Title: Crystal Orientation-Dependence of Shock-Induced Phase Transitions

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When a compressed material changes phase it doesn’t do so instantly. Instead it transitions through a mixed phase as it transforms to the end state phase for a given pressure, volume and temperature. Common phase diagrams show the phase boundaries as sharp lines when compression has been slowly applied and held for an infinite amount of time. When the compression is applied with high strain rate, however, the phase boundaries are no longer crisp as the kinetic effects of the crystal reorientation delay the transitions, resulting in regions of mixed phase. Molecular dynamics (MD) simulations recently have been used to examine the shock-induced transition in single crystal materials illustrating an orientation dependence of the transition stress, mechanisms, kinetics, and Hugoniot response. For example, the [100] orientation of iron had a simulated transition stress higher than the experimentally determined polycrystalline value of 13 GPa by 2 Gpa.

In December, the proton radiography team performed an HE-driven experiment with tin, shocking the sample to a peak pressure with an unsupported Taylor shock wave. Below is an 18-frame time sequence of the shock moving through the tin target: decaying pressure is indicated by contrast reduction.

As the pressure decayed, we measured shock positions (velocities) and relative densities directly off the radiographs. For each radiograph, a point on the Hugoniot was measured, resulting in 18 data points on the Hugoniot from one experiment. Unfortunately, we did not drive the tin sample hard enough to successfully force a phase transition.
Figure 2. Each radiograph yields a shock position (velocity) and relative density measurement, plotting out points on the Hugoniot as the pressure decays.

We propose a series of measurements using this newly developed technique on shock-loaded samples of different material composition and crystal orientations. Materials will include tin, iron, gallium, and zirconium. Through shock loading, we will dynamically compress polycrystalline samples as well as single crystals along different crystal planes. Since we are able to measure many points along the Hugoniot in one experiment, we will be able to determine Hugoniot response as a function of crystal structure and orientation by simply overlaying measured curves. Predicted transition stress differences are greater than 1%, which is greater than our achieved accuracy. We also intend to measure the length scale of the nucleating centers and volume fraction of mixed phase as a function of time for the targeted materials. We will use high accuracy bulk density measurements directly off the radiographs to determine the volume fraction of the two phases. Additionally, with quantitative relative density measurements, we will look for features in the region of the mixed phase, such as any ramping density change over time.

A preliminary shot design is pictured below. It consists of a 25mm plane-wave lens with a nearly 1.0 mm thick Stainless Steel ring and ¼ inch of PBX9501 booster. With this P-25 lens, the target sample is driven to high enough peak pressure (~400kbar) for all the target materials, Fe, Ga, Zr and Sn to completely transition phase. To optimize the radiography, the target samples will be 12.7mm (1/2 inch) diameter and 25mm thick.
We have run CTH simulations with a tin target sample and looked at the pressure profile down the center of sample. The pressures are relatively constant around the center plane. This is important to measure the most accurate shock velocities and densities. For the iron sample, a CTH run with a P25 lens in direct contact with a 12mm diameter x 20mm thick iron cylinder and is profiled below. The $\alpha \rightarrow \varepsilon$ phase transition is noticeable at approximately $3/4$ cm into the iron target.

We are presently running more CTH simulations with various shot configurations with and without 9501 booster, with stacked boosters, and with the suite of target materials.