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Shock Compression of Condensed Matter

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Shock Compression of Cryogenic Noble Gas Mixtures: Krypton - Xenon

Seth Root*, Rudolph J. Magyar, Raymond W. Lemke, and Thomas R. Mattsson

Sandia National Laboratories

Albuquerque, NM, United States

sroot@sandia.gov

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The Noble Gases

- **Understanding the high pressure – high temperature response of the noble gases provides insight into the behavior of filled – shell electronic configurations**
- **The noble gases represent ideal systems for liquid state theory**
- **Krypton – Xenon are miscible and provide a test system for developing Equation of State models for mixtures**

- **Understand the high – pressure behavior of a 70/30 Molar Mixture of Krypton/Xenon**
- **Perform shock – reshock experiments on the Z – machine**
- **Use DFT to examine regions not explored experimentally**

Previous work shows that integration of DFT, high-precision Hugoniot standards, and Z experiments constitutes a solid basis for understanding the high pressure response of materials.

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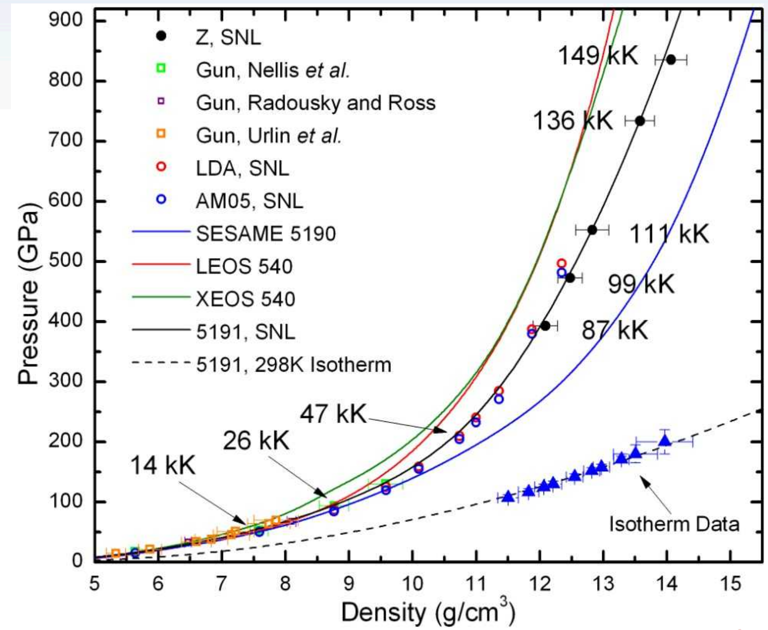
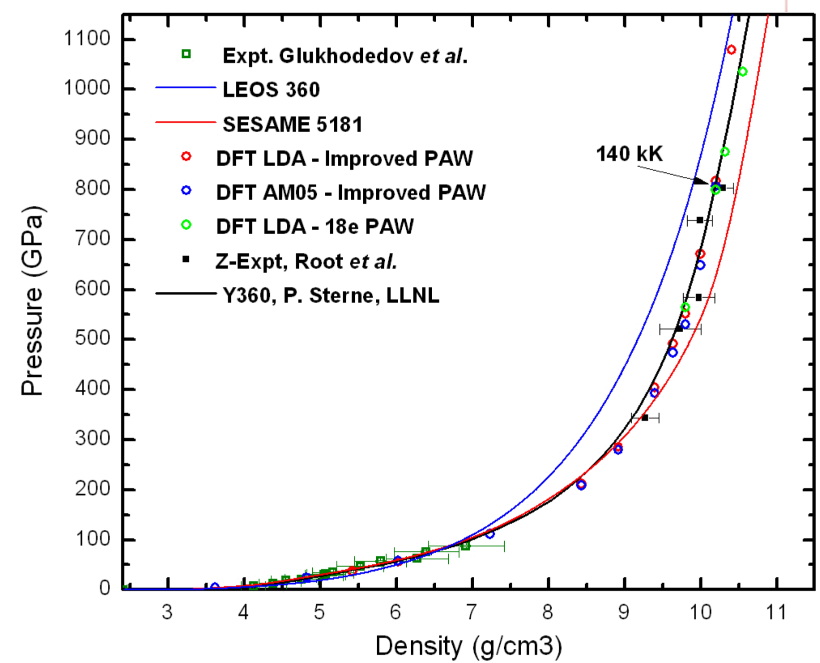
Pure Xe and Kr EOS Results

- **Measured the pure Xe and Kr Hugoniots to 8 Mbar**
- **Validated the use of DFT for calculating Hugoniots to Mbar pressures**
- **Results lead to development of new wide-range EOS models for xenon and krypton**
- **Xenon SESAME 5191, J. H. Carpenter (SNL)**
- **Krypton Y360, P. Sterne (LLNL)**
- **Understand noble gas mixtures: 70/30 molar mix Kr/Xe**



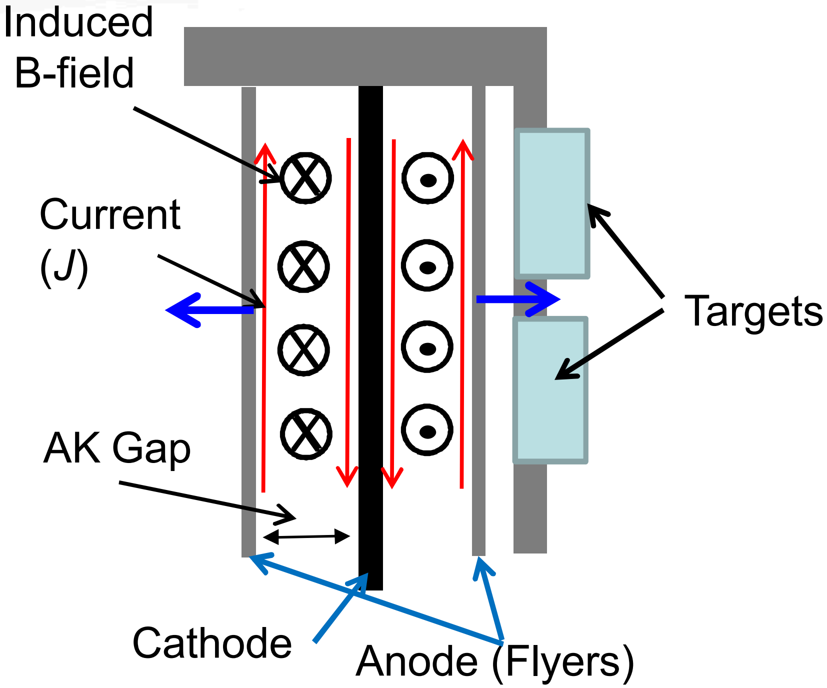


Xenon: S. Root *et al.*, Phys. Rev. Lett. 105, 085501 (2010).

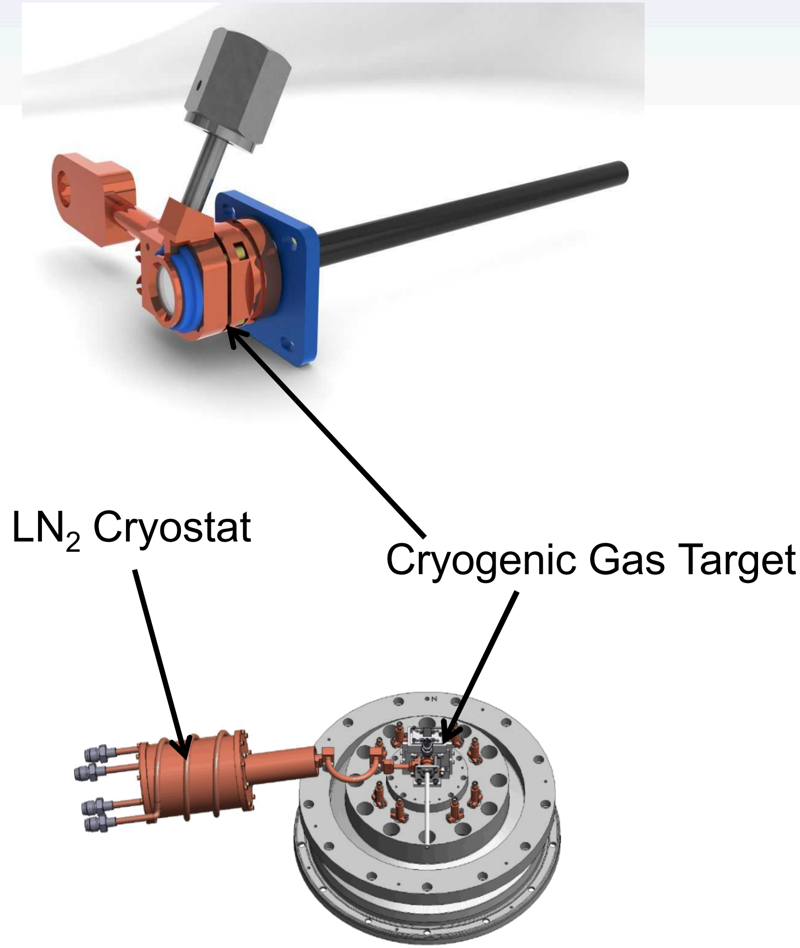
J. H. Carpenter *et al.*, EPJ Web of Conf. 10, 00018 (2010)

Krypton: S. Root *et al.*, SCCM 2011, Chicago, USA

Z-Experiment Setup

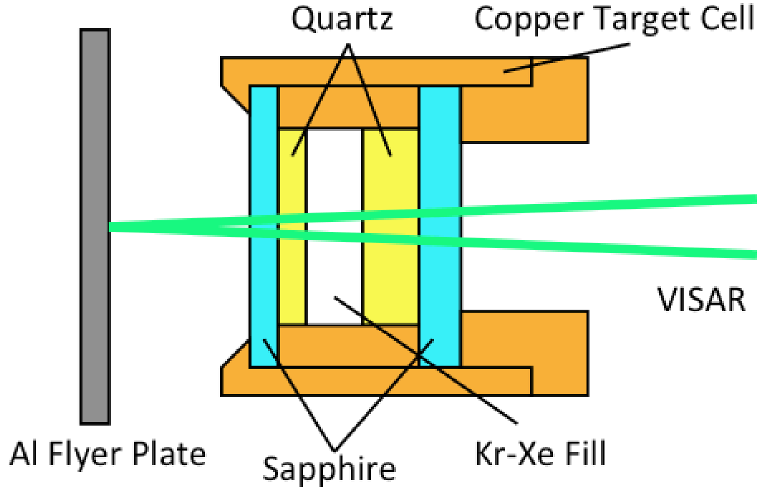


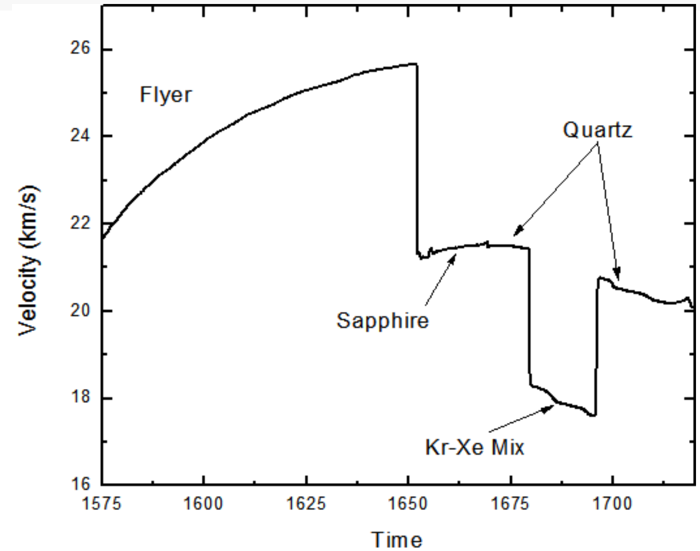
- Current pulse loops through shorting cap inducing a *B* – field.
- Resulting *J x B* force accelerates anodes (flyers) outward up to 40 km/s
- Asymmetric AK Gaps result in two different flyer velocities (two Hugoniot points per experiment



- Liquid Kr – 118 K, ρ_0 = 2.43 g/cm³
- Liquid Xe – 161.5 K, ρ_0 = 2.98 g/cm³
- Liquid Kr-Xe (70/30) – 161.5 K, ρ_0 = 2.46 g/cm³

Experimental Approach





- 70/30 Molar Mix Krypton/Xenon
- Initial Pressure 148 PSI
- Temperature = 161.5 K
- Mixed Liquid Density 2.46 g/cc
- Initial P-T repeatable for every experiment

- Sapphire windows to hold pressure
- VISAR measures flyer velocity
- Shock front reflective in Mix and Quartz – sapphire depending on pressure
- Multiple VPFs to reduce uncertainty

Target design allows for measurement of the reshock state

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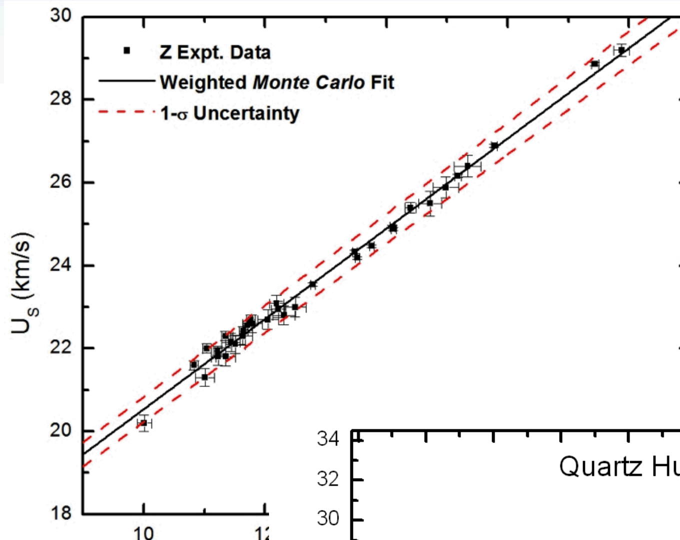
Quartz - Sapphire Us-Up Data and Fits

- Nearly 300 quartz and 34 sapphire Hugoniot data points
- Data includes uncertainty from Al and Cu Hugoniot standards
- Correlation Matrix propagates all uncertainties



Sapphire Fit

$$U_S = 9.664 + 1.088 U_P$$

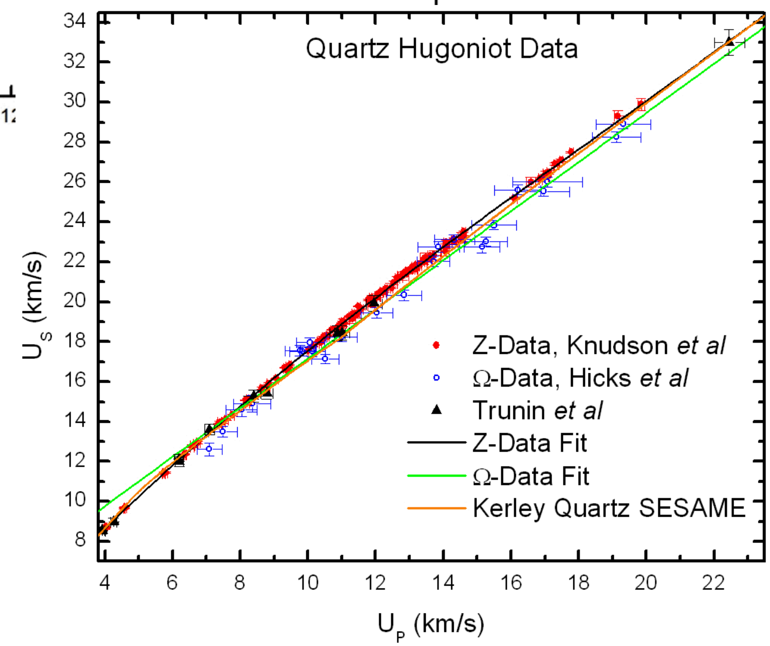
1	-0.9908
-0.9908	1

Sandia Z Quartz Cubic Fit:

$$U_S = 6.98 \times 10^{-3} U_P^3 - 0.0384 U_P^2 + 1.915 U_P + 1.559$$

Correlation Matrix:

U_P^3	U_P^2	U_P^1	U_P^0
1	-0.9976	0.9900	-0.9730
-0.9976	1	-0.9971	0.9848
0.9900	-0.9971	1	-0.9946
-0.9730	0.9848	-0.9946	1



Direct measurement of flyer and shock velocity leads to high precision data

- M. D. Knudson and M. P. Desjarlais, Phys. Rev. Lett. 103, 225501 (2009).
- D. G. Hicks *et al.*, Phys. Plasmas 12, 082702 (2005).
- R. F. Trunin, *Experimental Data on Shock Compression and Adiabatic Expansion of Condensed Matter* (2001).

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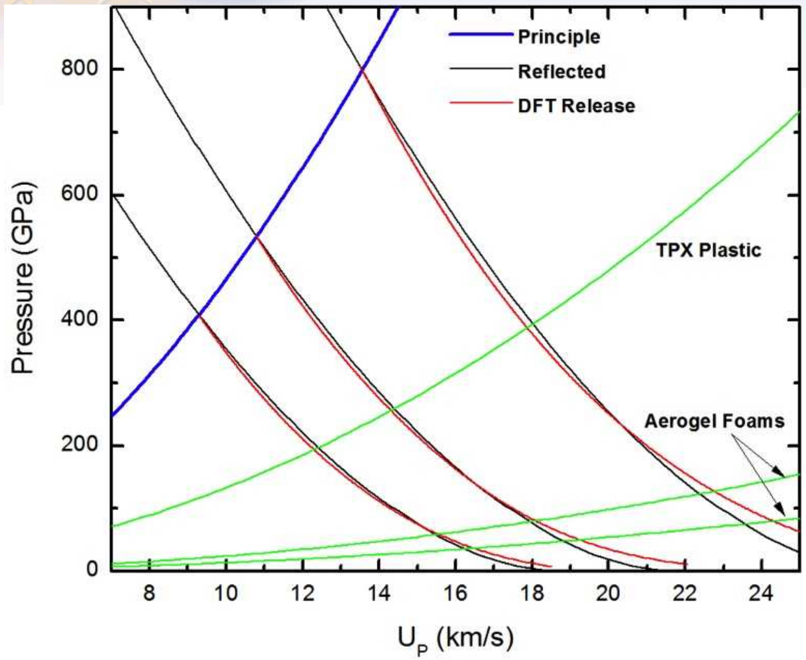
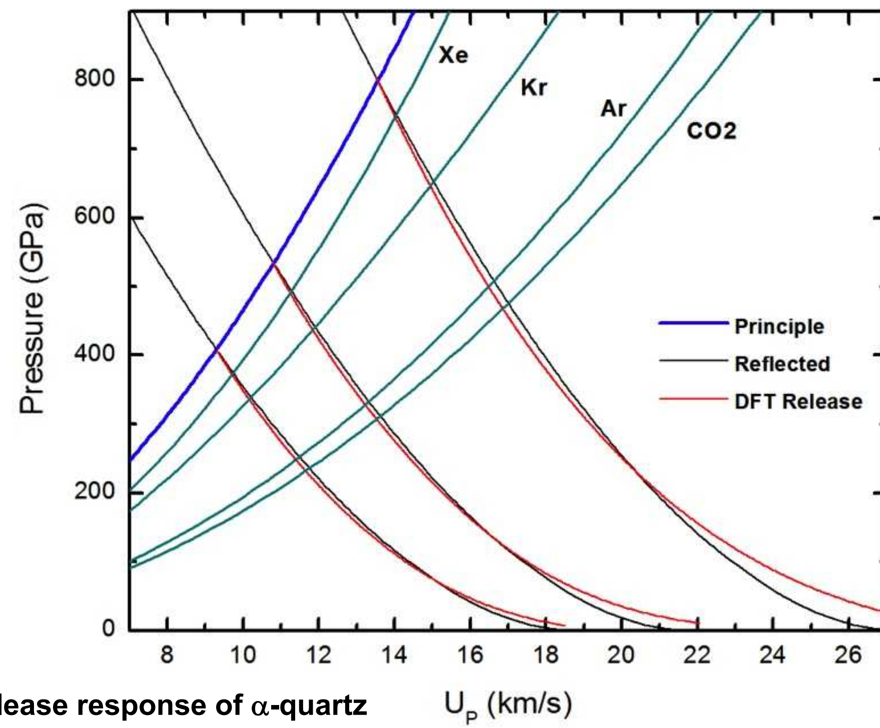
Release Paths



- **Quartz release measured using TPX and aerogel foam standards**
- **Density Functional Theory simulations used to calculate release paths**
- **New release model developed for quartz from experimental data**

- **Monte Carlo Impedance matching using the new quartz release model**
- **Monte Carlo impedance matching to sapphire reflected Hugoniot**
- **Correct for sapphire release using SESAME 7411**



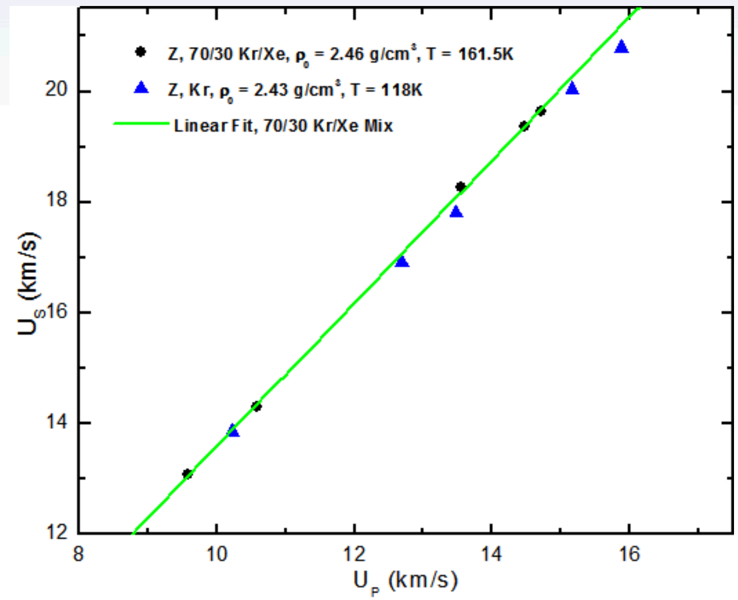
Experimental Results: Hugoniot

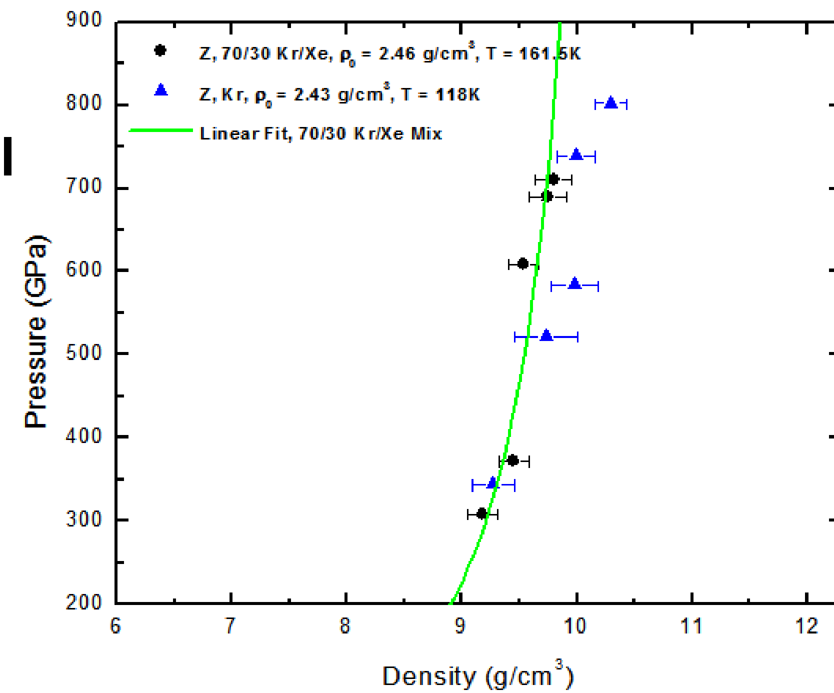
- **Measured the principle Hugoniot to 7 Mbar**
- **Monte Carlo analysis accounts for impedance standard uncertainty**
- **Experimental results similar to pure Kr**
- **Mix ρ_0 = 2.46g/cm^3, Kr ρ_0 = 2.43 g/cm^3**
- **Weighted Linear Fit to experimental data**

$$(0.705 \pm 0.213) + (1.290 \pm 0.018)U_P$$

Correlation Matrix

1	-0.9851
-0.9851	1





Density Functional Theory

- DFT-MD simulations performed using VASP 5.2.12*
- Electronic states occupied according to Mermin's finite-temperature formulation
- Projector augmented wave core functions (PAW) potential for core electrons – 8 valence electrons
- Calculate energy and pressure for a given density and finite temperature
- Solve the Hugoniot Condition: $2\left(E - E_{ref}\right) - \left(P + P_{ref}\right)\left(v_{ref} - v\right) = 0$

  - Initial conditions: ρ_0 = 2.46 g/cc, T_0 = 161.5 K, 30 atoms
  - AM05 exchange correlation functionals
  - Convergence tested: number of atoms, energy cut off
  - Methods demonstrated successfully on Xenon and Krypton

* G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993) and Phys. Rev. B 49, 14251 (1994).

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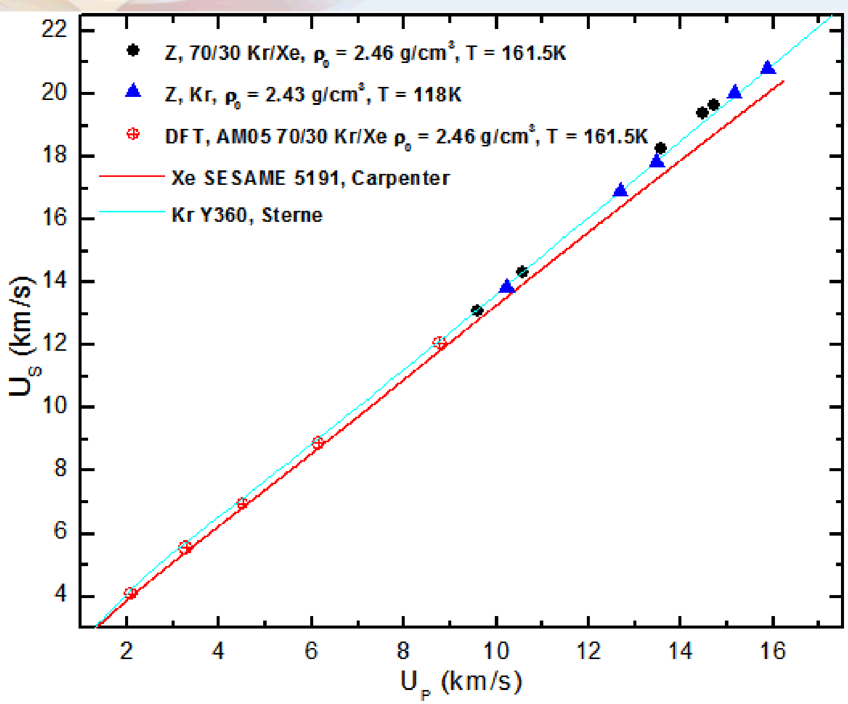
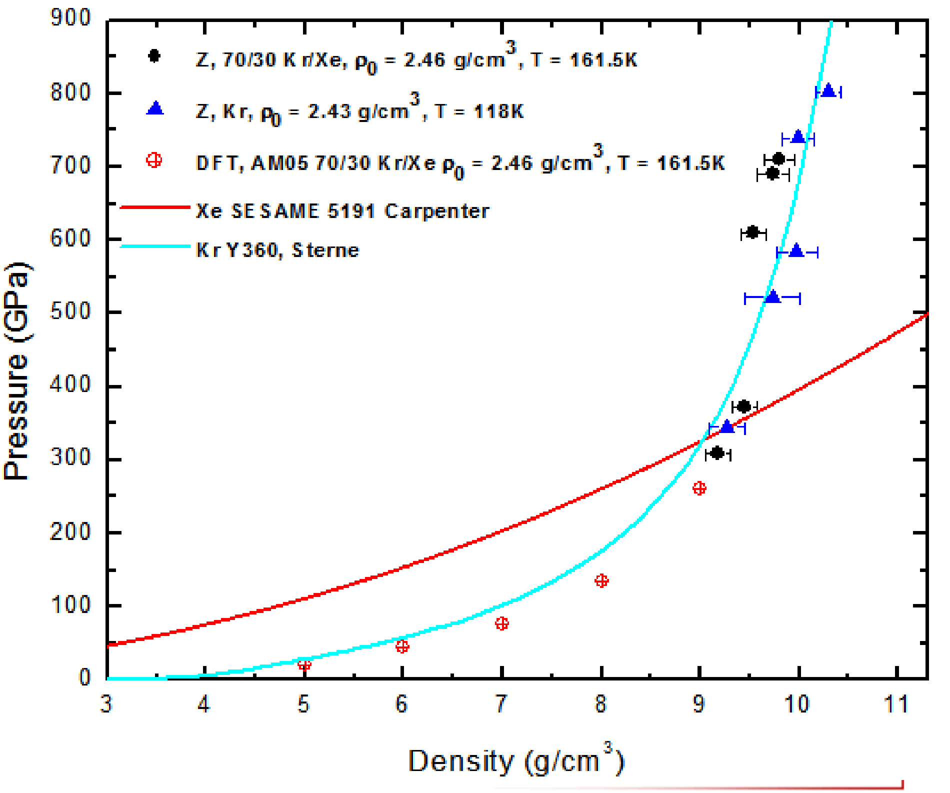
Comparison to DFT and EOS Tables



- **DFT simulations to 3 Mbar**
- **DFT results consistent with the experimental data**



- **The Kr Y360 EOS table reasonable reproduces the DFT and experimental data**
- **This applies only for this mixture ratio with these initial conditions!!**
- **The similar initial densities of the pure Kr and 70/30 Mix likely cause the similar results in this pressure regime**

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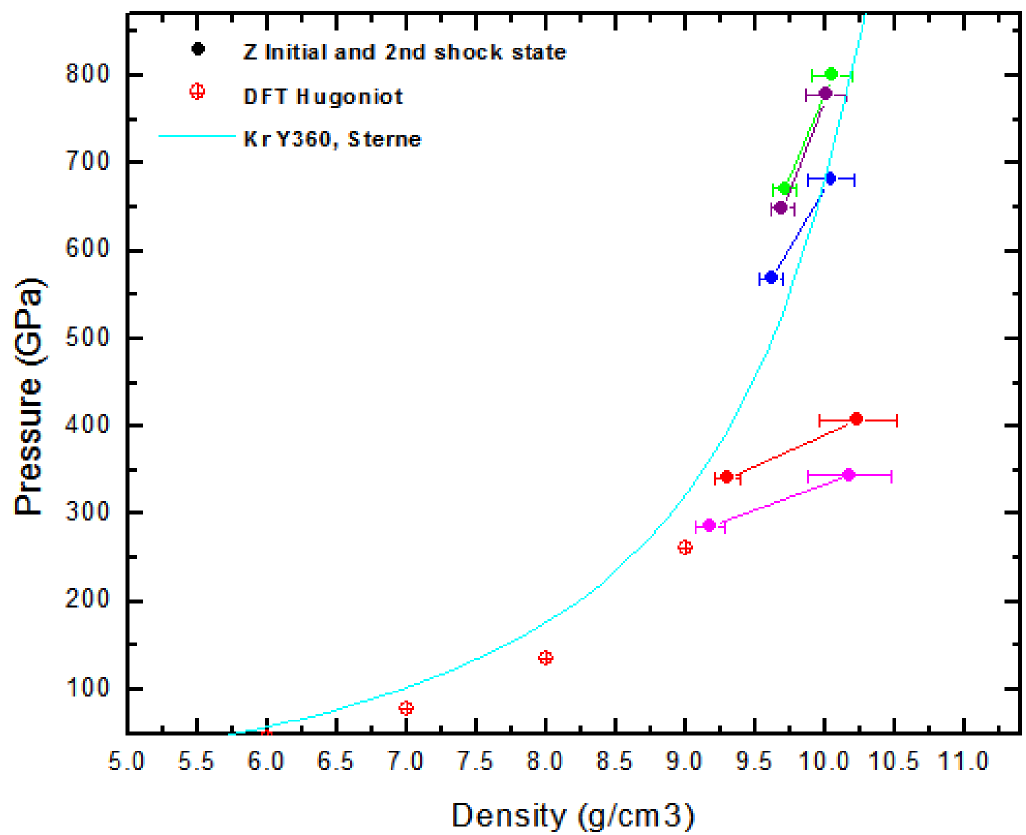
Second Shock State

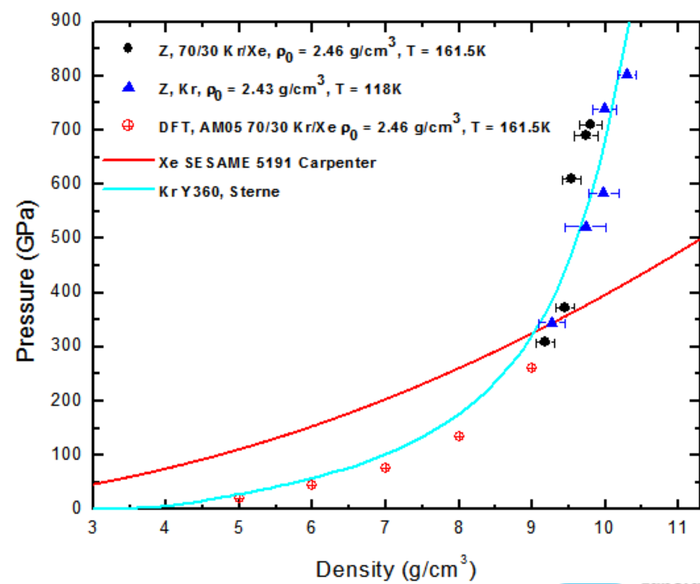
- **Experimental measured 2nd shock state to 8 Mbar**
- **Use linear fit to determine Mixture Hugoniot state prior to second shock (shock attenuation in the Kr/Xe sample)**
- **Monte Carlo Impedance Matching to the quartz Hugoniot**
- **Error bars larger because of uncertainty in initial state**
- **At pressures < 3.5 Mbar the 2nd shock is more compressible**
- **Above 5 Mbar the 2nd shock is less compressible**



Summary

- **Experimental measured the principle Hugoniot of a 70/30 Molar ratio mixture of krypton and xenon to 7 Mbar**
- **Determined the reshock state to 8 Mbar**
- **DFT simulations to calculate the low pressure (< 3 Mbar) region of the Hugoniot – results consistent with the experimental data**
- **The Y360 Krypton table reasonable describes the mixture Hugoniot, but only because of the initial density similarity**
- **Data can be used to understand mixture theory for EOS development**

The integration of DFT, high-precision Hugoniot standards, and Z experiments constitutes a solid basis for understanding the high pressure response of materials.



Acknowledgments

Krypton EOS Table
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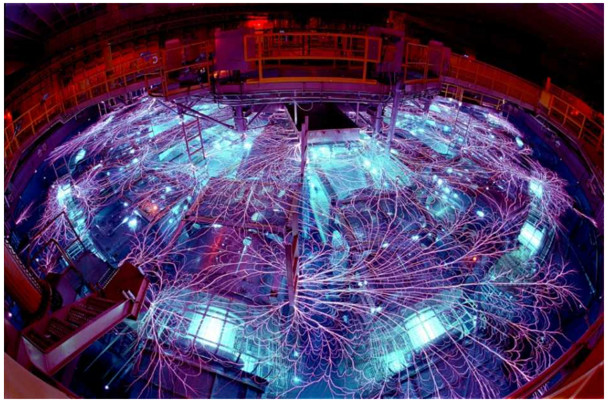
Keegan Shelton
Jose Villalva

Cryo-Target Assembly
Aaron Bowers
Nicole Cofer
Jesse Lynch

Diagnostics
Charlie Meyer

Designer
Devon Dalton

All Members of the Z-Operations Team and Target Fabrication



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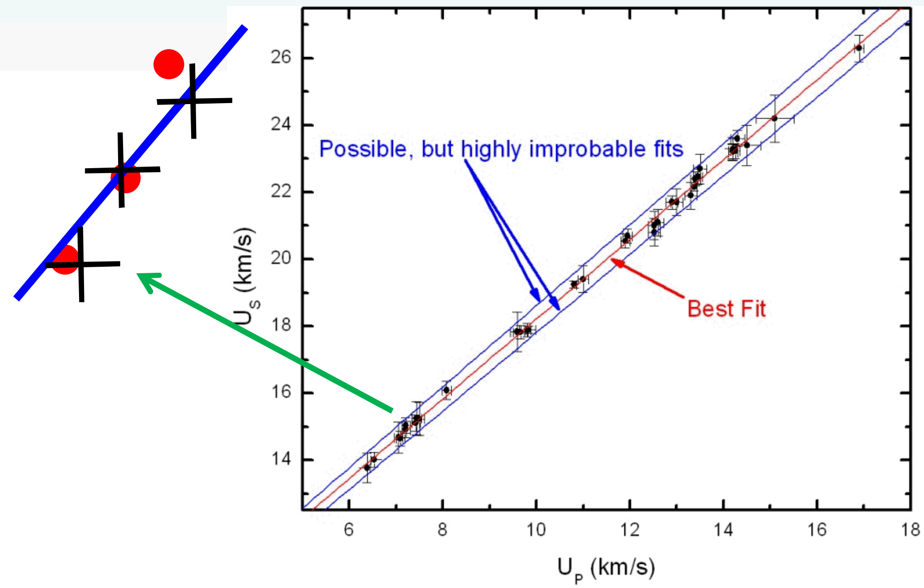
Monte Carlo (MC) Impedance Matching

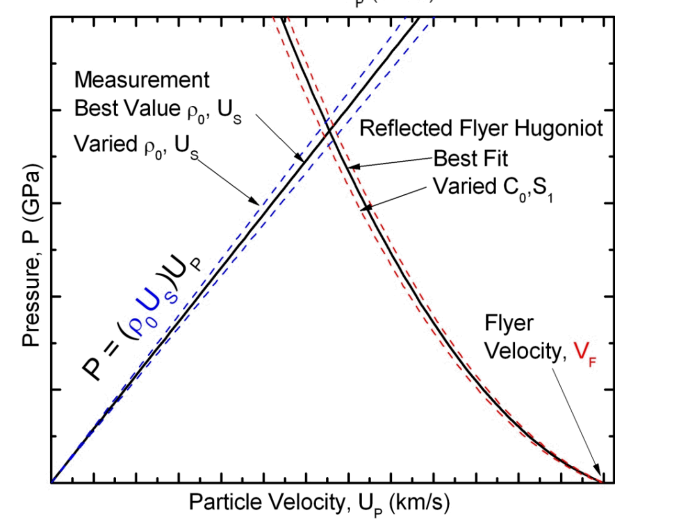
Aluminum

- Uncertainty in experimental data (Knudson *et al*., JAP 2003)
- Vary each U_S-U_P point by an uncorrelated random number with σ = expt. Uncertainty
- Solve for linear fit parameters
- Determine mean, σ, and correlation of fit parameters



Quartz

- Vary measured parameters (V_F, U_S, ρ_0) with uncorrelated random numbers, σ = experimental uncertainty
- Vary Al fit parameters using correlated random numbers
- Calculate U_P, P, and ρ
- Determine mean and σ



Monte Carlo **technique accounts for all experimental uncertainty and propagates the Al and Cu standards' error into the quartz data.**