Thermally Induced Damage in Energetic Materials

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The ability to correlate thermally induced damage in energetic materials to chemical ignition thresholds is an important goal for several DOE programs, including the Advanced Simulation and Computing Program (ASC), Joint Munition Technology Development Program (JMP), and C-2. We are addressing this problem by using both continuum and mesoscopic models and simulations, as well as drawing upon LANL's powerful experimental capabilities.

Energetic materials research at LANL on plastic-bonded explosives has a long history dating back to nearly the inception of the Laboratory. Much of the research tended to focus on several key areas including equation of state (EOS), mechanical properties, chemical ignition, and detonation propagation. Mechanical properties were studied primarily to gain confidence on explosive safety handling. As a result, operating temperatures for mechanical experiments were typically restricted to the vicinity of room temperature. A high-temperature measurement might reach 50 to 70°C, for example. These temperatures are well below that of thermal ignition for an explosive like PBX 9501, a primary DOE explosive. Only recently has considerable interest shifted to investigating the mechanical properties of explosives at much higher temperatures. The reason for the shift in interest is the need to correlate mechanical properties, such as damage to thermal ignition properties, which for PBX 9501 requires temperatures in the range of 160 to 200°C. Correlating mechanical properties to ignition is itself important because of the need to predict thermal ignition thresholds of an explosive in various low-velocity impact scenarios. In a low-velocity impact, the mechanical properties of the explosive have a dominating influence on the outcome of an initiated chemical reaction. The mechanical properties will determine if the reaction extinguishes, builds up to a full detonation, or results in something in between. To model such events requires coupling a thermal mechanical model with a thermal ignition model, which is the ultimate goal of the work described here.

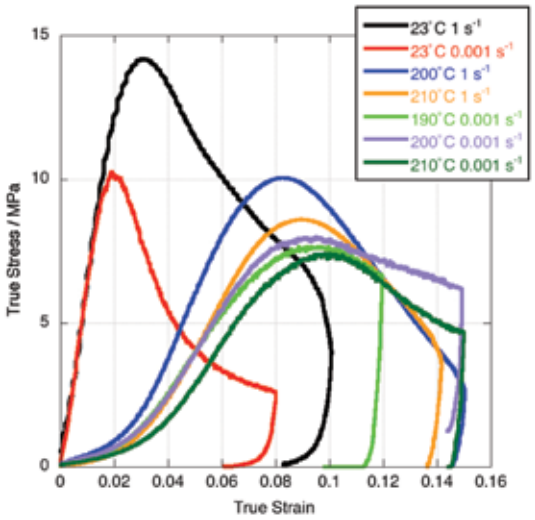

Fig. 1. Stress-strain curves for PBX-9501 measured by Rae, Parker, and Dickson [1].

Rae, Parker, and Dickson [1] have shown that high temperatures have a profound influence on the mechanical properties of PBX 9501. They measured the stress-strain behavior at room temperature and then again near 200°C, which is near the β−δ phase transformation. The β−δ phase transformation is a solid-solid transition occurring in the energetic component of PBX 9501, called HMX, and is accompanied by a 7% volume increase. Figure 1 shows several of their measured stress-strain curves where it is clear that a mechanism change occurs in going from room to high temperature. This mechanism change is potentially linked to the β−δ transformation, but other mechanisms may also contribute to the observed change in behavior. Interestingly, each proposed mechanism increases the level of damage in the explosive. Because of a large coefficient of thermal expansion mismatch between the PBX constituents, elevating the temperature results in a large increase in potential nucleation sites for damage. This will be exacerbated by the β−δ transformation. Upon straining the explosive, as in Fig. 1, these nucleation sites grow in size into fully macroscopic flaws that influence the mechanical stress-strain behavior.

Figure 2 is the solution of a LANL-developed continuum thermo-mechanical model. The model has the physics of a viscoelastic material that damages by the growth of shear cracks and porosity. It is clear that the same trend observed in the experiment is captured by the model if one lets the number density of nucleation sites increase with temperature, as expected. This is the first model known to capture this effect. The model relies heavily on measured thermo-mechanical properties of the explosive, and many of these properties were obtained by LANL's experimental groups. Nevertheless, for certain properties, macroscopic measurements are difficult. One such property is the microscopic interfacial debonding between the HMX and the polymer-binding matrix that occurs at elevated temperatures. To address this problem, we invoke a Direct Numerical Simulation (DNS) approach. DNS on PBX 9501 attempts to use micron-level radiography scans of the PBX 9501, obtained by B. Patterson at LANL, to obtain the microstructure. Using this microstructure and the properties of the explosive constituents, a finite-element simulation is then used to determine the

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underlying stresses, strains, and damage that occur in the explosive. The left part of Fig. 3 shows the DNS cell, where the lighter shaded areas are the HMX grains and the darker areas are either polymer binder, or a mixture of small HMX grains and binder. The right figure shows the thermal strains resulting when the temperature is increased by 100°C. The dark red regions are the new sites for damage nucleation. Using DNS we hope to provide quantitative input to the continuum model.

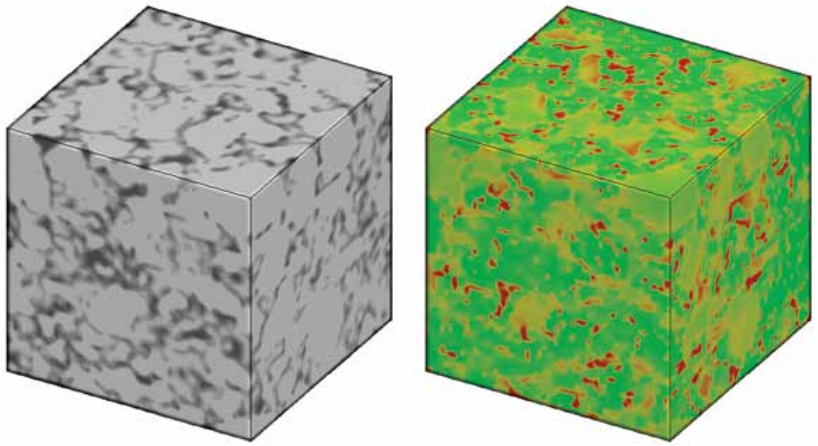

Fig. 3. A DNS representative volume element of PBX 9501 (left), and the corresponding thermal simulation (right), where the temperature has been increased by 100°C. The red regions have undergone substantial thermal straining. The box length is 750 μm .

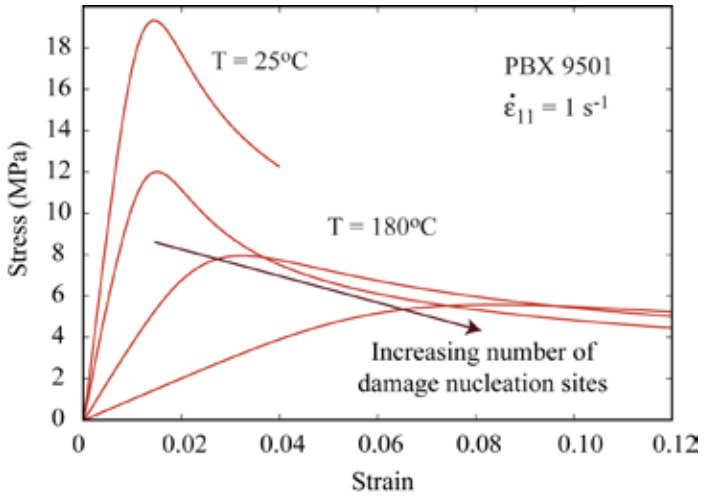

Fig. 2. Solution of our continuum model used for a study of effects of varying the damage nucleation site number density.

[1] Rae, P.J. et al., *Proceedings Fourteenth International Detonation Symposium*, 1304 (2010).