which consists of rolled aluminum and nickel foils in atomic ratio 1:1 by electric current, is considered. The electrodes are connected to the end faces of the cylinder and when the voltage is applied an electric current is flowing in the cylinder and is heating it. For mathematical formulation of the problem it is assumed that the sample is homogeneous and effective thermal characteristics of the material are determined by mole masses and densities of components. Heating and chemical reactions were modeled in a cylinder with length of 60 mm and diameter of 15 mm made from Ni and Al foils. The history of temperature distribution in the sample were analyzed. In case of absence of chemical reaction one can see that the higher is heating rate the more uniform is temperature distribution (the greater part of the sample reaches T_m) and heating lost zone near the end faces of the cylinder become smaller. Computation results for the case of taking chemical reaction between nickel and aluminum into account allow to conclude that process of thermal explosion occurs only in the case of enough high heating rate. It was evident that depending on heating rate the processes may differ in principle. If in case of high heating rate the reaction takes place all over the sample then in case of lower heating one can see combustion wave propagation from the center of the sample to its end and lateral surfaces.

References

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