NUMERICAL SIMULATION OF SOLID-PHASE CHEMICAL TRANSFORMATIONS IN THERMITE MIXTURES UNDER SHOCK-WAVE LOADING

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1- INTRODUCTION

Shock-wave loading is a promising and effective method for obtaining new materials with the desired structure and properties. A shock wave, acting on the reactive mixture, initiates chemical transformations and structural changes that can be predicted on the basis of joint experimental and theoretical studies. Using the same initial composition, it is possible to obtain materials with desired structures and properties.

Many studies on this subject have experimentally and numerically investigated the interaction of sulfur with metals in terms of the possibility of exothermic reactions under dynamic loads at high pressures and temperatures. Today, increasing interest is directed towards new energetic materials based on reactive mixtures, namely thermite compositions (thermites) for various applications. New energetic materials are being actively developed in all advanced countries (USA, France, Canada, China, etc.). Various types of nanostructured mixtures have been obtained at the Los Alamos National Laboratory (LANL) and technological universities. In particular, so-called "metastable intermolecular composites" (MIC) are used. MICs are mixtures of nanosized metal-oxidizer powders (Al/MoO3, Al/CuO, etc.) prepared using special methods (ultrasonic mixing, sol-gel technology, etc.).

The goal of this work is to investigate numerically the solid-phase synthesis of the Al/CuO thermite mixture under shock-wave loading using an improved mathematical model of a multicomponent medium and a software package.

2- FORMULATION OF THE PROBLEM

In this work, shock-wave loading of an aluminum-copper oxide (Al/CuO) thermite mixture placed in a steel cylindrical ampoule was simulated in three-dimensional space.

Combustion of the Al/CuO mixture proceeds according to the reaction:

$$3CuO + 2Al = Al_2O_3 + 3Cu \text{ with heat release of 4.08 kJ/g.}$$

Chemical reactions are simulated using a zeroth-order kinetic relation characterized by a constant rate of chemical transformations:

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

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

where T_i is temperature, P is the matched pressure of components, and T_η, P_η, K_p, K_0 are constants, η is the conversion degree.

For Al/CuO, the chemical reaction was started after performance of the criterion on temperature $T\eta$ = 435^{0}C (ignition temperature of the mixture, the experimental data), on pressure $P\eta$ = 1.6 GPa. The chemical transformation rate K_0 was set to 240.8 GJ/(kg*s), and the reaction acceleration factor at high pressures was Kp = 2.0. Shock-wave reaction initiation was simulated by the SPH method. The elastic-plastic flow was calculated using the weak variational formulation. The chemical reaction equations were integrated using the first-order Euler method.

LOADING CONDITIONS:

It is necessary to know the pressure of explosion products acting on the steel impactor versus time. In this work, it is assumed that the detonation process is stationary; the pressure of explosion products changes (drops) linearly over time. Under these assumptions, the change in pressure can be described by the equation:

$$P = P_0\left(1 - \frac{t - t_{imp}}{T_{imp}}\right)$$

3- NUMERICAL RESULTS

SHOCK-WAVE LOADING OF THERMITE MIXTURES

The shock-wave loading of an aluminum/copper oxide (Al/CuO) thermite mixture placed in a cylindrical steel ampoule was considered in the three-dimensional space. The height of the cylindrical sample was 95 mm and the diameter was 14 mm. The thickness of the ampoule walls was 3 mm; the upper and lower lids were 15 mm. The total height of the ampoule H was 125 mm; the external diameter of the ampoule was 20 mm. The mass concentration was 80% for copper oxide and 20% for aluminum powder. The crystal density of the composition Al/CuO ρ_{cr} = 5.10^9 g/cm^3.

The computer configuration of the ampoule with the mixture is shown in Fig. 1.

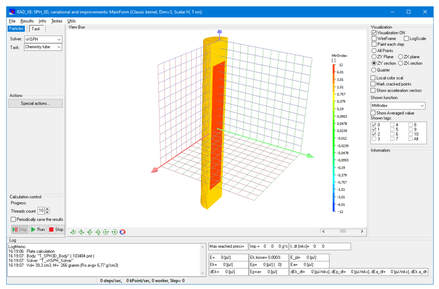
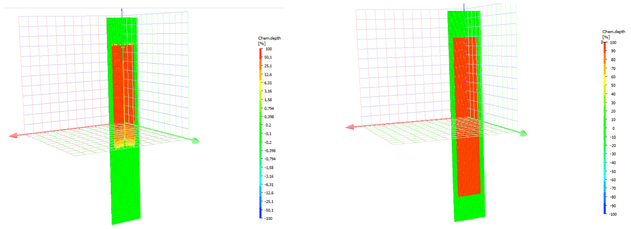


Figure 1. Computer configuration of the ampoule with the Al/CuO thermite mixture.

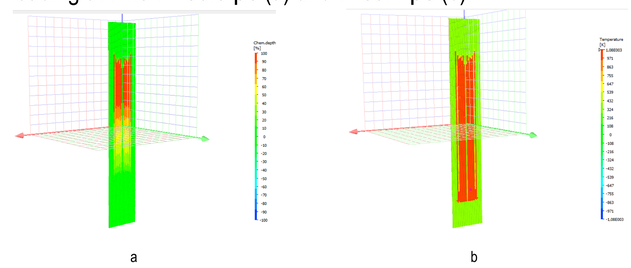
Figure 2 shows the conversion profiles for the Al/CuO thermite mixture at a pressure pulse of 4 GPa under shock-wave loading at time t = 24.8 μs (a) and t= 118 μs (b).



a b

Figure 2. Conversion profiles for the Al/CuO thermite mixture at a pressure pulse of 4 GPa and time t = 24.8 μs (a) and t= 118 μs (b).

Figure 3 shows the conversion profiles for the Al/CuO thermite mixture at at a pressure pulse of 3 GPa under shock-wave loading at time t = 30.5 μs (a) and t= 59.1 μs (b).



a b

Figure 3. Conversion profiles for the Al/CuO thermite mixture at a pressure pulse of 3 GPa and time t = 30.5 μs (a) and t= 59.1 μs (b).

4- CONCLUSIONS

A numerical study of the solid-phase chemical transformations in the Al/CuO thermite mixture under shock-wave loading has shown that the initiation of chemical transformations in the shock wave, further development and completion depend significantly on the amplitude and duration of the shock wave. It was found that insufficient pressure pulse can lead to incomplete reaction of starting components, or insufficiently compacted final product.

Numerical computations were carried out using the developed mathematical models, which can investigate and predict the behavior of reactive mixtures to obtain materials with desired properties and characteristics, as well as can continuously monitor changes in the parameters of the test system exposed to high temperatures and pressures.

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