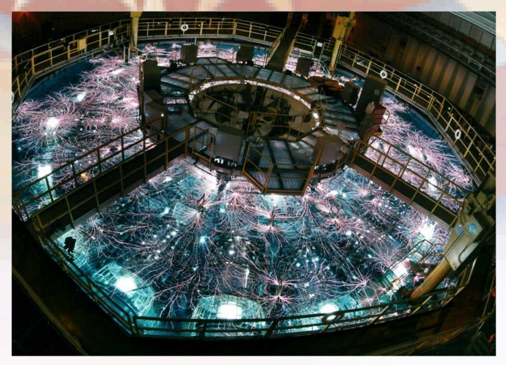
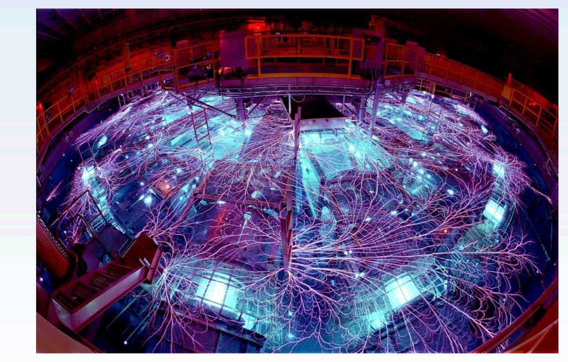
SAND2011-5940C

Liquid Krypton Hugoniot at Megabar Pressures





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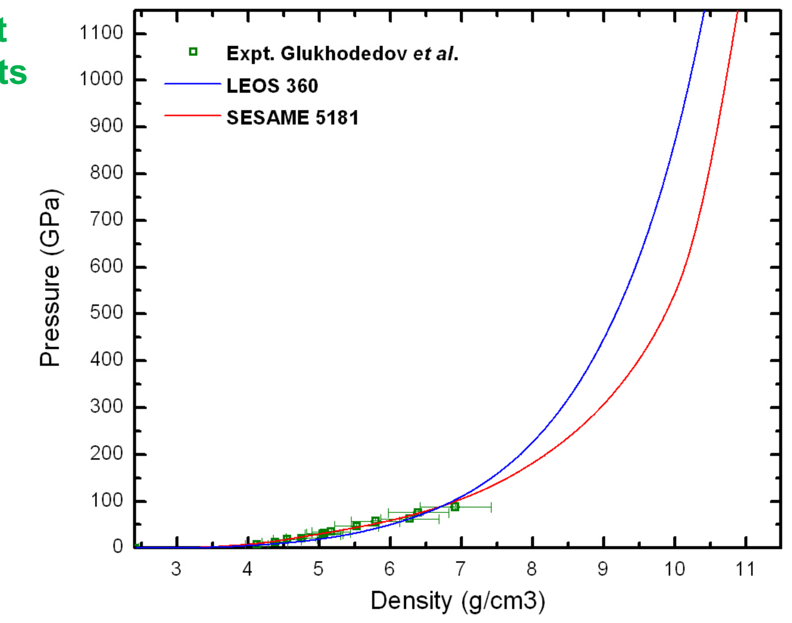
Shock Compression of Krypton

- 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

- Use Density Functional Theory simulations to calculate the krypton Hugoniot
- Experimentally measure the liquid krypton Hugoniot
- Use the DFT and experimental results to validate an EOS model

Density Functional Theory

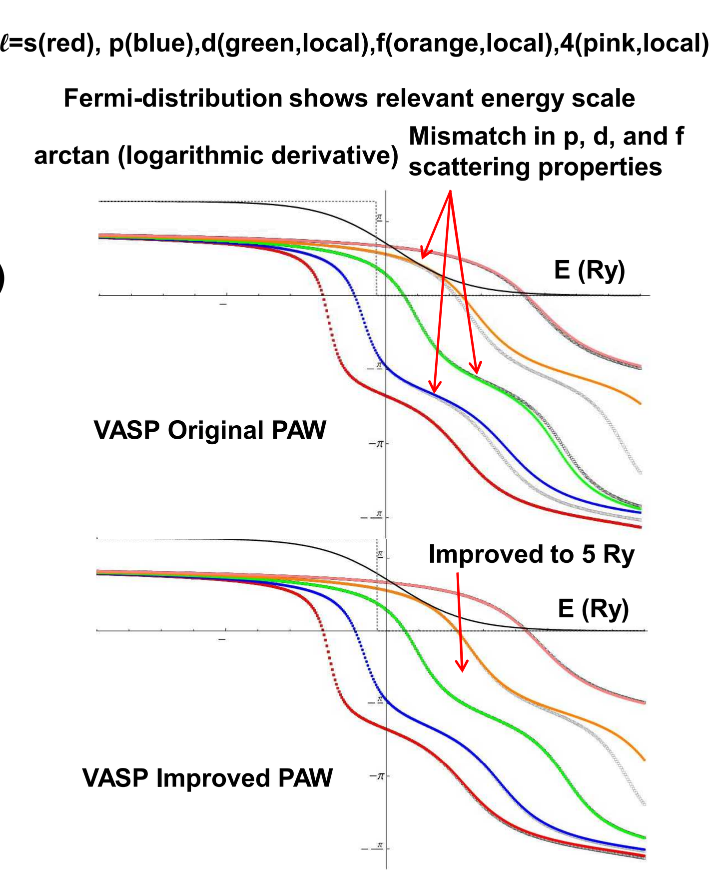
- DFT-MD simulations performed using VASP 5.1.40*
- Electronic states occupied according to Mermin's finite-temperature formulation
- Projector augmented wave core functions (PAW) potential for core electrons – 8 valence electrons
- Calculate energy and pressure for a given density and finite temperature
- Solve the Hugoniot Condition: $2(E-E_{ref})-(P+P_{ref})(v_{ref}-v)=0$

- Initial conditions: ρ_0 = 2.41 g/cc, T_0 = 118 K, 32 atoms
- LDA and AM05 exchange correlation functionals
- Convergence tested: number of atoms, energy cut off
- 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).

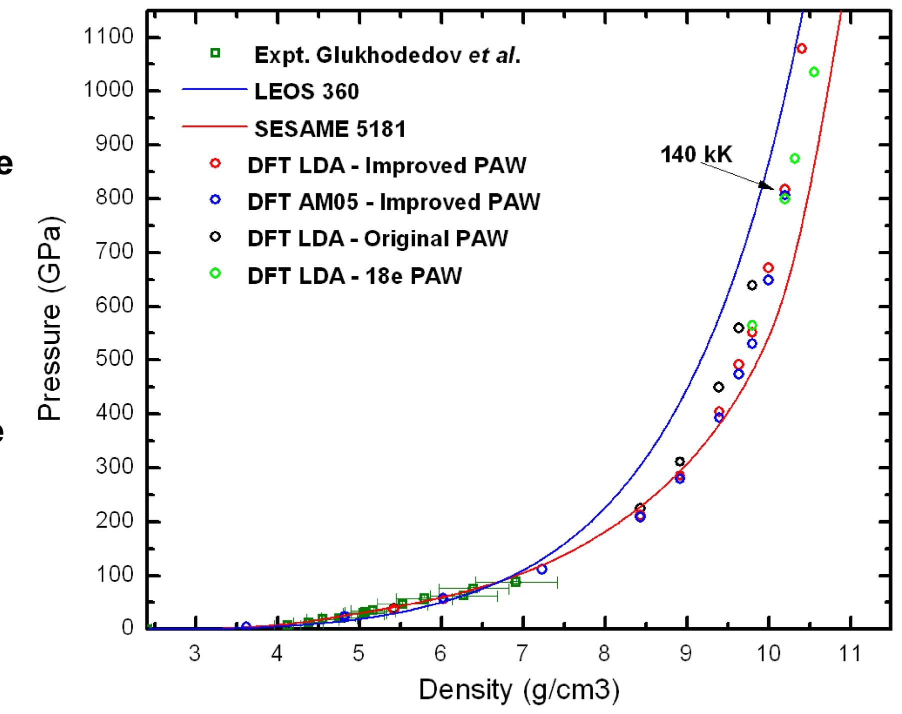
PAW Potential Improvement

- 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 original VASP 8e PAW is adequate for low T, but mismatch in logarithmic derivative as T (energy) increases
- The improved VASP 8e PAW has improved scattering properties at high energy and temperature
- Matches scattering properties to 5 Ry (68 eV)



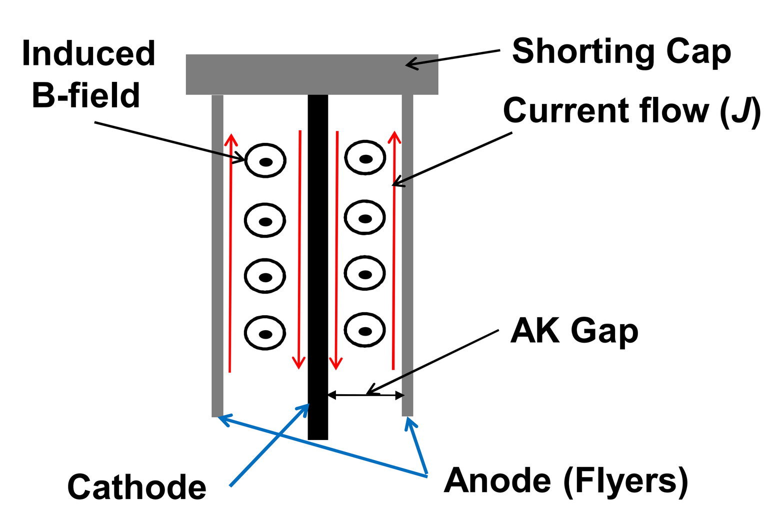
DFT Results

- DFT Results consistent with experimental Hugoniot data < 1 Mbar
- SESAME 5181 and the DFT results agree up to 4 Mbar
- Original VASP PAW trends stiffer
- At high T the PAW potential for core electrons is incorrect
- Core electrons can be excited out of the potential
- A modified PAW (with 18 valence electrons) developed for high T
- The 18e PAW agrees with the improved 8e PAW results to 8 Mbar

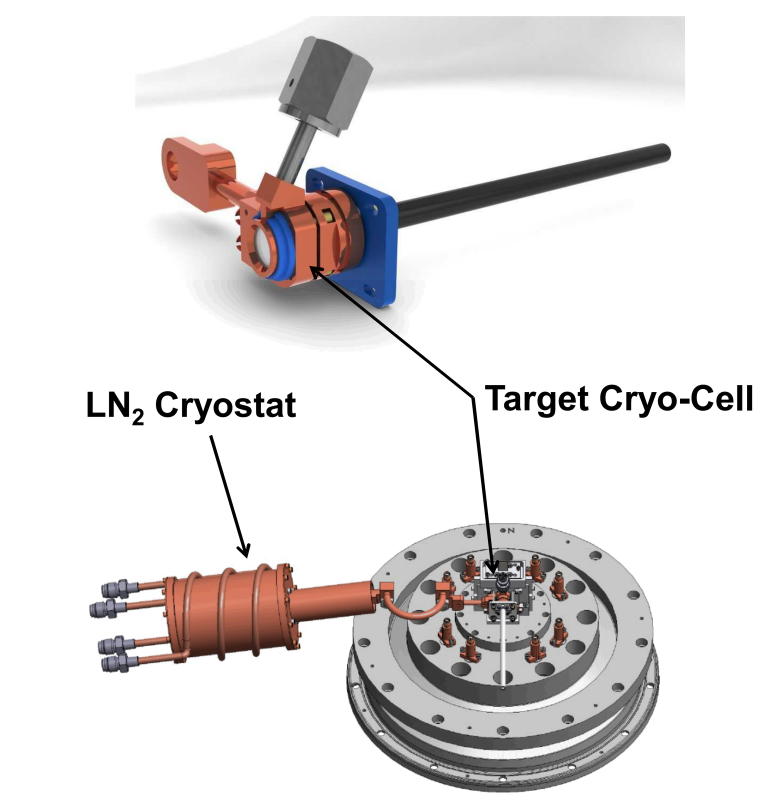


Need experimental data to validate the DFT simulations and EOS tables

Z-Experiment Setup

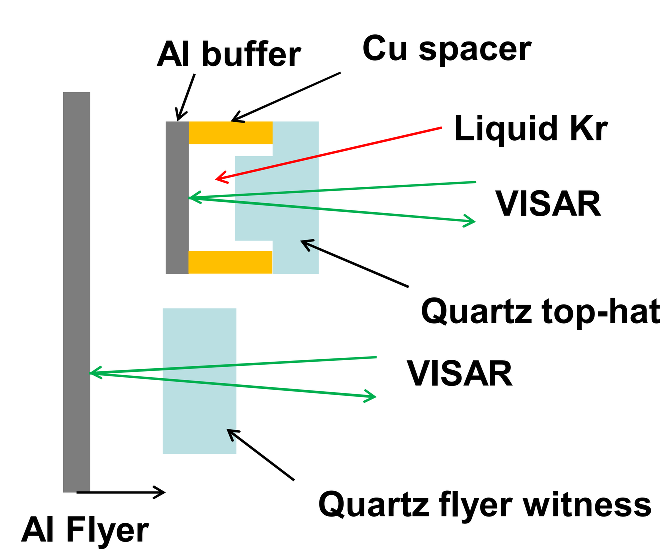


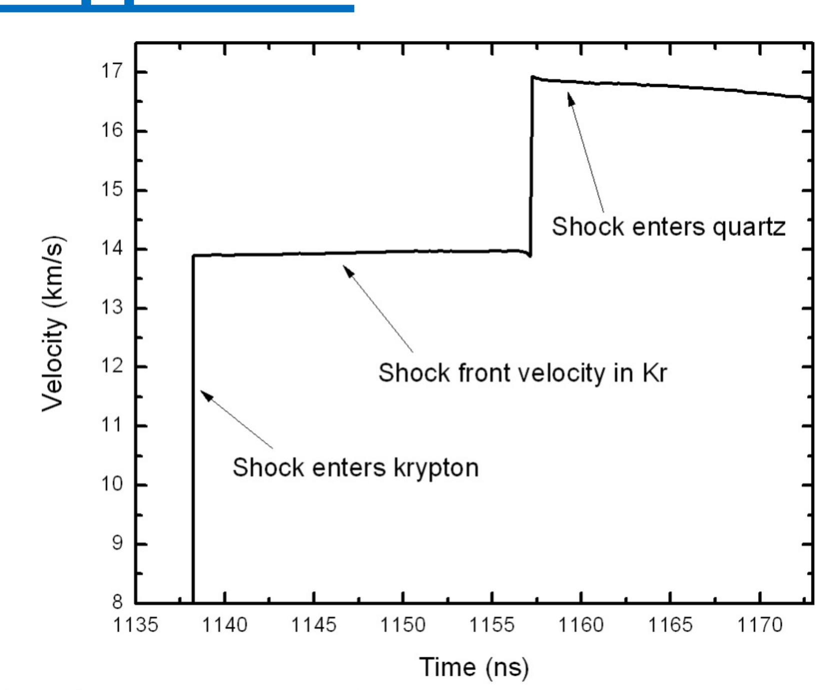
- Current pulse loops through shorting cap inducing a *B* – field.
- Resulting *J x B* force accelerates anodes (flyers) outward up to 40 km/s
- Asymmetric AK Gaps result in two different flyer velocities (two Hugoniot points per experiment)



- Target filled to ~16.7 PSI high purity Kr gas
- Cooled to 118 K with LN_2

Experimental Approach



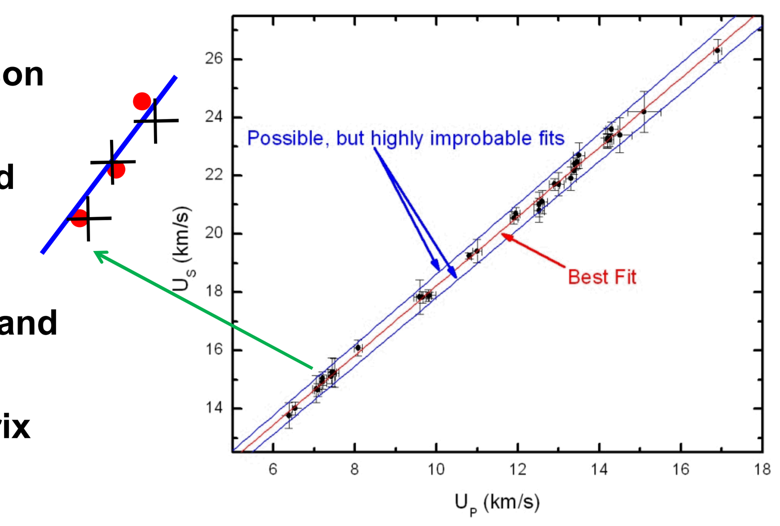


- Temperature = 118 K, Kr ρ_0 = 2.426 g/cc, Sample size ~ 250 μm
- Typically 4 different VPFs on target – reduce uncertainty
- Shock front in Kr is reflective – direct measurement of shock velocity
- Measure flyer velocity directly on the quartz flyer witness
- Starting from liquid provides a well-characterized,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

Monte Carlo (MC) Impedance Matching

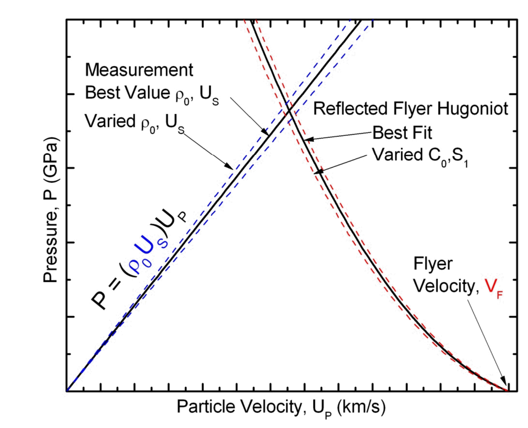
Aluminum

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



Krypton

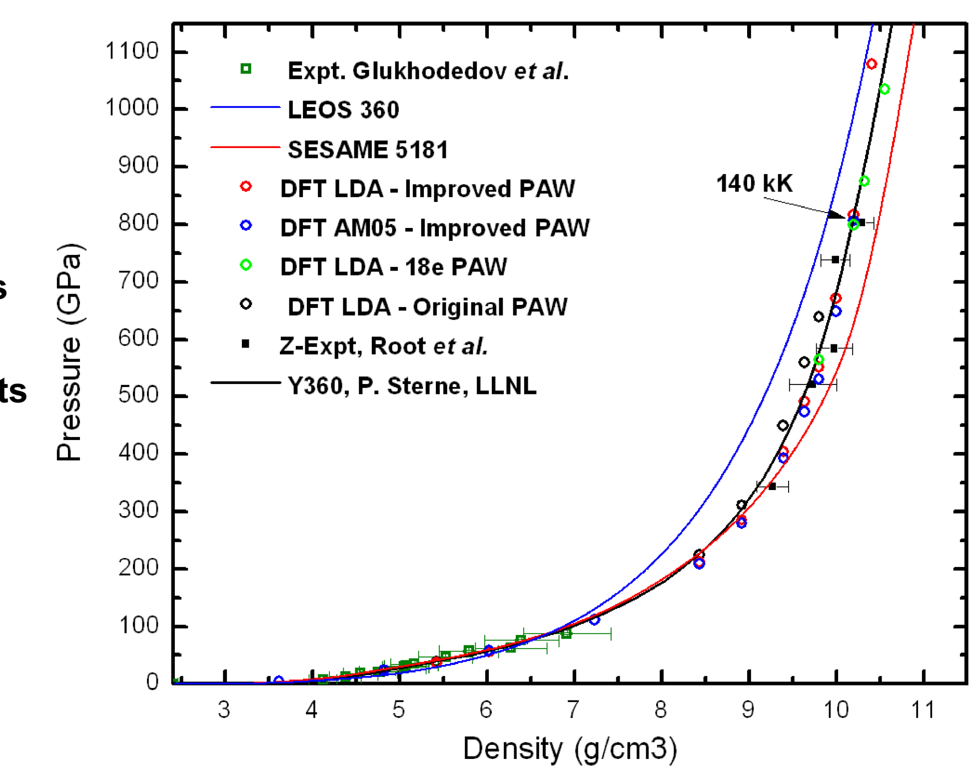
- Vary measured parameters (V_F, U_S, ρ_0) with uncorrelated random numbers, σ = experimental uncertainty
- Vary Al fit parameters using correlated random numbers
- Calculate U_P, P, and ρ
- Determine mean and σ



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

Experimental Results

- Hugoniot determined to 8 Mbar
- Used reflected Al Hugoniot to calculate Kr state
- Using SESAME 3700 release shifts density lower ~ 1%
- Improved PAW and 18e PAW results agree with experimental data
- Original VASP PAW too stiff
- SESAME 5181 agrees to 4 Mbar



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

Summary

- Experimentally measured the liquid Kr Hugoniot to 8 Mbar
- Demonstrated the need for accurate PAW potentials at high temperatures
- Validated DFT results to 8 Mbar
- Showed that SESAME 5181 is reasonable to 4 Mbar
- Sterne's Y360 EOS reliably reproduces the Hugoniot to multi-Mbar pressures

Acknowledgments

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