A BURN MODEL BASED ON HEATING DUE TO SHEAR FLOW: PROOF OF PRINCIPLE CALCULATIONS

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Preliminary modeling calculations with the finite element material dynamics computer program EPIC using an ignition model incorporating heating due to shear show that this type of model can successfully predict ignition in a ballistic impact test in which a small wafer of energetic material is squeezed between an anvil and a striker. Both experiment and model indicate that ignition occurs at the periphery, in the region of large shear, rather than at the center, the region of high pressure.

INTRODUCTION

Preliminary modeling calculations for a ballistic impact test show that an ignition model incorporating heating due to shear successfully predicts the ignition pattern observed in the experiments, that is, ignition occurs in regions of high shear, and not necessarily high pressure.

The reaction model addresses ignition due to combined compression and shear in plastic bonded explosives composed of energetic crystals interspersed in a back-bone of a polymeric binder. Both compression and shear dissipate plastic energy. Instead of uniformly heating the explosive, the resulting heat is localized in a number of discrete hot spots, the temperature of which is determined by the competition between energy dissipation and heat conduction to the cooler surrounding material. Both the elastic energy and the heat conducted from the hot spots are assumed to heat the material uniformly. A simple Arrhenius relation is then used to express the bulk rate of decomposition of the energetic material involved in the hot spot in terms of its temperature. The model also allows for liquefaction of the material once the buildup of decomposition products in the pore increases the pressure to the level of the macroscopic mean stress. Since the dissipation of plastic energy due to both compression and shear ceases after liquefaction, the model provides a natural way of limiting the extent of mechanically-induced ignition in the reaction process.

In the ballistic impact test, a small wafer of energetic material is squeezed

between an anvil and a striker. When a friction-inducing material that prohibits sliding is introduced between the sample and the two surfaces squeezing it, the central region of the wafer is subjected to high pressures, but little shear, whereas the periphery undergoes large shear, but low pressures. The experimental result, as well as the model, show that ignition occurs at the periphery, in the region of high shear, not in the central high-pressure region.

Several constitutive models have been implemented by Flis[1] in the 1997 version of EPIC[2], a Lagrangian material dynamics computer program. The models include the reaction model proposed by Guirguis[3].

The original implementation of the Guirguis reaction model only allowed for a constant yield stress (reduced by the burn fraction) material so Flis also re-implemented the Guirguis model and included a variant of a constitutive model developed by Zerilli[4] for polytetra-fluoroethylene (PTFE) and also a modified Zerilli-Armstrong[5] model originally applied to PTFE and PTFE/Al mixtures. The implementation has not been completed, but it is at the stage at which some preliminary calculations, up to the point of ignition, can be performed.

REACTION MODEL

The reaction model addresses heterogeneous materials consisting of explosive grains interspersed with binder and pores filled with burned explosive. The model is described by the following three equations. The first equation says that the plastic energy is dissipated in hot spots and that heat conduction cools the hot spots:

$$f_h \rho C_V \frac{dT_h}{dt} = f_h \frac{dW^e}{dt} + \Phi - h(T_h - T) \quad (1)$$

The heat conduction is confined to a single element (cell) and is not a general heat conduction throughout the material. It is also an approximate expression. The second equation assumes that the elastic energy heats all the material uniformly:

$$(1 - f_h) \rho C_V \frac{dT}{dt} = (1 - f_h) \frac{dW^e}{dt} + h(T_h - T) \quad (2)$$

The third equation is the Lee-Tarver rate equation with the ignition term replaced by an Arrhenius kinetics expression:

$$\frac{df}{dt} = Ae^{-E/kT_h} + \sum_i G_i f^{x_i} (1 - f)^{y_i} p^{z_i} \quad (3)$$

In Eq, (3), p is the pressure. The independent variables are T_h, the microscopic hot spot temperature, T, the macroscopic average temperature, and f , the mass fraction of reaction products. In addition to the material parameters (G_i, x_i, y_i, z_i) required for the Lee-Tarver growth term (right hand term in Eq. 3), four additional material parameters are required: f_h , the mass fraction of material involved in hot spots; h, the heat conduction constant; and the Arrhenius constants, A and E. W^e is the elastic energy per unit volume and Φ is the rate of plastic work per unit volume.

In practice, the average temperature

TABLE 1. CONSTITUTIVE EQUATION PARAMETERS USED IN BALLISTIC IMPACT TEST MODEL.

c_0 (GPa)	0
c_1 (GPa)	4.025
K_0 (MPa)	41.6
K_1 (MPa)	0
n	0.07
β_0 (K^{-1})	0.0201
β_1 (K^{-1})	2.64×10^{-4}
γ_0 (K^{-1})	0

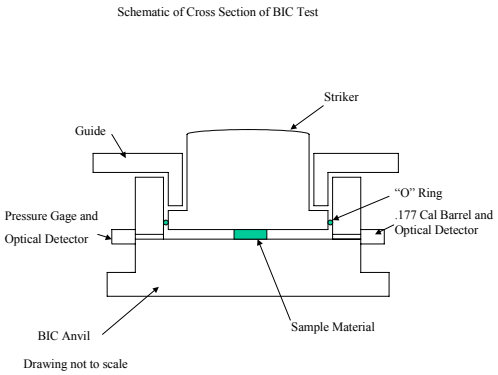

FIGURE 1. SCHEMATIC OF BALLISTIC IMPACT EXPERIMENT.

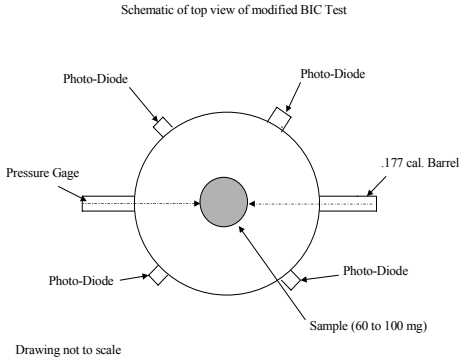

FIGURE 2. TOP VIEW OF BALLISTIC IMPACT EXPERIMENT.

and the elastic energy can be assumed negligible. A simple model is used to describe the localization of plastic energy. The mass fraction of material involved in the hot spots is assumed constant, a single parameter that depends on the microstructure of the explosive. It is usually a small number of the order of 1 – 3%, the precise value of which is to be determined by fitting the model predictions to basic ignition experiments. Three additional parameters are required to characterize the thermo-chemical behavior of the explosive composite - the thermal conductivity coefficient, which theoretically may be obtained from the thermal conductivity of the unreacted material, but must be considered a fit parameter for practical purposes, and the Arrhenius constants, which can be determined by measuring the bulk rate of decomposition of the energetic crystals. A constitutive model is also required to calculate the material deformation resulting from the mechanical load applied, subject to the appropriate boundary conditions of the problem, from which the plastic energy dissipated can be calculated.

The model allows for liquefaction (loss of shear strength) of the material when the pore pressure reaches the value of the surrounding medium ambient pressure. At this point Φ vanishes. This provides a natural way of limiting the reaction, but also adds a serious complication to implementation in a code which is not structured to handle multiphase materials. Specifically, the pore pressure, p_i , must be tracked, as well as the

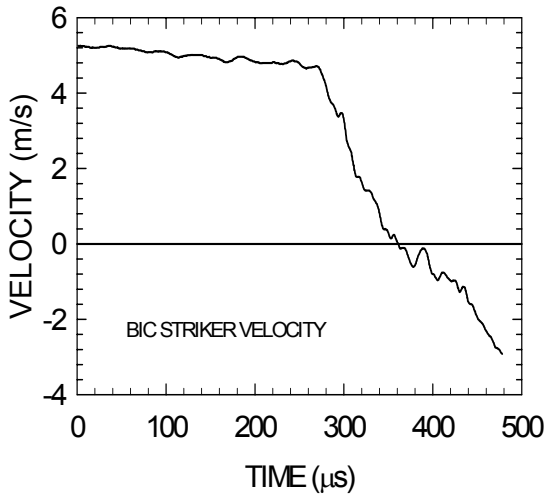

FIGURE 3. STRIKER VELOCITY VS. TIME.

skeletal pressure, p, and the machinery to calculate the pore pressure must be included (volume of pores, mass of reaction products and binder, equations of state to calculate pore pressure from these quantities).

The equation of state model also contains dissipative effects in the form of a bulk viscosity of the form

$$\sigma_{ii} = -3p(\rho,T) + 3\kappa\dot{\varepsilon}_{ii} \qquad (4)$$

where $p(\rho,T)$ is the equilibrium equation of state and κ is a bulk viscosity.

CONSTITUTIVE MODEL

The plastic component of the deformation is described by the equation

$$\sigma = c_0 + c_1 e^{-\beta T} + (K_0 + K_1 e^{-\gamma T})\varepsilon^n \qquad (5)$$

where

$$\beta = \beta_0 - \beta_1 \ln\dot{\varepsilon}$$
$$\gamma = \gamma_0 - \gamma_1 \ln\dot{\varepsilon} \qquad (6)$$

and c_0, c_1, K_0, K_1, n, β_0, β_1, γ_0, γ_1 are constants. The values of the constants used in the ballistic impact experiment model are given in Table 1.

BALLISTIC IMPACT EXPERIMENT

Figure 1 shows a schematic diagram of the ballistic impact experiment. In this experiment, a striker is dropped from a predetermined height on to a thin disk of test material placed on the anvil. The acceleration of the striker is monitored with an accelerometer and integrated to obtain its velocity and position. The sample height, radius and radial velocity at the edge of the cylindrical sample at the moment of initiation may be determined. Initiation is determined by four fast photo-diodes located on the interior walls of the Ballistic Impact Chamber as shown in Figure 2.

It has been shown experimentally that initiation during impact always occurs at or near the edge of the impacted sample. This result applies to all crystalline explosives impacted with essentially undeformable anvils. The outer perimeter region of the sample is the region of maximum shear, shear deformation and minimum pressure. Initiation never has been observed in the center of the impacted sample where the pressure is highest.

Figure 3 shows the velocity vs. time for the striker in an experiment performed by

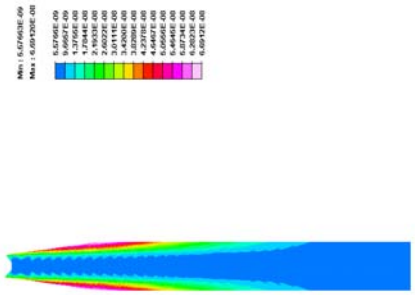

FIGURE 4. SIMULATION OF BALLISTIC IMPACT EXPERIMENT. RADIAL CROSS SECTION OF DISC SHAPED SPECIMEN IS SHOWN AT 100 μS. AXIS OF SPECIMEN IS VERTICAL AT RIGHT OF FIGURE. ANVIL (NOT SHOWN) IS HORIZONTAL AT THE BOTTOM, STRIKER (NOT SHOWN) COMES IN FROM TOP. BURN FRACTION CONTOURS ARE SHOWN.

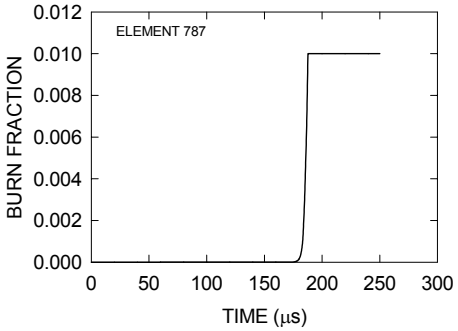

FIGURE 5. BURN FRACTION VS. TIME FOR A CELL NEAR OUTER PERIPHERY OF SAMPLE. APPROXIMATE LOCATION OF CELL IS IN AREA OF LARGEST BURN FRACTION AS SHOWN IN FIG. 4.

Namkung and Coffey[6] on PBXN-109. The sample had an initial radius of 6.35 mm and thickness of 1.75 mm. Observation of light output from the sample indicates reaction starting at around 200 μs.

BALLISTIC IMPACT EXPERIMENT MODELING

Model calculations for the ballistic impact experiment were performed to determine the feasibility of doing such simulations with a Lagrangian code. The experimental velocity, depicted in Figure 3 was used as a boundary condition at the top surface of the sample in the calculation. The anvil is simulated as a rigid boundary at the bottom surface. The sample is squeezed to $1/20^{th}$ or less of its original thickness, not an easy model for a Lagrangian code.

The results up to this point indicate that it is marginal, but feasible, to do such a simulation to obtain ignition parameters for energetic materials. Much more to the point, these calculations are able to model ignition in the ballistic impact test in which it is demonstrated that shear is the most important factor in the ignition of an energetic material.

A generic explosive (that is, typical parameters not specific to any one explosive were used) was modeled for the feasibility study for a number of reasons, not the least of which was the lack of a complete set of data for any one explosive. In any case, the constants are good enough to enable a rough "proof of principle" calculation.

The parameters A (5×10^{19} s^{-1}) and E (220 kJ/mole) were obtained from reaction data on pure HMX[7], h (1×10^{10} $W/m^3/K$) was estimated by assuming a characteristic conduction time constant of 500 μs, and f_h was

set arbitrarily to 0.01. The bulk viscosity coefficient was set to zero for these calculations. The model was set up in EPIC using sample dimensions and striker velocity vs. time data for tests on PBXN-109 performed by Namkung and Coffey. The equation of state parameters for a Mie-Gruneisen equation were obtained from Hugoniot data for PBXW-110 provided by Sutherland[8]. The Gruneisen parameter (0.8) was calculated from the specific heat, bulk modulus, and thermal expansion coefficient for PBXW-110. The constitutive equation used was that which was hardwired by Flis into the code. This was the modified Zerilli-Armstrong model, described above, for PTFE. The constants for the model are given in Table 1.

Figure 4 shows a typical model at 100 μs. The beginnings of reaction are shown at the outer periphery of the sample at the position shown in typical experiments. The ignition reaction burn fraction becomes significant (0.01) at about 180 μs, about the time it is observed in the PBXN-109 experiment. After 180 μs it increases rapidly (see Fig. 5), but it is limited to the value of the fraction of hot spots, 0.01, by a parameter input to the model. Only the ignition term (that is, the Arrhenius term in Eq. (3)) is turned on in this model. The constants for the growth terms must be determined from separate experiments.

CONCLUSIONS

The simulation of the ballistic impact test for a generic explosive can be done up to the point of ignition. Pressures of 15 –30 kbar occur at the center of the sample. Current reaction models generally will show ignition at these pressures in spite of the fact that ignition does not occur in the actual experiment. The Guirguis model showed ignition occurred at the outer perimeter of the sample where it should have and no ignition in the high pressure region at the center where it should not have.

ACKNOWLEDGEMENTS

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