Pulsed Power
Extreme Environments

Shock-wave exploration of the high-pressure phases of carbon

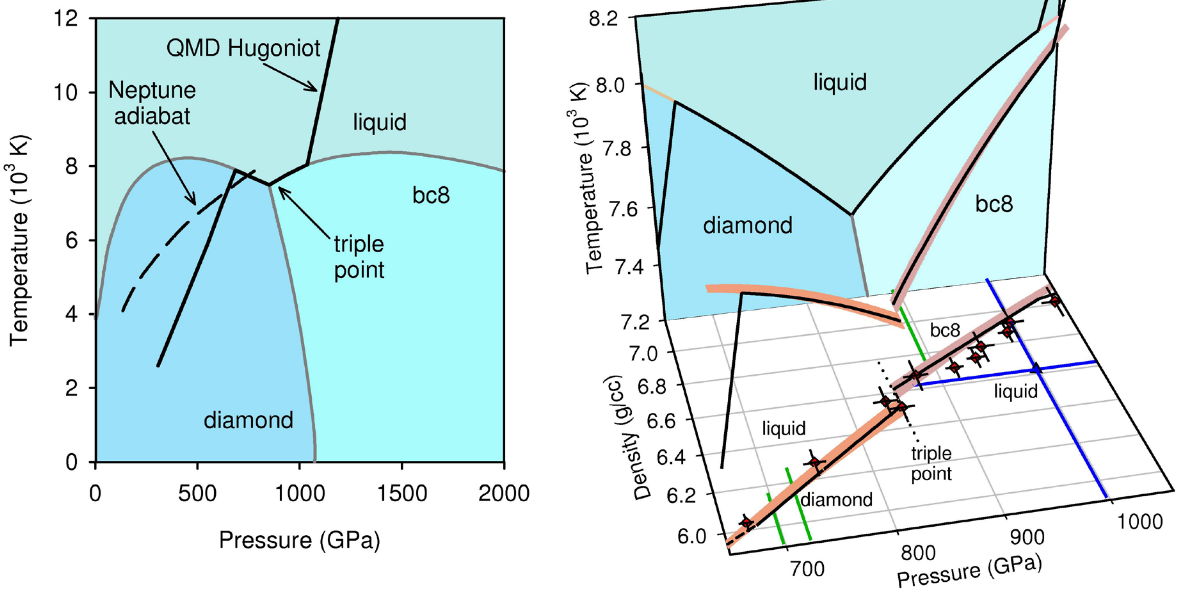

Figure 1: (Left) Phase diagram for high energy density carbon. Solid black line, QMD Hugoniot from this work; dashed black line, predicted adiabat for Neptune (Uranus similar). (Right) QMD predictions near the triple point for the diamond-liquid (orange band) and bc8-liquid (magenta band) coexistence regions in density – pressure – temperature space. Also shown are projections in the pressure – temperature (back wall) and pressure – density (floor) planes. The black line is the QMD predicted Hugoniot. The Hugoniot lies within the solid – liquid coexistence over the entire pressure range of ~690 to 1060 GPa, inclusive of the diamond – bc8 – liquid triple point at ~850 GPa. Experimental data are shown in the pressure – density plane; colors and symbols as in Fig. 2.

Melting of diamond under pressure at the Sandia Z machine

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Diamond is being considered as one of the ablator materials for inertial confinement fusion (ICF) capsules. Consequently, understanding the melt properties of diamond along the Hugoniot, the locus of end states achievable through compression by large amplitude shock waves, is critical for designing capsules and drive pressure pulse-shapes that minimize the possibility of micro-structural effects during the implosion phase of the capsule; such effects could lead to heterogeneities that would seed instabilities capable of quenching the implosion. In support of the National Ignition Campaign, detailed quantum molecular dynamics (QMD) calculations were performed in the vicinity of the melt transition using the Vienna *ab-initio* simulation package. Concurrently, a series of ultra-high velocity impact experiments were performed at the Sandia Z machine to determine the melt properties of diamond along the Hugoniot.

The QMD calculations predicted the onset and completion of diamond melt along the Hugoniot at pressures of ~690 and ~1060 GPa (6.9 and 10.6 million times atmospheric pressure), respectively (see Fig. 1). Additionally, and possibly more significantly, these calculations also suggested the existence of a diamond-bc8-liquid triple point within the shock melt coexistence region at a pressure of ~850 GPa. As shown in Fig. 2, the resulting Hugoniot near melt exhibits four distinct regions, with significant differences

in shock velocity throughout the coexistence region. However, as seen in Fig. 2a, data obtained from recent experimental studies performed at ultra-intense laser facilities elsewhere were of insufficient accuracy to provide quantitative comparison with these predictions.

A series of 15 flyer plate impact experiments were performed on polycrystalline diamond samples on the Sandia Z machine over the pressure range of 550 to 1400 GPa. The relatively large lateral area of the flyer plates permitted simultaneous loading of three diamond samples, each substantially larger than samples used in previous studies, which enabled precise measurement of the shock wave velocity. Furthermore, measurement of the impact velocity in these experiments enabled precise inference of the particle velocity. These aspects of the experiment enabled roughly an order-of-magnitude improvement in accuracy as compared to recent laser studies, as illustrated in Fig. 2, and enabled quantitative comparison with QMD predictions. These results validate the QMD calculations and provide compelling evidence for the existence of the triple point along the Hugoniot, which is the first experimental evidence of a high-pressure solid phase of carbon beyond that of diamond.

This work dramatically improves the understanding of the melt properties of carbon in this high energy density regime. In addition to being essential in the design of capsules for ICF applications, these data and QMD calculations should also provide for more accurate equation-of-state models for carbon in the regime of interest to planetary physicists. In particular, improved models for carbon may lead to better models for the interiors of Neptune and Uranus that may provide insight into the source of the unusual magnetic fields observed for these two planets.

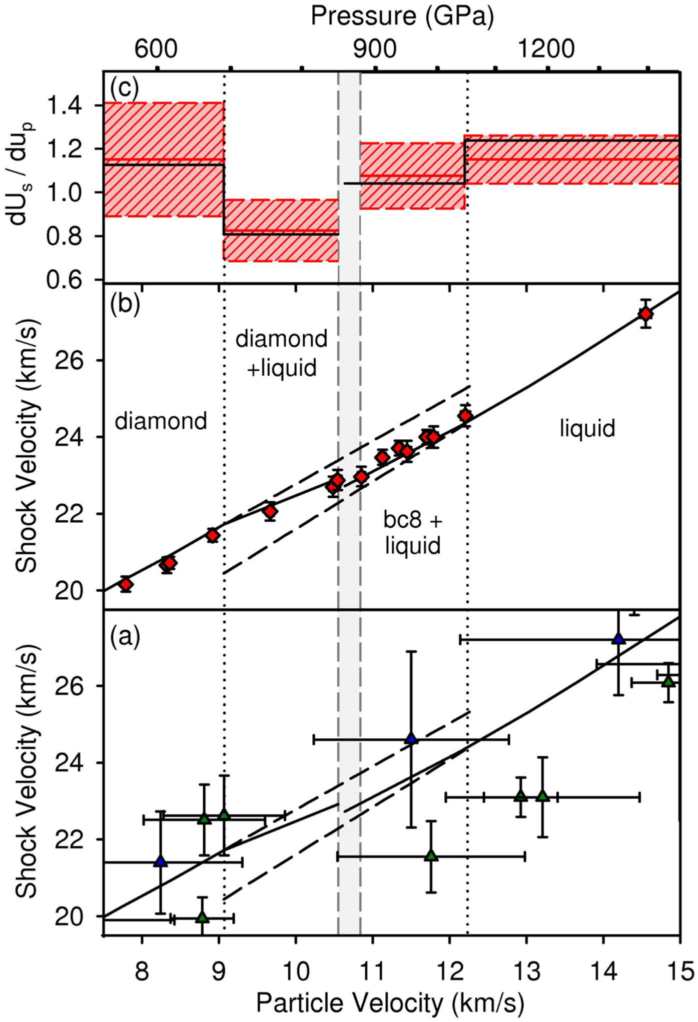

Figure 2: (a) and (b) Diamond Hugoniot in shock velocity, U_s, versus particle velocity, u_p. Solid line, QMD Hugoniot, this work; dashed line, QMD metastable solid and liquid Hugoniots, this work. Experimental data: blue and green triangles, laser driven data; red diamond, this work. (c) Comparison of the U_s-u_p slopes from QMD calculations (solid black line) and a piecewise linear fit to the experimental data (solid red line). Also shown are the uncertainties in the slopes of the fit (dashed red line). Gray region indicates the experimental bounds for the diamond-bc8-liquid triple point.

Sandia National Laboratories

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND2008-5080P

NNSA National Nuclear Security Administration

08/2008