Mechanical Engineering Doctoral Defense

Investigation of shock-induced material transformations using first principle calculations and classical force field molecular dynamics

School for Engineering of Matter, Transport and Energy

Jing Hu
Advisor: Jay Oswald

Abstract

Material behavior under high strain rate deformation have always been an interesting topic. Under this extreme impact, possible structure changes such as phase transformation, chemical reaction, densification occur in materials. It is helpful to develop a fundamental understanding of structure-property relationship, which help to build a theoretical model and speeding up material design process. Despite the shock experiment techniques have been widely developed, numerical approaches such as first principal calculations and molecular dynamics simulations have demonstrated their power in predicting shock behavior and revealing structure-property relationship in an economic and feasible manner. In this work, I will investigate the mechanical properties and shock responses of three materials, polyurea, silicate glass, and erythritol, among which polyurea and silicate glass are proposed to be protective materials, while erythritol is proposed to be a surrogate of the explosive material pentaerythritol tetranitrate. First principal calculations and classical molecular dynamics will be carried out to predict the shock Hugoniot, and other thermomechanical properties. The simulations will also explore potential shock-induced phase transformations in these three materials and seek to draw connections between shock-driven transformations and the underlying chemical composition and material structure.

April 12, 2022; 9 AM;
Zoom Link: https://asu.zoom.us/j/9982622965