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Predictions for Multi-Scale Shock Heating Of a Granular Energetic Material

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ABSTRACT

It is well established that thermal energy localization resulting from the rapid deformation of granular explosives is important for mechanical ignition and sustained combustion of these heterogeneous reactive materials. Localization occurs at the grain scale due to processes such as inelastic deformation, intergranular friction, and fracture. Modeling has long been used to better understand the interplay of localized heating and ignition at the grain scale and the bulk system response. This modeling necessarily involves the coupling of physical phenomena occurring over disparate length and time scales. Bulk models used to describe mechanically induced transition to detonation for both pressed and granular explosives fail to estimate the magnitudes of high frequency stress and temperature fluctuations occurring during shock compaction. As such, the development of subgrid scale models is an important & challenging issue. Here we try to estimate the magnitude of these fluctuations, within the frame work of a continuum bulk model.

Recently, Gonthier [1] described a modeling approach that can resolve key features of hot-spot formation in a manner compatible with both grain scale contact mechanics and bulk compaction energetics. The approach involves estimation of the bulk material response, evolution of the material structure (e.g., grain size and packing), a localization strategy for depositing bulk dissipated energy at the grain scale, and a model for the grain scale response. It assumes that the bulk material response is experimentally well-characterized and can be accurately predicted by the bulk model. Bulk dissipated energy is thermalized at localization sites centered at intergranular contact surfaces [Fig.1]. The grain scale response tracks the evolution of hot-spot temperature subject to the localization strategy. The integrity of bulk model predictions is maintained by requiring that the integrated mass, momentum, and energy at the grain scale locally equals that given by the bulk model. This constraint is consistent with the common interpretation that the bulk response is an average manifestation of the grain scale response.

In this study, we modify the localization strategy of Refs.[1,2] to account for compressive heating and phase change occurring at the grain scale. For simplicity, we consider an inert material; combustion and multiphase flows would require a much more intensive analysis. In the range of piston speeds analyzed here, the compression doesn't have significant effect on grain temperature compared to plastic deformation. Also, phase change may significantly affect hot-spot energetics, particularly at low impact speeds. We use the model to predict and resolve the temperature field in the vicinity of intergranular contact surfaces for dynamic compaction of the high-explosive HMX. Though not shown here, our model predictions are compared with detailed mesoscale simulations [3] for the variation in plastic strain, solid pressure, and porosity within the compaction zone for various impact speeds. Mesoscale simulations can provide useful information about hot-spot fluctuations at the grain scale, especially in the absence of experimental data, but are computationally expensive and fine scale structure is difficult to numerically resolve.

Mathematical Model

The comprehensive model consists of a bulk model and a meso-scale model. A detailed description of the model is given in Ref.[1&2].

The bulk model consists of conservation equations for mass, linear momentum and total energy of the granular solid, along with evolution equations for solid volume fraction ϕ, and no-load solid volume fraction $\tilde{\phi}$. Here $\tilde{\phi}$ is the equilibrium value of ϕ in the absence of an applied load. Constitutive relations needed to mathematically close the model equations are obtained from quasi-static and dynamic compaction data and shock Hugoniot curves for granular HMX. The modified evolution equation of internal energy for the granular material is partitioned into thermal (irrecoverable) and recoverable components. It is important to note that while the bulk model does not attribute dissipation to specific processes it does accurately reflect the experimentally measured net dissipated work and, thus, constrains the partitioning of energy at the grain scale.

The localization model of Gonthier [1] is adopted and modified to account for compressive heating and phase change [2]. The localization strategy is consistent with mesoscale simulations and grain contact mechanics which indicate that the applied bulk load is transmitted through the material by intergranular contact. This contact results in elastoplastic deformation and friction near contact surfaces. The bulk dissipated mechanical energy is the integrated effect of these grain scale dissipative mechanisms. As shown in Fig. 1, we track the evolution of thermal energy within solid regions surrounding intergranular contact surfaces referred to as localization spheres of radius, r_0. We attribute compaction induced thermal energy to plastic work and deposit it over a volume of radius $r_c(x,t) \leq r_0$ centered at the contact surface where r_c is the radius of the localization center. We equate the volumetric rate of work done by the plastic flow stress P_Y to the bulk volumetric compaction induced dissipated energy for the evolution of r_c. Compressive heating is assumed to uniformly affect all material within a localization sphere. In our localization model, we further assume that $(dr_0 / dt)/D$ << 1.0 and take r_0 to be a constant. The non-linear evolution equation of internal energy within a localization sphere, with bulk energy redistributed at intergranular contacts, is solved to obtain the local grain temperature distribution.

The energy equation is solved for either the temperature distribution in pure solid/liquid phase or the evolution of liquid phase $\hat{\chi}$, during the phase change. We assume an isothermal phase change with a constant latent heat of fusion, q_m^0 and same specific heat, c_v for solid and liquid phases [3].

REPRESENTATIVE RESULTS

Predictions are given in this section for localized grain heating of inert HMX (ϕ_0= 0.81) by steady compaction waves; these predictions are then compared to the predictions of Menikof and Kober [3] obtained by detailed mesoscale simulations. To this end, the model equations are expressed in a steady frame attached to moving waves using the transformation $\xi = x - Dt$ and $v = u - D$, where D is the wave speed. Here, the compaction zone structure is described for a compaction wave corresponding to a piston impact speed of u_p = 106 m/s. This speed is chosen to demonstrate some interesting features that are also observed in the mesoscale simulations. Here, we use the Haye's EOS for HMX [4]; other constitutive relations used in this work are given in [1].

The transformed bulk and grain scale model equations are numerically solved using a Method of Lines technique. Second-order central differencing is used to approximate the radial derivatives on a N_r = 100 node grid, and the resulting system of ODEs in ξ are integrated using the implicit routine ODE15s contained in the MATLAB software package.

Figure 2 gives compaction zone predictions for u_p = 106 m/s and D = 748.2 m/s. Fig.2(a) gives the variation of ϕ and $\tilde{\phi}$ along the compaction zone. At lower piston speeds, not shown here, unsteady two-wave structures are predicted consisting of a fast propagating viscoelastic precursor followed by a slower viscoplastic wave. Such two-wave structures are analogous to elastoplastic waves in solids that possess a Hugoniot elastic limit; here, however, the precursor is dissipative due to inelastic compaction. Remnants of such a precursor are evident in the figure. Some noteworthy features in this figure are: 1) the viscoelastic region of the wave (for which $\tilde{\phi} = \phi_0$) induces a weak hot-spot near the intergranular contact surface [r = 0 μm in Fig. 2(b)] which is rapidly quenched by thermal conduction prior to the onset of viscoplastic heating; 2) the plastic work induced by the viscoplastic wave is highly localized near the contact surface, resulting in a peak hot-spot temperature of 970.3 K. Temperatures of this magnitude would trigger prompt combustion initiation; in fact, DDT tube-tests with granular HMX show evidence of detonation transition for comparable piston speeds. Importantly, the melting shown here has resulted in a significant 100.4 K reduction in hot-spot temperature. The predicted magnitude of compressive heating is nearly four orders of magnitude less than compaction heating, and is thus unimportant for a low speed impact. At higher piston speeds, conduction becomes insignificant as viscoplastic deformation rate is much higher.

FIGURES

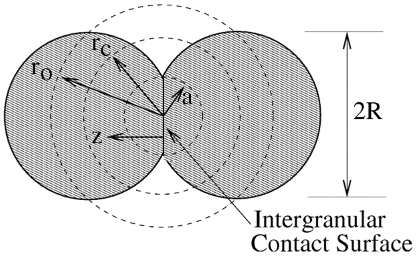

Figure 1: Illustration of the grain contact geometry

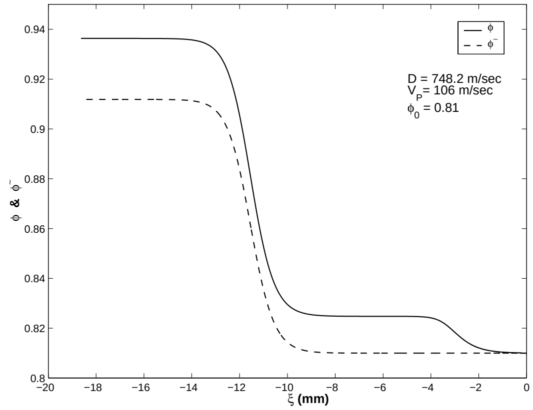

Fig. 2(a)

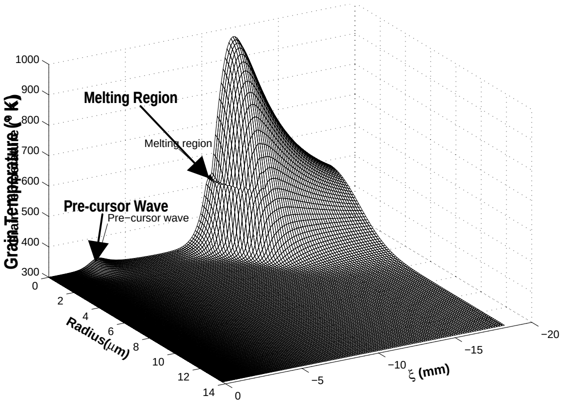

Fig. 2(b)

Figure 2: Compaction zone structure for inert HMX with u_p = 106 m/s: (a) solid volume fraction and (b) grain scale temperature.

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