

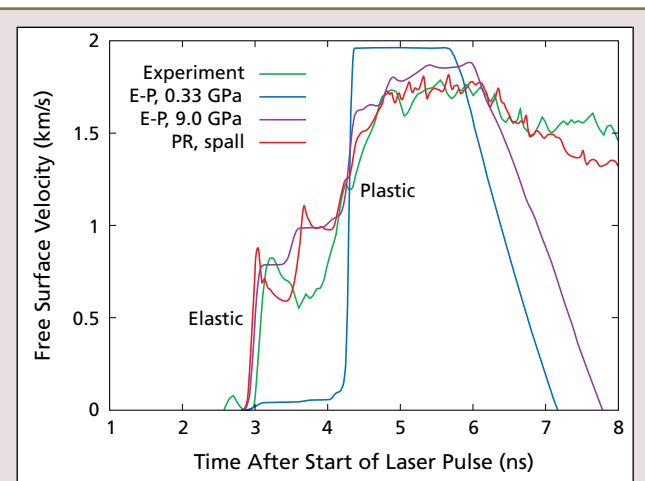
for compressed states because the  $c/a$  predictions included no data for the STP state.

To predict the elastic constants, we made similar quantum mechanical calculations as the crystal was distorted (strained) by compression along different crystal directions and by shearing different pairs of faces. In each case, we used the electron states to calculate stress on the crystal; the elastic constants are the rates with which stress changes with strain. We repeated the calculations for several different compressions, giving the elastic constants as functions of compression. Again, the values we predicted for STP agreed reasonably well with the measured values, giving us confidence that our predicted variation with compression is also reasonable.

### Measuring Crystal Properties

The rate of plastic flow, which is related to the elastic strain or stress that the material can support before flow occurs (also called the yield stress), depends greatly on the time available for crystal defects to move—and therefore on the thickness of the component.

We used LANL's Trident laser to induce shock waves in beryllium crystals 40- to 100- $\mu\text{m}$  thick—similar to the 150- $\mu\text{m}$  thickness of the ignition capsule—and studied the shape of elastic waves that run ahead of the shock. From these waves, we inferred parameters in a plasticity model that represents the properties of the defects accurately.



Velocity history from the free surface of a beryllium crystal, compared with simulations using different models of plasticity. Elastic-plastic (E-P) simulations are the simplest models of plasticity; 0.33 GPa is a typical flow stress on microsecond time scales. The elastic wave breaks out at the correct time, but the amplitude is too low and the shape of the plastic wave is incorrect. Increasing the flow stress to 9 GPa improves the amplitude but not the shape. The plastic relaxation (PR) model reproduces the shape of the elastic wave more accurately; this model did not include work hardening, so the rising part of the elastic wave shows stronger reverberations in the simulation than we observed experimentally. The PR simulation also included spall, improving the match after the peak of the plastic wave. Note that more accurate simulations of the elastic wave also improve the match in the plastic region.

For a range of drive pressures, the elastic wave outruns the shock. Wave amplitude is set by yield stress and its precise shape gives more details that constrain parameters in the plasticity model. Plastic flow occurs as defects—dislocations and twin boundaries—move along planes in the lattice of atoms (the slip systems) that comprise the crystal. The average speed of a defect's movement across a plane depends on the elastic shear stress resolved over that plane; generally, several different slip systems may be active simultaneously as a crystal deforms. The stress required to activate slip systems may vary, as may the population of defects able to mediate strain in each slip system. Our studies included these variations with experiments on beryllium crystals of different orientations.

Having developed a plasticity model for single beryllium crystals, we can predict the response of a given microstructure to loading and heating. Because it is crucial to test the predictions, we will obtain elastic-