Shock-Shear Modeling for Energetic Materials

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Two widely used theories of HE shock initiation use only pressure as the primary variable regulating the rate of reactive burn. However, due to limited successes, it is clear that relevant physics is missing, which is hypothesized to be shear. There is a need to replace pressure with the full stress tensor in the reaction progress variable. The required experiments have been undertaken by the WX Division, and T Division addresses the theoretical analysis.

The Ignition and Growth (IG) model developed by Lee and Tarver [1] and the Forest Fire (FF) model of Forest [2], are two widely used theories of high explosive (HE) shock initiation. Both theories require knowledge of the equation of state (EOS) of the reactant HE, the final gaseous product HE, and a reaction progress variable, which is a measure of the fraction of the HE converted from the reactant to the product phase. Other more subtle ingredients in the analysis include the assumption of pressure-temperature equilibrium of the reactant-gas mixture. In both models, only the pressure is the primary variable that regulates the rate of the reactive burn. The simplicity of this assumption results in a relatively easy parameterization procedure, thus contributing to the model's wide usage. These reactive burn models can reproduce important ignition properties like, for example, run distance to detonation as a function of the pressure. Because IG and FF have only pressure-dependent progress variables (i.e., shear is absent) they are known for working well in planar geometries. Less conspicuous, these models also tend to work well for bare or lightly covered explosives that have suffered an impact from an external insult [3,4]. As successful as these models have been, they do suffer from well-known shortcomings and have documented limited domains of applicability.

The IG and FF reactive burn models almost always require a new parameterization as the loading scenario changes, or as properties like HE porosity or density are altered–a clear indication that relevant physics is missing. They also show limited success at predicting the behavior of impacted HEs having thick cover plates [5]. Frey et al. [3] observed that for thick-cased explosives the threshold velocity for ignition was always lower than that predicted by the pressure-dependent-only reactive burn models. They hypothesized that shear was the missing physics required to bring the theory into agreement with thick plate experiments. Moreover, Howe [6] provided further evidence that the initiation mechanism in the penetration of thick-plated HEs is macroscopic shear occurring in the vicinity of the penetration. Another important point is that the limitations of these models seem to be most pronounced in weak-ignition problems. This is an important issue for the Department of Defense (DoD) because explosive safety and accident scenarios are almost always in this regime. Accident scenarios are typically accompanied by the occurrence of shear-driven damage in the HE, which in turn increases the sensitivity to explosive initiation (and the ensuing violence of the reaction) by introducing additional sites for "hot spot" activity. These include, for example, shear cracks, which by frictional heating can provide substantial temperature rises conducive to initiation. As a final point, when hot spot mechanisms are listed, many more potential hot spot mechanisms are commensurate with shear loading (frictional sliding between impacting surfaces, localized adiabatic shear bands, viscous heating of materials rapidly extruded between impacting surfaces, heating at shear crack tips, plastic deformation, etc.) than are with volumetric deformation (adiabatic compression of trapped gas in pores). All of these observations point to the need for replacing the pressure with the full stress tensor (thus including shear) in the reaction progress variable. While this is a goal of known importance, the theoretical research required to achieve this may be classified as rather infantile. The requirements for a successful theoretical project are very clean experiments for which the shear states are well understood. LANL's WX Division will undertake these experiments (Fig. 1 shows the two geometries) and ADTSC researchers in T-Division will address the theoretical analysis.

A combination of HE reactive burn and thermo-mechanical (strength, damage, viscoelasticity) models are envisioned for this work. The

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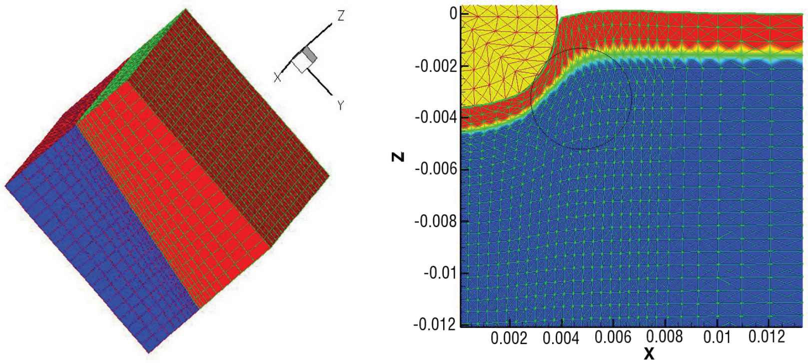

Fig. 1. Oblique impact configuration for introducing longitudinal and shear waves into the target HE (left). The impact direction is along the z-axis. Blunt impact configuration where a conical penetrator impacts a metal plate-covered HE sample (right). Impact is from above. In this configuration shear will be important in the neighborhood of the enclosed region.

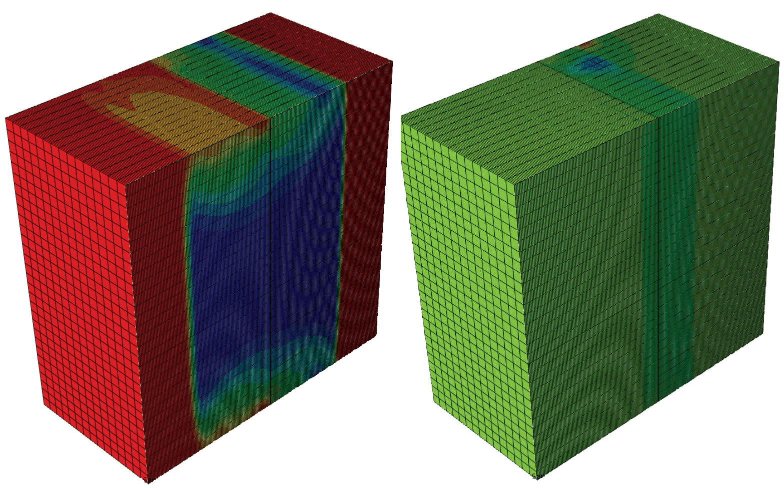

Fig. 2. Longitudinal (left) and shear shocks (right) propagating into Mock 90021 after being impacted with a Kel-F 81 impactor. The time is 1.8 ms after impact.

model viscoSCRAM was implemented into a Finite Element Model (FEM) code and shock-shear test geometries were simulated. The crucial question addressed this year was, since explosives are known to produce considerable damage by shear crack growth: Can a shear wave propagate any substantial distance into the HE? That answer was shown to be affirmative because under large confining pressures (thus away from lateral surfaces in these experiments) shear crack growth is impeded. The model viscoSCRAM has pressure-dependent shear crack growth, and thus was used to shed some light on this issue. Because chemical reaction was omitted in this study, the simulations were done on a well-characterized HE simulant called Mock 90021. Figure 2 shows waves propagating into the sample. A weak (in contrast to the longitudinal wave) shear wave is clearly observed. For early times, near the center of the target, damage was minimal. For later times, cracking from outer surfaces creep into the central regions and diminish the shear wave. In future work shear and pressure-driven initiation needs to replace the IG/FF physics implemented in our simulation codes. This work offers the possibility of true advancements in our understanding of the initiation process.

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