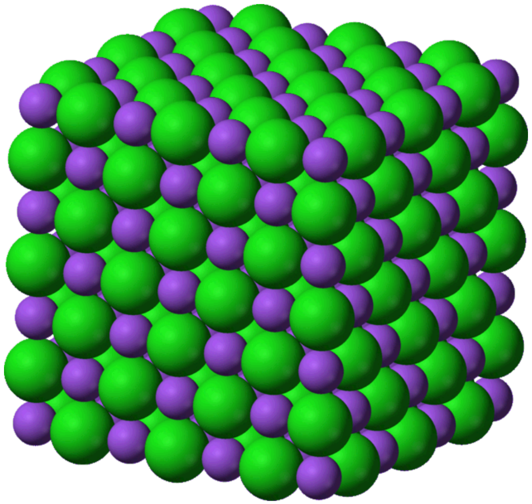
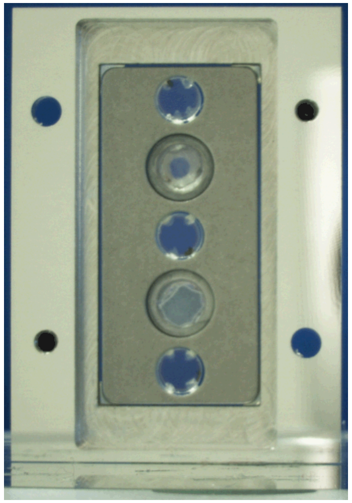
SAND2014-17082PE

Lithium Deuteride:
First principles calculations and Z experiments

Marcus D. Knudson
Sandia National Laboratories, Albuquerque, NM



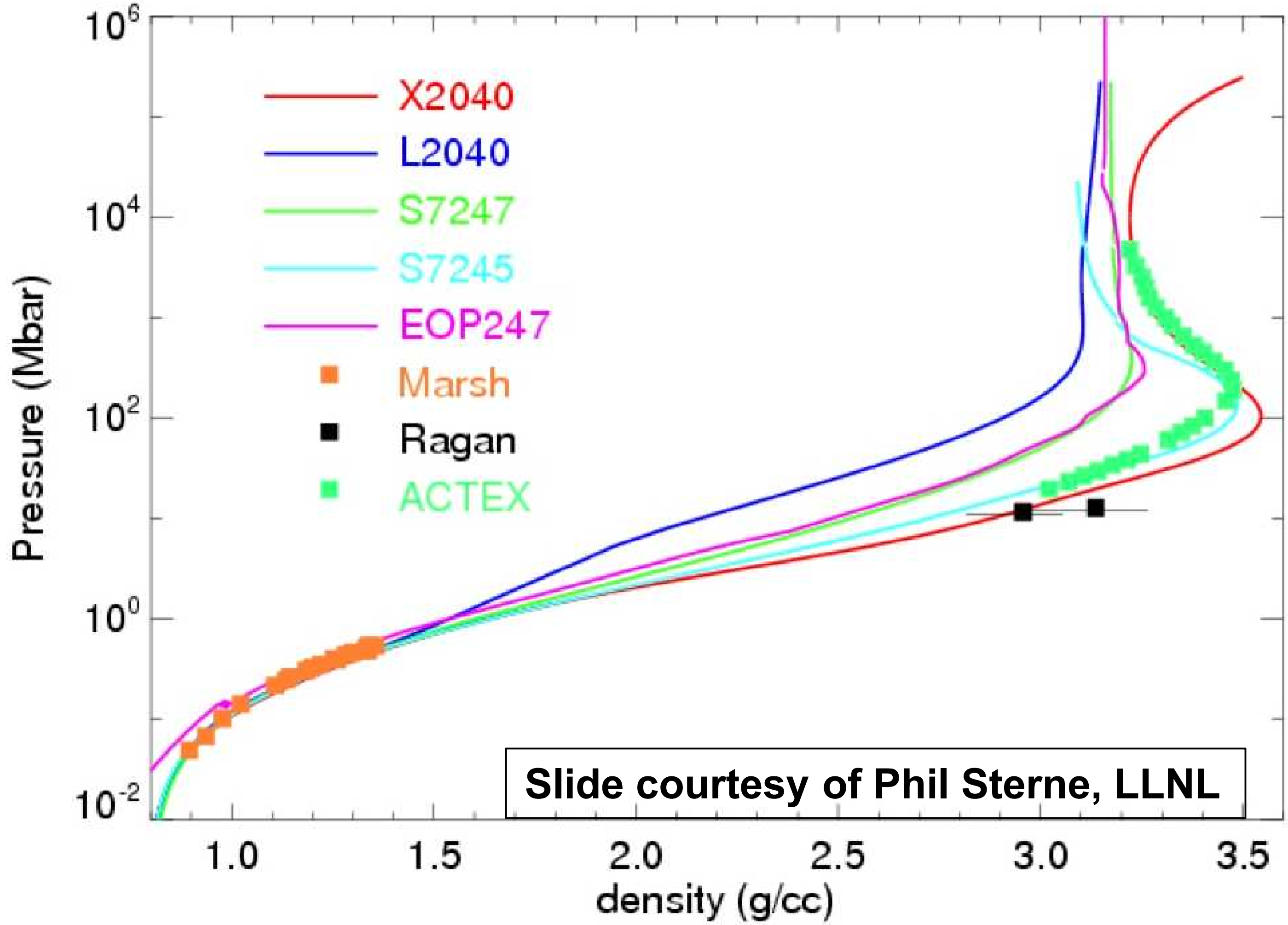


Co-PIs: Mike Desjarlais (SNL), Thomass Mattsson (SNL), Amy Laziki (LLNL)

Marcus D. Knudson, (505) 845-7796, mdknuds@sandia.gov

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

EOS models predict a wide range for the Principal Hugoniot of LiD

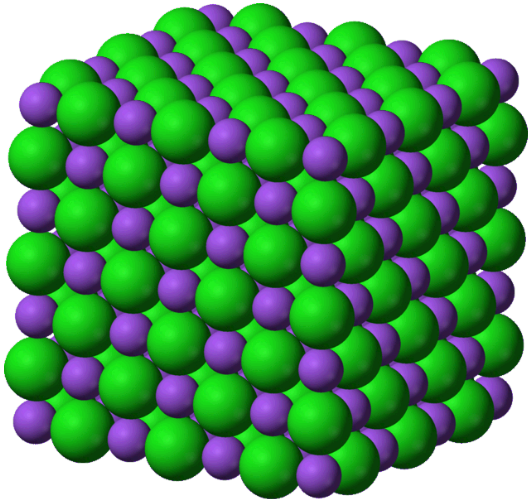


Both explosively driven data (Ragan) and ACTEX theory favor the more compressible EOS models that use atom-in-jellium for electron-thermal terms

First-principles QMD calculations

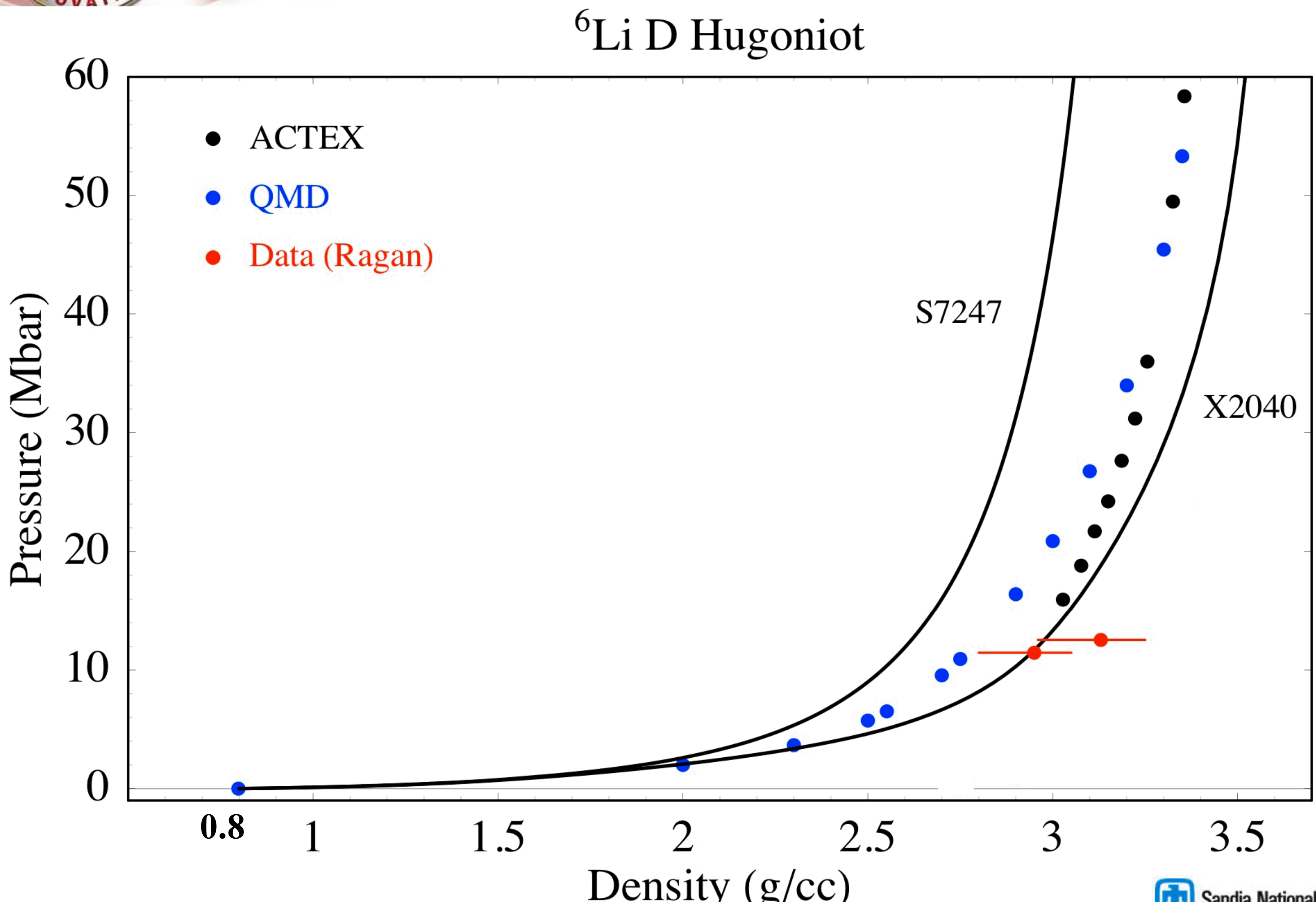
- Quantum molecular dynamics (QMD) calculations
  - Density functional theory, thermal ions and electrons
- Zero-point contributions to the reference state are calculated from the phonon density of states
- ^{6}Li and D are modeled with all electron potentials, carefully constructed to have good high energy scattering properties
- Satisfy the Rankine-Hugoniot relations

Lithium deuteride at ambient has the NaCl (rock salt) structure: two interlaced
FCC lattices;   5 eV band gap: single crystal samples are transparent



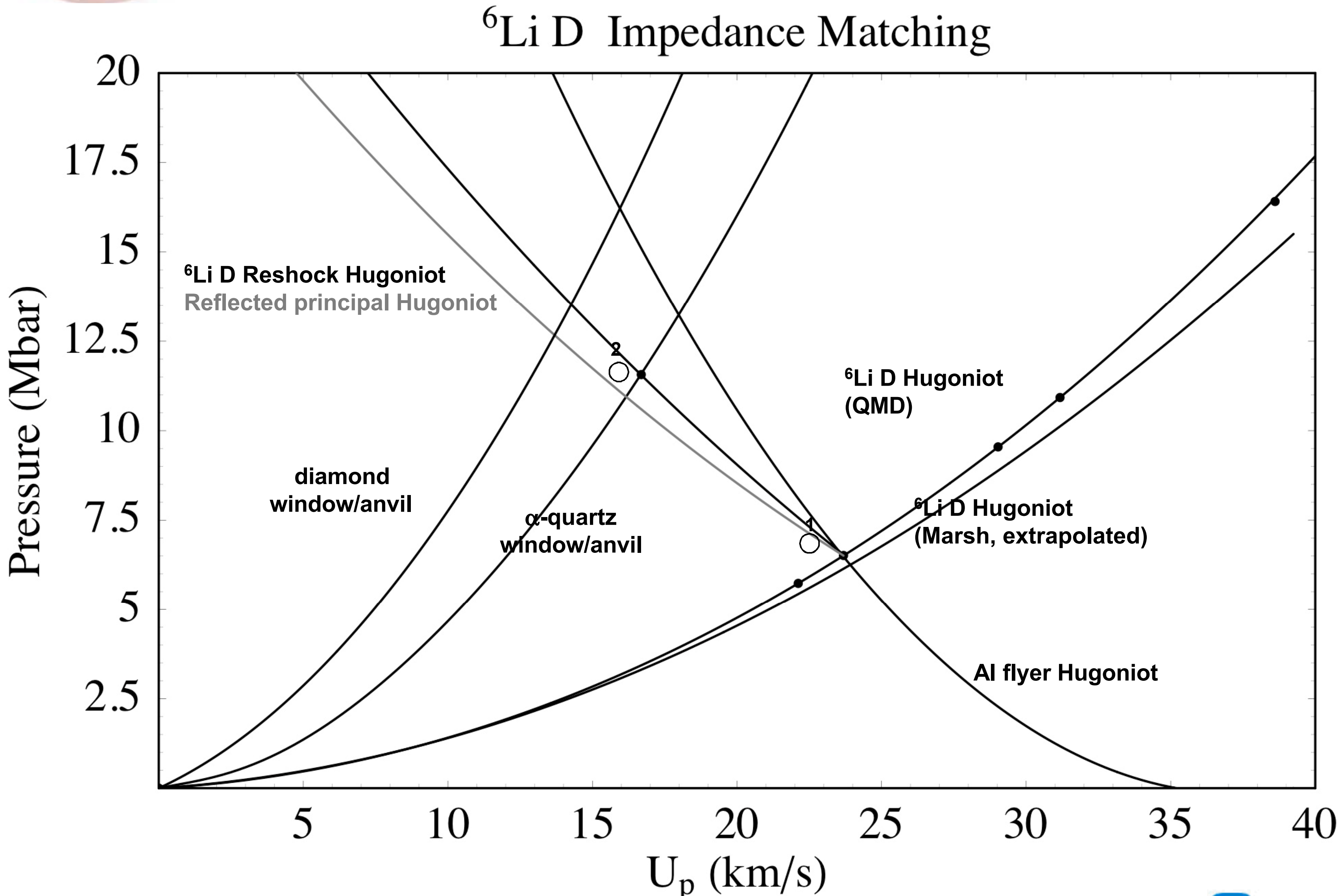
Lithium deuteride come in single crystals, (packed) powders, or pressed into cakes. We will use single crystals and pressed cakes

Our QMD calculations agree with X2040 at low pressure, and merge with ACTEX at higher pressures

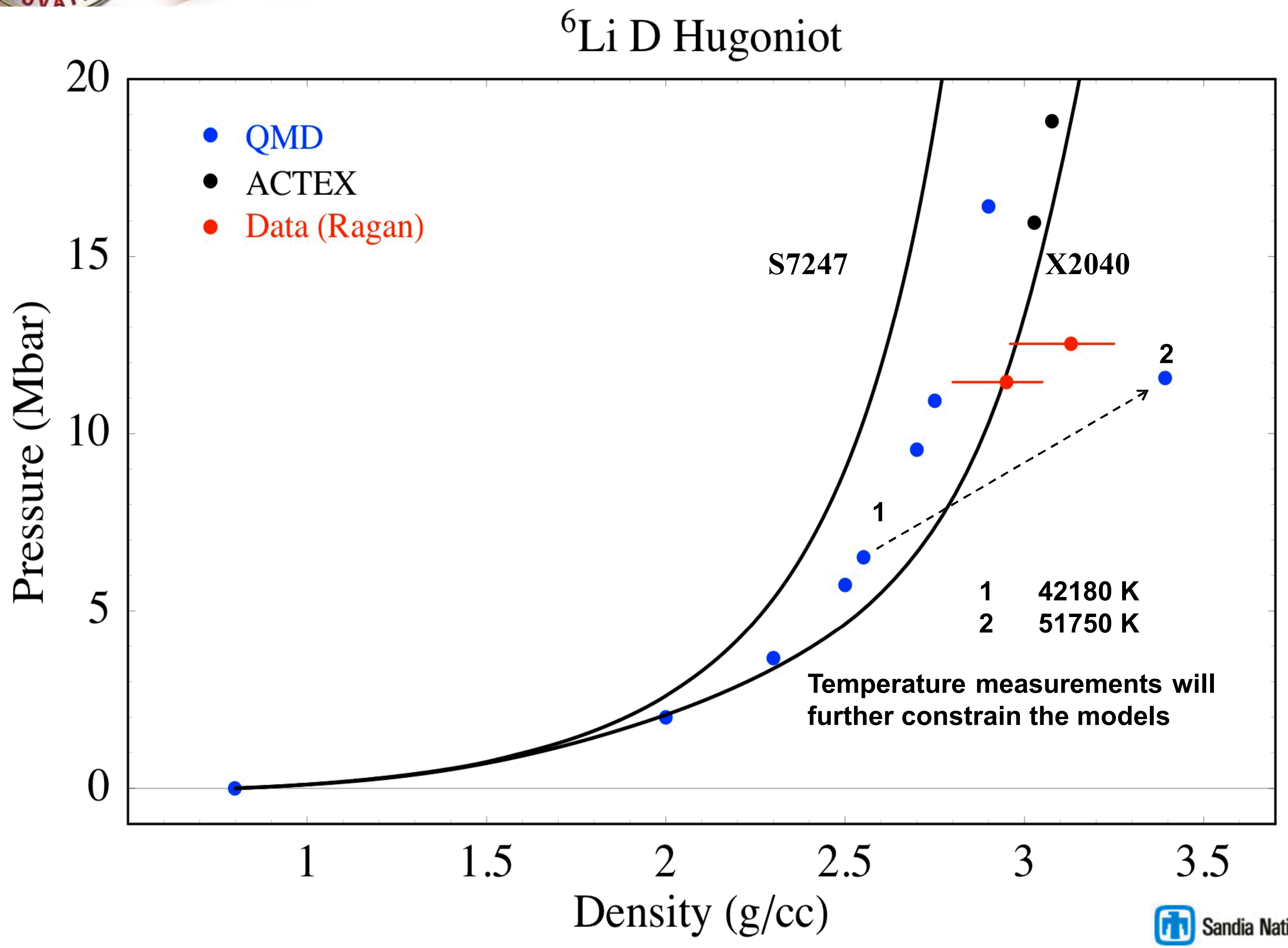


Sandia National Laboratories

Z can reach relevant pressures on first shock and reshock from quartz to distinguish models



First and second shock data from Z will constrain the next generation LiD EOS



We obtained single crystal LiD crystals from University of Utah crystal growth lab

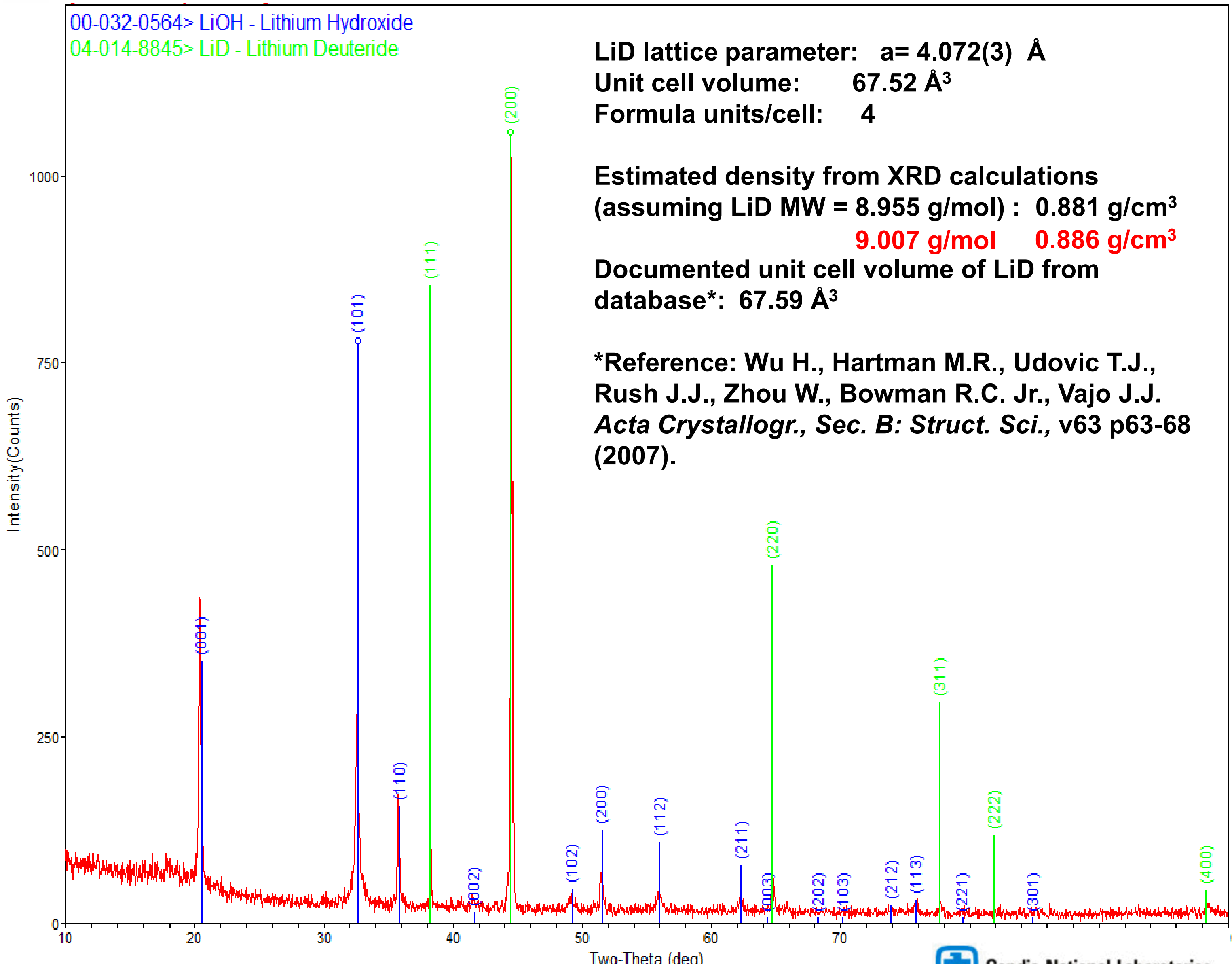
ICP-MS of the LiD sample to determine isotopic concentration:

^{6}Li	2.2-2.4%
^{7}Li	97.6-97.8%

Natural isotopic concentration:

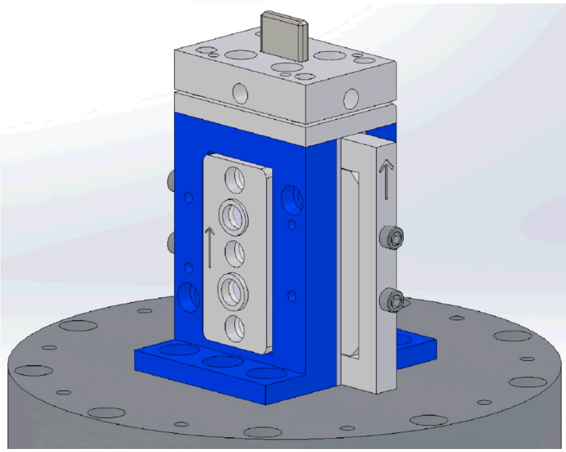
^{6}Li	7.6%
^{7}Li	92.5%

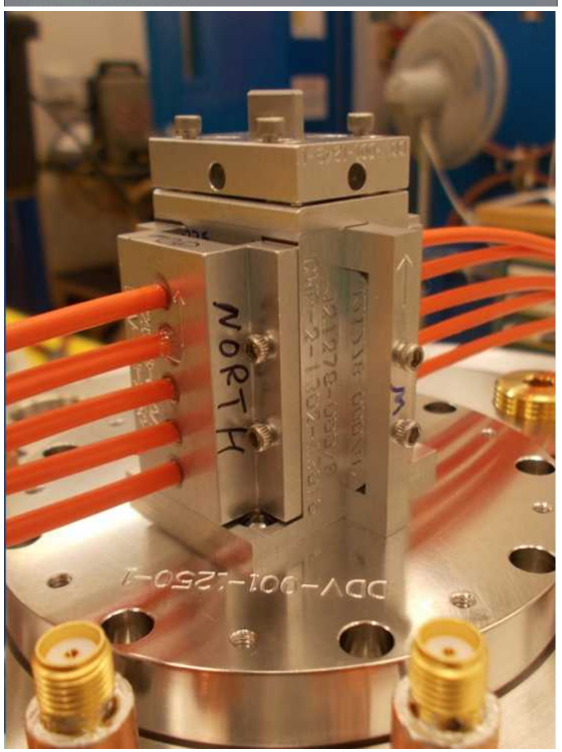
These samples are ^{7}Li rich - nearly ^{7}LiD

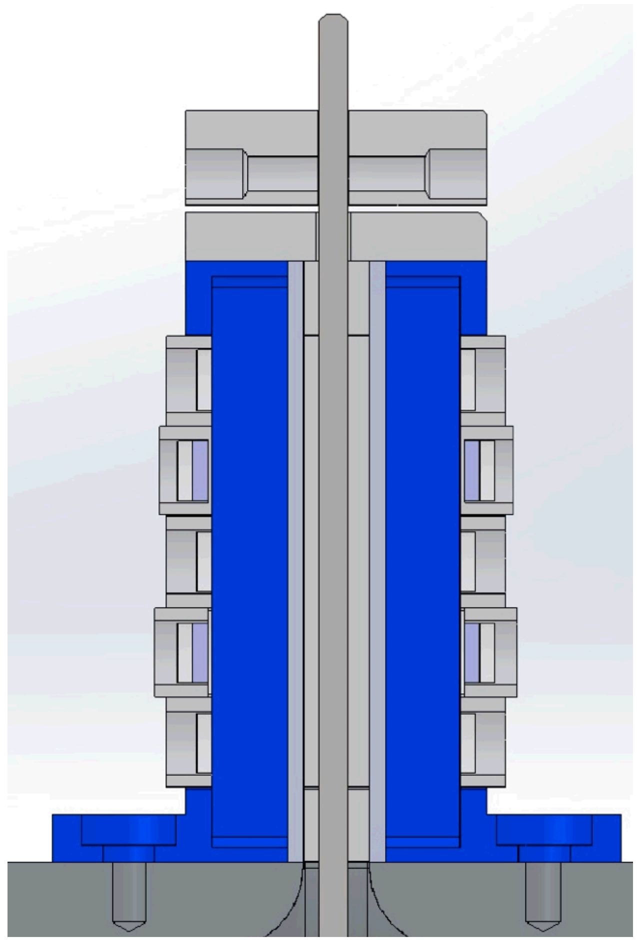


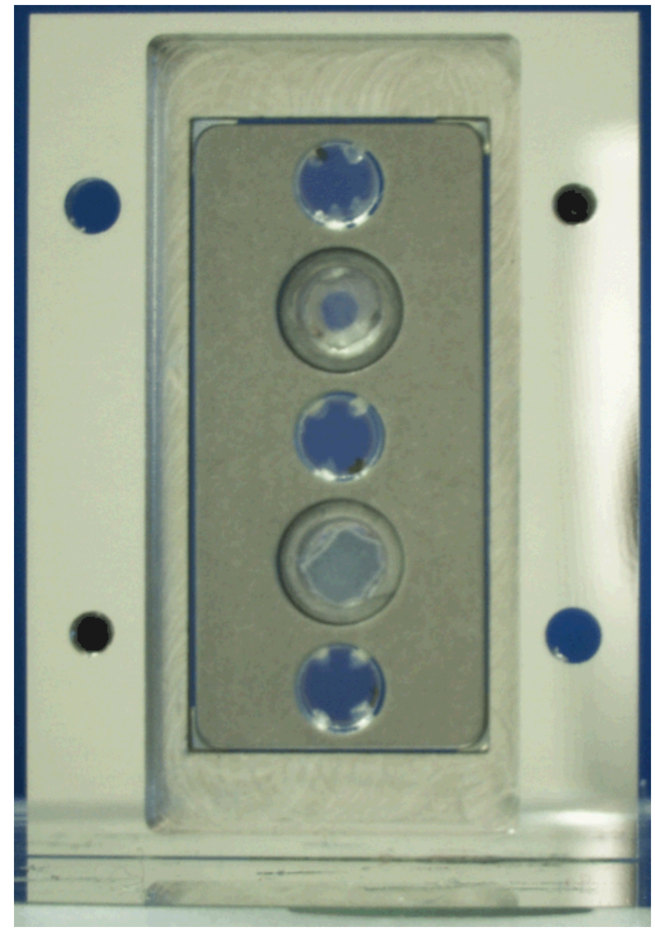
Sandia National Laboratories

Experiments take full advantage of our high-accuracy shock and release data on quartz





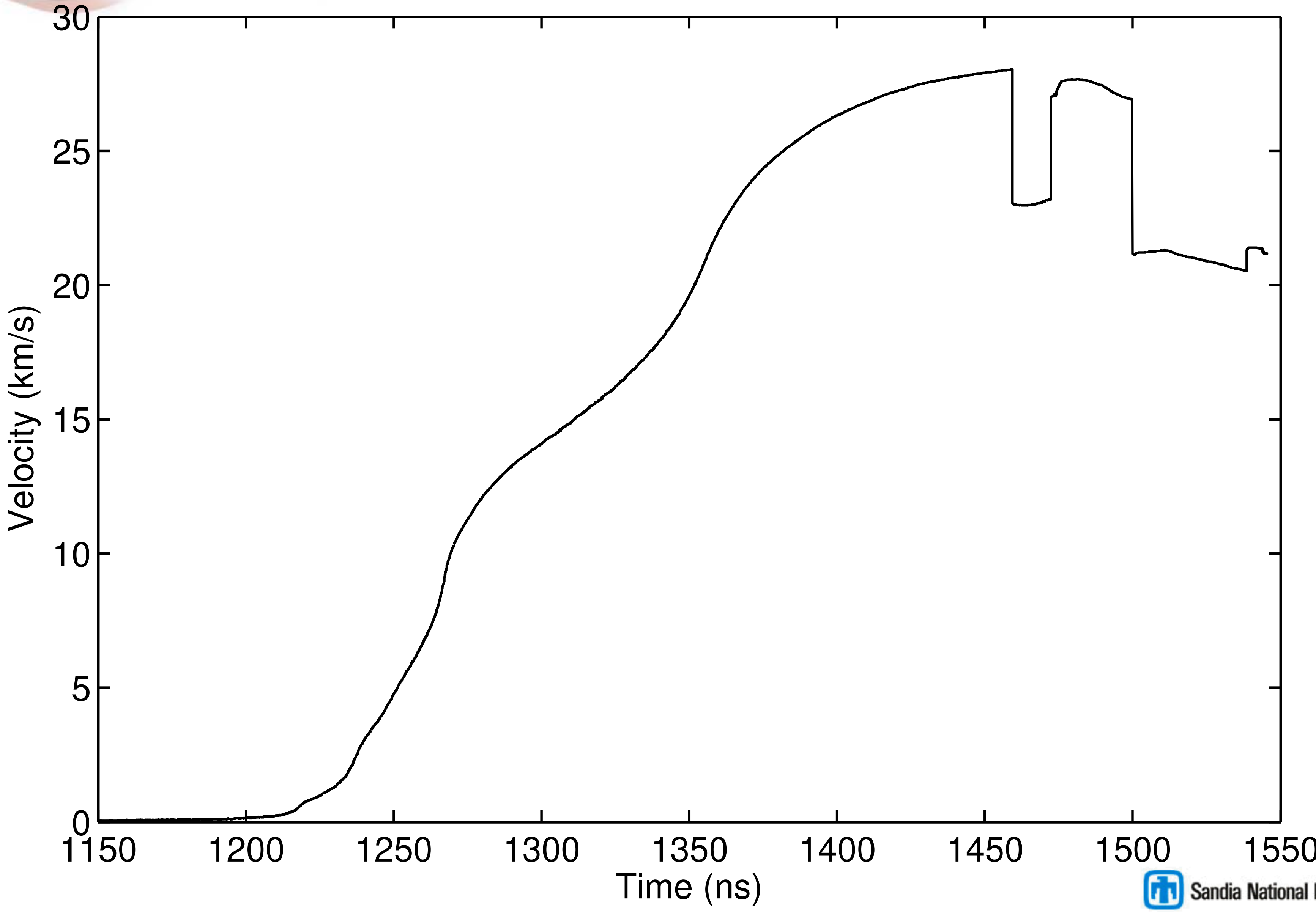




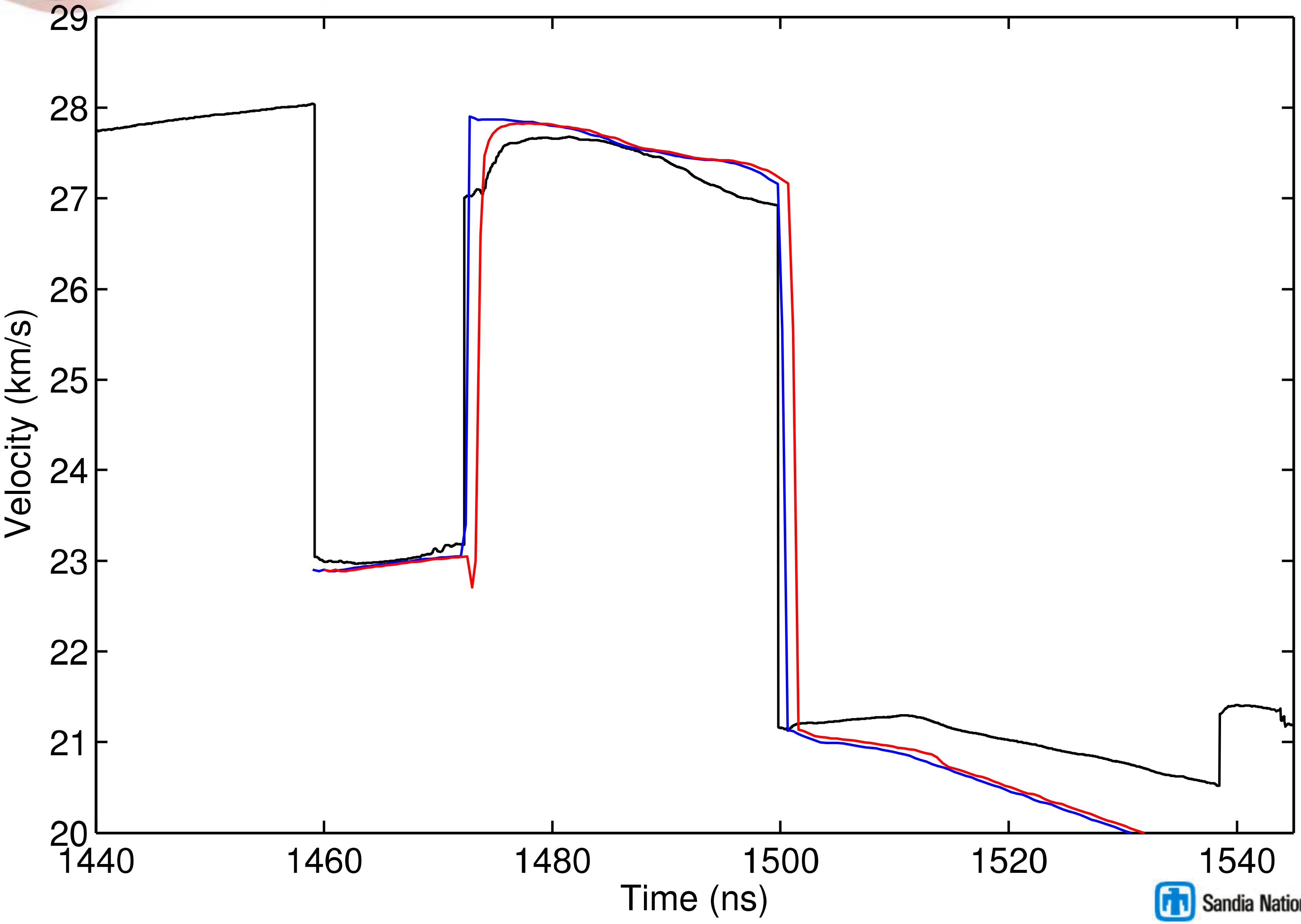
Four samples total, two per side

Experiments in collaboration with LLNL

Quality VISAR data obtained through flyer plate launch and shock propagation through samples

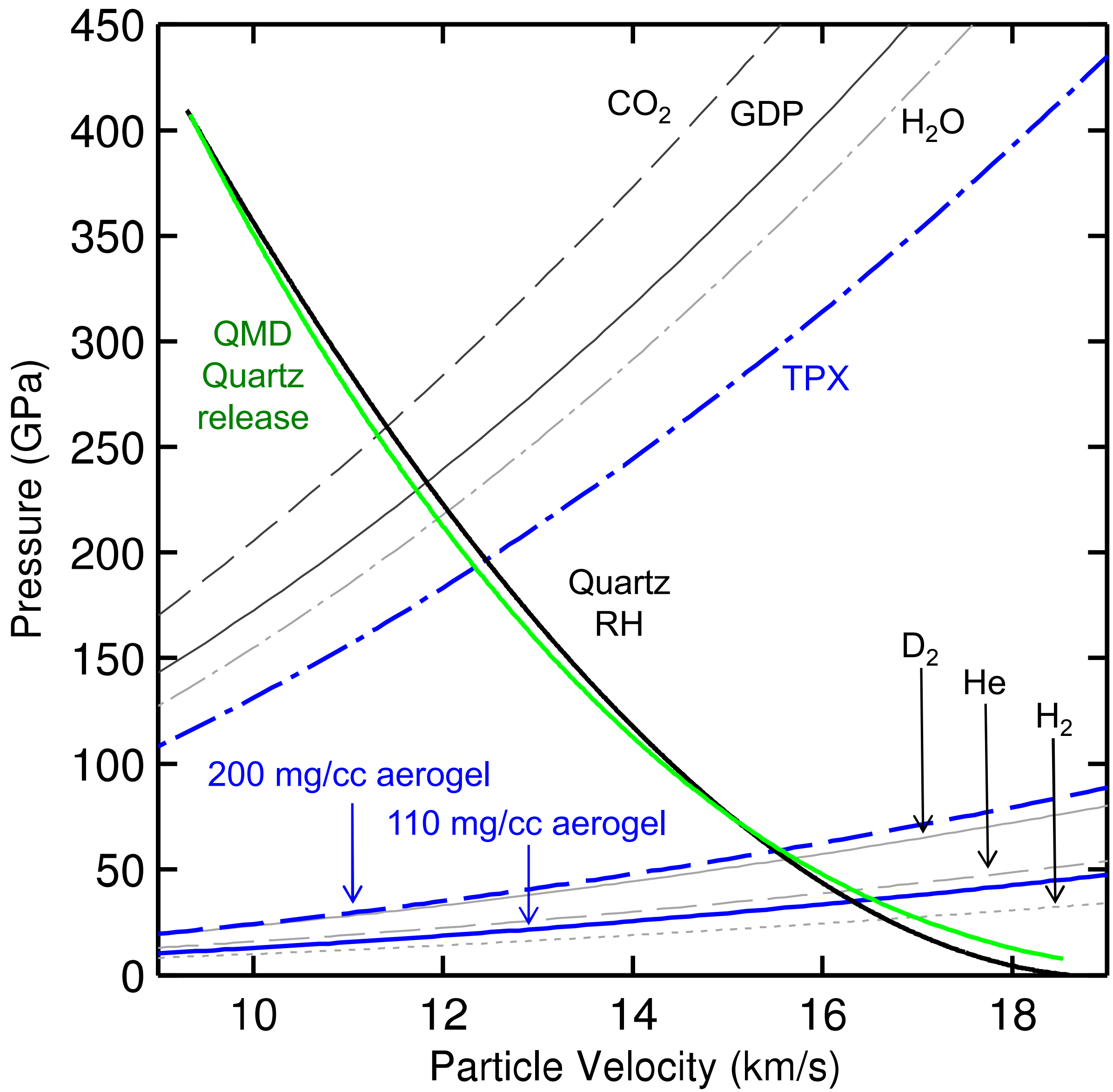


Evidence of small gaps between the quartz and LiD samples effect wave propagation and analysis



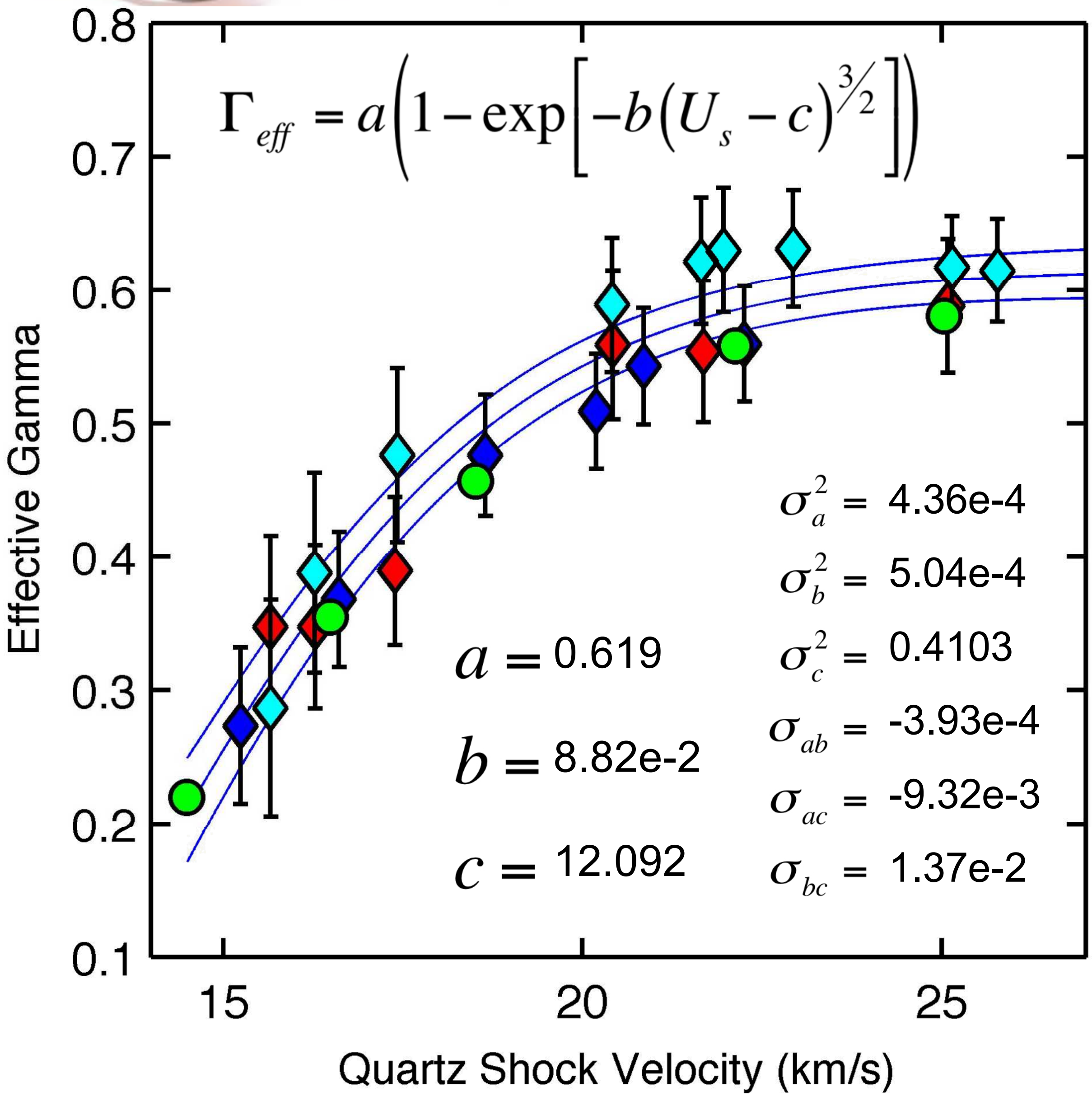
Recent work has validated the use of quartz for impedance matching experiments

- Quartz melts at ~100 GPa into a conducting fluid
  - Shock front becomes reflective
- Quartz is quickly becoming a high pressure shock wave standard
  - Helium, hydrogen, deuterium, water, GDP, carbon dioxide, xenon, krypton, …
- For accurate results there is a need to understand the off-Hugoniot response of quartz
  - Errors in u_p will be magnified by a factor of $(\rho/\rho_0 -1)$



Sandia National Laboratories

Γ_{eff} exhibits similar trend for all release standards and shows very good agreement with QMD trend

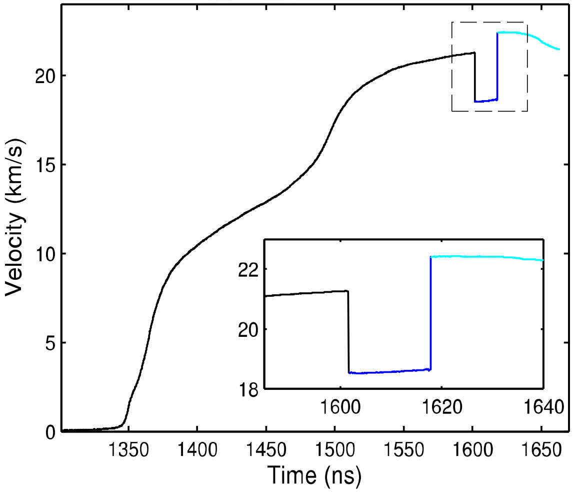


The similar trend in Γ_{eff} for all three release standards suggests that the Mie-Grüneisen, constant Γ_{eff} model with linear U_s-u_p Hugoniot reference adequately describes the release path to quite low pressure states

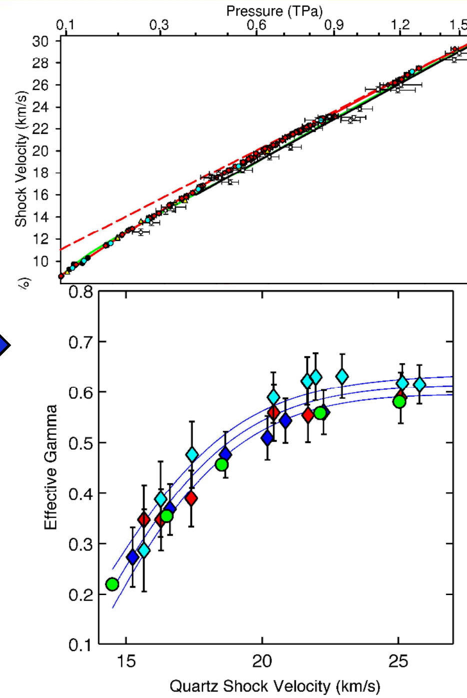
These results corroborate the QMD release calculations, albeit with a slightly higher Γ_{eff} for a given quartz shock velocity

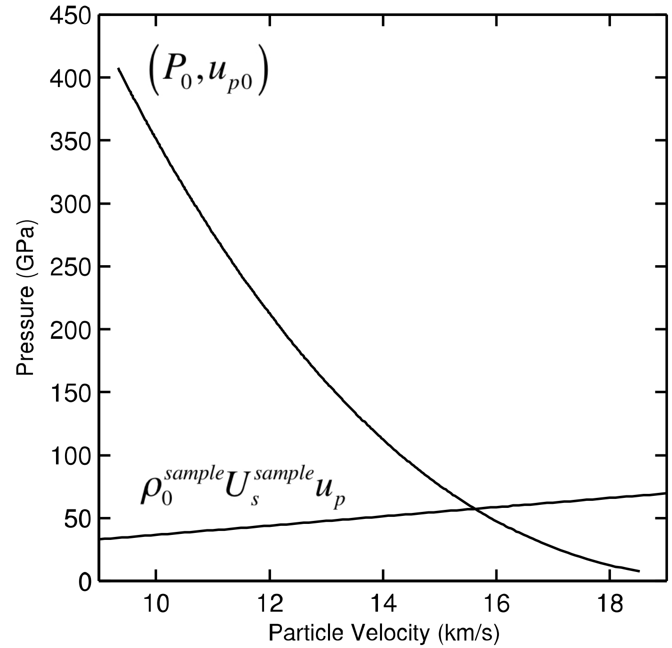
Sandia National Laboratories

Simple analytical model for impedance matching with quartz into lower impedance material



measure U_s^{quartz} and U_s^{sample}





U_s^{quartz} determines:

$$(P_0, u_{p0}), \qquad C_0 = \frac{P_0}{\rho_0 u_{p0}} - S u_{p0}$$

$$\Gamma_{eff} = a\left(1 - \exp\left[-b\left(U_s - c\right)^{3/2}\right]\right)$$

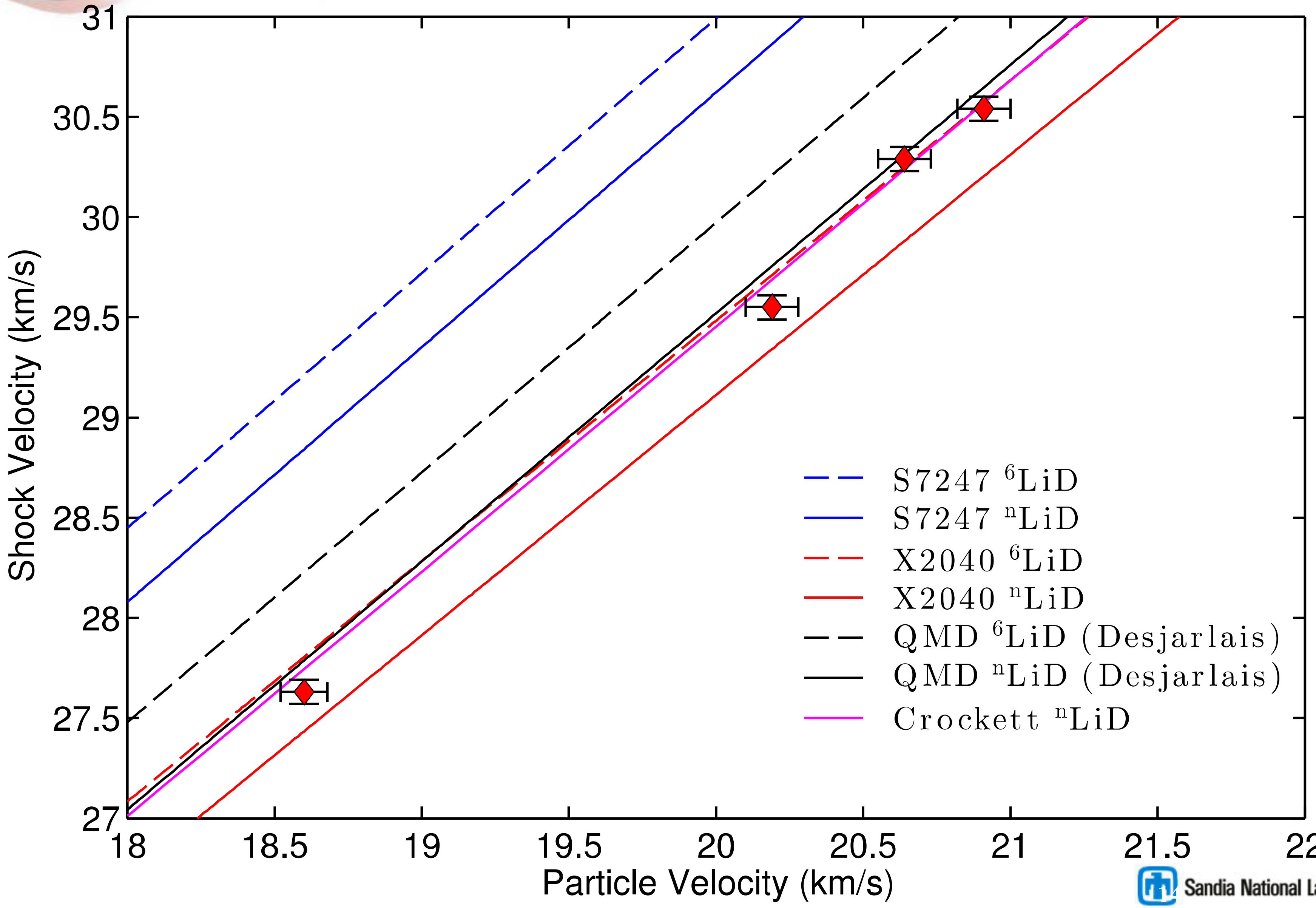
Solve the set of coupled ODEs:

$$P = P_H + \frac{\Gamma_{eff}}{V}\left(E - E_H\right), \qquad dE = -PdV$$

$$C_s^2 = -V^2 \left.\frac{\partial P}{\partial V}\right|_s, \qquad u_p = u_{p0} + \int_{P_0}^{P} \frac{VdP}{C_s}$$

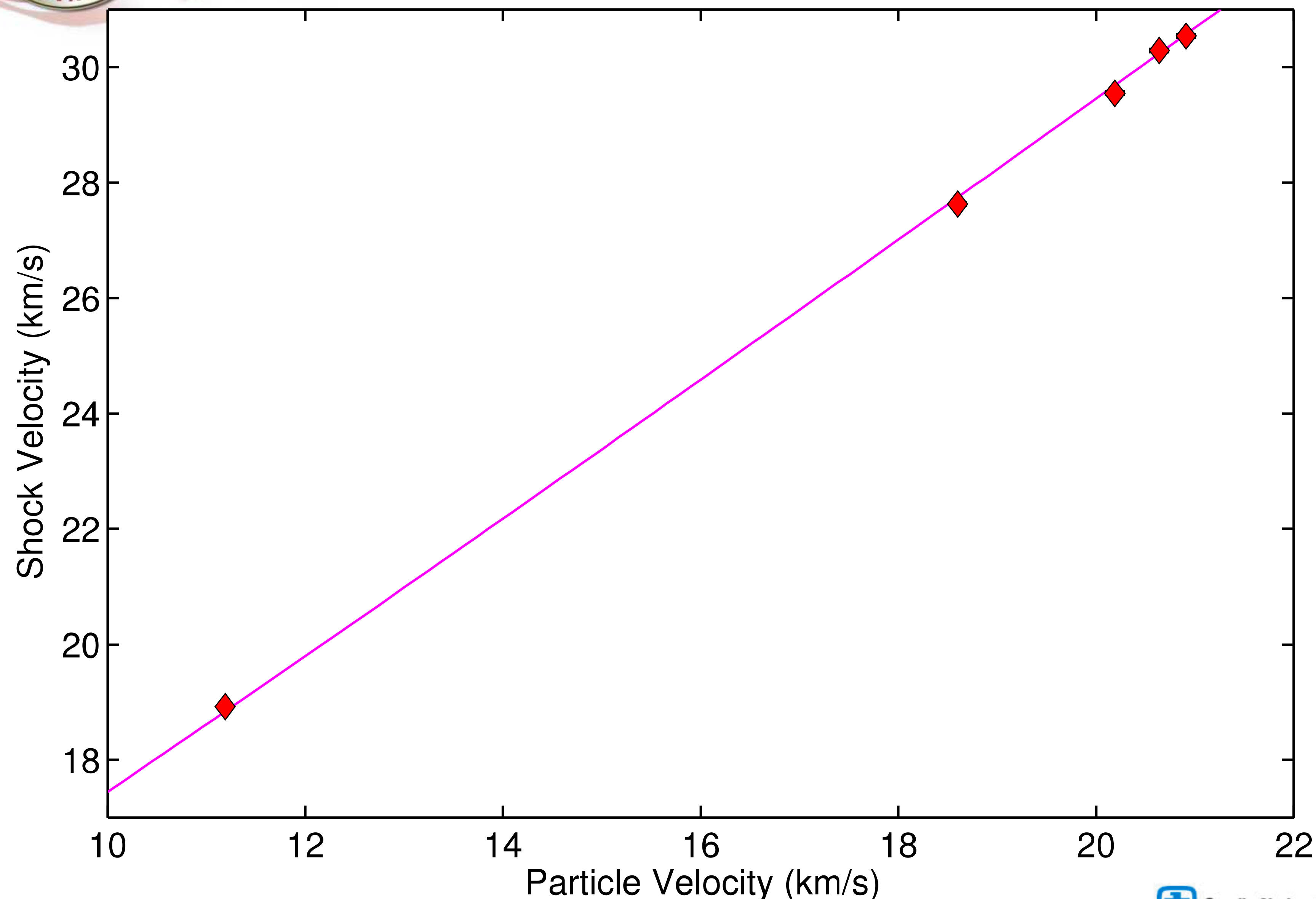
Sandia National Laboratories

High-precision Hugoniot data obtained in the 450-550 GPa regime on the Principal Hugoniot



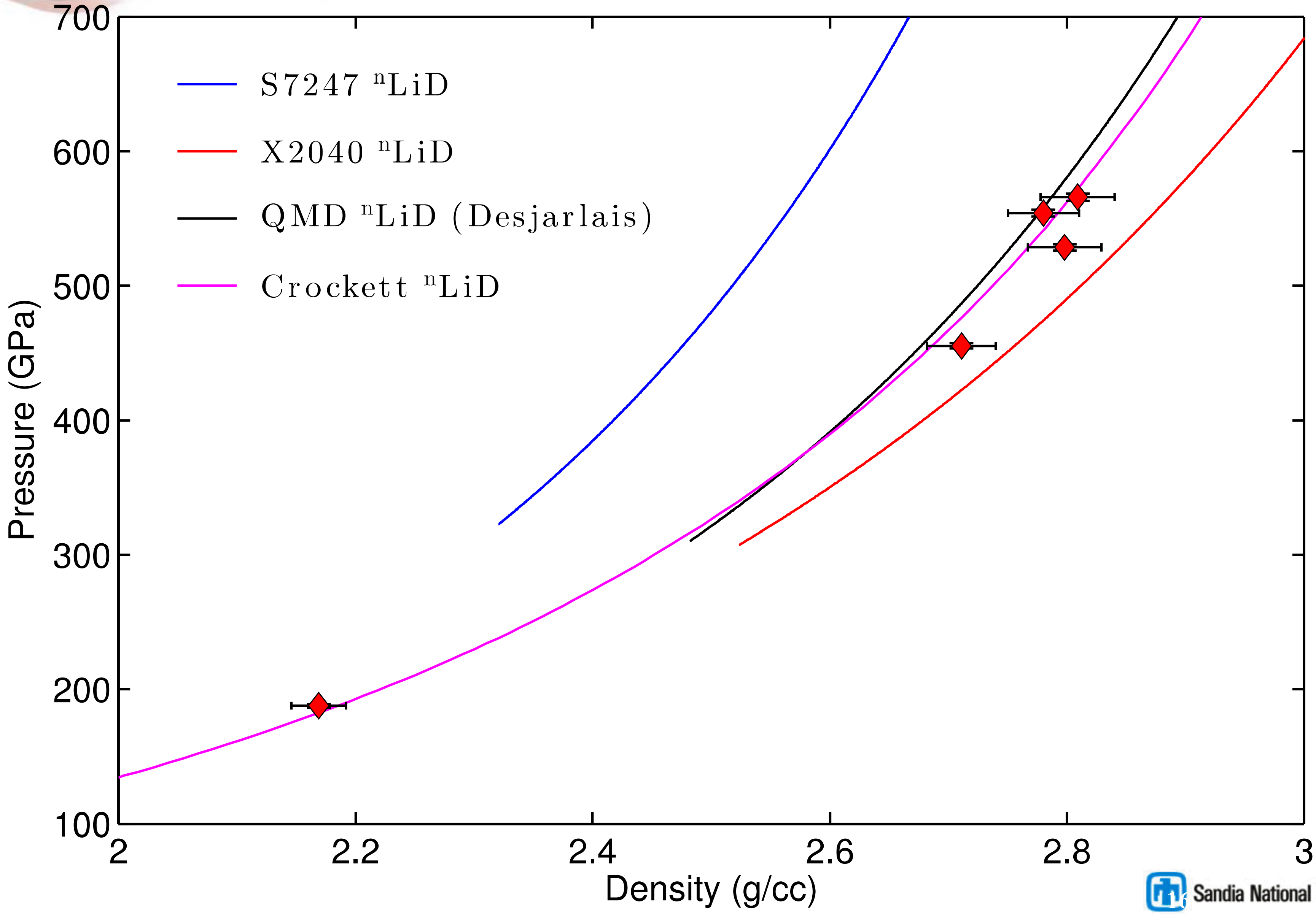
Sandia National Laboratories

Failed shot (incorrect pulse shape) also provided data at ~190 GPa

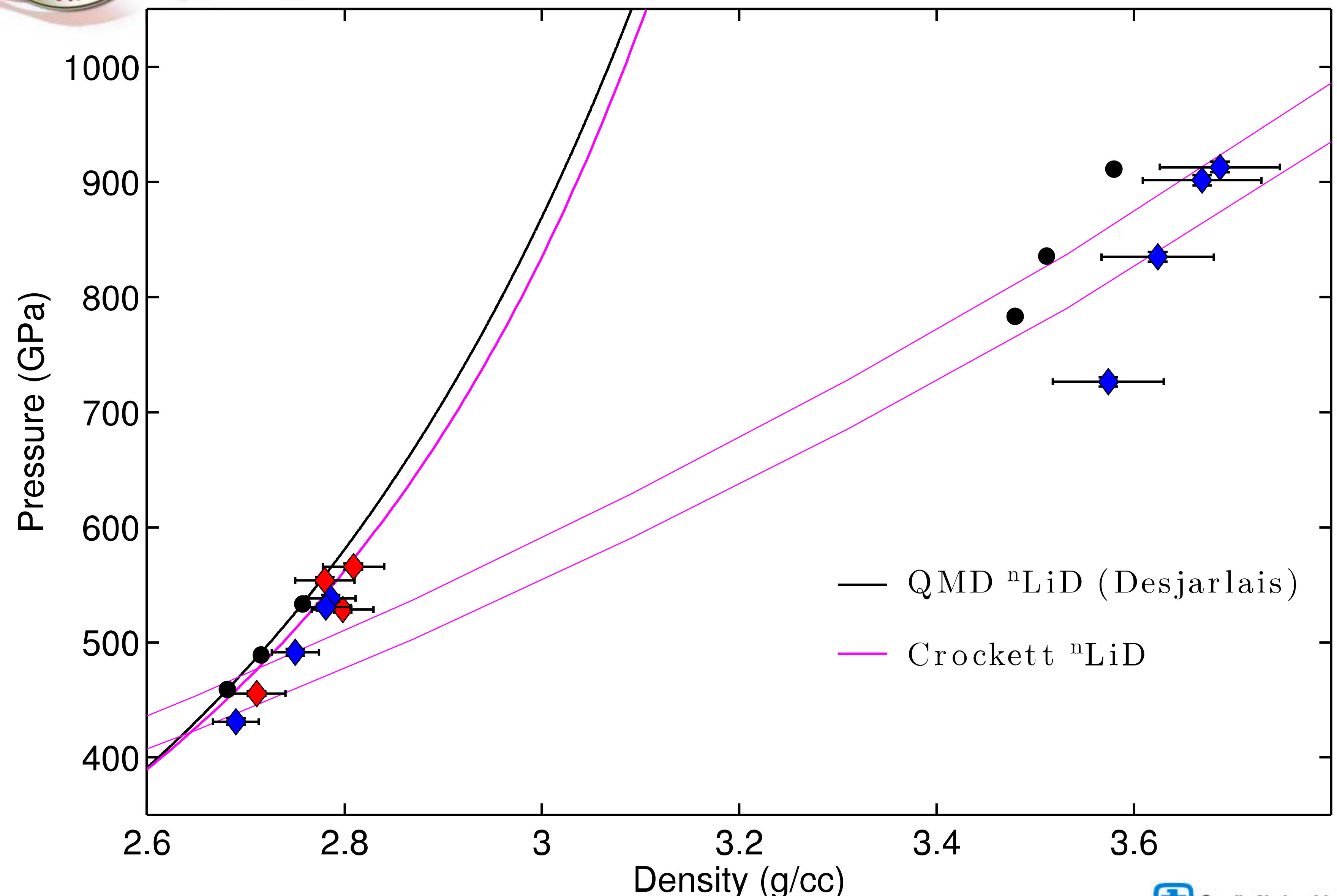


Sandia National Laboratories

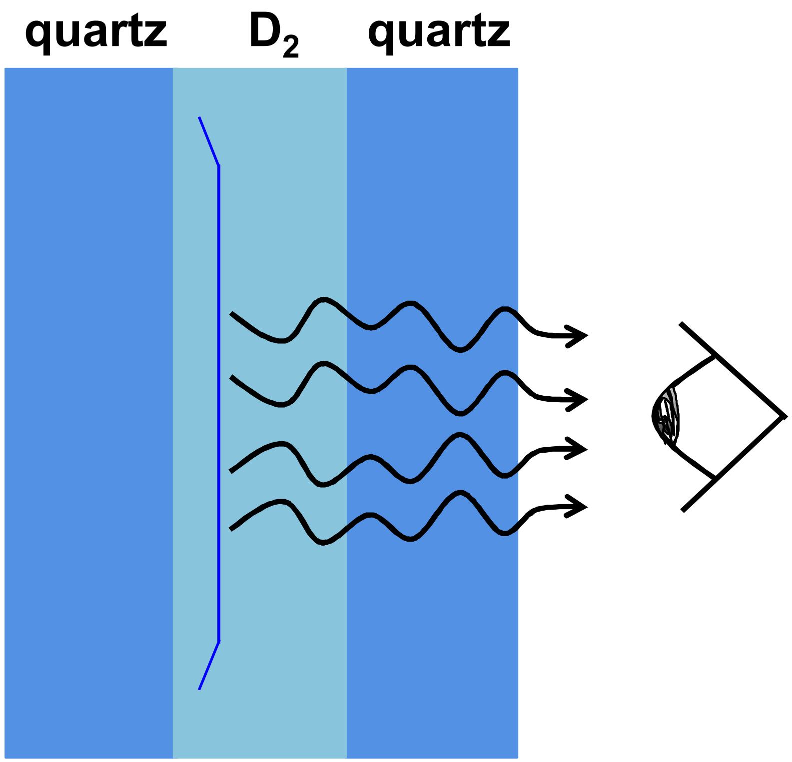
Z data seems to be systematically softer than the QMD and recent LANL Hugoniot

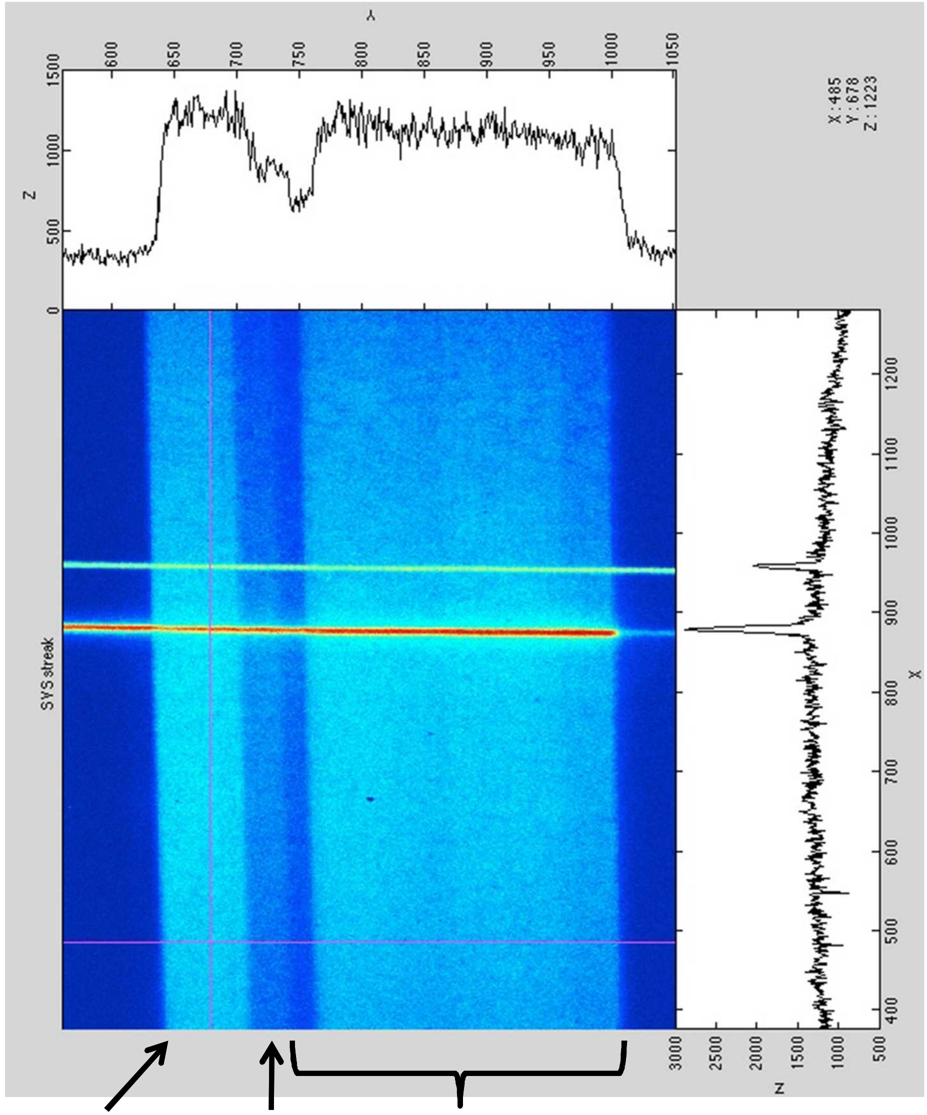


This is exacerbated in the re-shock data, however the results are very sensitive to initial refractive index



Visible emission dispersed in wavelength and time to infer temperature along the Hugoniot

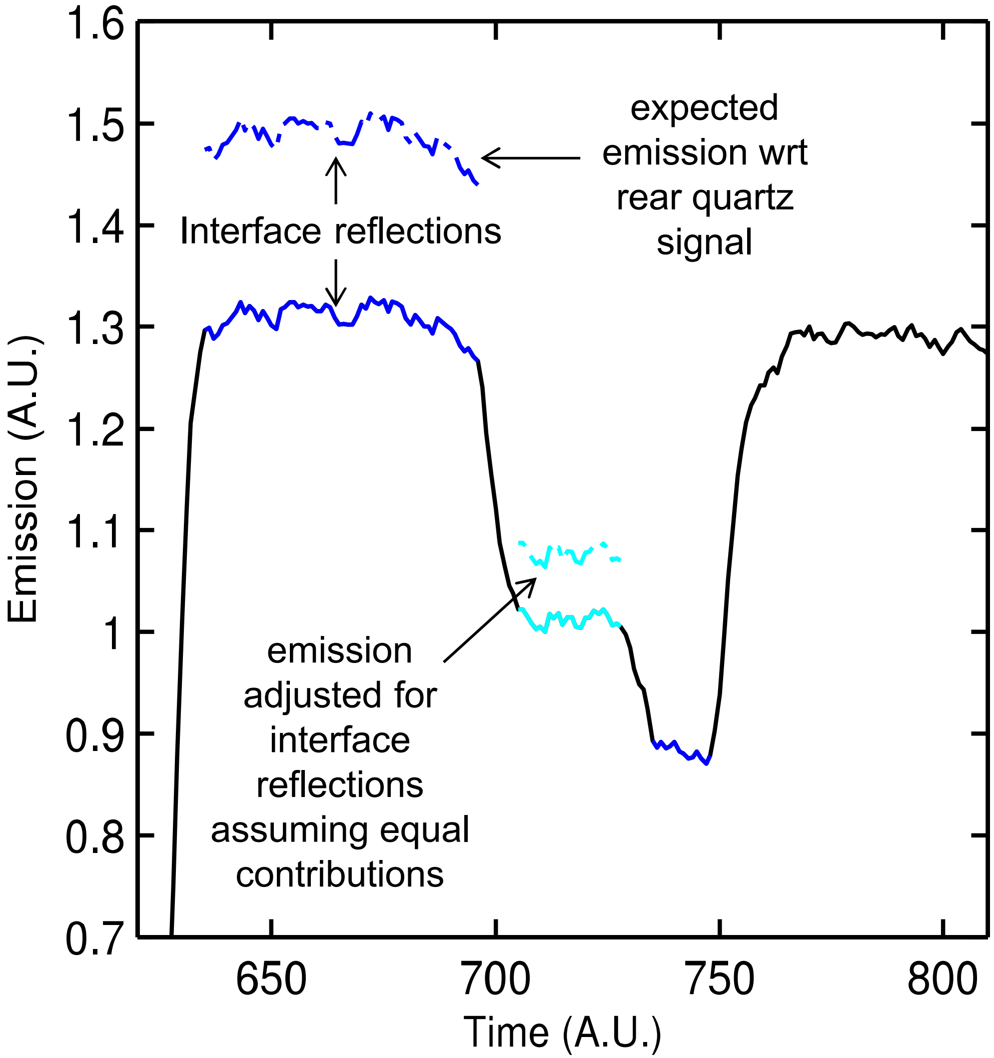


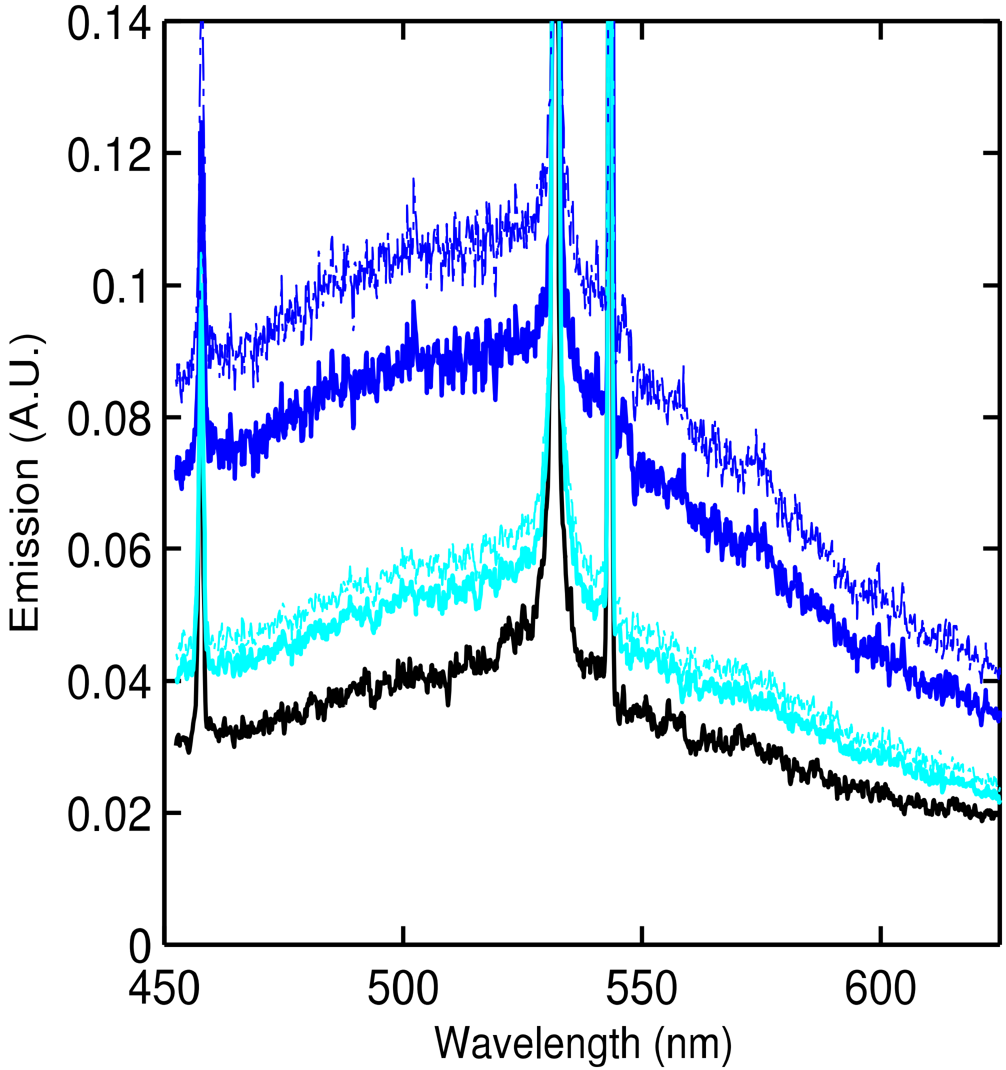


Quartz emission used both as a relative calibration and to correct for effect of reflections at quartz/sample interfaces

Sandia National Laboratories

Quartz emission on either side of the D_2 is used as a relative calibration to account for interfaces



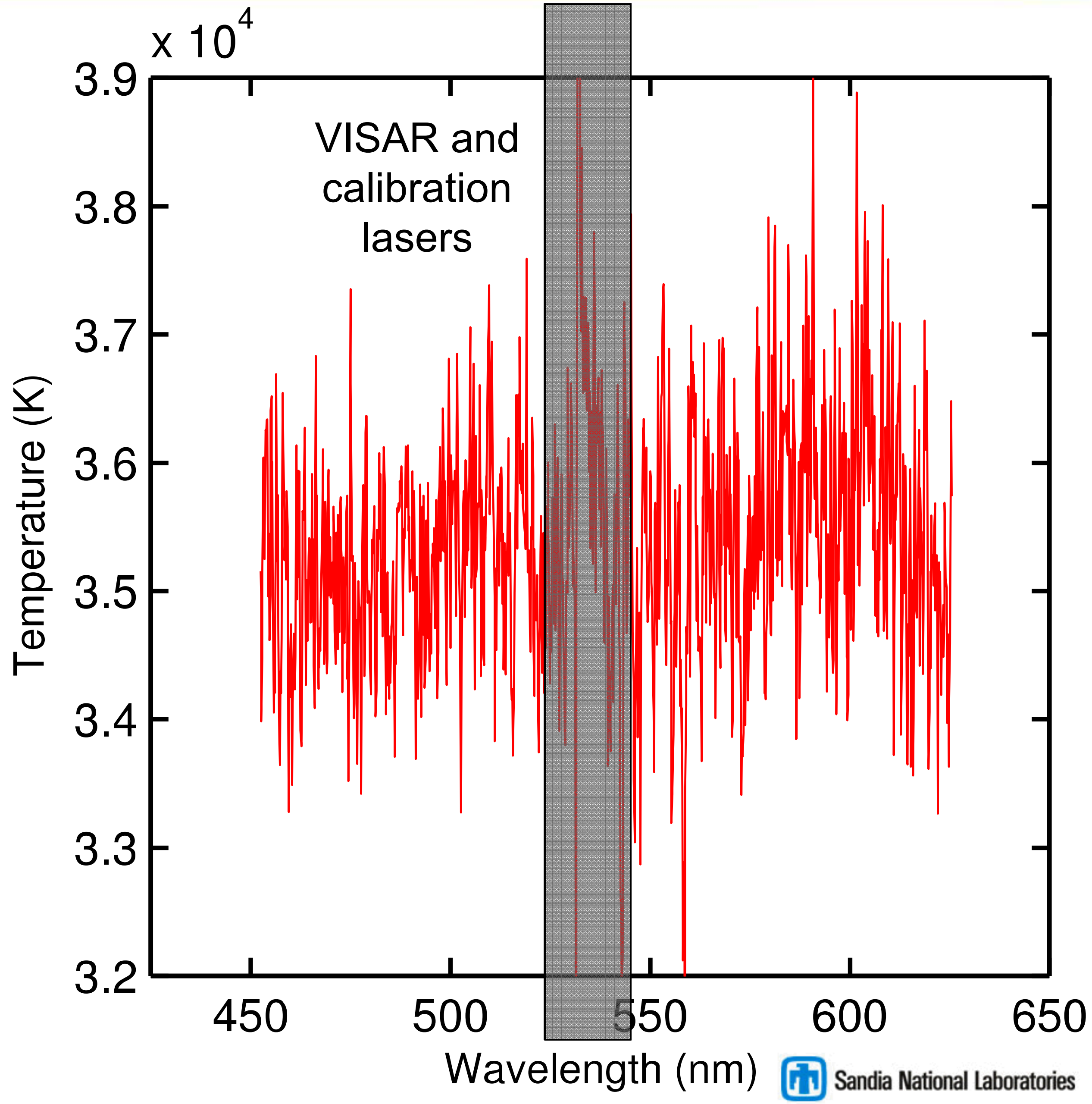


Calculation is done at each wavelength over a few hundred nm wavelength range

Emissivity for quartz and deuterium are determined from QMD calculations and are wavelength dependent

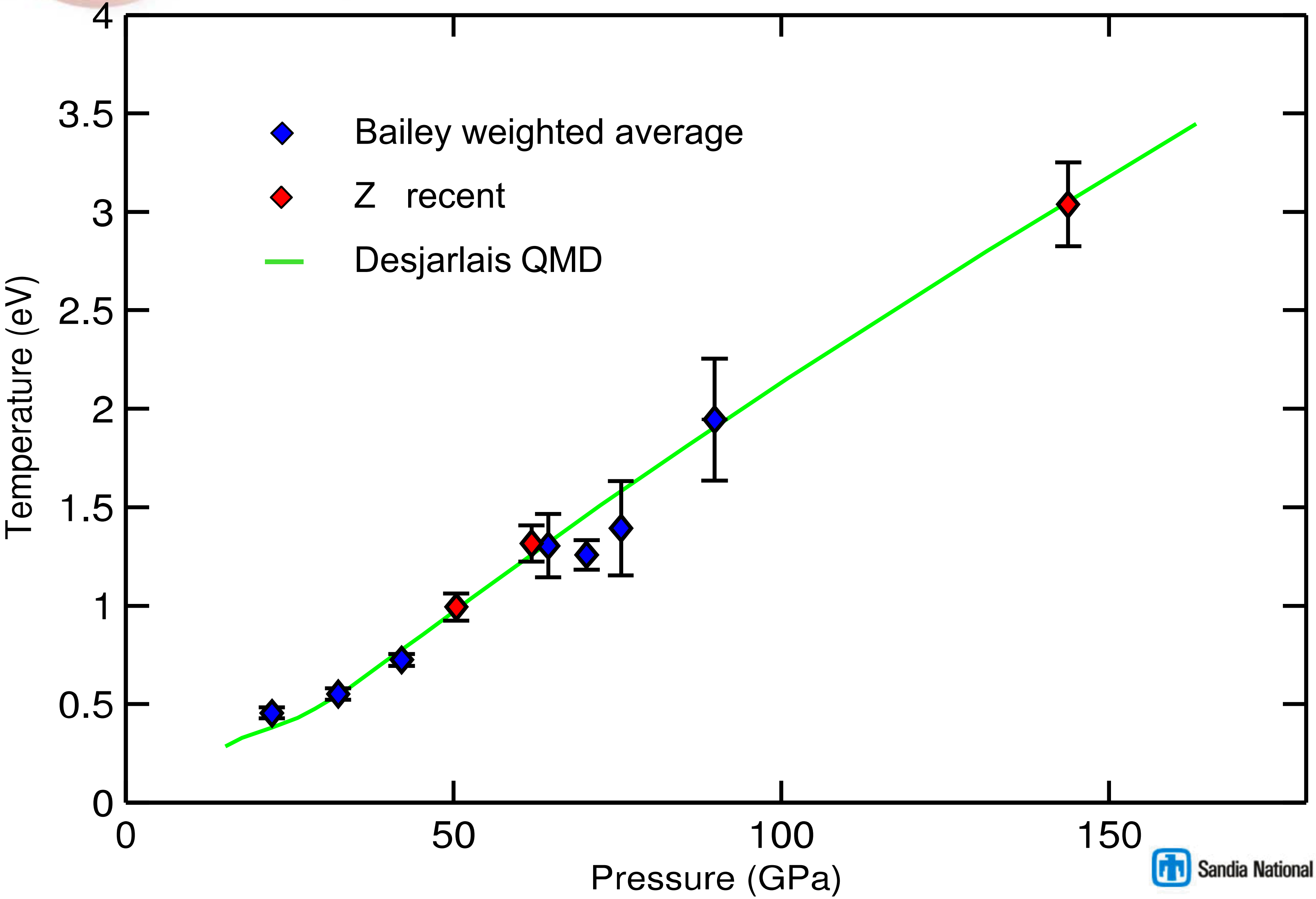
Wavelength independent response suggests that the method used to correct for reflections at the interfaces is reasonable

Technique was recently employed with data from LiD which further corroborate the method



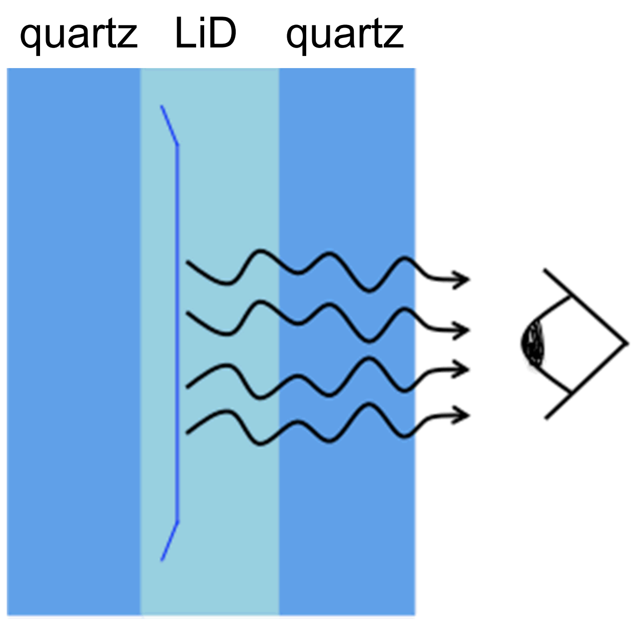
Sandia National Laboratories

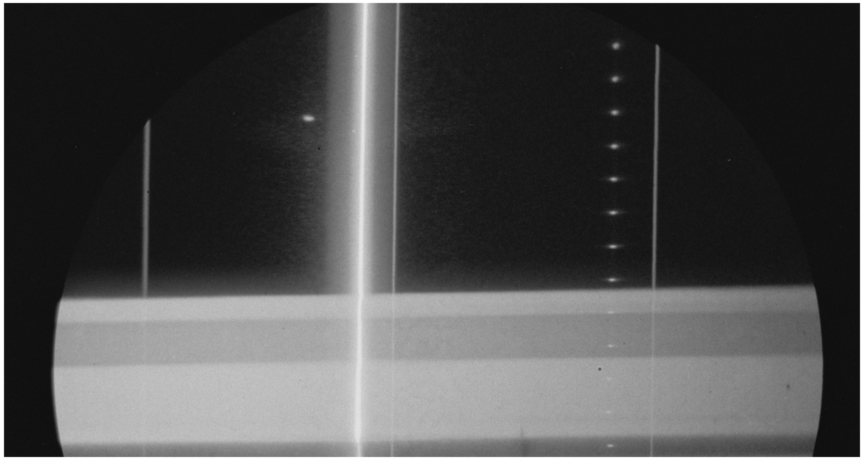
Temperature measurements are in very good agreement with QMD and previous data

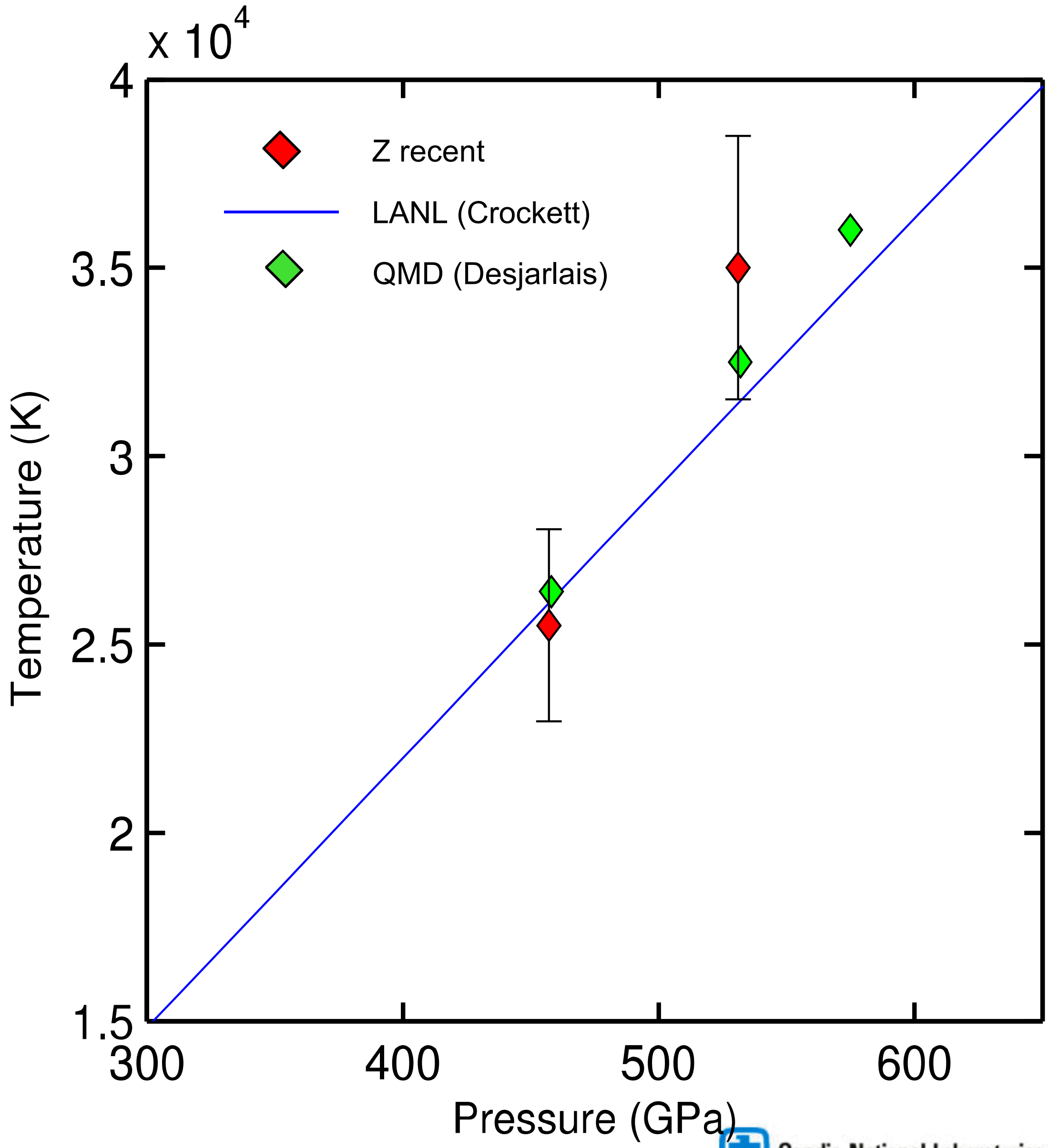


Sandia National Laboratories

Similar method used to extract temperature data for LiD

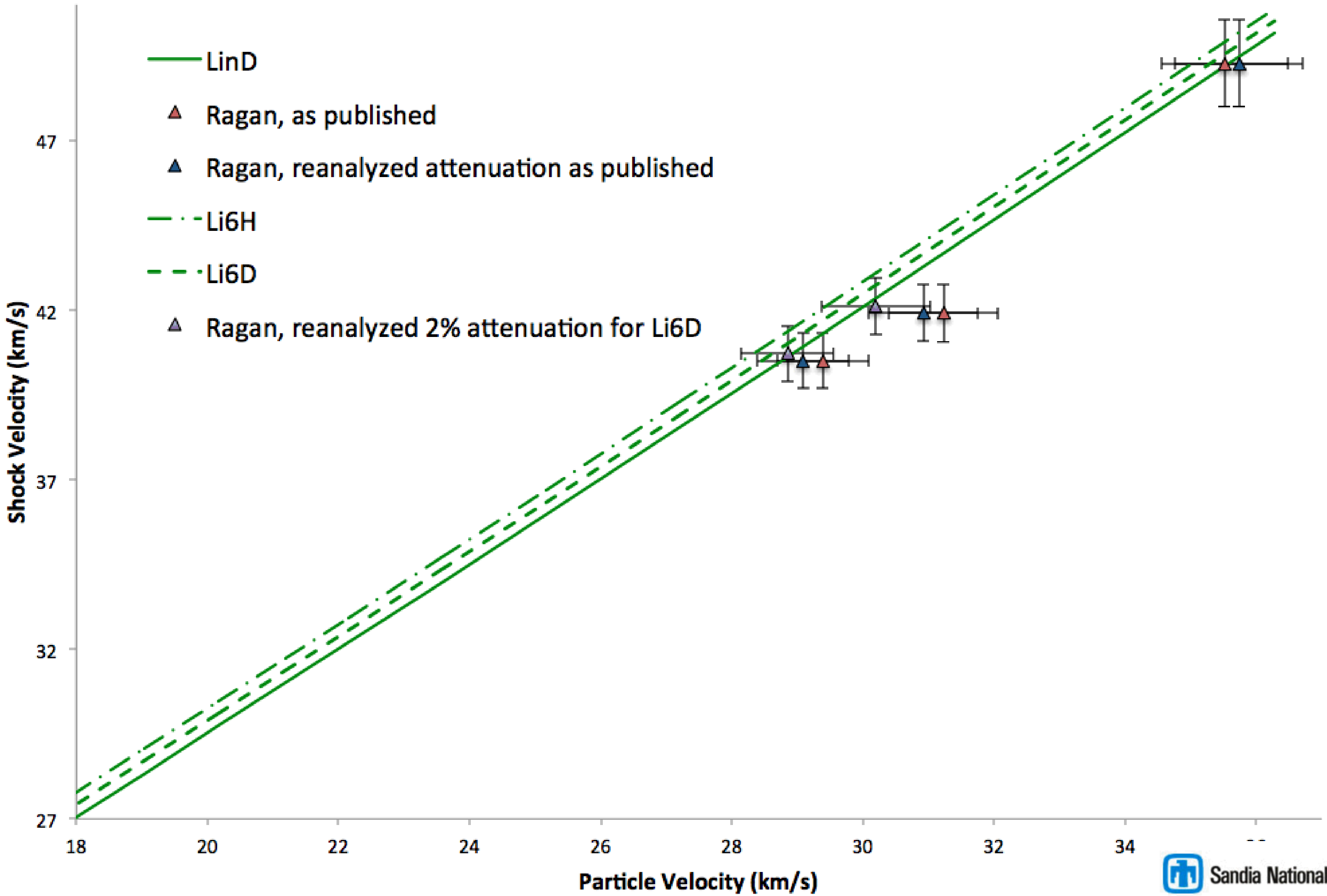






Sandia National Laboratories

Reanalysis of Ragan data is consistent with the recent QMD Hugoniot at high pressure



Conclusions

- LiD Hugoniot measurements have been made in the 190-550 GPa range
- LiD re-shock measurements have been made in the 700-900 GPa range
- LiD temperature measurements have been made on the Hugoniot in the 450-550 GPa range
- All of these measurements are reasonably consistent with the recent QMD Hugoniot and re-shock calculations of Desjarlais and the recent table produced by LANL (Crockett)