

***In situ* Mechanical Studies of Plastic Bonded Explosive, Multiscale 3D Imaging and Modeling**

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It is well known that the microstructure of materials has a large effect upon its mechanical properties. Understanding that relationship is the key to understanding how the formulation affects the ultimate characteristics of the material. One material in which this is particularly important is plastic bonded high explosives (PBX). HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine) is a high explosive used in a variety of PBX formulations. It is typically mixed into a binder and pressed into the desired shape. During formulation, air pockets may be left behind which can affect the explosive properties and shock sensitivity of the material. The formulation chemistry governs the microstructural morphology of the material, which in turn, controls the long-term mechanical and chemical performance of the material. Changes in microstructure with either age or with loading can increase the material's sensitivity, performance & safety and must be understood for lifetime performance prediction. Uniaxial loading of PBX formulations using HMX crystals has been explored in order to understand the role of binder stiffness upon material performance.

The use of 3D and 4D X-ray tomography (CT) at the micro and nanoscale is critical to understanding how the formulation of the binder can affect the mechanical properties of the system, the formation of voids at the crystal-binder interface, or formation of voids within the crystals themselves. X-ray microCT images are used to understand and quantify the formation of these voids based upon processing. Additionally, *in situ* CT experiments at various size scales were carried out using laboratory-based X-ray micro and nanoscale computed tomography on the loading of PBX materials at various size scales. Loading of bulk HE shows that minute changes in the binder chemistry can change binder stiffness leading to a 'rolling' response within soft materials to delamination between the binder and the crystals in stiffer formulations. Decreasing the imaging field of view, experiments were also conducted to explore the delamination between individual crystals by adhering two HMX crystals together with the binder and completing before and after tensile testing tomographic images. Finally, increasing the resolution even further, nano-scale CT experiments were completed in which a single HMX crystal was imaged before and after loading to explore the fracture mechanics within a crystal¹. Not only does X-ray CT provide 3D images to understand the mechanical response, but directly converting the 3D images to meshes allows for the modeling and simulation of mesoscale thermomechanical responses. Modeling the delamination behavior between individual crystals can elucidate cohesive parameters important for accurately capturing void creation in larger scale simulation of polycrystalline samples. This effectively allows us to better calculate the local strain within the material to better predict which surfaces are most likely to fail. Linking the processing to the microstructure, the microstructure to the mechanical performance, and then to the explosive performance is critical to creating stable PBX formulations.

References:

[1] B.M. Patterson *et al*, Exp Mech (2016), p. 1.

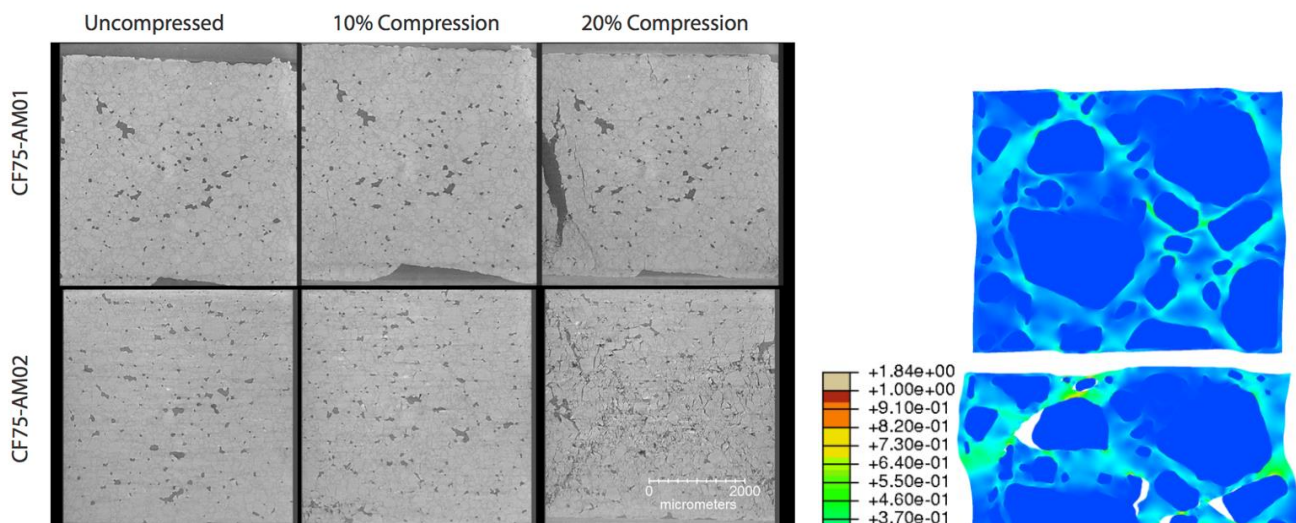


Figure 1. (above): Reconstructed X-ray CT slices as a comparison of two binder formulations upon the mechanical response at increasing strain. The top sample, AM01 has a softer binder, the bottom, AM02, is stiffer. Delamination is seen in the stiffer binder with conical fracture seen within the specimen.

Figure 2. Maximum principal strain during simulated macroscale compression of HMX crystals within a polymer binder. At increasing loads, the binder is stiff enough to delaminate from the crystals. This has the unfortunate effect of increasing the sensitivity of the material and weakening the bulk structure.

Figure 3. Reconstructed slice through two HMX crystals after pull testing. The crystals were bonded with NPE binder and then epoxied into the load cell. The material primarily pulls apart at the crystal binder interface, but voids and crack are seen throughout that lead to intracrystalline fracture.

