Shock Compression of Liquid Noble Gases to Multi-Mbar Pressures

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Summary: The Sandia National Laboratories' Z-machine is the ideal platform for performing multi-Mbar shock compression experiments to study materials under extreme conditions. For many materials, the current equations of state models in these high P-T regimes have no data for comparison. By combining the Z-experimental results with quantum molecular dynamics simulations, we determine high precision Hugoniots—data critical to EOS development.

Introduction

The high P-T behavior of noble gases is of considerable interest because of their use in z-pinch liners for fusion studies and for understanding astrophysical and planetary evolution. However, our understanding of the equation of state (EOS) of the noble gases at extreme conditions is limited. A prime example is the liquid xenon Hugoniot. Previous EOS models rapidly diverged on the Hugoniot above 1 Mbar because of differences in the treatment of the electronic contribution to the free energy. Similar divergences are observed for the krypton and argon EOS. By combining shock compression experiments and density functional theory (DFT) simulations, we can determine the thermo-physical behavior of matter under extreme conditions.

Shock compression experiments performed using Sandia's Z-Accelerator determine the principal Hugoniot of cryogenically-cooled liquid xenon, krypton, and argon in the Mbar regime. Under strong shock compression, an insulator to metallic state transition occurs and the shock front becomes reflective allowing for a direct measurement of the sample's shock velocity using laser interferometry. DFT simulations at these extreme conditions show good agreement with the experimental data – demonstrating the attention to detail required for dealing with elements with relativistic core states and d-state electrons. The results from shock compression experiments and DFT simulations are presented for liquid Xe to 840 GPa, for liquid Kr to 800 GPa, and for liquid Ar to 600 GPa

Method

The Sandia Z-machine is a pulsed power accelerator capable of producing currents and magnetic fields in excess of 20 MA and 10 MG, respectively [1]. The large current and field densities generate intense magnetic pressures that are capable of accelerating flyer plates up to 40 km/s [2]. For these experiments, the target consists of a copper cell filled with a front drive plate of either Z-cut alpha quartz or aluminum and a quartz rear window. The cell is filled with a high purity noble gas and cooled to the gas-liquid transition using liquid nitrogen and helium. The temperatures for the targets were Xe = 163.5 K, Kr = 118 K, and Ar = 85 K. Shock velocities in the liquefied nobles are measured using laser interferometry. The Hugoniot state is determined using a Monte Carlo analysis method that accounts for systematic error in the standards and for correlations.

Results and Discussion

Figures 1-3 show the Z experimental data and DFT simulation results along with prior data and current EOS models for Ar, Kr, and Xe. For all three nobles, the current EOS models reproduce the low pressure (<1 Mbar) Hugoniot data and above 1 Mbar, the EOS models diverge from each other. For Ar, the DFT simulations trend to higher densities above 1 Mbar than do the EOS models. The Z experimental data were analyzed using reflected quartz Hugoniot as well as a release model and the Hugoniot was determined to ~6 Mbar. Both analysis methods clearly show that Ar trends softer than the EOS models predict. For Kr and Xe, the DFT simulations above 1 Mbar are bracketed by the EOS models. The Z

experimental data again validate the DFT predictive simulations and demonstrate that the EOS models are no longer accurate in regions where no data previously existed. For Xe, it is important to note that 4 of 5 experiments used quartz for the impedance matching standard. The 5th point near 730 GPa was impedance matched to aluminum highlighting that the results are independent of the impedance matching standard.

Conclusion

The principal Hugoniots for liquid Ar, Kr, and Xe were measured to several Mbar with high precision. Experimental results validated the use of DFT simulations for extreme conditions. The combined experimental and DFT results provide a solid basis for the development of new EOS for these materials.

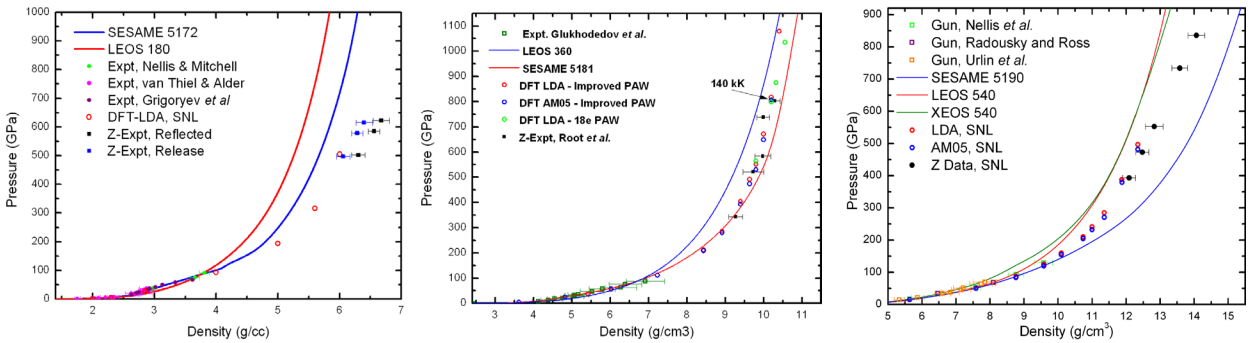

Figure 1. The r – P Hugoniot data for Ar, Kr, and Xe (left to right). Plots include current EOS models, prior experimental data, Z – data, and various DFT simulations.

References

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