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Sandia National Laboratories

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Shock Compression Response of the Light Noble Gases: Neon and Helium

Seth Root*, Luke Shulenburger, Kyle Cochrane, Heath Hanshaw, Andrew Lopez, Keegan Shelton, Jose Villalva, and Thomas R. Mattsson

Sandia National Laboratories

Albuquerque, NM, United States

sroot@sandia.gov

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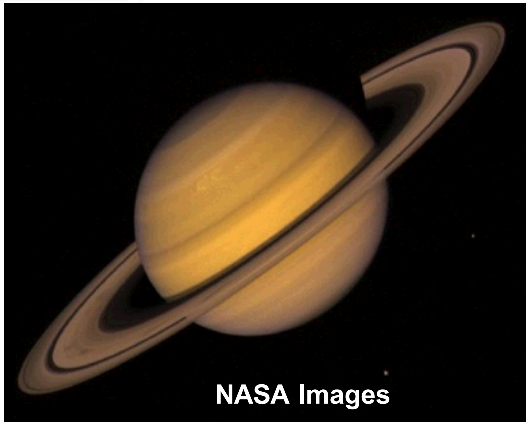
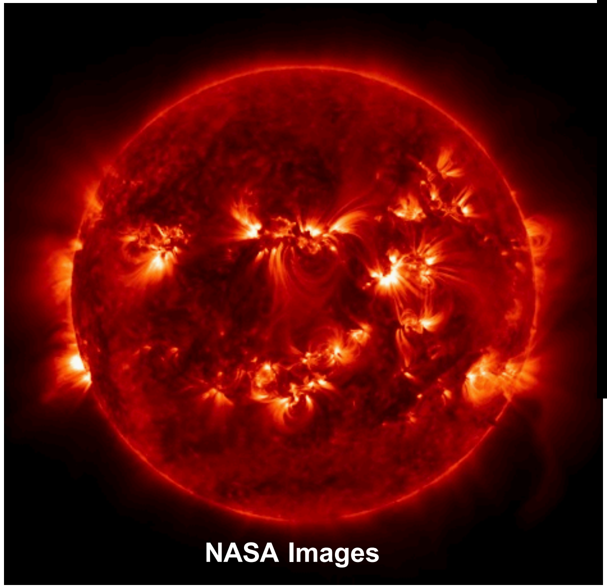
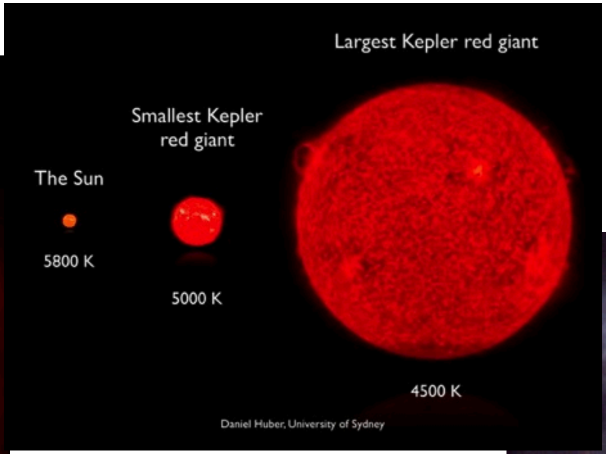
Helium and Neon in Astrophysical Systems

- Helium and Neon are 2nd and 5th most abundant elements in the universe
- Helium plays an important role in the evolution of stars and gas giant planets
- For massive stars (>8 solar masses) neon affects the internal structure

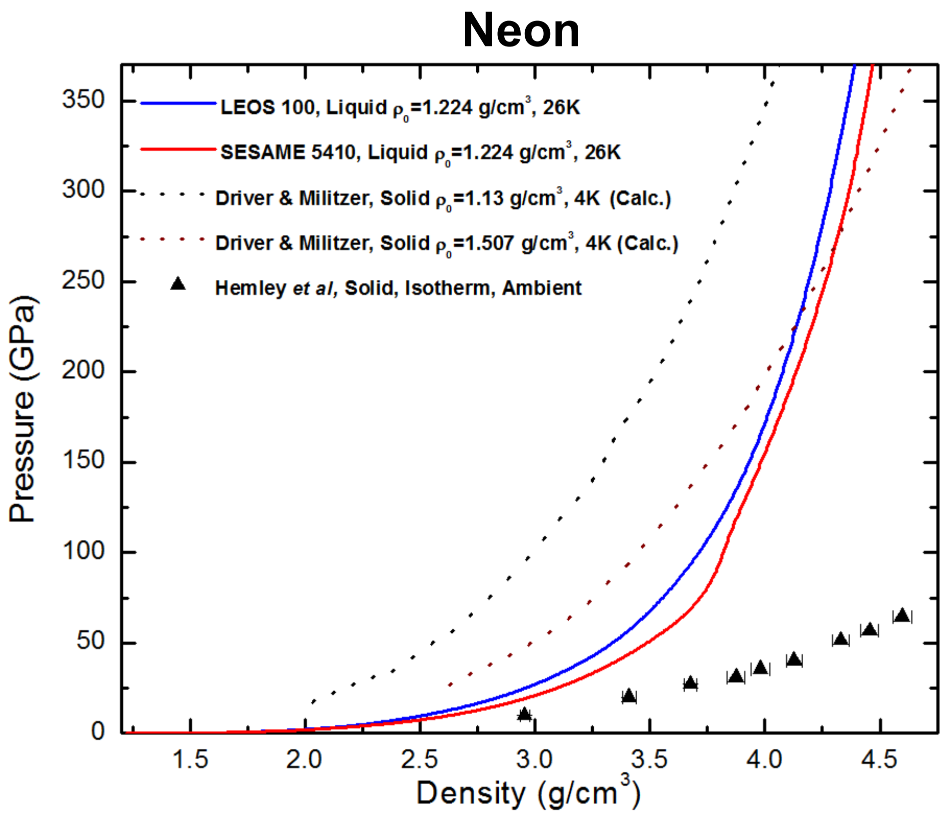






Neon Studies at High Pressures

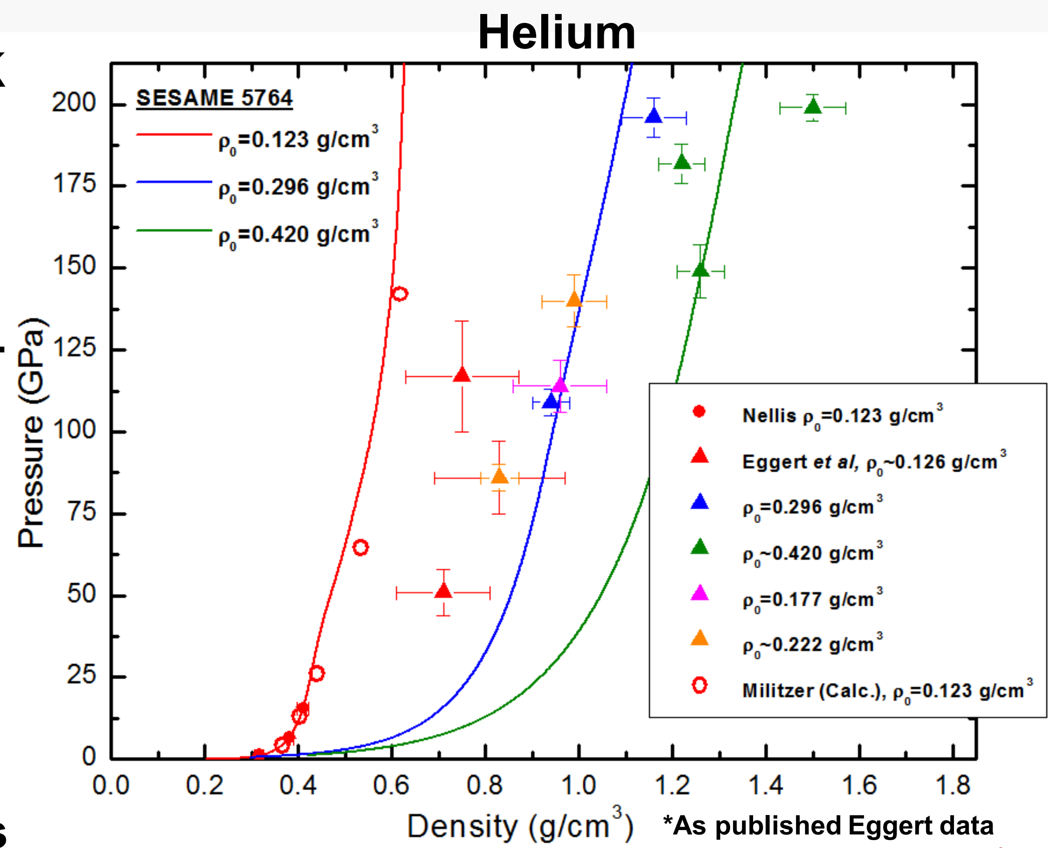
- Very limited data on neon at extreme conditions
- DAC data on solid neon to 110 GPa
- Driver and Militzer performed DFT and Path Integral Monte Carlo for several initial densities on Hugoniot
- Tabular EOS models exist: SESAME 5410 and LEOS 100, but made without any experimental data



R. J. Hemley *et al.*, Phys. Rev. B **39**, 820 (1989)
K. P. Driver and B. Militzer, Phys. Rev. B **91**, 045103, (2015)

Helium Data at High Pressures

- Nellis *et al.* (1984) performed 3 experiments on liquid He at 4.3 K
- Eggert *et al.* (2008) performed several experiments on pre-compressed He at various ρ_0
- Militzer performed PIMC and DFT simulations to calculate the He Hugoniot from the initial state of Nellis.
- Laser data showed over 6-fold compression
  - – a large difference compared to PIMC/DFT (PBE) calculations
- Kerley developed the SESAME 5764 table using the shock data from Nellis *et al.*



Colors represent similar initial density

W. J. Nellis *et al.*, Phys. Rev. Lett. **53**, 1248 (1984)
J. Eggert *et al.*, Phys. Rev. Lett. **100,** 124503 (2008)
B. Militzer, Phys. Rev. Lett. **97**, 175501 (2006)
G. I. Kerley, KTS04-2, Kerley Technical Services (2004) – SESAME 5764

NEON

DFT Simulations **Z Experiments**

High Pressure – High Temperature Behavior

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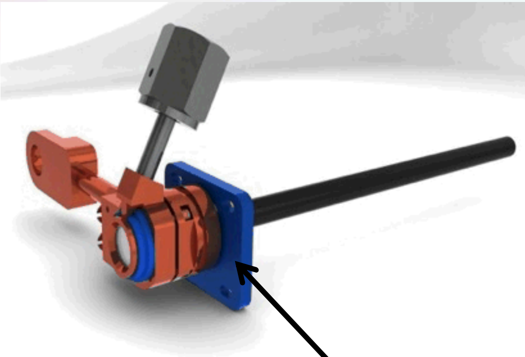
Density Functional Theory Calculations for Neon

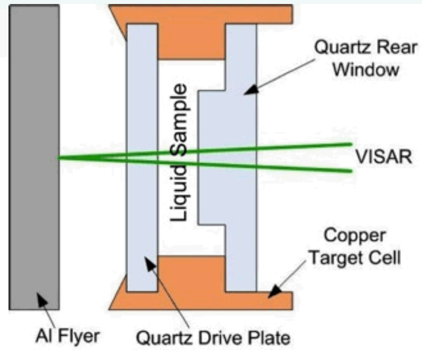
- DFT-MD simulations performed using VASP 5.3.3*
- Electronic states occupied according to Mermin's finite-temperature formulation
- Projector augmented wave core functions (PAW) potential for core electrons – 8 valence electrons, s2p6, (Ne_GW_02Oct2006)
- Calculate energy and pressure for a given density and finite temperature
- Solve the Hugoniot Condition: $2(E - E_{ref}) - (P + P_{ref})(v_{ref} - v) = 0$

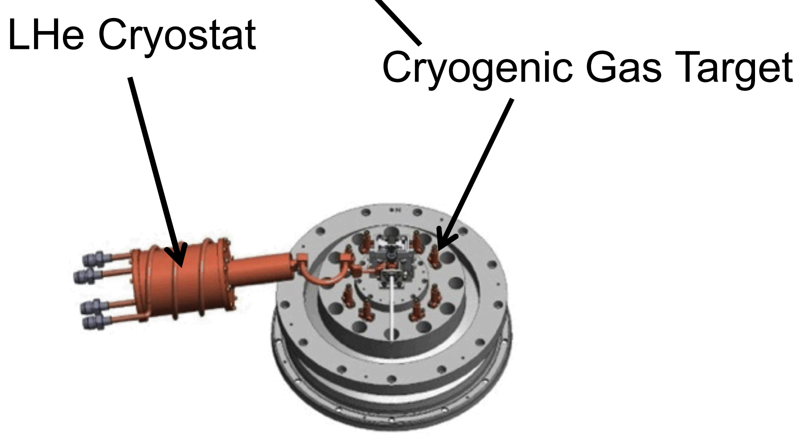
- **Initial conditions: ρ_0 = 1.224 g/cc, T_0 = 26 K, 108 atoms**
- **LDA exchange correlation functional**
- **Energy cut-off = 800 eV**
- **Methods demonstrated successfully: H_2O, C, MgO, quartz, Ar, Kr, Xe**

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

Neon Experimental Initial Conditions

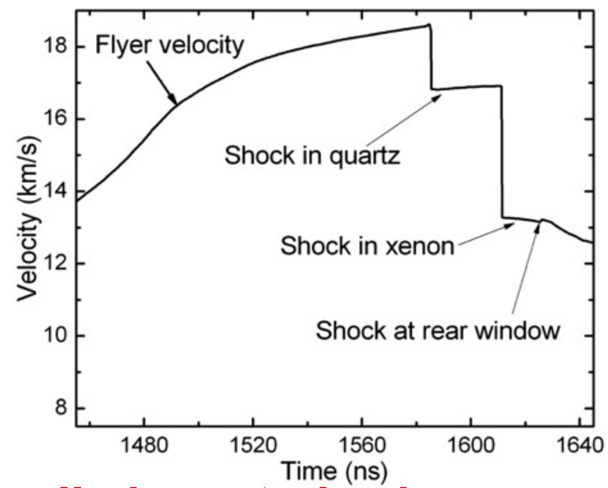






Liquid Neon Experiment

- T_0 = 26 K, ρ_0 = 1.224 g/cc
- n = 1.09
- Reflective shocks in the quartz and neon sample
- Multiple VPFs for improved precision



- **Starting from liquid state provides a well-characterized, reproducible initial state for all experiments**
- **Direct measurements of shock velocities leads to high accuracy results**

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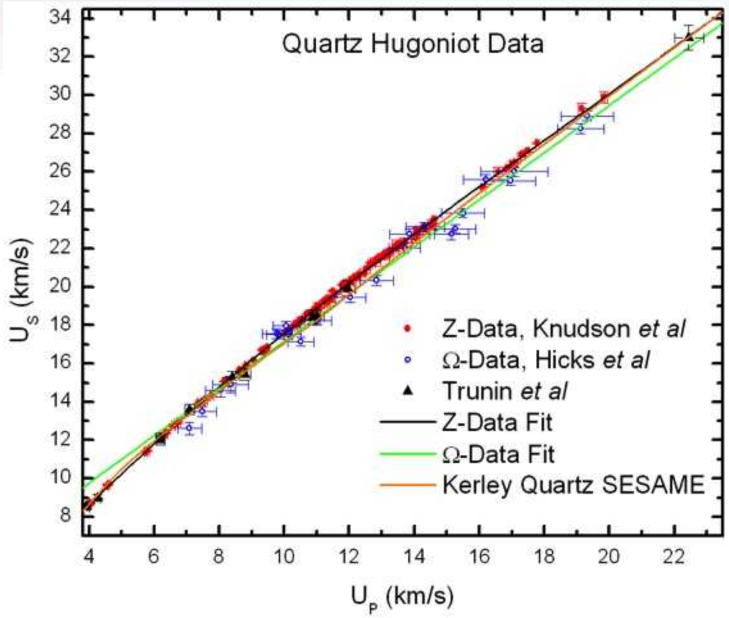
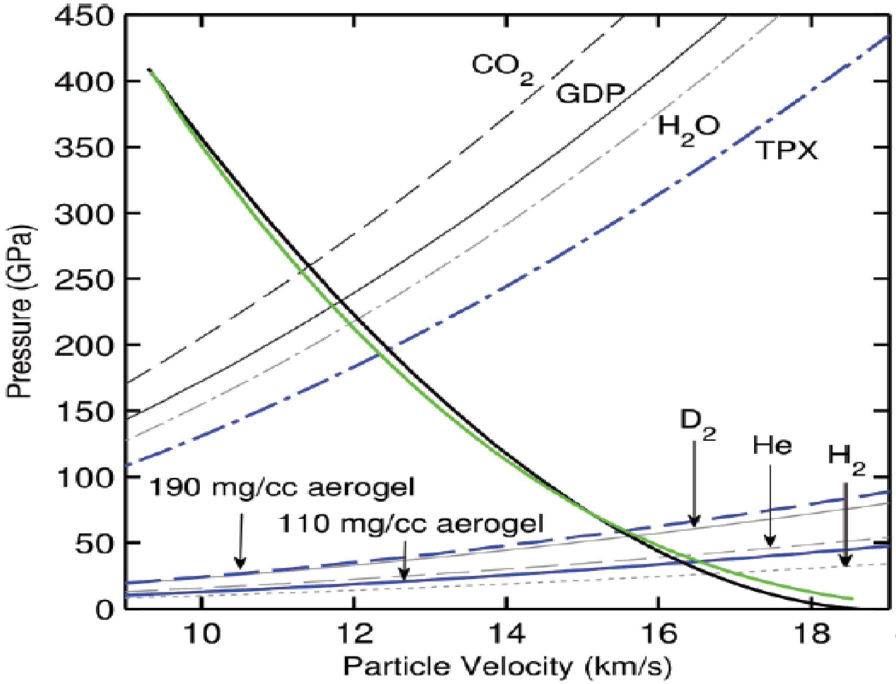
Quartz Hugoniot and Release



- **Monte Carlo Analysis method to determine He and Ne Hugoniot states**
- **Nearly 300 quartz Hugoniot data points**
- **Determine an effective Gruneisen Γ as a function of quartz Hugoniot state**
- **Calculate the quartz release path**

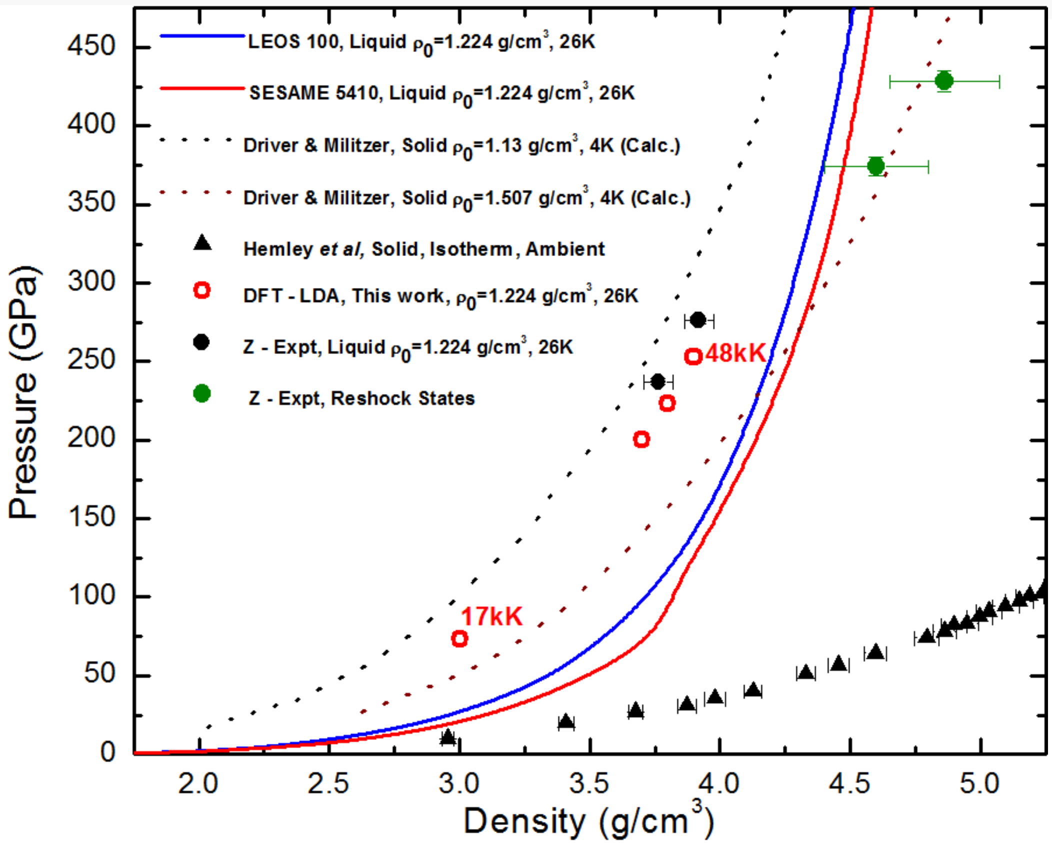


M. D. Knudson and M. P. Desjarlais, Phys. Rev. B **88**, 184107 (2013)

- **For lower density gases: reflected versus release difference is significant**
- **Thermal contraction in quartz is small (~0.5% at 2K) –only a density change for impedance calculation**
- **Accurate/Precise Standards = Accurate/Precise Results**

Experimental and Calculation Results: Neon

- Peak shock pressures of 275 GPa and 237 GPa
- Reshock state pressures of 374 GPa and 430 Gpa and ~4 times compressed from ρ_0
- DFT-LDA to 250 GPa
- The DFT results are consistent with the experiments
- Driver & Militzer calculations are consistent with data
- EOS tables had no data to use for their construction



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HELIUM

DFT Simulations → **Z Experiments**

High Pressure – High Temperature Behavior

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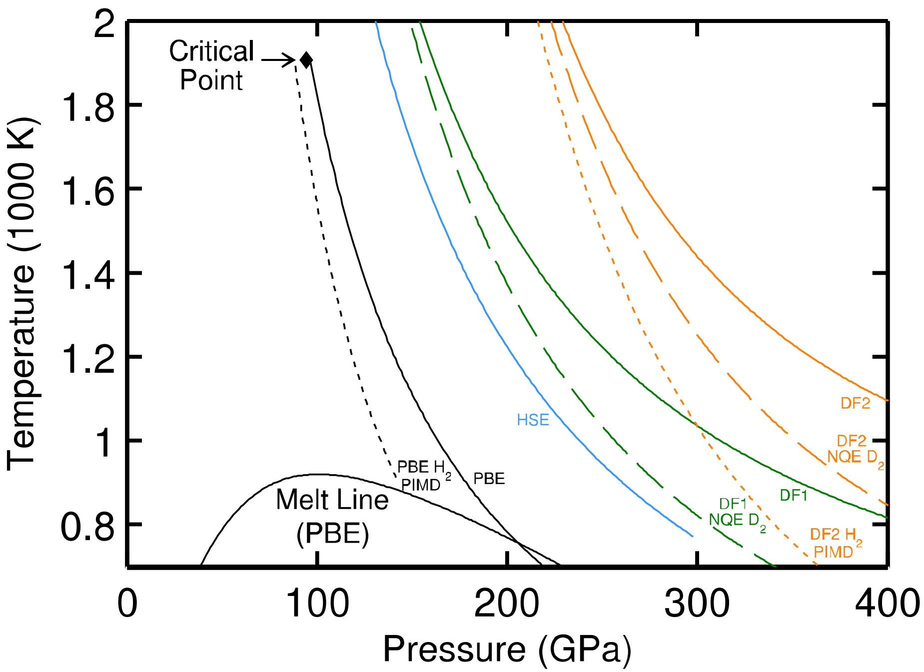
DFT Methods for Helium

- For light elements, exchange correlation functionals and quantum nuclear effects have a significant effect on the DFT simulation



The phase boundary for the liquid-liquid phase transition in hydrogen spans a broad range depending on XC functional and quantum nuclear effects.

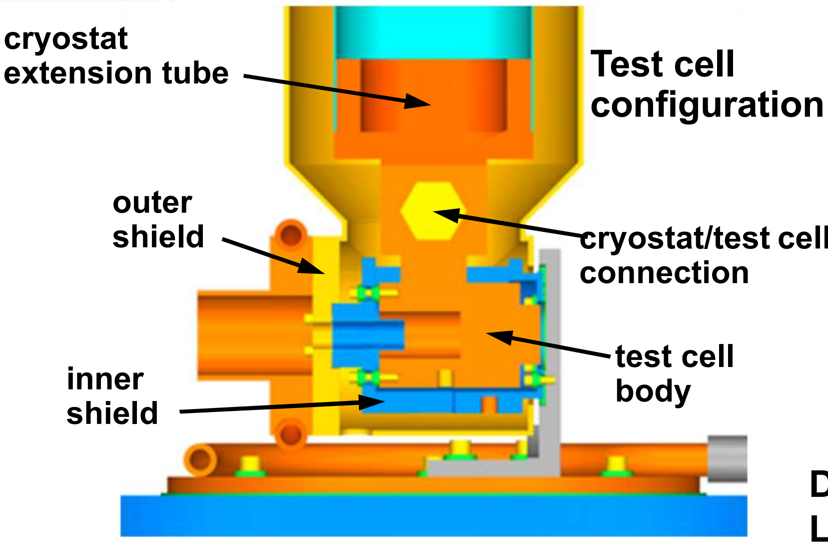
M.D. Knudson et al, SCIENCE, accepted (2015).

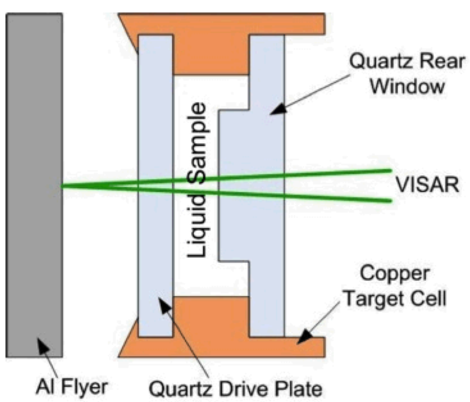
- **VASP (5.3.3)**
- **van-der Waals corrected functional, DF-2, [Lee et al, 2010] (for hydrogen, the functional that agreed best with Z data at high temperature**
- **108 atoms, PAW core functions**
- **Complex k-point sampling (1/4,1/4,1/4)**
- **Finite temperature DFT [Mermin]**
- **Nuclear treatment**

  Standard MD
  Path-integral discretization (in progress)

The combination of van-der Waals functionals and quantum nuclear effects should provide a high-fidelity description of He

Helium Experiments

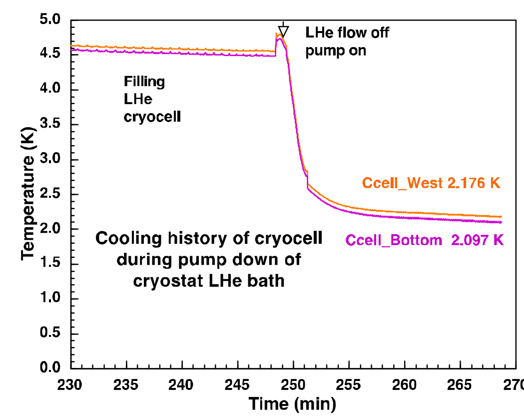




Liquid Helium Experiment

- T_0 = 2.14 K, ρ_0 = 0.147 g/cc
- n = 1.03
- Reflective shocks in the quartz and helium sample
- Multiple VPFs for improved precision

Details on the cryostat and cooling methods in A. Lopez *et al*, SCCM 2015 (the talk previous)



- **Starting from liquid state provides a well-characterized, reproducible initial state for all experiments**

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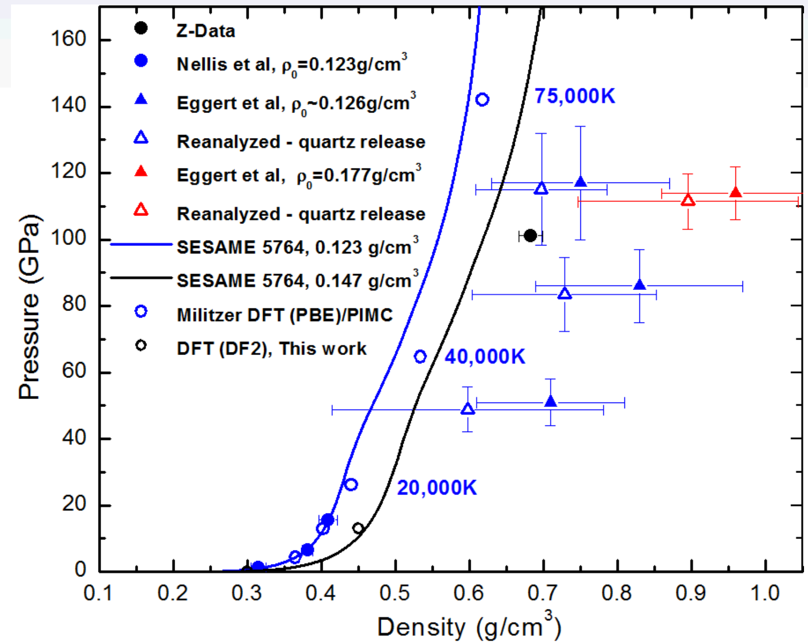
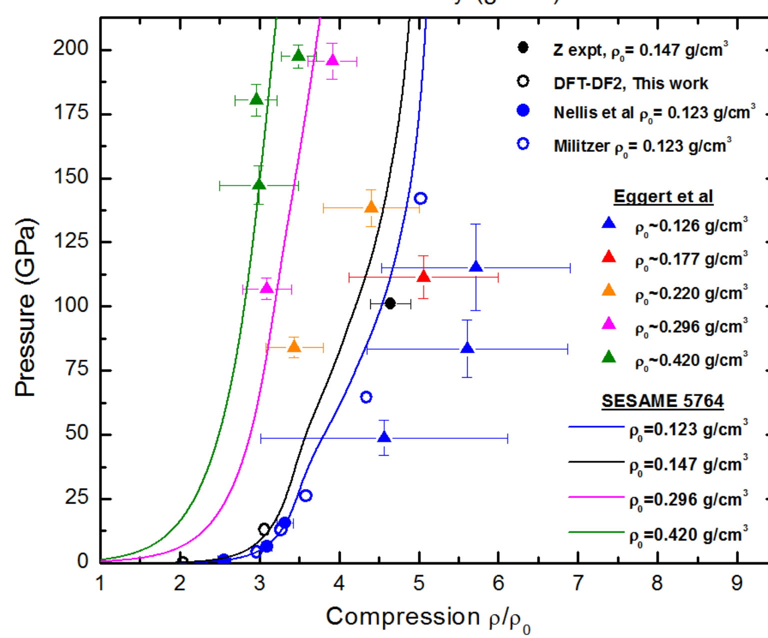
Helium Results

- **Direct measurement of shock velocities and high precision Hugoniot standards provide accurate & precise data**
- **Z – experimental Hugoniot point reached 101 GPa**
- **Z data shows 4.64 compression**
- **Our DFT simulations using DF2 XC show good agreement with the Kerley EOS**
- **Reanalyzed Eggert *et al* data shows higher compression when compared to Militzer's calculations**
- ***More work needed!***





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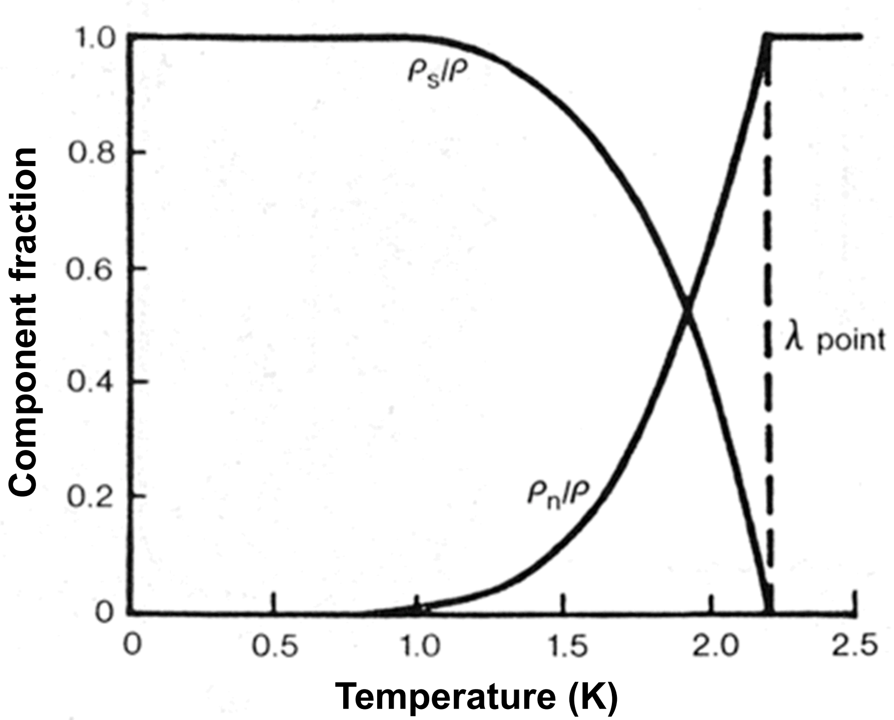
SUMMARY

- First experimental data set on Neon
  - Hugoniot state up to 3.2 compression and 275 Gpa
  - Reshock state up to 4 compression and 430 Gpa
- DFT simulations using LDA show good agreement with the experimental data
- Measured a Hugoniot state for liquid Helium at 4.65 compression and 101 Gpa
- Our preliminary DFT simulations using the DF2 XC functional show reasonable results
- More experiments on Helium upcoming
- Currently working on Path Integral Monte Carlo calculations for Helium at higher pressures and temperatures

Extra Slides

The quantum liquid ^{4}He II behaves as a mixture of a normal fluid and a superfluid component

As the temperature is reduced below the λ-point, more He atoms occupy the ground state



The normal fluid consisting of He atoms in excited states carries all the entropy of the liquid and has normal viscosity

The superfluid component consisting of He atoms in the ground state of the Bose-Eistein condensate has zero entropy and very little viscosity

The normal and superfluid components are completely mixed and do not interact

A superfluid He II film with vanishing viscosity can move up the walls of a He bath fill tube by frictionless flow until it reaches a hotter region and evaporates

At 2.14 K, the sample is predominately normal Liquid Helium

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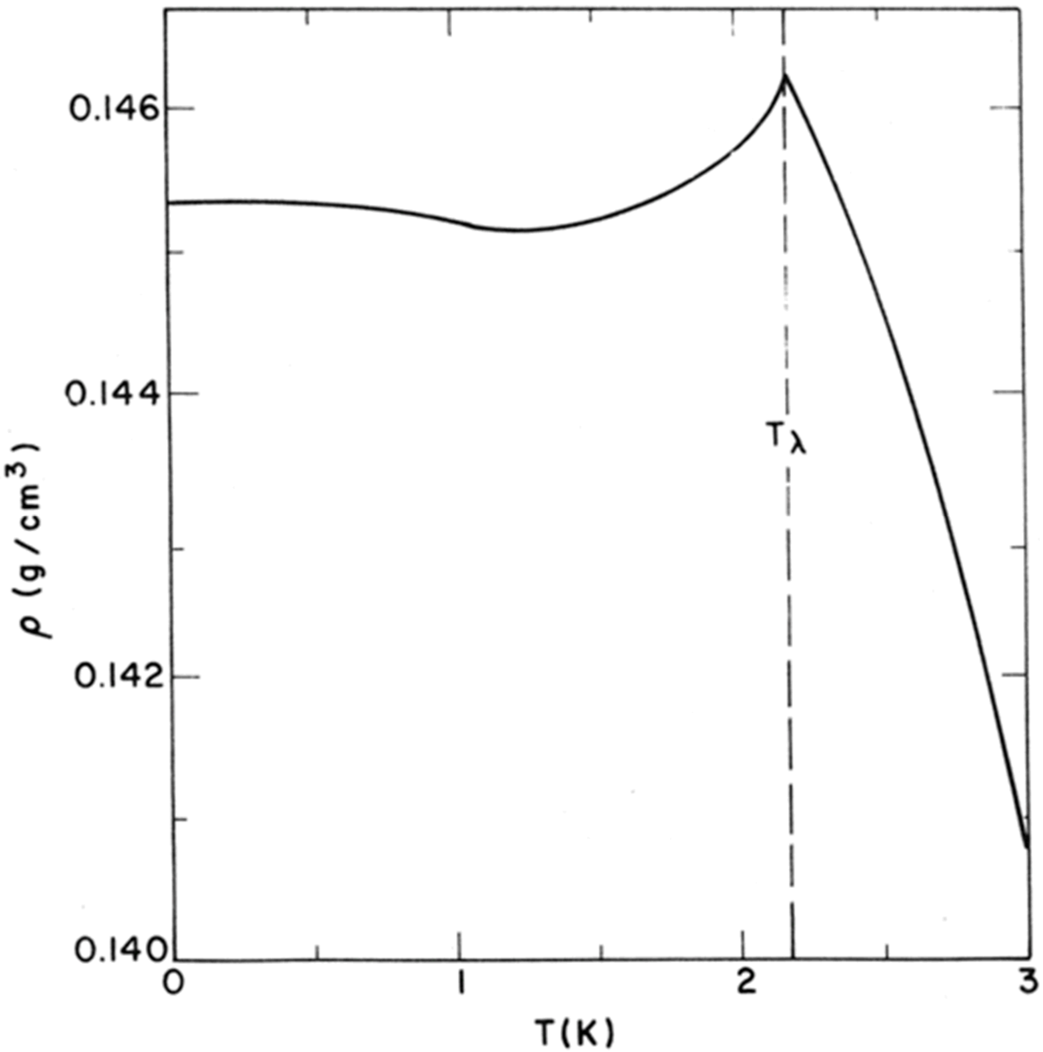
A superfluid He II sample has the advantage that its density as a function of temperature is relatively constant below the λ-point



Below T_λ = 2.177 K, it does not require a super accurate temperature measurement to determine the initial LHe sample density to 0.1%

Also, the LHe sample density does not vary significantly with small (100 mK) temperature fluctuations