SAND2015-4919C

SCCM, J5: EOS VII : Multiphase Systems
Tuesday, June 16 @ 11:15-30 AM Grand Ballroom I/J Tampa 2015

A New Equation of State for α-Quartz

R.J. Magyar
And
J. Carpenter

Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

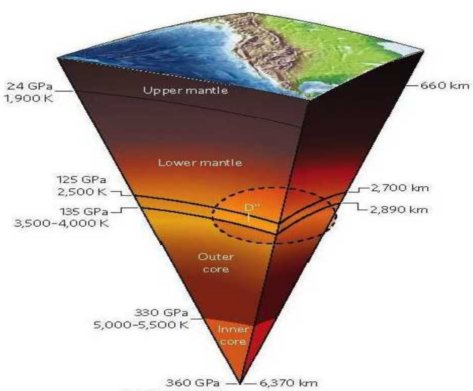
Materials Properties are Needed to Model Complex Phenomena through Equations of State

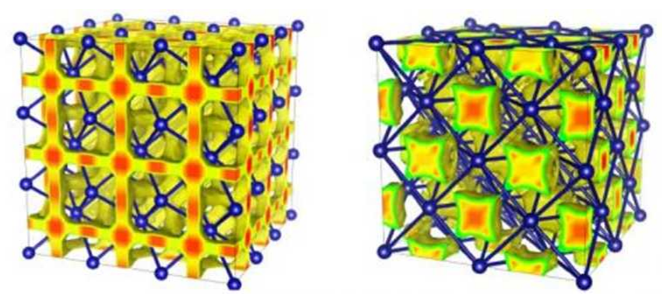
Pressure, density, temperature, phase….

- Materials science
- Planetary collision science
- Geoscience
- Inertial confinement fusion

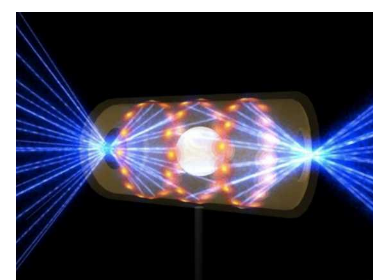
Information to build equations of state

- Low temperature experiments diamond anvil cell < a few kK
- High temperature plasma physics where degeneracies are negligible





Super ionic water

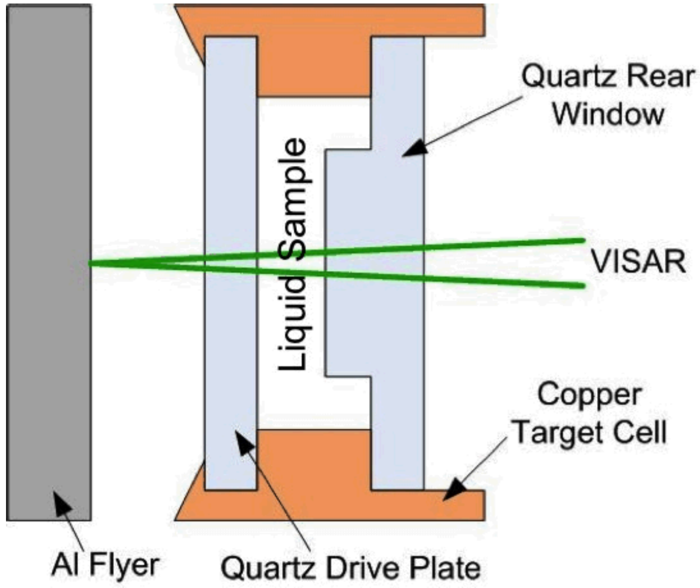


Sandia National Laboratories

The Z-Machine Relies on Impendence Matching to Determine Many of these Properties.

- Achieves Pressures greater than 10 Mbar (1 TPa).
- Recent work on Xenon reached a state 840 GPa and 149kK
- Compare to diamond Anvil cell – up to 300 GPa and several kK

Indirectly but Accurately Measures **Pressures and Densities**



- Evaluation through comparison with shock compression data
- impedance match (IM) standards
- errors in the standard affect predictions
- Quartz has recently become an IM standard of choice in the several 100 GPa regime.

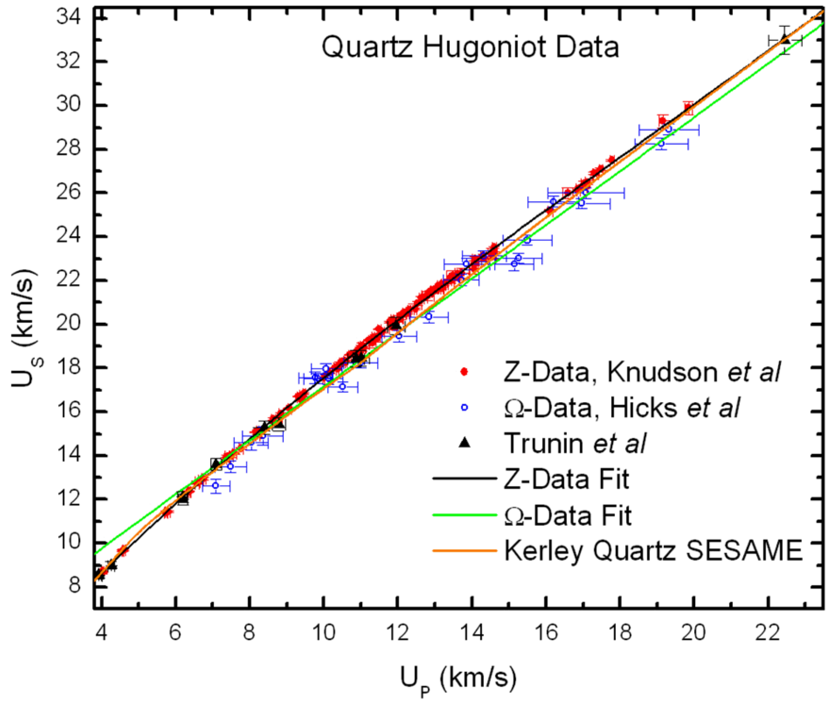
VISAR main diagnostics

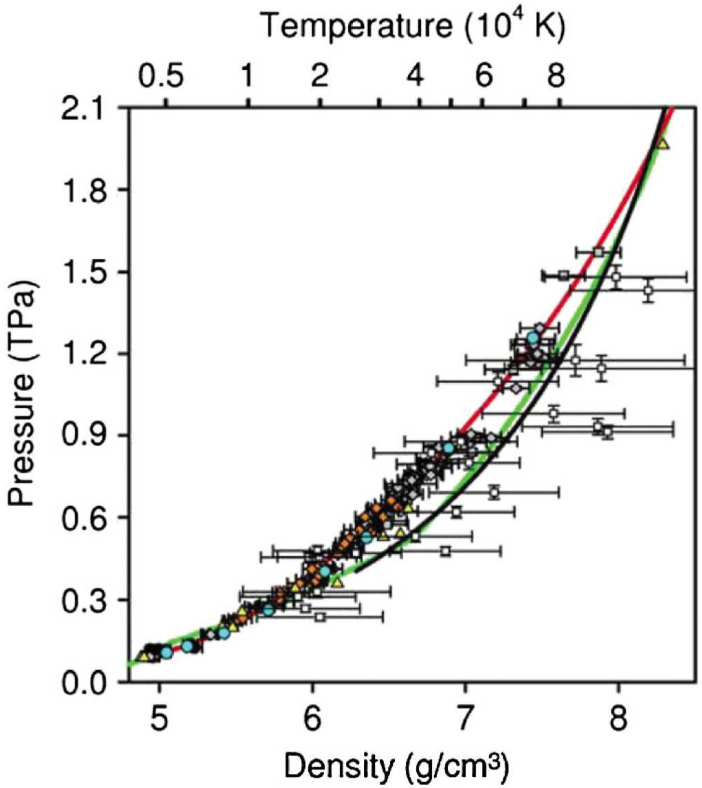
Flyer velocity, time of impact

Arrival at interfaces and breakout

Shock velocity in samples

High Accuracy EOS for Quartz Window (SiO_2) is Needed for High Fidelity Shock Experiments.

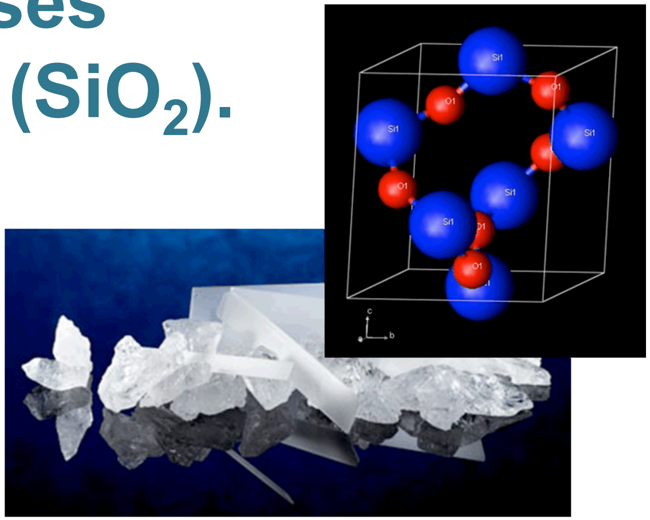


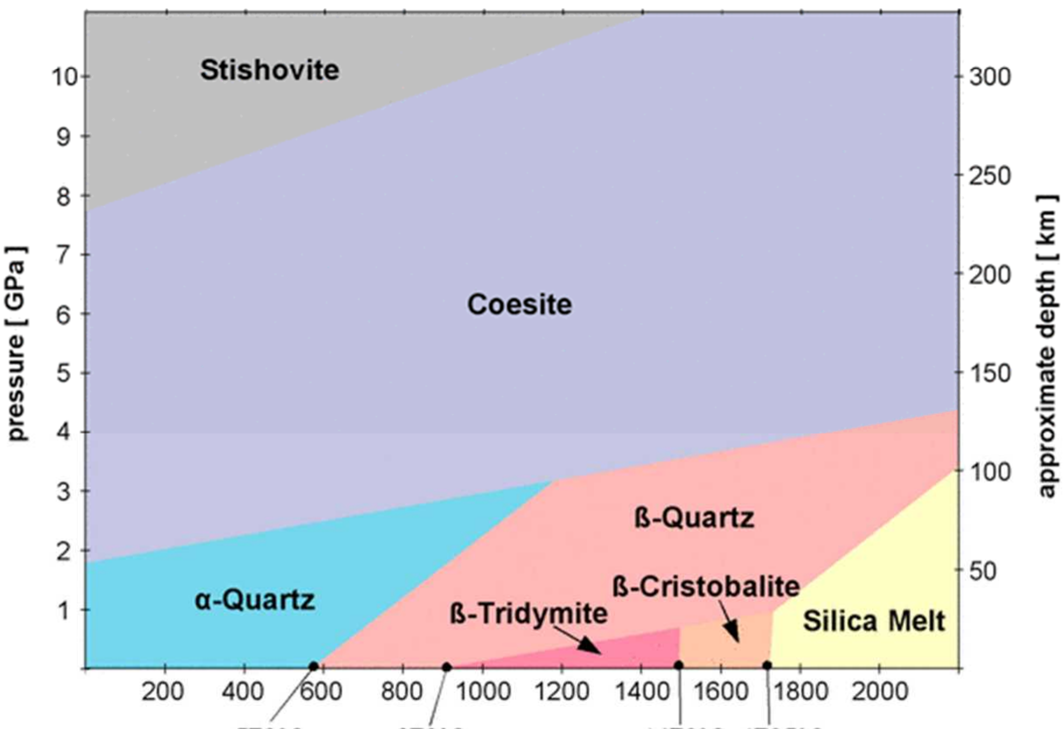


Errors in the IM standard produce systematic errors up to 12% and 23% in the density of deuterium and helium in the 100–200 GPa pressure range, respectively.

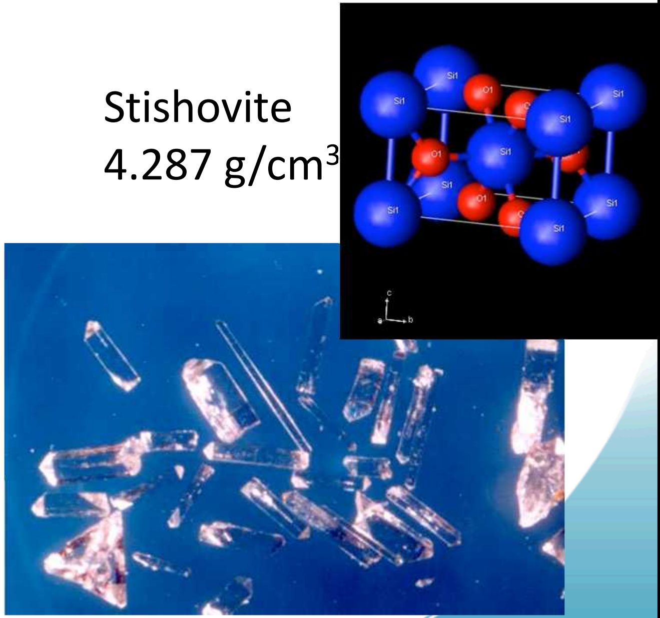
The Principle Hugoniot Traverses Several Polymorphs of Quartz (SiO_2).

Alpha Quartz
2.648 g/cm^3



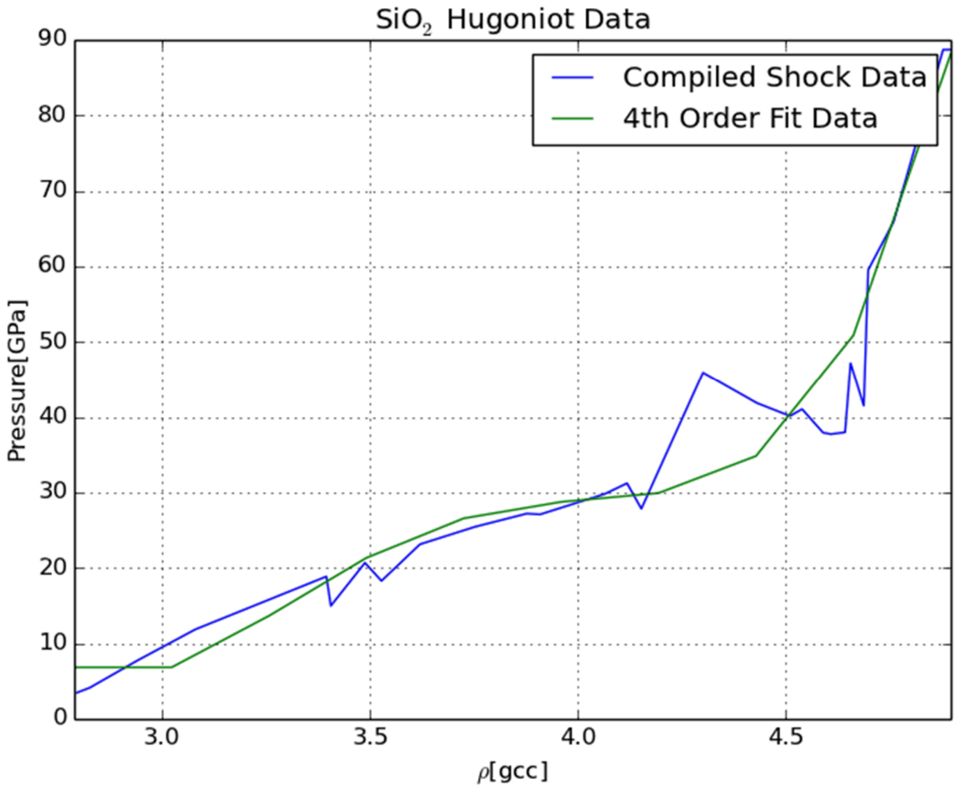


Stishovite
4.287 g/cm^3



Sources of Reference Data Span the Relevant Thermodynamic Conditions.

1. Diamond Anvil Cell alpha-quartz and stishovite
2. JANAF thermo data data from NIST
3. Hugoniot for Alpha and Stishovite (LASL shock data handbook, http://www.ihed.ras.ru/rusbank/)
4. Z- release data (M. D. Knudson and M. P. DesjarlaisPhys. Rev. Lett. 103, 225501, M. D. Knudson and M. P. Desjarlais Phys. Rev. B 88 184107 (2013))
5. Melt (Kanzaki, Jackson, Ahrens, Belonoshko, and others)
6. DFT-MD (Sandia – K. Cochrane)
7. Inferred vapor dome (Kraus et al. J. OF GEO. RES., 117, E09009



Sandia National Laboratories

Equation of State Modeling is often Described in Terms of a Separation of Helmholtz Free Energies.

$$F(\rho, T) = F_{cold}(\rho) + F_{ionic}(\rho, T) + F_{electronic}(\rho, T)$$

Cold Curve, thermal ionic, and thermal electronic

Multi phase EOS

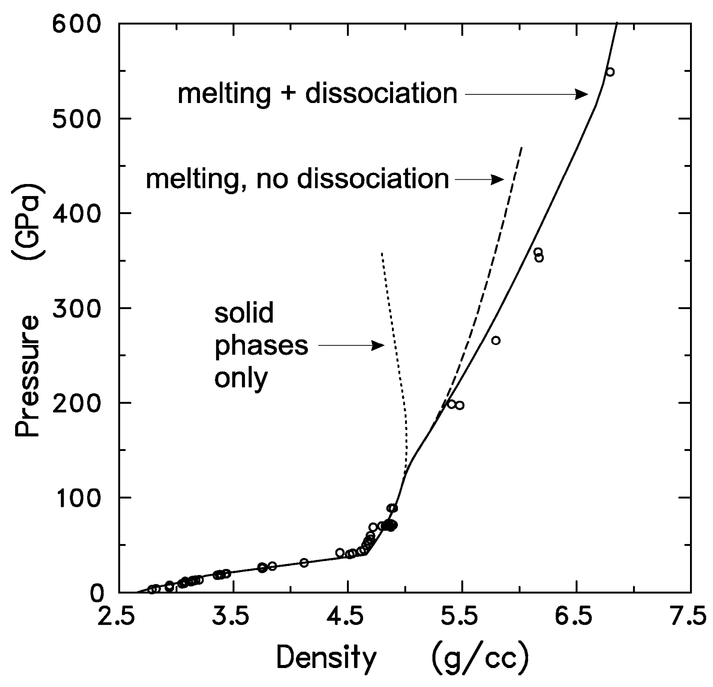
- Number of phases (solid 1 – solid 2 – fluid)
- 2 Triple points
- 1 Critical point
- 5 number of phase boundaries

Solid Model Describes Two Solid Phases.

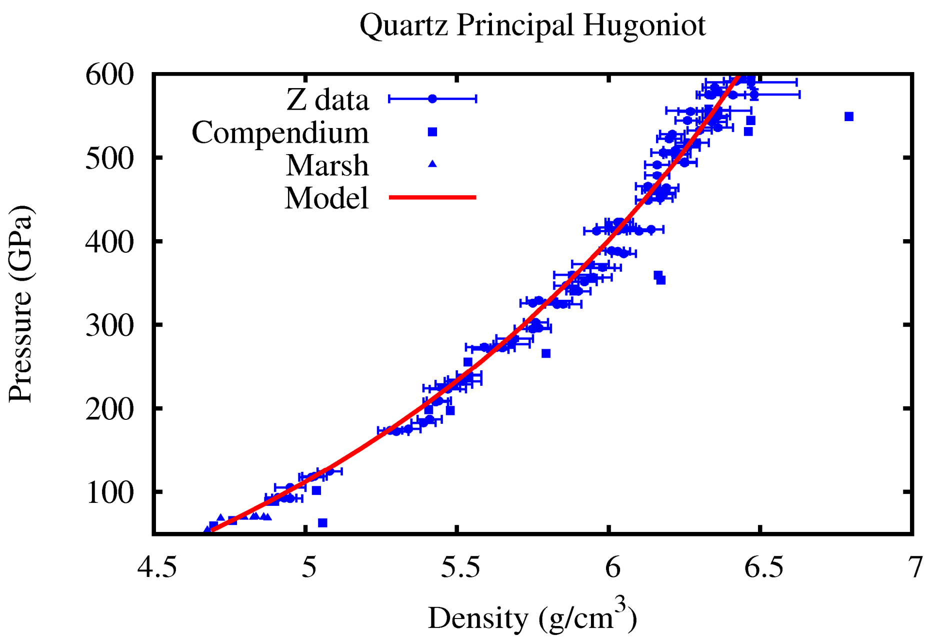
- General multiphase model with an arbitrary number of phases in an arbitrary phase diagram, under only a few restrictions for connectivity of phases
- 2 solid phases included (alpha and stishovite). The Hugoniot crosses both and these two have significantly differing densities.
- Melt curve
- The cold curve: Vinet-Holzapfel-Thomas-Fermi-Kirzhits model. Good for cold compression of metals, matches Thomas-Fermi and Vinet in appropriate limits.
- Expansion model needed (sigma<1) series expansion.
- Atomic model is a Debye Ionic model
- Electronic thermal model is a generalized metal electric

Fluid Model Does not Explicitly Include Dissociation.

- Fluid phase describes both liquid and gas states.
- No explicit dissociation model - Analysis of the Hugoniot has revealed that this dissociation model development is likely unnecessary.



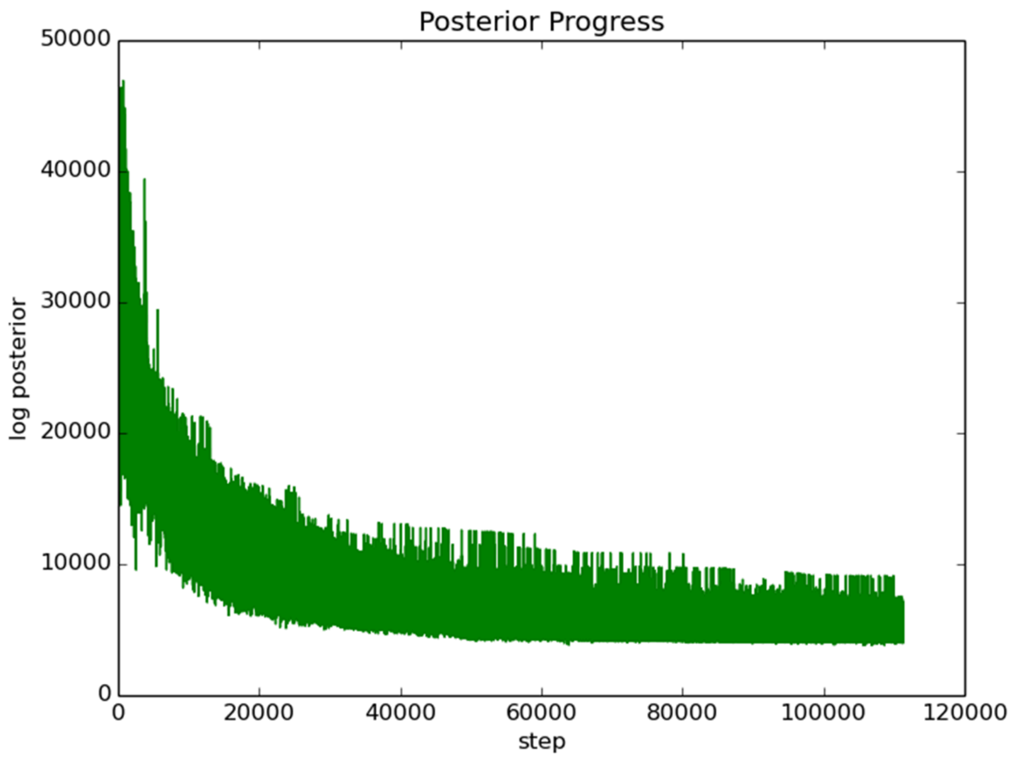
[Kerley, KPS99-4, 1999]



Our model – no dissociation

Sandia National Laboratories

The Parameters are Fit using Several Approaches.

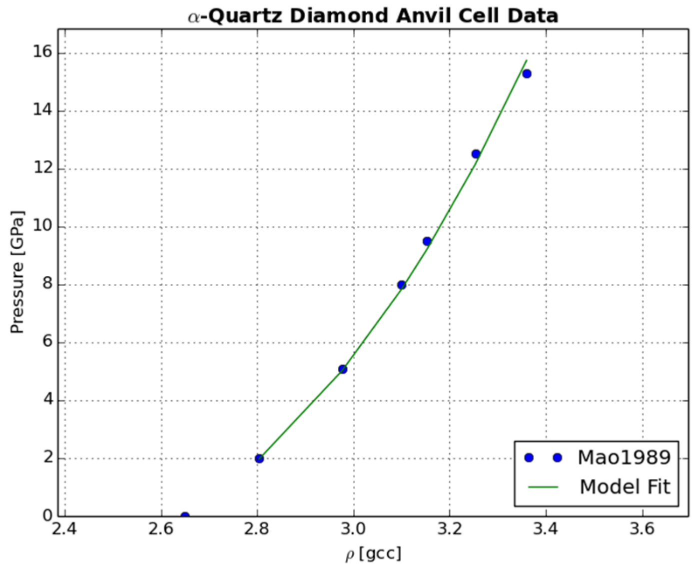


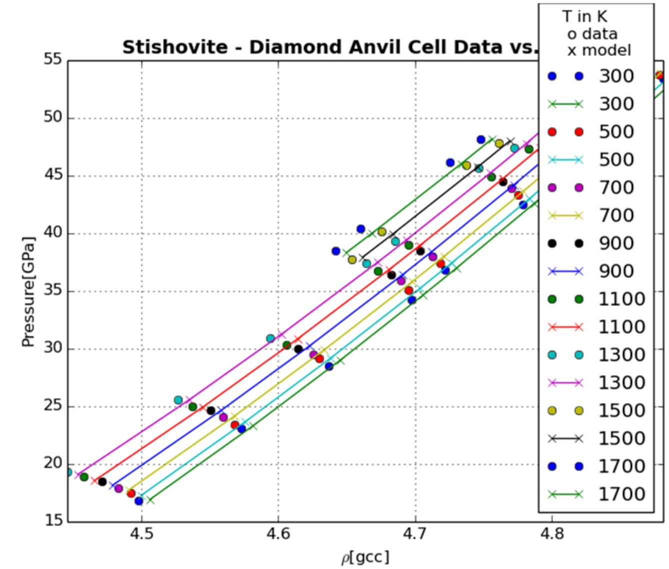
30-35 params to fit

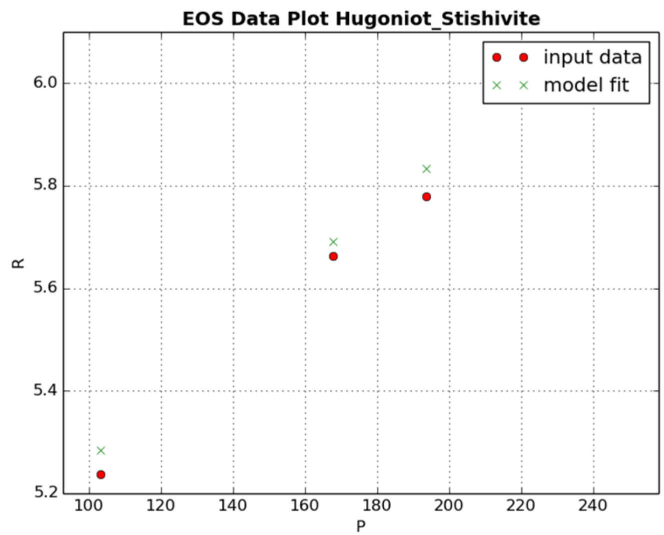
Two methods :

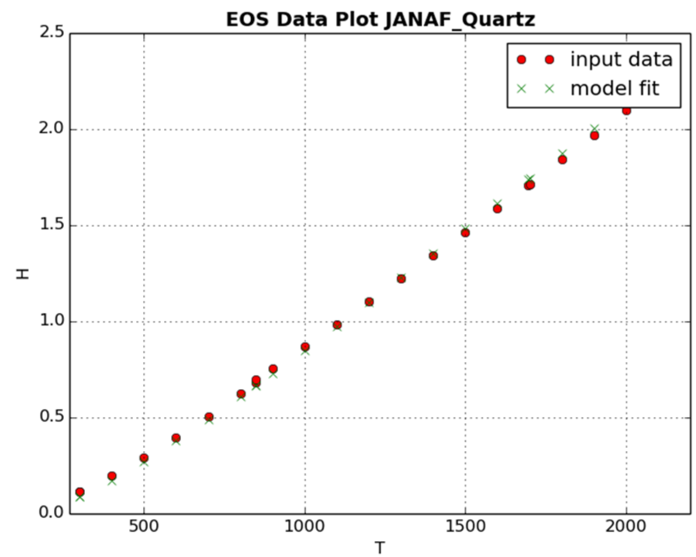
1. Run stochastic Dirichlet process within a Bayesian framework
2. Gradient optimization

Current Choice of Fitting Parameters Describes Several Data Sets Well.

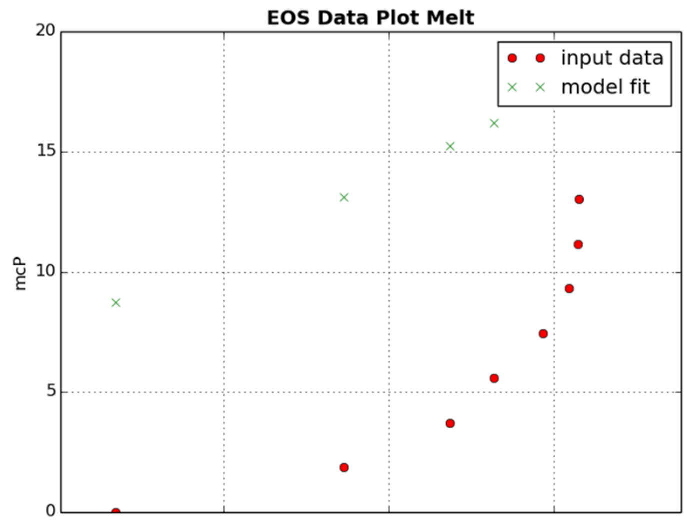


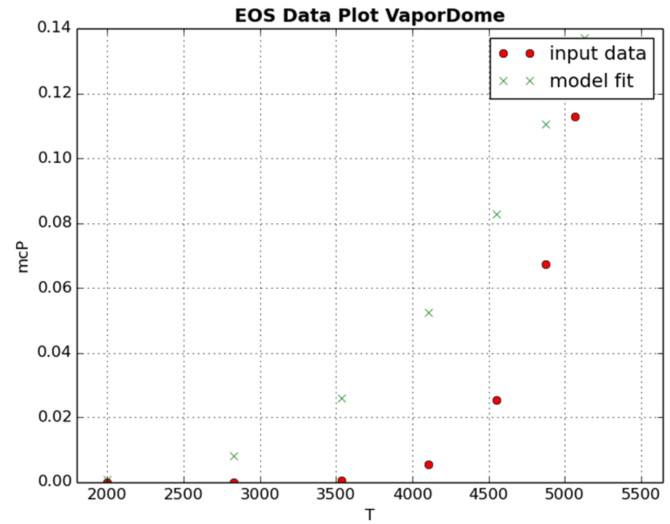


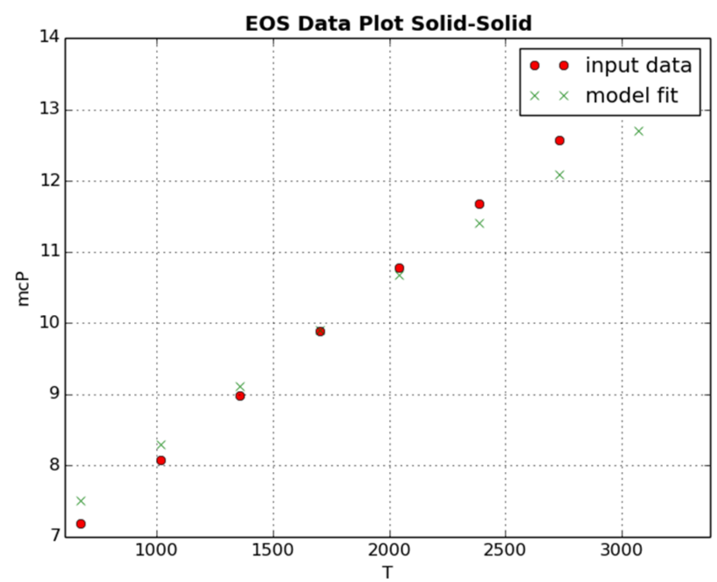




However, Data Sets Such as the Vapor Dome and Melt Curves are Not Converged







Additional variational degrees of freedom are being added through multiple melt models in the fluid and alpha phases

Sandia National Laboratories

Summary and Future Work

- We are developing a multi phase EOS for alpha quartz windows for use in the analysis of shock experiments on Z
- The new model includes 2 solid phases.
- 2 melt models are required to match the 2 melt boundaries.
- Currently, we are optimizing parameters.
- Initial results demonstrate reasonable agreement with input data.
- Release data will be included in later iterations.
- Developing a high accuracy equation of state optimized along the Hugoniot will enable even higher fidelity analysis of Z-shots.