MODELLING AND EXPERIMENTAL INVESTIGATION OF REACTIVE SHEAR BANDS IN ENERGETIC SOLIDS LOADED IN TORSION

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MODELLING AND EXPERIMENTAL INVESTIGATION OF REACTIVE SHEAR BANDS IN ENERGETIC SOLIDS LOADED IN TORSION

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Motivated by the long term goal of developing munitions which are insensitive to accidental initiation and the short term goal of understanding shear banding in reactive materials, this paper considers the behavior of energetic and inert solids subjected to simple shear loading. Data from a torsional split-Hopkinson bar (TSHB), built for this study, was reduced to calibrate a constitutive law for stress, including the effects of strain and strain rate hardening and thermal softening. A one dimensional finite difference study of shear localization was performed. The effects of thermal conductivity, viscoplastic heating and Arrhenius kinetics were modeled. Results revealed shear localization and reaction initiation in the explosives simulated. Experimental failure of the inert solids, however, occurred at shear strains significantly lower than those predicted by theory. This has been attributed to the presence of failure mechanisms other than macroscale shear localization, which were not included in the theoretical model. While the tested energetic materials did not undergo macroscale shear localization or initiation under the conditions considered, the study may have intrinsic value for less brittle materials which may undergo macroscale shear localization or even for brittle materials, which could shear localize on a microscale. A full literature review and detailed discussion of this study is given by Caspar (1996); a partial list of relevant reference material is at the end of this abstract. Some details of this study follow here.

Initiation of reaction in energetic solids due to mechanical insult is an important, yet poorly understood mechanism. In a typical event, a sharp blow will result in an input of mechanical energy into the solid which will initially manifest itself in the form of internally propagating stress waves. These waves will interact with themselves, material interfaces, and boundaries, all the time dissipating mechanical energy into thermal energy. Should the dissipation rate be sufficiently high and concentrated, it may be possible to initiate a temperature-sensitive exothermic chemical reaction, which can lead to detonation in the solid.

In order to understand this process, it is imperative to have accurate constitutive equations. Additionally, before full scale implementation in large scale design codes, it can be beneficial to test the constitutive equation in a much simpler code. With such a model one can quickly and unambiguously focus on the performance of the constitutive equation in a simple computational environment which contains the key modeling ingredients: experimentally verified stress-strain-strain rate relations, finite rate exothermic temperature-sensitive chemical kinetics, and thermal diffusion.

A photograph of the TSHB used to determine the stress-strain-strain rate is reproduced in Figure 1. This apparatus is capable of deforming materials in simple shear at shear strain rates of 10^2 to 10^4 s^{-1}.

Figure 1: Photograph of the torsional split Hopkinson bar (TSHB).

This technique is often used to determine material characteristics for metals, in which failure often occurs due to a mechanism known as shear localization. Shear localization is one of the least understood initiation mechanisms in solid explosives. If shear localization were to occur, it would be likely to appear in the TSHB configuration studied here.

Figure 2 is a sketch of the shear localization process. In Figure 2a, a portion of an undeformed material

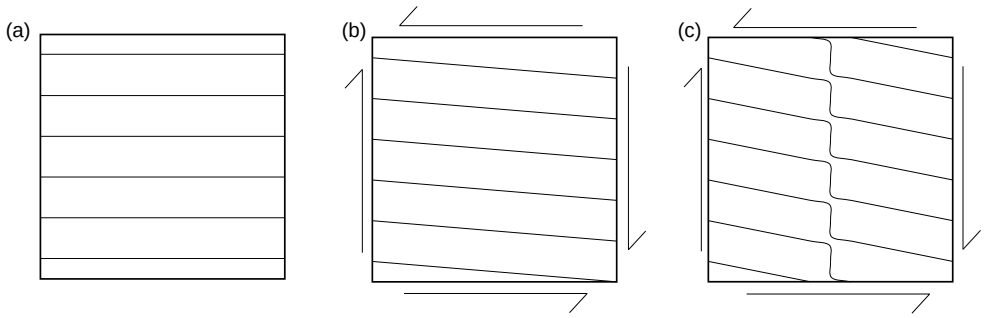

Figure 2: Schematic of the shear localization process. (a) Undeformed grid lines, (b) Homogeneous deformation, (c) Shear localization

is sketched with thin lines inscribed on its surface. When this material is sheared, these lines begin to slope at a uniform angle, as seen in Figure 2b, reflecting what is known as homogeneous deformation. Increased straining into the plastic range results in material hardening. In addition, if there is a geometric discontinuity or other material weakness, straining near that discontinuity will occur at a higher strain rate, which also hardens the material. This increased local deformation, however, also causes plastic heating of the material. If the straining occurs at high strain rates (typically greater than $10^2\ s^{-1}$), there is not enough time for the generated heat to be conducted away. The local increase in temperature results in thermal softening of the material. If this process dominates over the hardening due to strain and strain rate effects, the material strength decreases. As a result of this local softening, deformation is localized into a thin planar region, as depicted in Figure 2c. This final process is known as shear localization or shear banding. Due to the potential concentration of thermal energy in a shear band, it is hypothesized that this could trigger a reaction, which could spread through the material.

A simple model for this reactive shear banding process was developed for a thin walled cylindrical incompressible material and is given below:

$$\rho\frac{\partial v_\theta}{\partial t} = \frac{\partial \tau}{\partial z}\ , \tag{1}$$

$$\rho\frac{\partial e}{\partial t} = \tau\frac{\partial v_\theta}{\partial z} - \frac{\partial q_z}{\partial z}\ , \tag{2}$$

$$\frac{\partial u_\theta}{\partial z} = \gamma\ , \tag{3}$$

$$\frac{\partial u_\theta}{\partial t} = v_\theta\ , \tag{4}$$

$$\frac{\partial \lambda}{\partial t} = Z\,(1-\lambda)\exp\left(-\frac{E}{RT}\right), \tag{5}$$

$$\tau = \alpha\ T^\nu\ \gamma^\eta\ \left|\frac{\partial \gamma}{\partial t}\right|^{\mu-1}\frac{\partial \gamma}{\partial t}\ , \tag{6}$$

$$q_z = -k\frac{\partial T}{\partial z}\ , \tag{7}$$

$$e = m_A e_A + m_B e_B\ , \tag{8}$$

$$e_A = c_A T + e_A^o\ , \tag{9}$$

$$e_B = c_B T + e_B^o\ , \tag{10}$$

$$m_A = 1-\lambda\ , \tag{11}$$

$$m_B = \lambda\ . \tag{12}$$

Here t is time, z is the axial distance, v_θ is the velocity in the circumferential direction, τ is the shear stress, e is the internal energy, q_z is the heat flux in the axial direction, u_θ is the displacement in the circumferential

direction, γ is the shear strain, λ is the reaction progress variable ($0 < \lambda < 1$), and T is the temperature. The parameters Z, E, and R are, respectively, the kinetic rate constant, the reaction activation energy, and the universal gas constant. Also α is a stress constant; subscripts A and B refer to the unreacted and reacted material, respectively; e_A and e_B are the internal energies; m_A and m_B are the mass fractions; c_A and c_B are the specific heats; and e_A° and e_B° are the energies of formation. Equation (1) models the conservation of linear momentum in the circumferential direction. Equation (2) models the conservation of energy. Equation (3) is the definition of strain. Equation (4) defines velocity as the time derivative of displacement. Equation (5) is an Arrhenius kinetics law. Equation (6) is a constitutive law for stress, where ν, η, and μ are the exponents which characterize the thermal softening, the strain and strain rate hardening, respectively. These coefficients were chosen to fit experimental data found as part of this study. Equation (7) is Fourier's law of heat conduction. Equation (8) is a mixture law. Equations (9) and (10) are the caloric state equations. Lastly, Equations (11) and (12) define the mass fractions in terms of the reaction progress.

These equations are supplemented by appropriate initial and boundary conditions and then cast in dimensionless form. It can be shown formally shown that the equations are parabolic and thus suitable for solution via a time-marching technique. They are solved numerically by first replacing all terms involving spatial derivatives with second order accurate finite difference approximations. The resulting system of equations is a set of N non-linear ordinary differential equations in time, where N is related to the user-chosen resolution of the finite difference grid. These equations are then integrated implicitly using the standard package, LSODE, to generate time dependent solutions at each grid point. The code has been verified on a number of test problems with known exact solutions; grid refinement studies verify that the numerical approximations converge to the exact solutions at a rate roughly proportional to the square of the spatial grid size.

Figure 3 gives a comparison of the experimentally observed and numerically predicted shear stress and shear strain characteristics for an inert simulant of the pressed explosive PBX. From this figure, it is seen

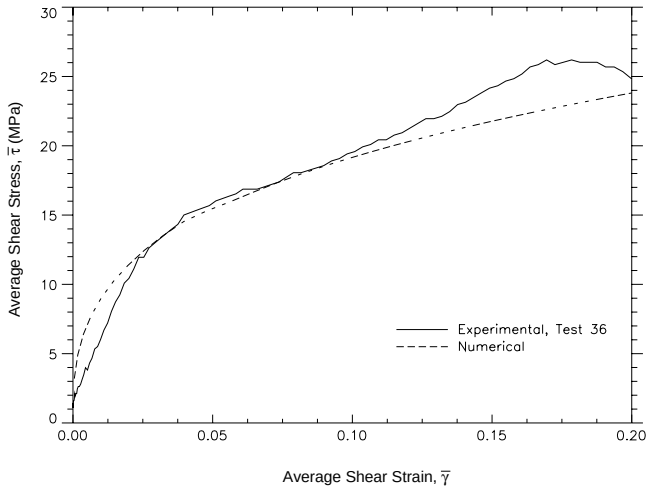

Figure 3: A comparison of the experimental and numerical results for PBX pressed simulant.

that the model predicts the shear stress and shear strain characteristics fairly accurately until just before failure. Not shown in Figure 3 however, the model does not predict localization to begin until a nominal shear strain of 4.63 is reached, as compared with the experimentally observed brittle failure at 0.20 shear strain. So, the PBX pressed simulant does not fail due to macroscale shear localization.

Figure 4 plots the theoretical predictions of the time-evolution of the spatial temperature distribution for a reactive material, PBXN-109. The effects of including reaction proved to have little effect on the results prior to initiation, when compared to a simulation in which reaction was neglected. As was anticipated by the nonreactive case, reaction in the reactive test did occur shortly following the onset of localization. It was predicted that appreciable reaction did not commence until the reaction temperature was reached, at which time reaction quickly initiates in the localized hot spot. It is important, however, to state that the nominal shear strain reached at initiation is approximately 6.4, whereas the simulant failed after a shear strain of 0.2

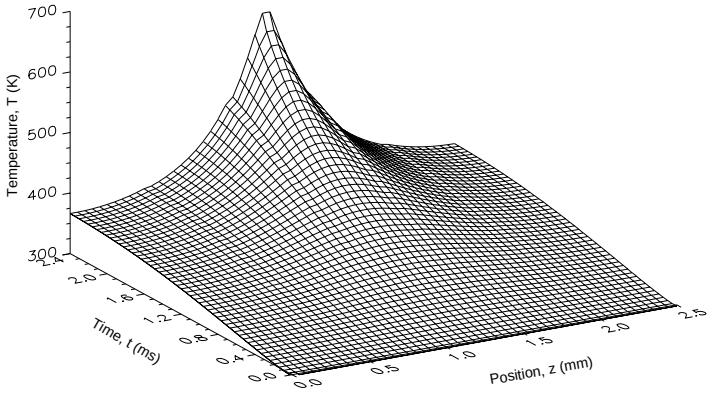

Figure 4: Evolution of the temperature field for PBX 9501 with reaction.

experimentally. While indeed, this is a weakness of the present model for the system studied, we reiterate that a theory presented here, when applied to brittle materials on a microscale, or to more ductile materials, may through blending simple chemistry and mechanics, may have great promise in gaining understanding of initiation of reaction in complex materials.

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