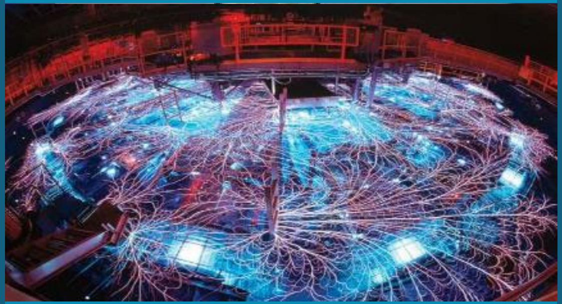
SAND2022-9025C

Sandia National Laboratories

Principal Hugoniot and temperature measurements in liquid neon at multi-megabar pressures



PRESENTED BY

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22nd Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter
July 11-15, 2022
Anaheim, California

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Acknowlegements

OMEGA experiments – Julie Fooks (target assembly), Roger Janezic (cryo support), Jared Hund (target fabrication) and EP operations

Z experiments – Jeff Gluth and Ed Scoglietti (Z VISAR support), Andrew Lopez and Keegan Shelton (Z cryo support), Z operations team

Summary

Neon is the 5th most abundant element in the universe and is an important constituent in planetary atmospheres of gas giant planets

Due to large bandgap and closed shell, it poses difficulties for molecular dynamics methods

- Previous calculations[1] have shown that bandgap persists to >10^6K and >15 g/cm^3
- No shock data exists for neon to benchmark molecular dynamics simulations

Principal Hugoniot was measured using laser-driven shocks on OMEGA Laser Facility and impact experiments on Z facility

- Experiments ranged from 120-560 GPa
- Reshock pressures measured to 600 GPa

DFT-MD calculations of principal Hugoniot made up to 500 GPa

Experiments and DFT in excellent agreement above 150 GPa

- Insufficient data to compare at lower pressures

Shock temperature measurements agree well across all tables and experiments

[1] Driver and Militzer, Phys Rev B **91**, 045103 (2015)

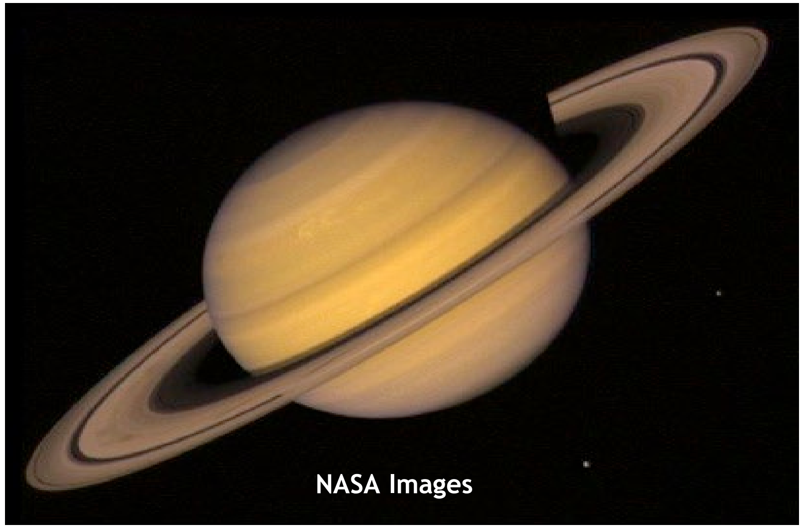
Understanding neon is important for astrophysical models

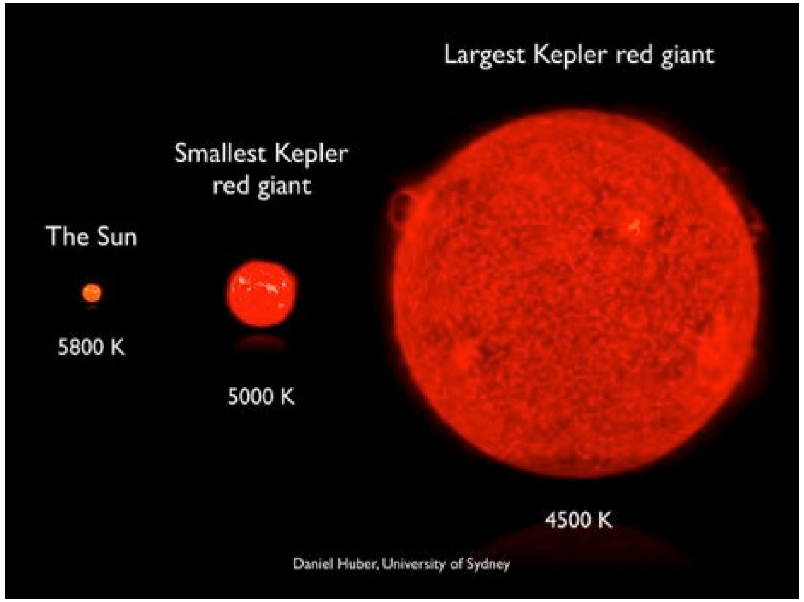
5th most abundant element in universe

Key constituent of gas giant interiors – may help explain difference in temperature between Saturn and Jupiter[1]

Affects internal structures of stars >8 solar mass

Knowledge of properties at extreme conditions will help improve models of planetary and stellar formation and interiors





[1]McWilliams, *et al*, PNAS **112** (26), 7925-7930 (2015)

OMEGA target designs enabled measurement of two Hugoniot states, reshock state, and decaying shock temperature on single shot

Two OMEGA cryo target designs were used for experiments

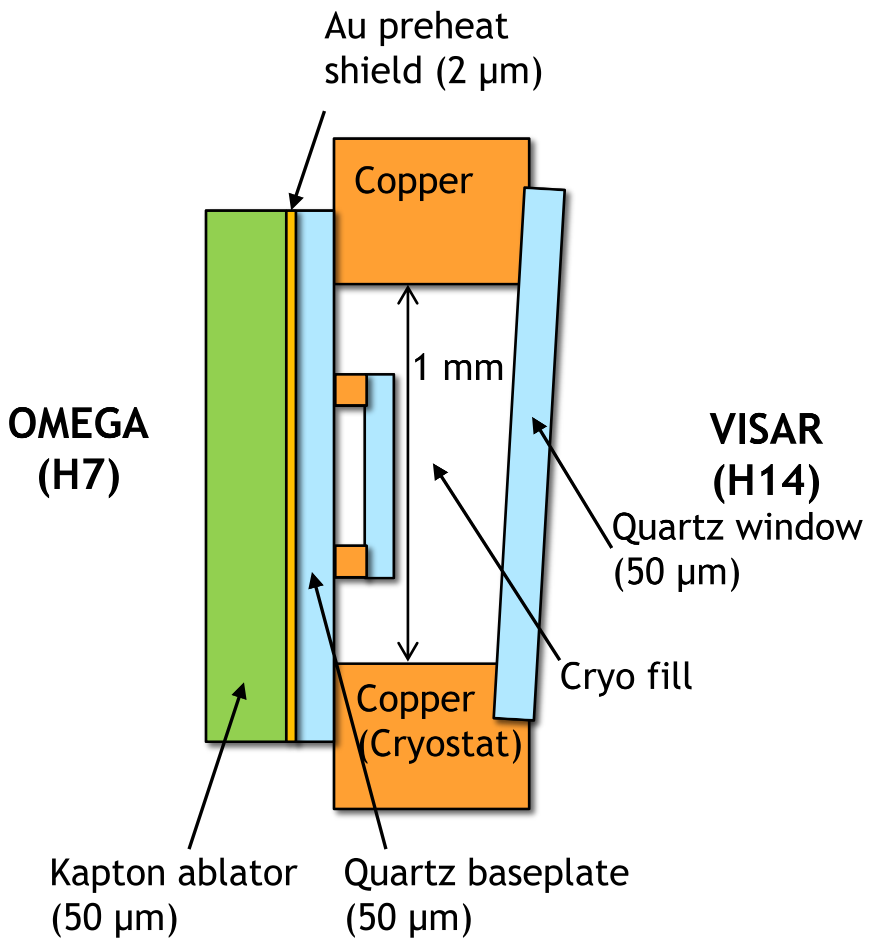
- Updated design included thin quartz reshock anvil to enable two principal Hugoniot and one reshock state on single shot
- Hugoniot results determined using quartz release model[1]
- Targets cooled to initial temperature of 26K for initial density $\rho_0 = 1.224\ g/cm^3$

Reflecting shocks recorded with VISAR in both quartz and neon for direct measurement of shock velocity at all impedance match locations

Decaying shock used to extract temperature with SOP

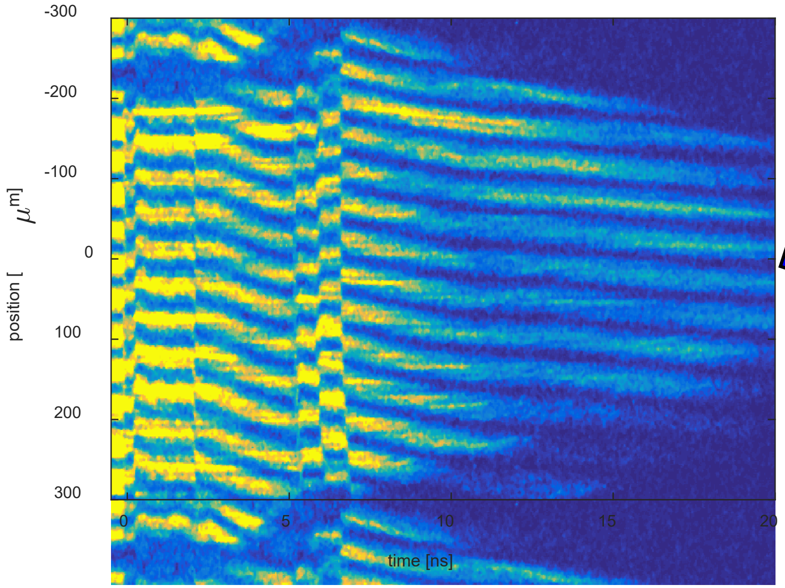
- Additional shots on shot day used thick quartz samples for relative SOP calibration

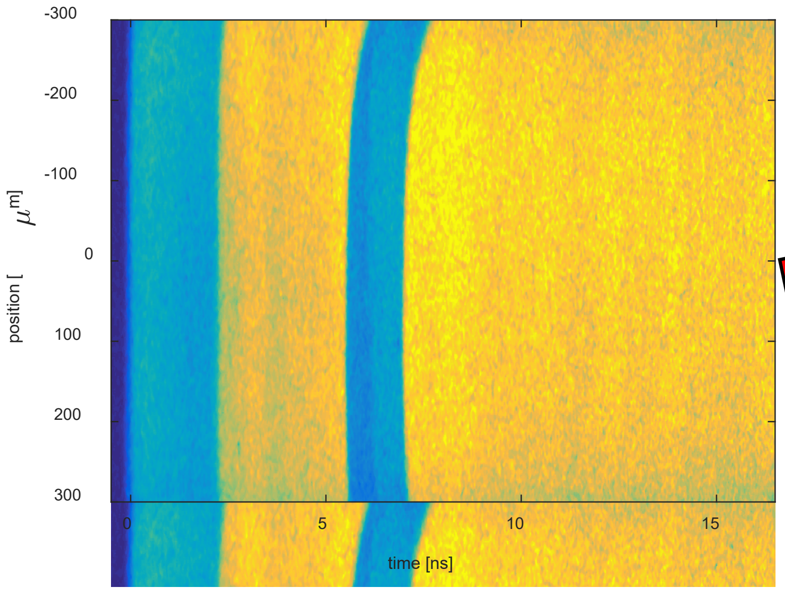
Laser intensities up to 900 PW/m^2 used to drive shocks in samples

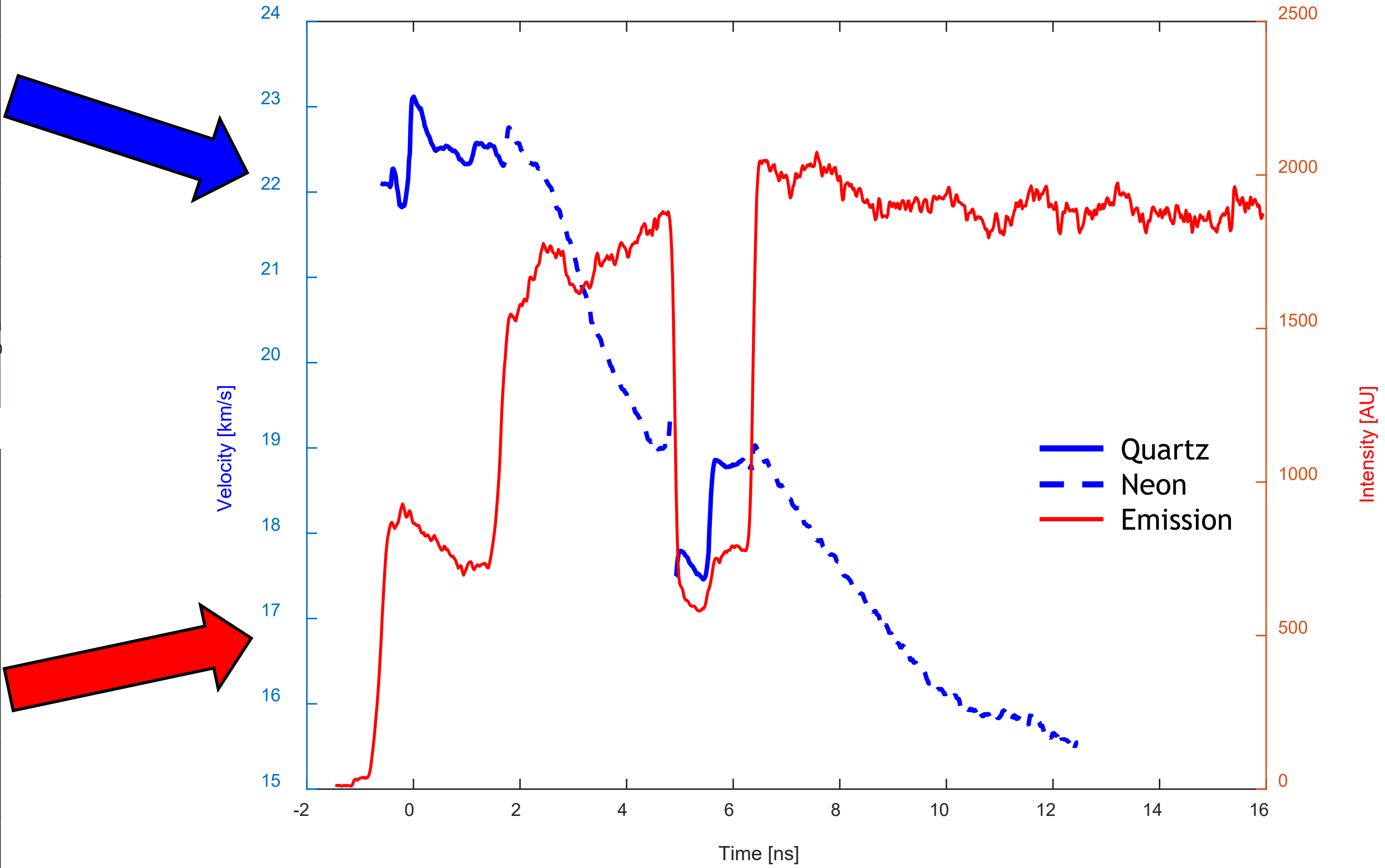


[1]Desjarlais, Knudson,and Cochrane, J. Appl. Phys. **122**, 035903 (2017)

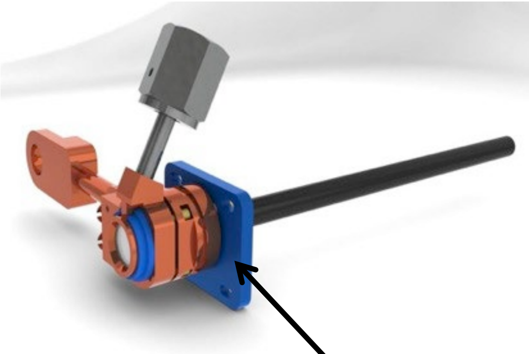
Exceptional data quality was recorded for OMEGA shots

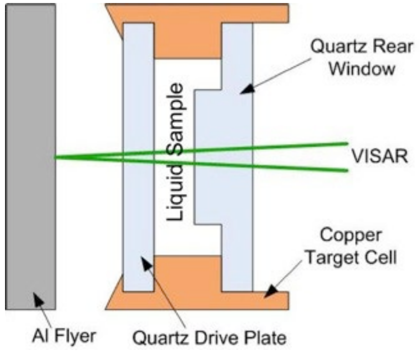






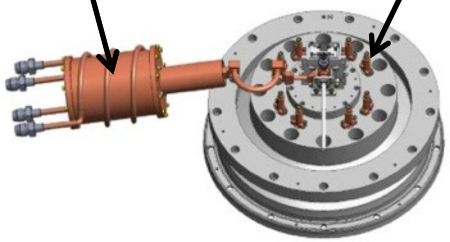
Neon Experimental Initial Conditions





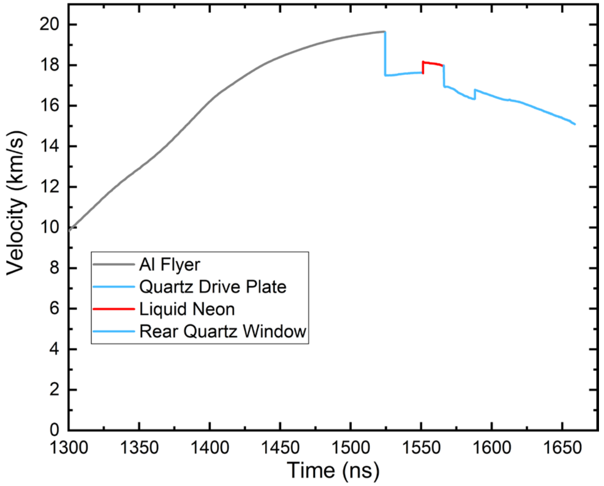
LHe Cryostat

Cryogenic Gas Target



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**

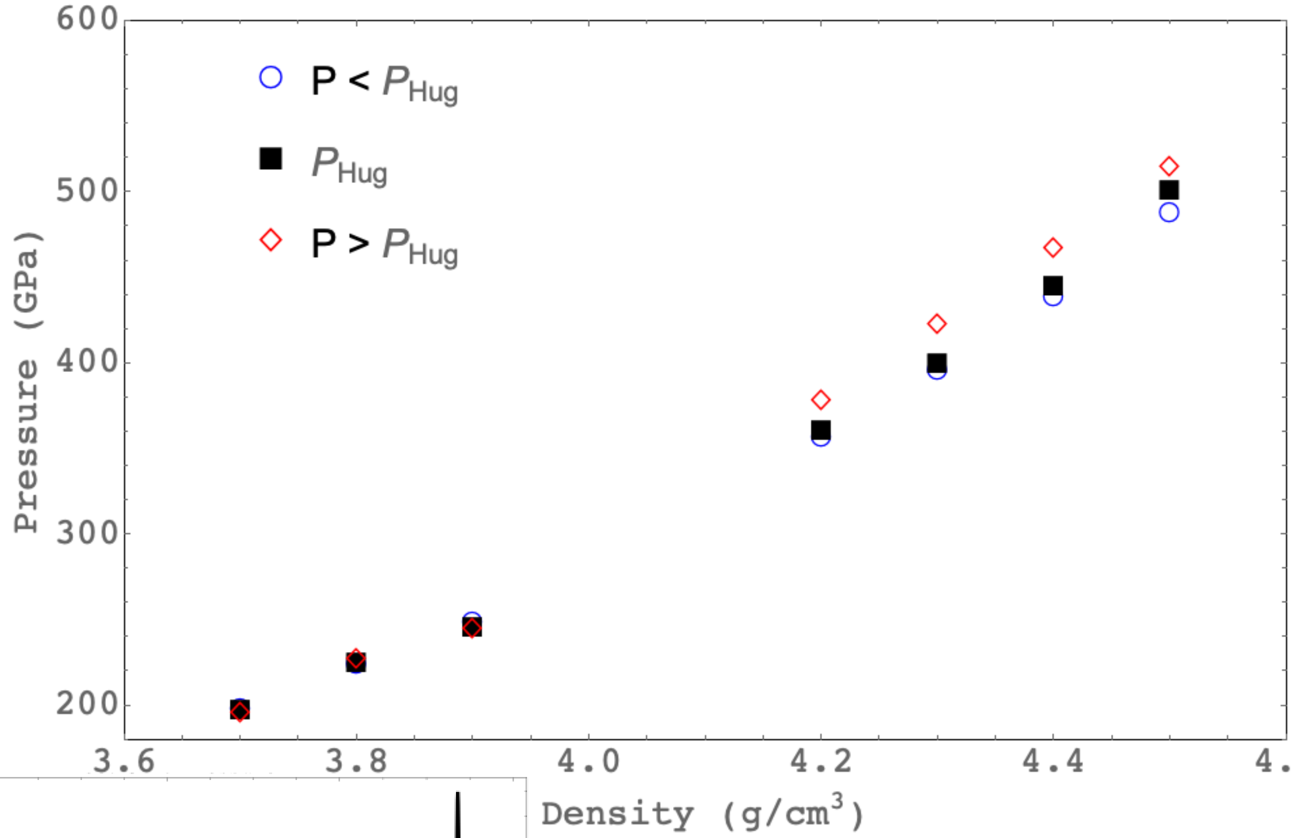
Use density functional theory (DFT) calculations to simulate Hugoniot

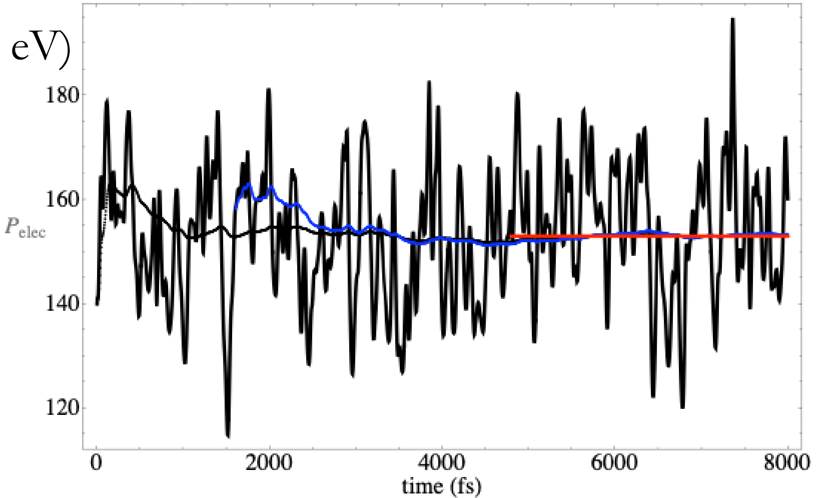
First-principles simulations DFT

- VASP – plane-wave code w PAW core-functions
- Use of DFT codes simulating warm dense matter
  - M. P. Desjarlais Phys. Rev. B **68**, 064204(2003)
- Great care in convergence
  - A. E. Mattsson et. al. Modeling and Simulation in Material Science and Engineering **13**, R1 (2005)

Assemble reference system

- 108 atoms
- 8 valence electrons
- AM05 potential
- Cutoff energy = 800 eV
- Baldereschi Mean Value Point
- Equilibrate at constant temperature and volume
- Equilibrated for ~2 ps at 0.2 fs
- Significant questions about band gap (DFT ~ 12 eV)
- Reference = 26 Kelvin, 1.224 g/cm^3
- Velocity scaled thermostat
- Hugoniot
  - Overshoot and undershoot P(T,ρ)
  - Interpolate





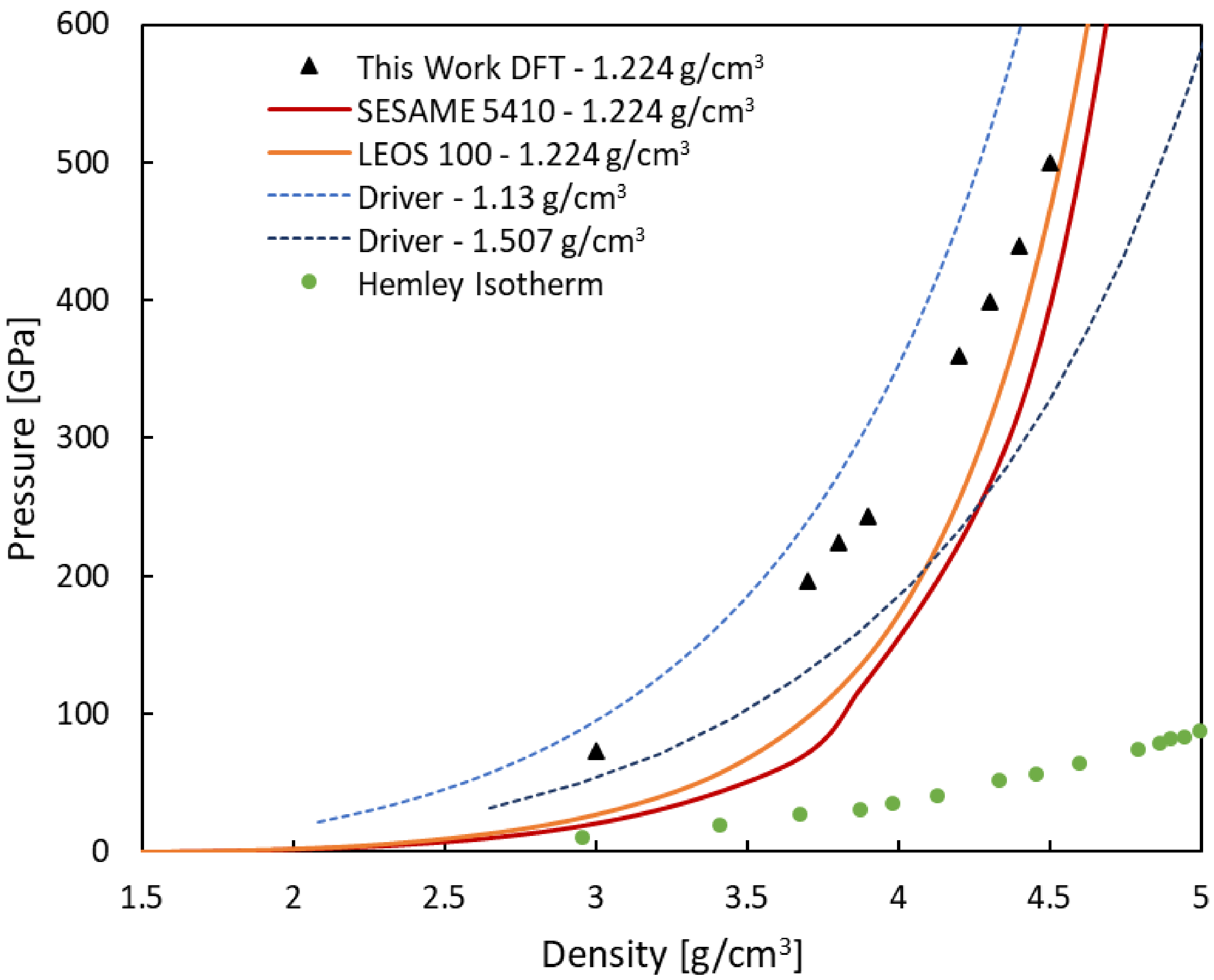
Existing EOS tables had no benchmarking data when developed and do not agree with DFT calculations

DFT calculations do not agree with existing EOS tables

Calculations by Driver and Militzer for solid Ne have similar shape to our calculations from different initial densities

- Consistency between independently computed DFT Hugoniots is promising

Experiments are needed to benchmark DFT calculations and EOS tables

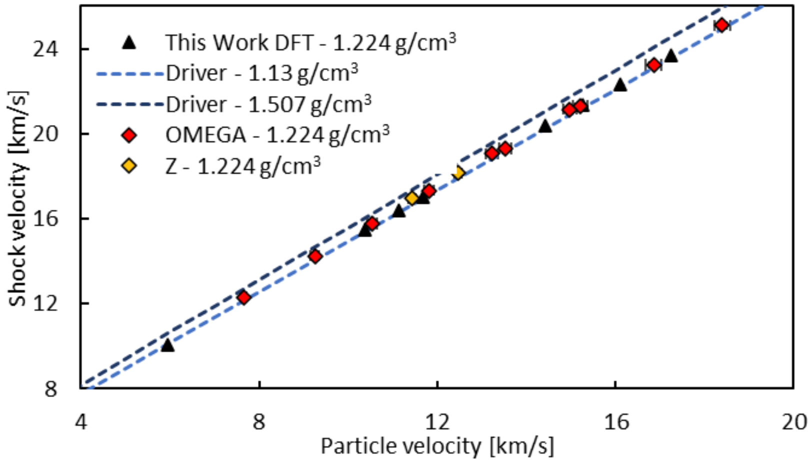


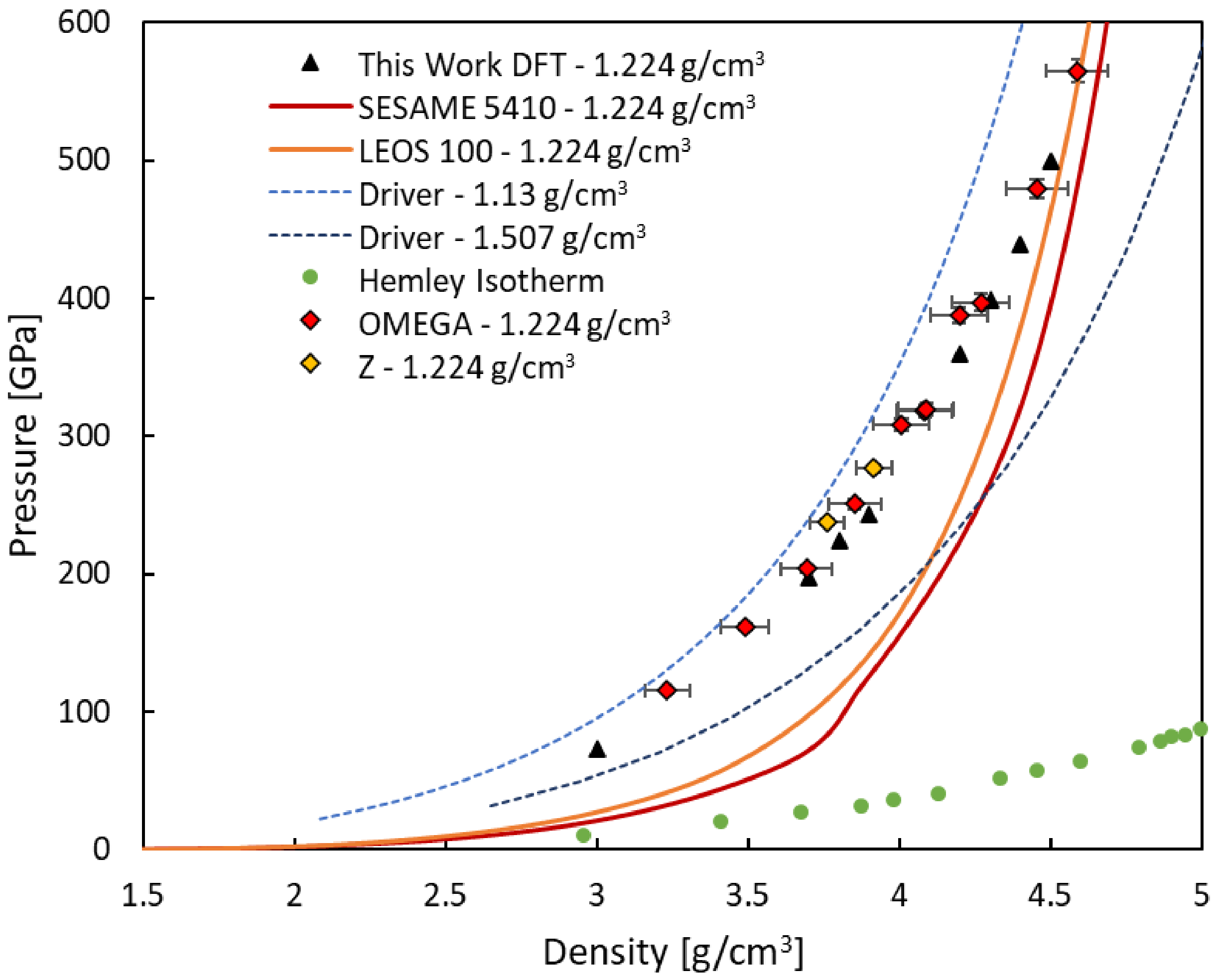
The experimental results agree well with the DFT calculations of the principal Hugoniot

DFT, OMEGA, and Z results are in excellent agreement

- Experiments were done on two different platforms, but used same standard (quartz)
- Agreement indicates that gold preheat shield on OMEGA targets was sufficient to mitigate hard x-ray and hot electron generation

Us-up data shows good agreement between our results and calculations by Driver and Militzer





Temperature measurements

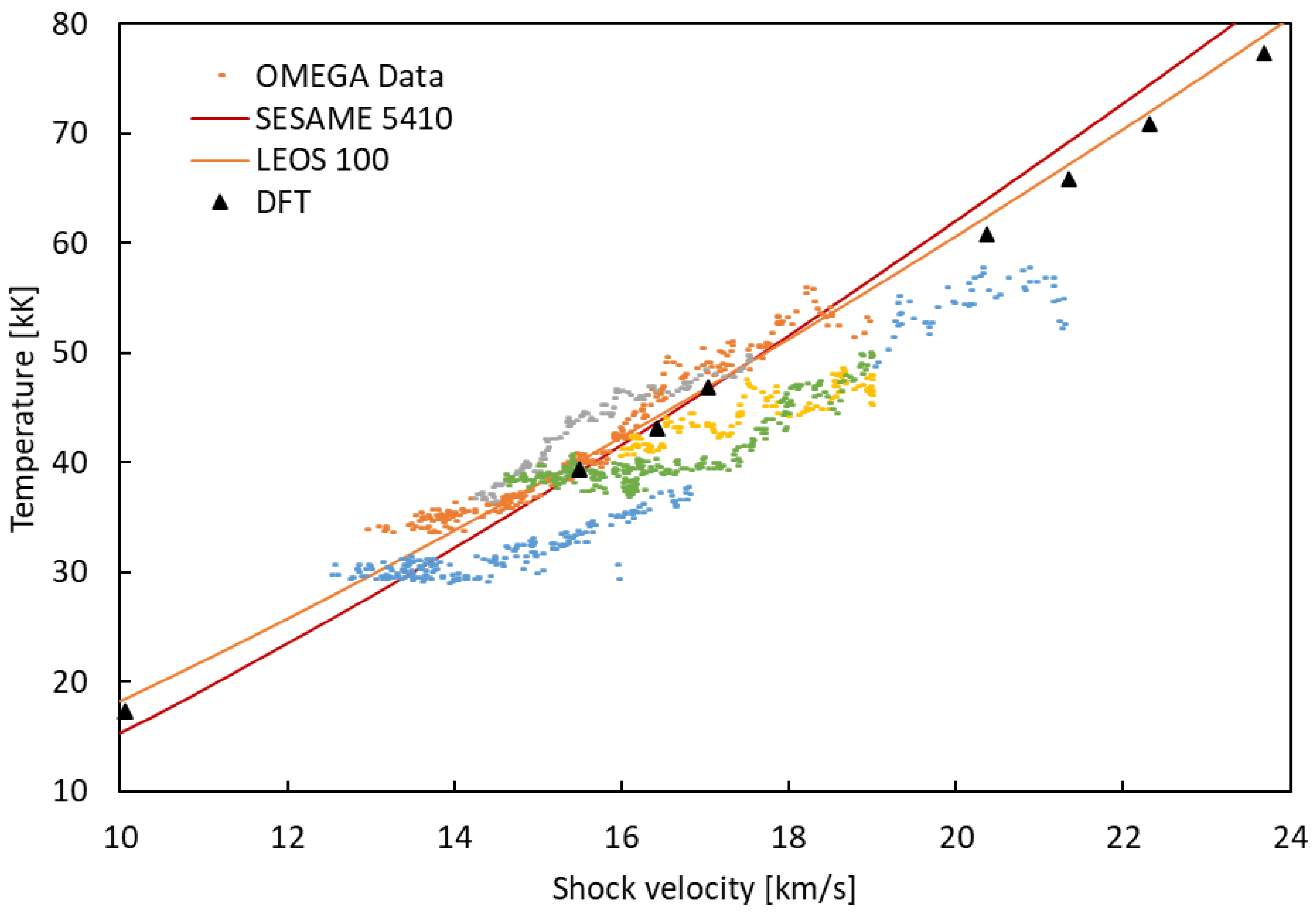
OMEGA data agrees well with DFT calculations of the shock temperature

Calculated Hugoniots from SESAME and LEOS also agree well with the experimental and DFT results in T-Us plane

- Interesting result when considering the significant difference in compression
- Likely an incorrect C_V used in tables allowed for accurate temperature, but incorrect compressibility

Higher pressure temperature measurements not valid due to potential scattering of emitted light off surfaces inside target

- Emission and reflectivity increased with decreasing pressure within initial neon region on all shots with new design



Summary

We performed a combined experimental and computational study to measure the Hugoniot and temperature of liquid neon in the pressure range 70-560 GPa

The principal Hugoniot was measured using laser-driven shocks on OMEGA Laser Facility and impact experiments on Z facility

- Experiments ranged from 110-560 GPa
- Experiments from both facilities are in good agreement

DFT-MD calculations of principal Hugoniot made up to 500 GPa

- Due to large bandgap and closed shell, it poses difficulties for density functional theory methods
- Bandgap does not close over entire range of experiments

Experimental and DFT Hugoniots agree well for pressures above 150 GPa

- Existing SESAME and LEOS tables do not accurately represent compressibility

Shock temperature measurement agree well with DFT, SESAME, and LEOS