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Shock Compression of Condensed Matter
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Liquid Krypton Hugoniot at Megabar Pressures

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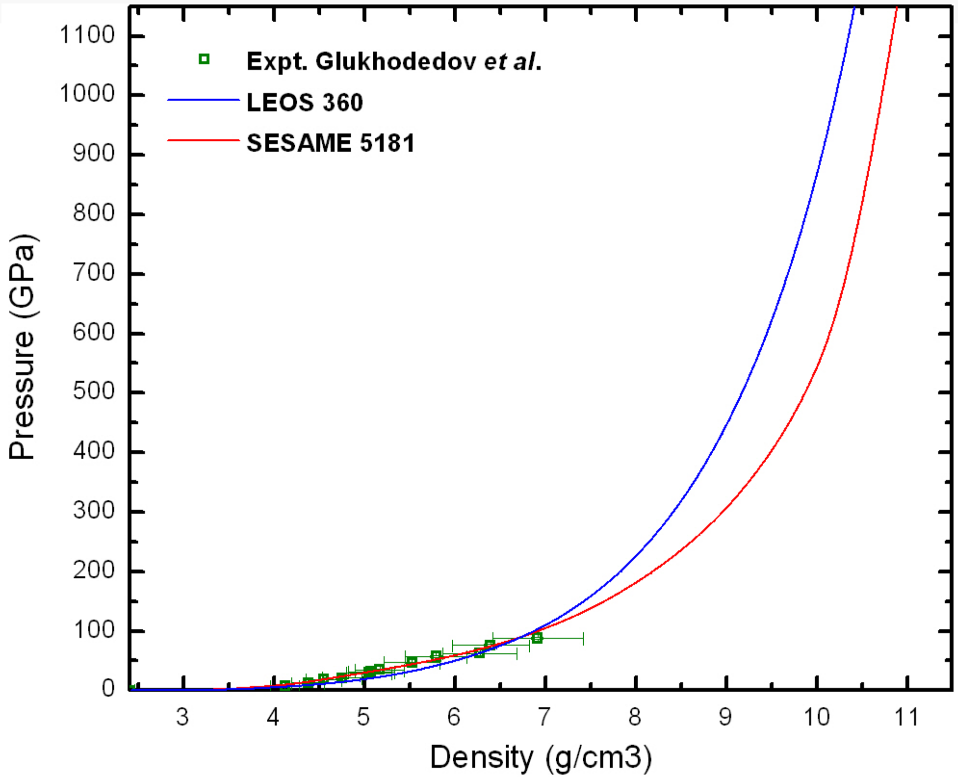
Shock Compression of Krypton

- Krypton is a model element to study high pressure effects on filled-shell electron configurations

  - Liquid Kr Hugoniot experimentally determined to 100 Gpa
  - Current EOS tables show good agreement below 100 Gpa
  - EOS tables diverge above experimental data



Objectives

- Validate the use of Density Functional Theory simulations to calculate high pressure – high temperature Hugoniots and predict the Kr Hugoniot
- Experimental determine the liquid krypton Hugoniot to Mbar pressures
- Use the DFT and experimental results to validate the tabular EOS

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Density Functional Theory

- DFT-MD simulations performed using VASP 5.1.40*
- Electronic states occupied according to Mermin's finite-temperature formulation
- Projector augmented wave core functions (PAW) psuedo-potential for core electrons
- Calculate energy and pressure for a given density and finite temperature
- Solve the Hugoniot Condition: $$2(E - E_{ref}) - (P + P_{ref})(v_{ref} - v) = 0$$

  - LDA and AM05 exchange correlation functionals
  - Typically 32 atom simulations – 16 atoms at highest temperatures
  - Convergence tested: number of atoms, energy cut off
  - DFT simulations performed without knowledge of experimental results
  - Methods demonstrated successfully on Xe, H_2O, C, quartz

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

PAW Potential Modification

- Scattering properties an issue first discovered in our work on Xe (Root et al., PRL **105**, 085501 (2010))

- PAW core potential/function (color) should display same scattering properties as the full electron atom (gray)

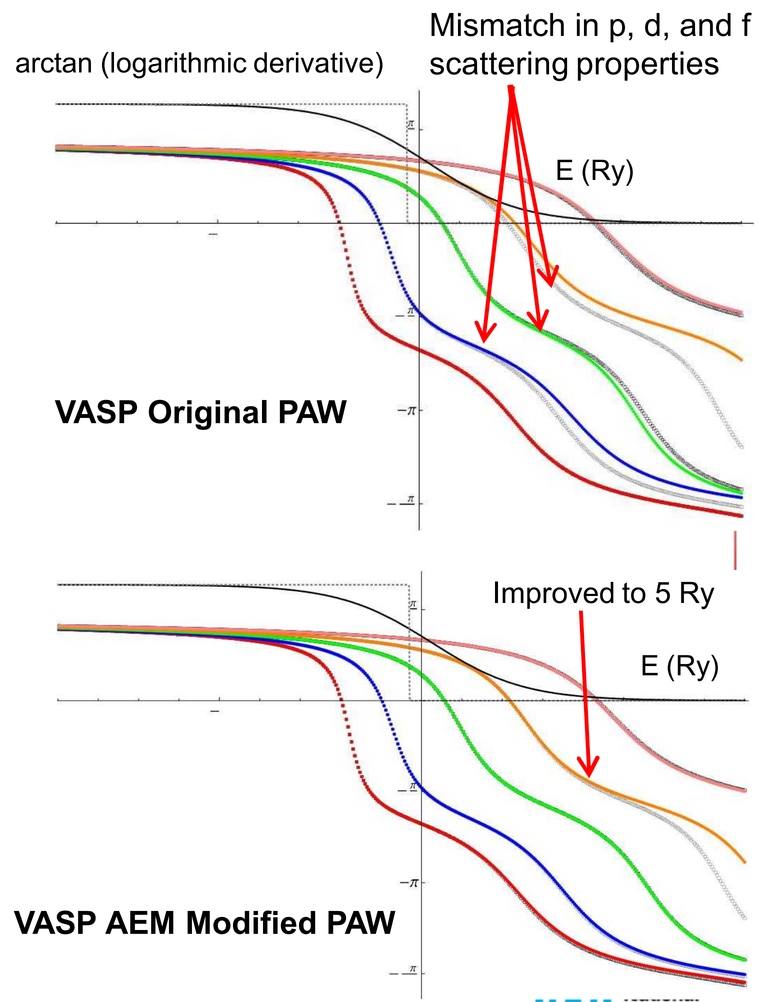
- The standard VASP 8e PAW is adequate for low T, but mismatch in logarithmic derivative as T (energy) increases

- The new VASP 8e PAW (AEM) has improved scattering properties at high energy and temperature

- Matches scattering properties to 5 Ry.

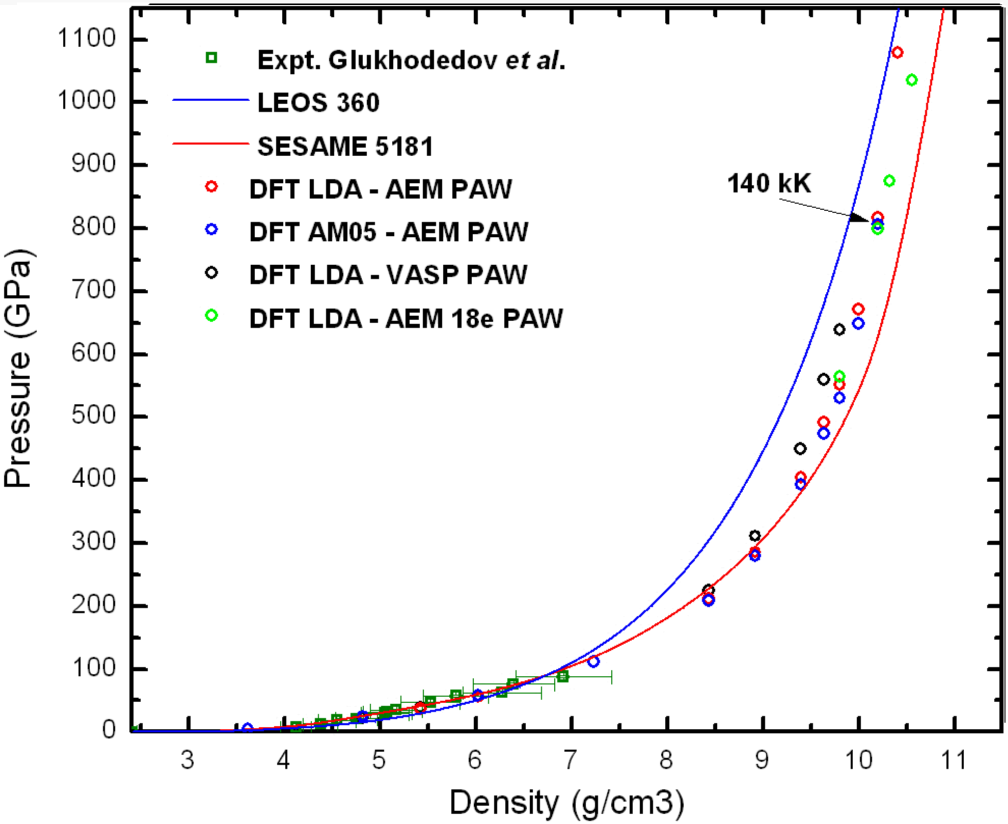
ℓ=s(red), p(blue),d(green,local),f(orange,local),4(pink,local)

Fermi-distribution shows relevant energy scale



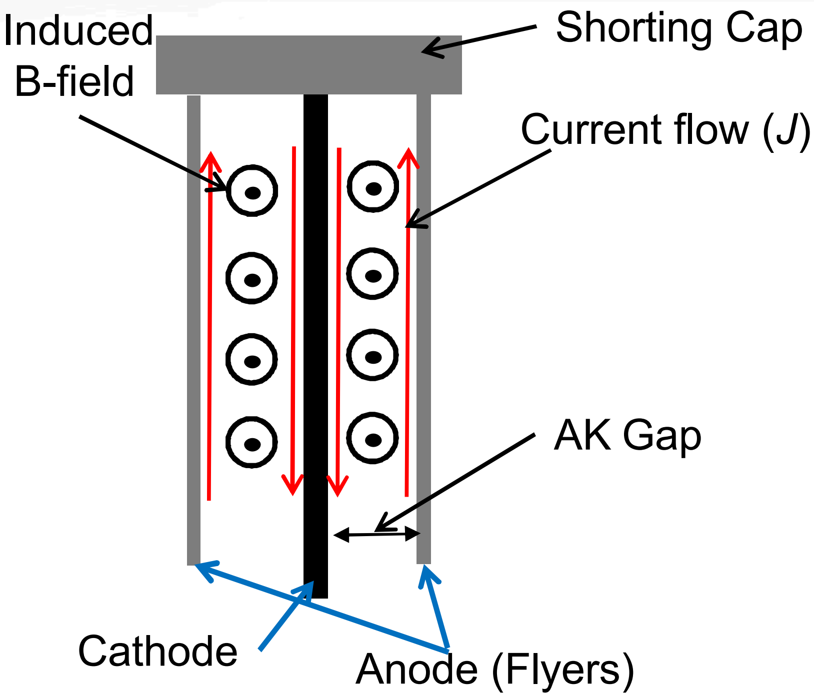
DFT Results

- DFT Results consistent with experimental Hugoniot data < 1 Mbar
- SESAME 5181 and the DFT results agree up to 4 Mbar
- The VASP PAW agrees with gun data but deviates from AEM PAW > 3 Mbar
- At high T the PAW pseudo-potential for core electrons is incorrect
- Core electrons can be excited out of the psuedo-potential
- A modified PAW (with 18 valence electrons) developed for high T
- The 18e PAW agrees with the AEM PAW results to 8 Mbar

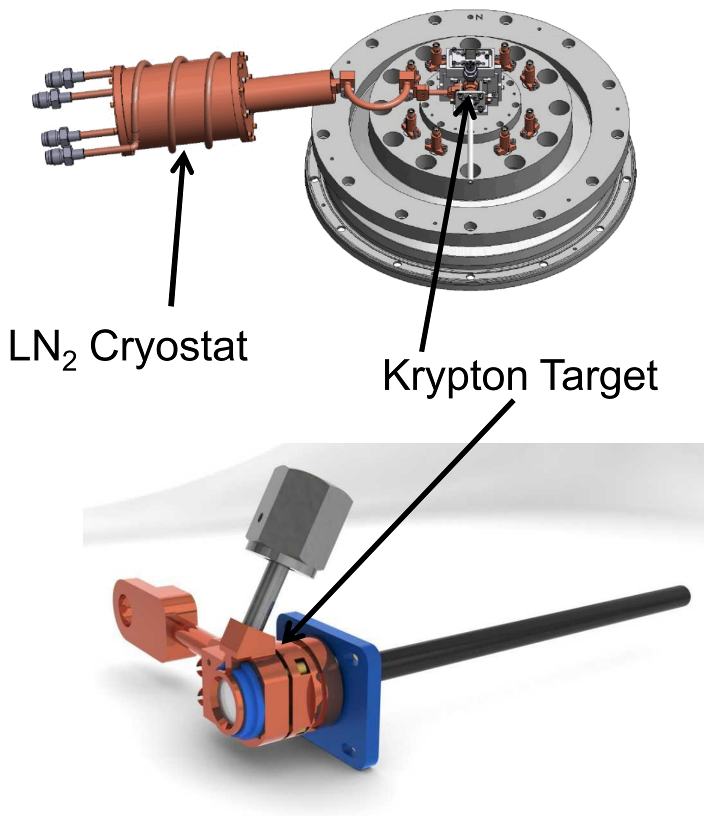


Need experimental data to validate the DFT simulations and EOS tables

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



- Target filled to ~16.8 PSI high purity Kr gas
- Cooled to 118 K with LN_2

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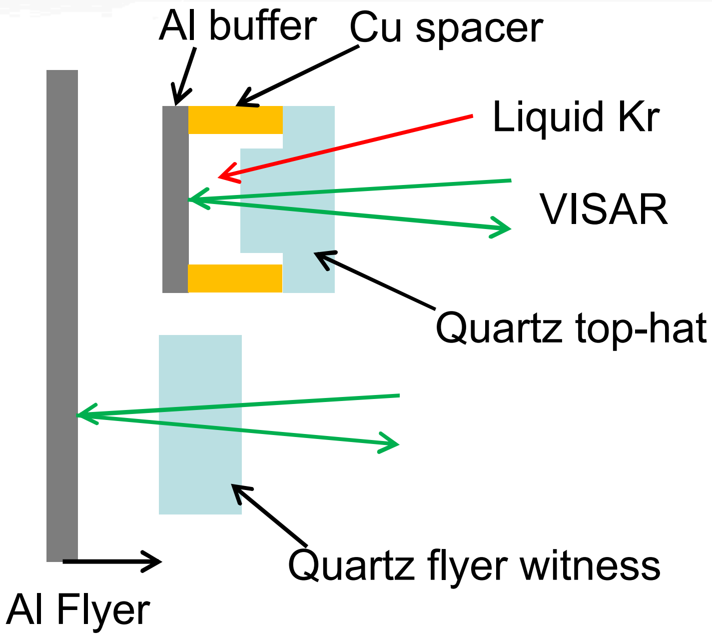
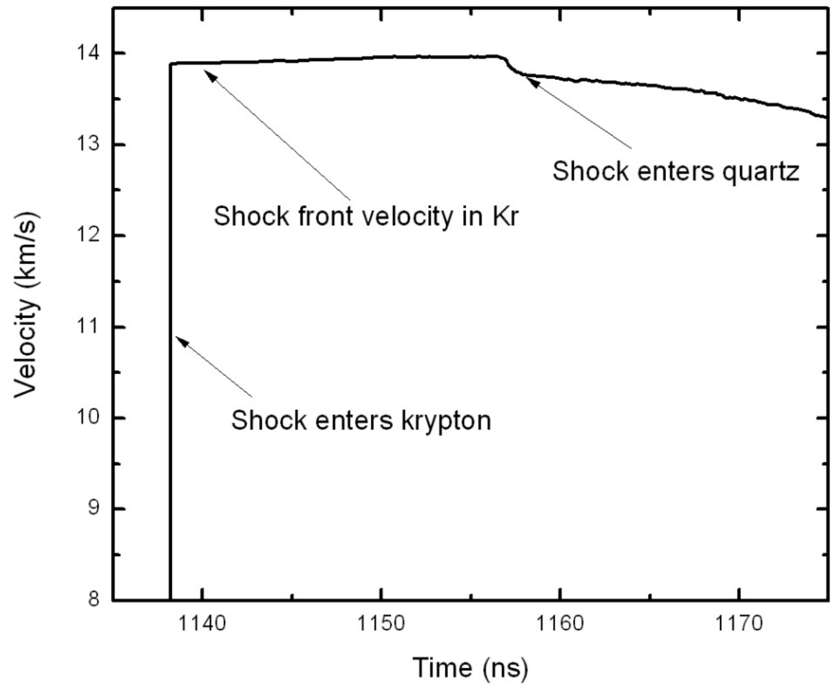
Experimental Approach





- Temperature = 118 K, Kr ρ_0 = 2.426 g/cc, Sample size ~ 250 μm
- Typically 4 different VPFs on target – reduce uncertainty
- Shock front in Kr is reflective – direct measurement of shock velocity
- Measure flyer velocity directly on the quartz flyer witness
- Starting from liquid provides a well-characterized, uniform initial state that is repeatable from experiment to experiment

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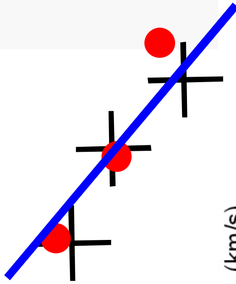
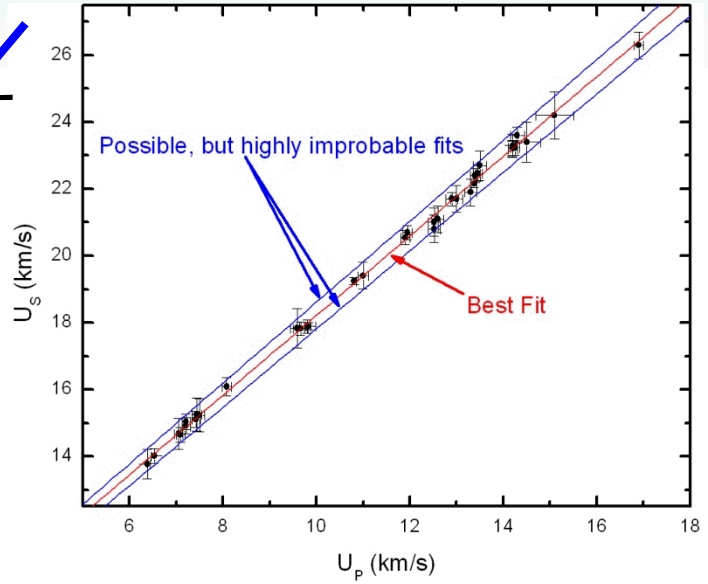
Monte Carlo (MC) Impedance Matching

Aluminum

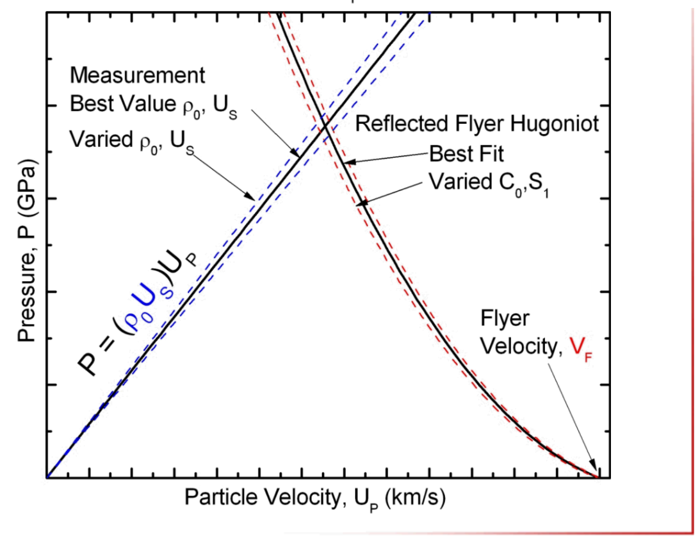
- Uncertainty in experimental data (Knudson *et al.*, JAP 2003)
- Vary each U_S-U_P point by an uncorrelated random number with σ = expt. Uncertainty
- Solve for linear fit parameters
- Determine mean, σ, and correlation of fit parameters





Krypton

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



Monte Carlo technique accounts for experimental uncertainty and propagates error in the Al standard into the resulting Kr data.

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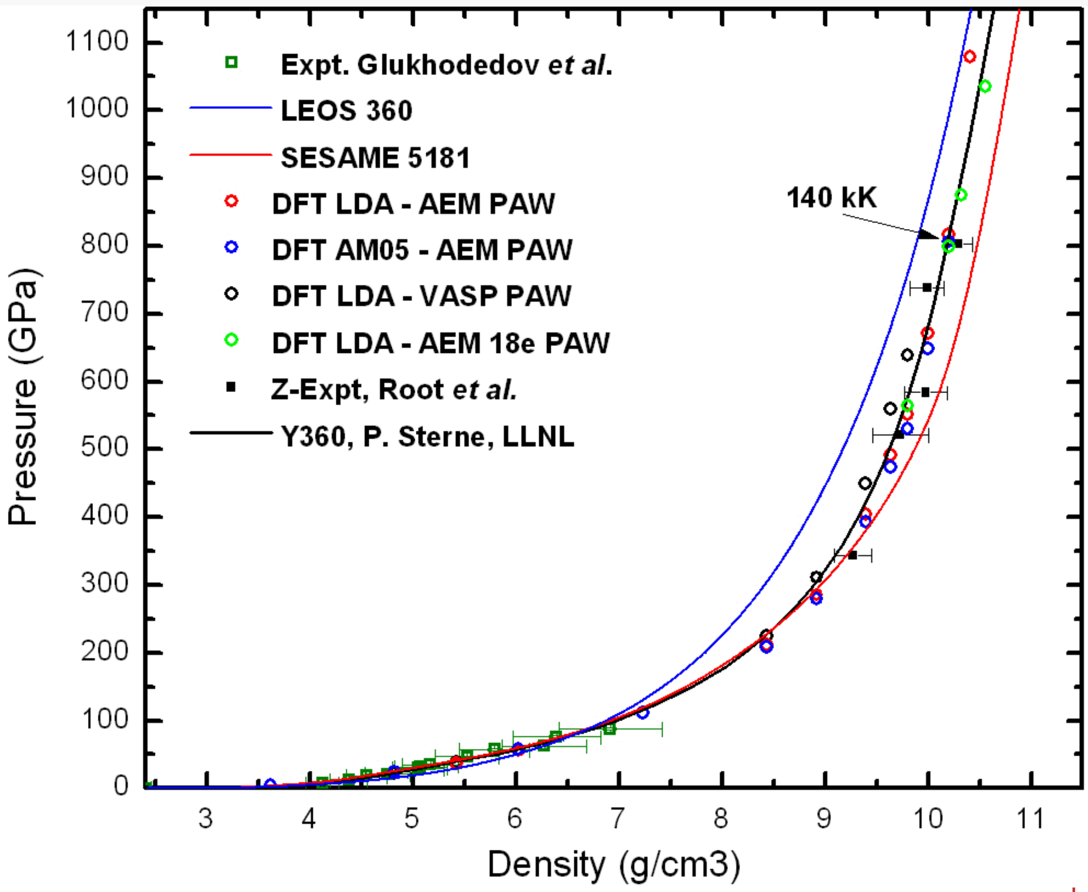
Experimental Results

- Hugoniot determined to 8 Mbar
- Used reflected Al Hugoniot to calculate Kr state
- Al density at 118 K used
- Using SESAME 3700 release shifts density lower ~ 1%
- AEM PAW results agree with experimental data
- VASP PAW too stiff
- SESAME 5181 agrees to 4 Mbar



New EOS is needed for situations above 4 Mbar

- Phil Sterne (LNLL) developing Y360 using DFT and Z-Expt. Results

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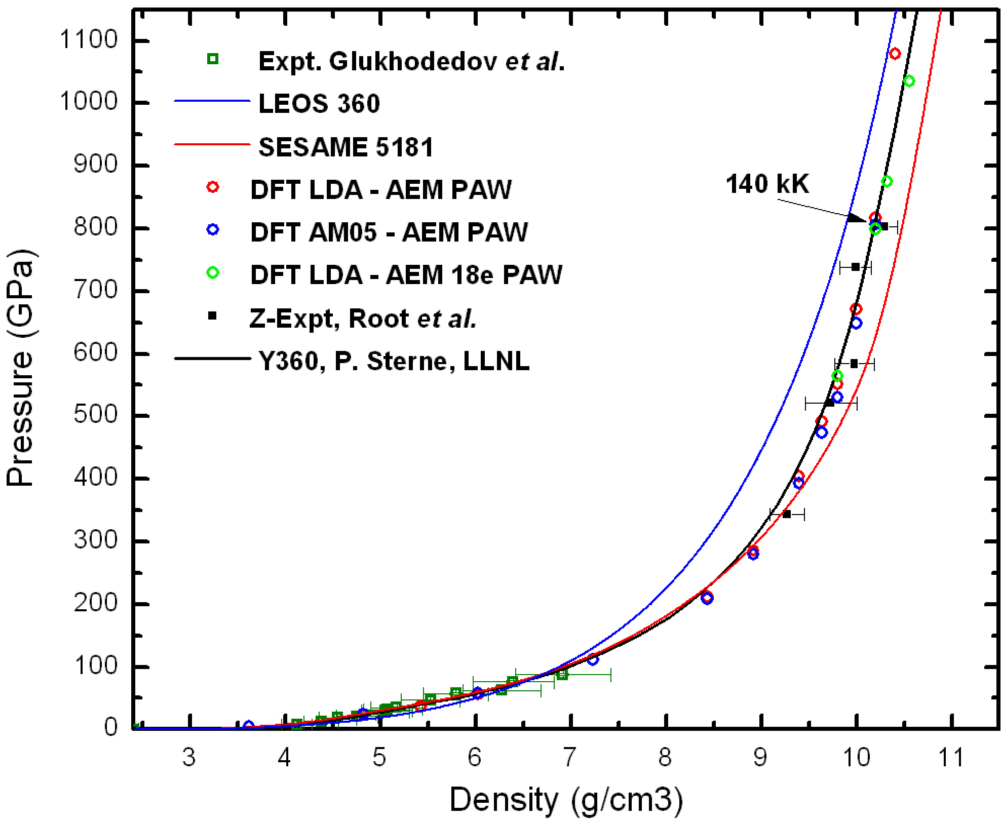
Summary



- Measured the liquid Kr Hugoniot to 8 Mbar
- Demonstrated the need for accurate psuedo-potentials
- Validated DFT results to 8 Mbar
- Showed that SESAME 5181 is reasonable to 4 Mbar
- Sterne's Y360 EOS reliable reproduces the Hugoniot to multi-Mbar pressures

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