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Title: An Introduction to Equation of State & Shock Physics Research

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An Introduction to Equation of State & Shock Physics Research

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A general introduction to Equation of State (EOS) and Shock Physics Research will be presented. The goal is to provide the audience with an overall sense of what is involved in producing a complete Equation of State (single and multi-phase) and what advanced methods (DFT, QMD, etc..) are being utilized to better constrain the thermodynamic models. I will also present a variety of shock data results and show how these results are utilized in validating our EOS. The general interest of this work spans disciplines: Physicists, Chemists, Material Scientists, Mechanical Engineers, Geophysicists, and Applied Mathematicians.

Abstract

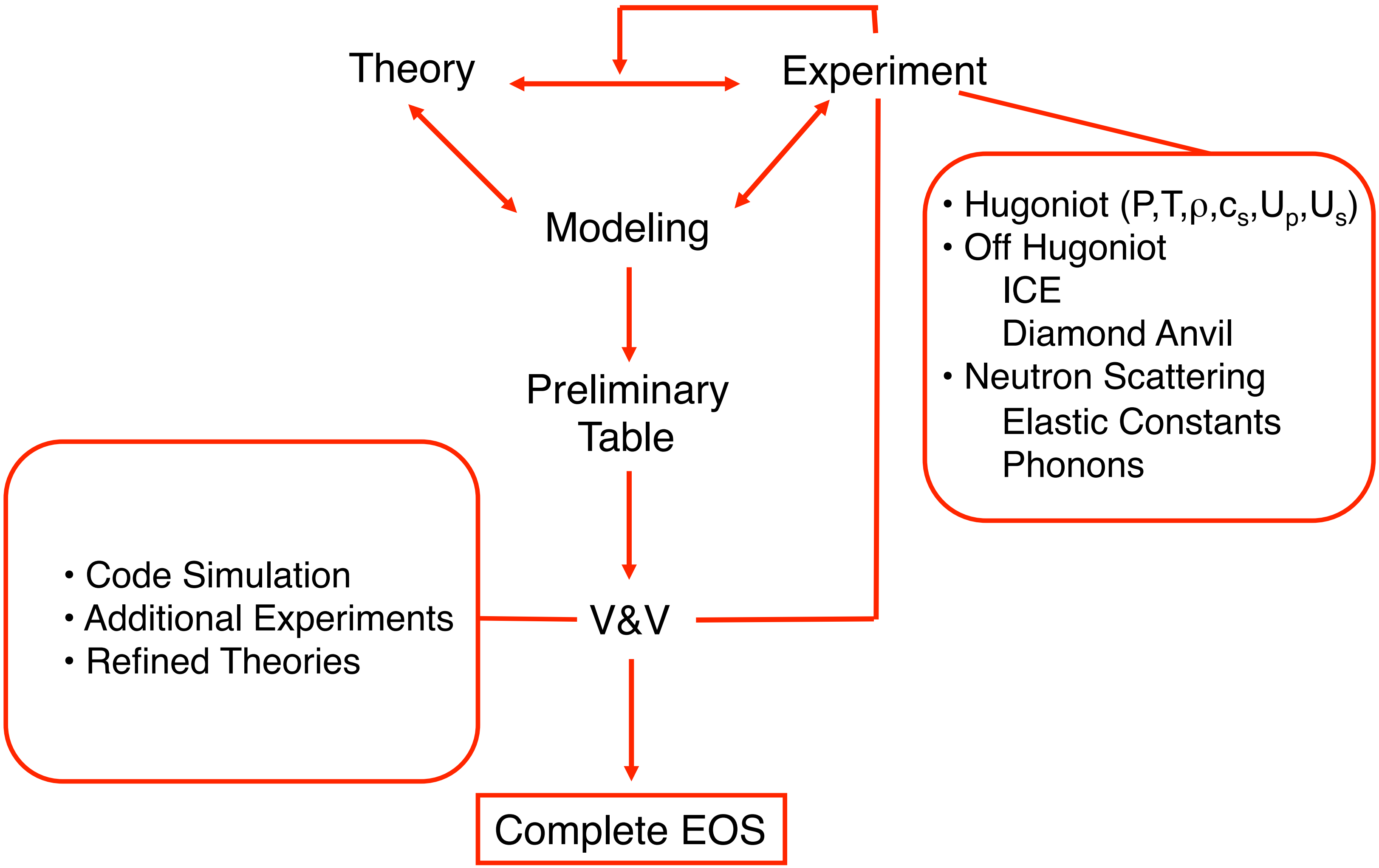
A general introduction to Equation of State (EOS) and Shock Physics Research will be presented. The goal is to provide the audience with an overall sense of what is involved in producing a complete Equation of State (single and multi-phase) and what advanced methods (DFT, QMD, etc..) are being utilized to better constrain the thermodynamic models. I will also present a variety of shock data results and show how these results are utilized in validating our EOS. The general interest of this work spans disciplines: Physicists, Chemists, Material Scientists, Mechanical Engineers, Geophysicists, and Applied Mathematicians.

Introduction

- A brief overview of Equation of State modeling.
- Introduction to the shock physics and the conservation laws.
- An example of the Equation of State modeling applied to Germanium.

Equation of State

Standard Approach to Making an EOS



Equation of State

Scope of the Problems

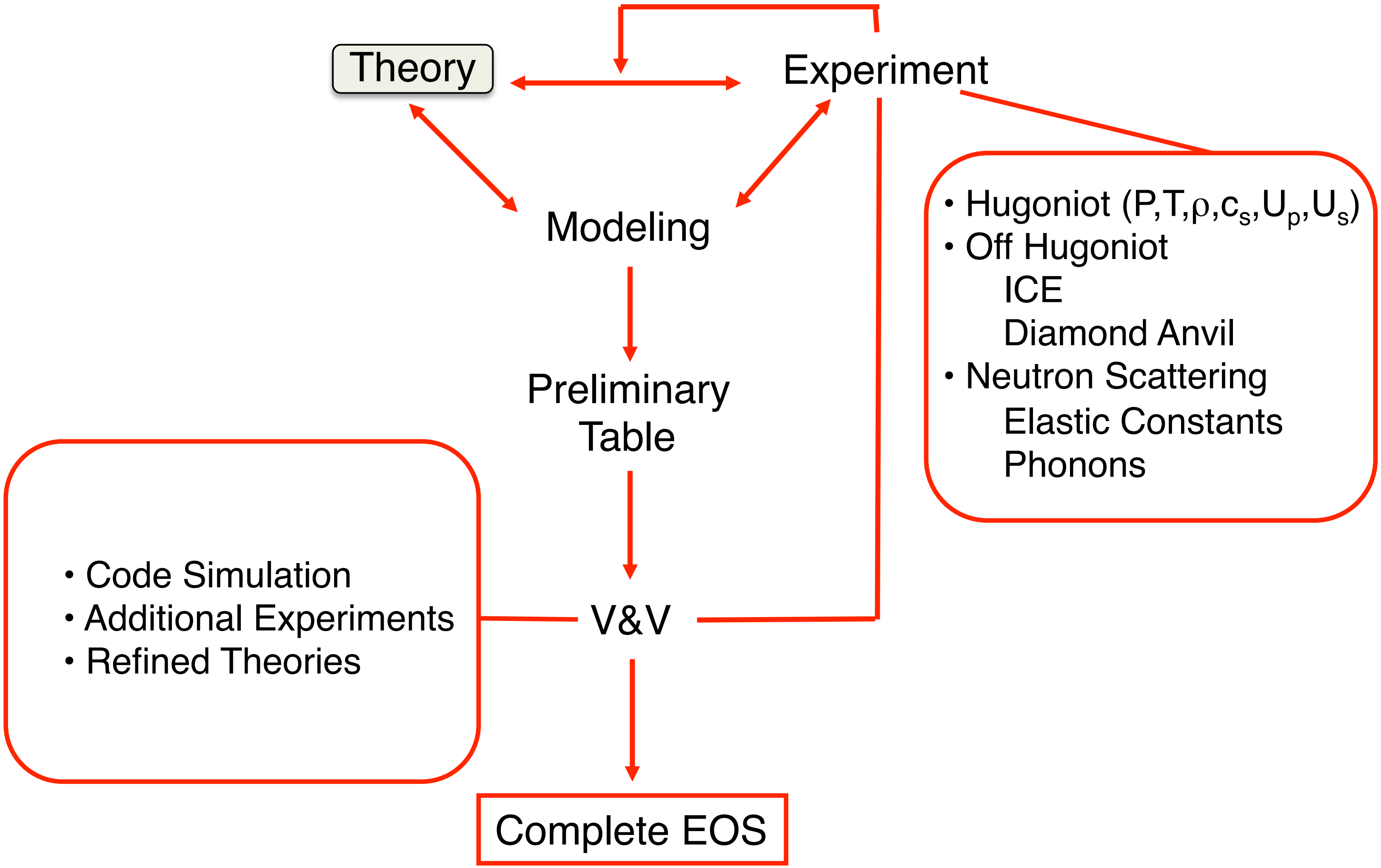
- Wide Variety of Complex Materials
  - Actinides (Pu, U, etc.)
  - Elemental Metals
  - Alloys and Chemical Compounds
  - Molecular Solids and Liquids
  - Polymers, Foams, Composites, and Geological
  - High Explosives
- Ambient to Astrophysical Conditions ($10^{-6} < \rho/\rho_o < 10^5$, $0 < T < 10^5$eV)
- Nonequilibrium Processes (melting & refreezing)
- Large Ranges of Interpolation Between Models
- Incomplete Experimental Information

Solutions

- More Basic Theory
- Improved Modeling
- Increased Support for Experiments

Equation of State

Standard Approach to Making an EOS



Three-term Decomposition of Free Energy

$$F(V,T) = \phi_0(V) + F_{\text{ion}}(V,T) + F_{\text{el}}(V,T)$$

$\phi_0(V)$ cold curve contribution (Vinet analytic form)

$F_{\text{ion}}(V,T)$ cold + thermal ionic contribution (Debye model)

$F_{\text{el}}(V,T)$ thermal electronic contribution (Thomas Fermi Dirac)

Questions: Is this free energy too simple? Should we include anharmonic, electron-phonon and/or a more complicated electronic part?

$$G^s(P, T_m(P)) = G^l(P, T_m(P))$$

Basic thermodynamic quantities

$$F = E - TS$$

$$dF = dE - TdS - SdT$$

$$= -SdT - PdV$$

$$dF = \left(\frac{\partial F}{\partial T}\right)_V dT + \left(\frac{\partial F}{\partial V}\right)_T dV$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_V \longleftarrow \text{Entropy}$$

$$P = \rho^2 \left(\frac{\partial F}{\partial \rho}\right)_T \longleftarrow \text{Pressure}$$

$$E = F + TS = F - T\left(\frac{\partial F}{\partial T}\right)_V \longleftarrow \text{Internal energy}$$

Basic thermodynamic quantities

$$C_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V = \left(\frac{\partial E}{\partial T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V$$ ← Specific heat at constant volume

$$C_P = \left(\frac{\partial H}{\partial T}\right)_P = T\left(\frac{\partial S}{\partial T}\right)_P$$ ← Specific heat at constant pressure

$$B_T = V\left(\frac{\partial^2 F}{\partial V^2}\right)_T = -V\left(\frac{\partial P}{\partial V}\right)_T$$ ← Isothermal bulk modulus

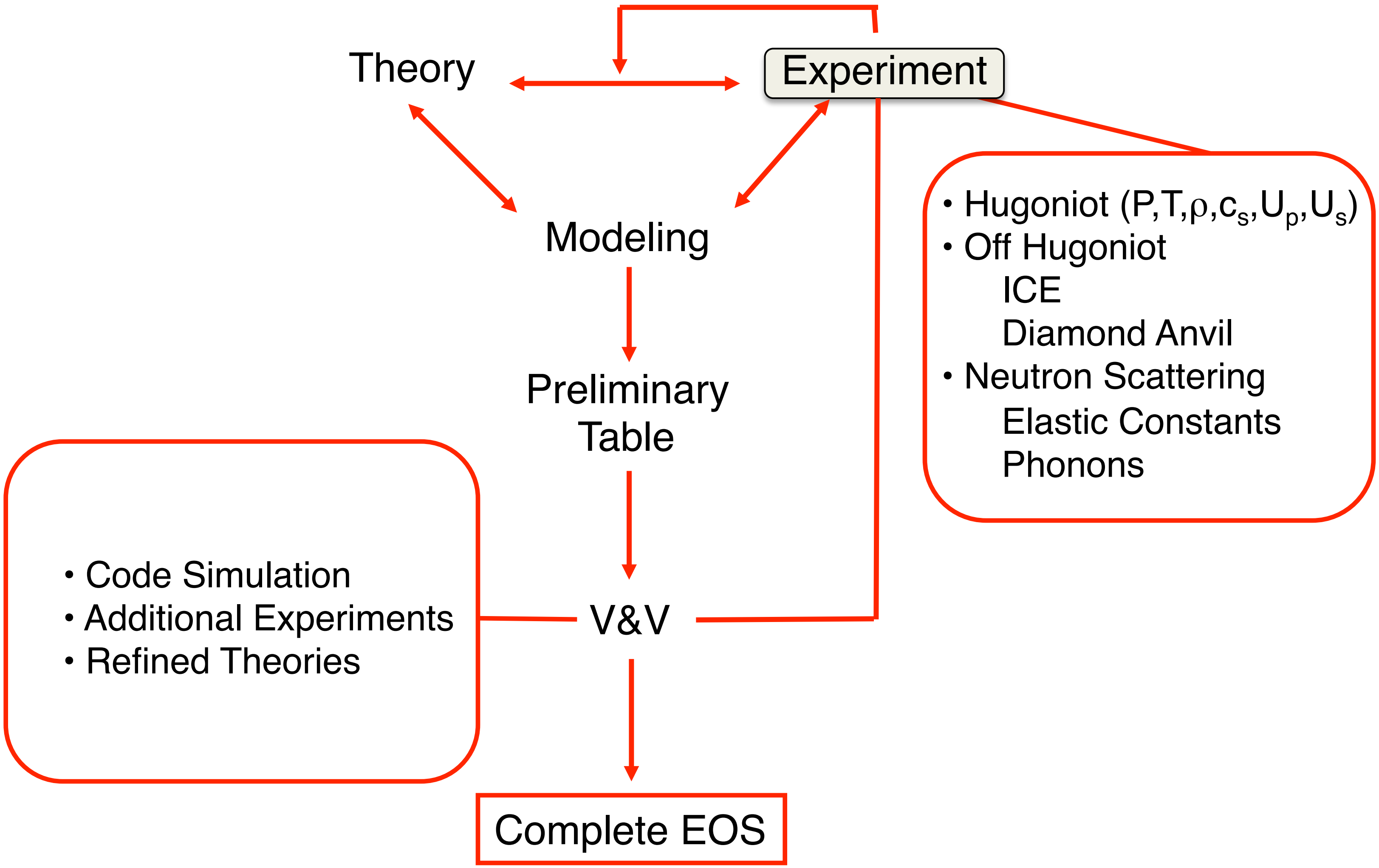
$$B_S = -V\left(\frac{\partial P}{\partial V}\right)_S$$ ← Adiabatic bulk modulus

$$\frac{B_S}{B_T} = \frac{C_P}{C_V}$$

$$\gamma = \frac{\alpha B_s V}{C_p}$$

Equation of State

Standard Approach to Making an EOS



Experimentally Measured Data

- **Near-ambient Pressure Data**
  - Density
  - Melt and Boiling Point
  - Thermal Expansion
  - Acoustic Data
  - Specific Heat
  - Phonon / Elastic Moduli
  - Isobaric

Experimentally Measured Data

- **High Pressure Data**
  - Melt Curve
  - Shock (Dynamic High Pressure)
  - Diamond Anvil (Static High Pressure)
  - Phonon/Elastic Moduli
- **Other Data**
  - Vapor curve
  - Critical Point

Shock Physics

Characteristic features of shock wave compression

Breadth of Problems

- **Pressure range: ~1-10^4 GPa**
- **Time scales: ~10^{-13} - 10^{-5} s**
- **Directionality of loading**
- **Non-isotropic compression**
- **Large temperature rise (assuming thermal equilibrium)**
- **Nonlinear coupling between wave propagation and material response**

Shock wave experiments at different length scales: Recent achievements and future challenges, Y. M. Gupta, AIP Conf. Proc. 505, 3 (2000)

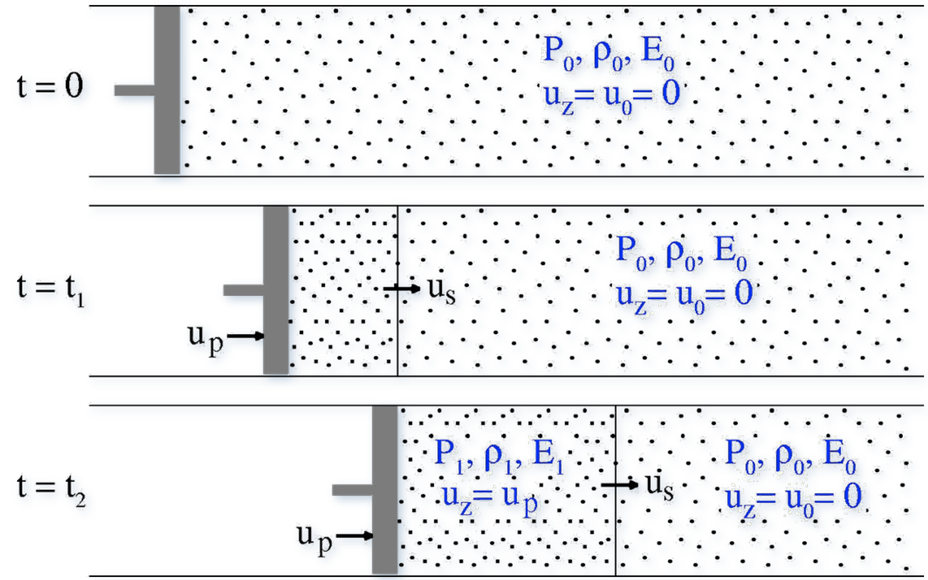
Shock Physics 101: Rankine-Hugoniot ("jump") relations

The initial and final states are linked through the conservation of mass, momentum, and energy:

$$\varepsilon = 1 - \frac{\rho_0}{\rho_1} = 1 - \frac{V_1}{V_0} = \frac{u_p}{u_s}$$

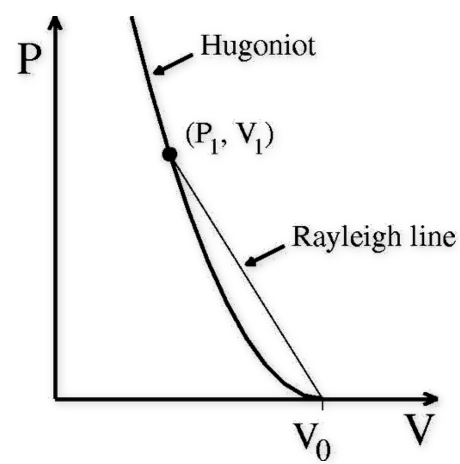
$$P_1 = P_0 + \rho_0 u_s u_p$$

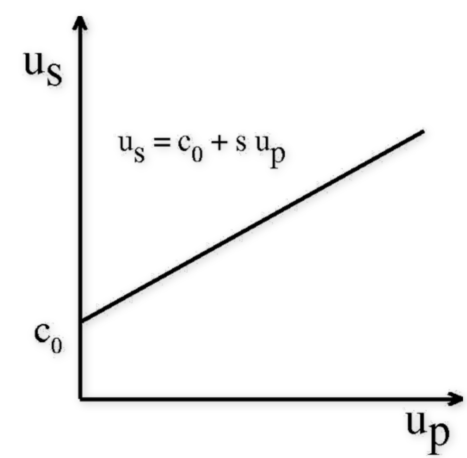
$$E_1 = E_0 + \frac{1}{2}(P_1 + P_0)(V_0 - V_1)$$



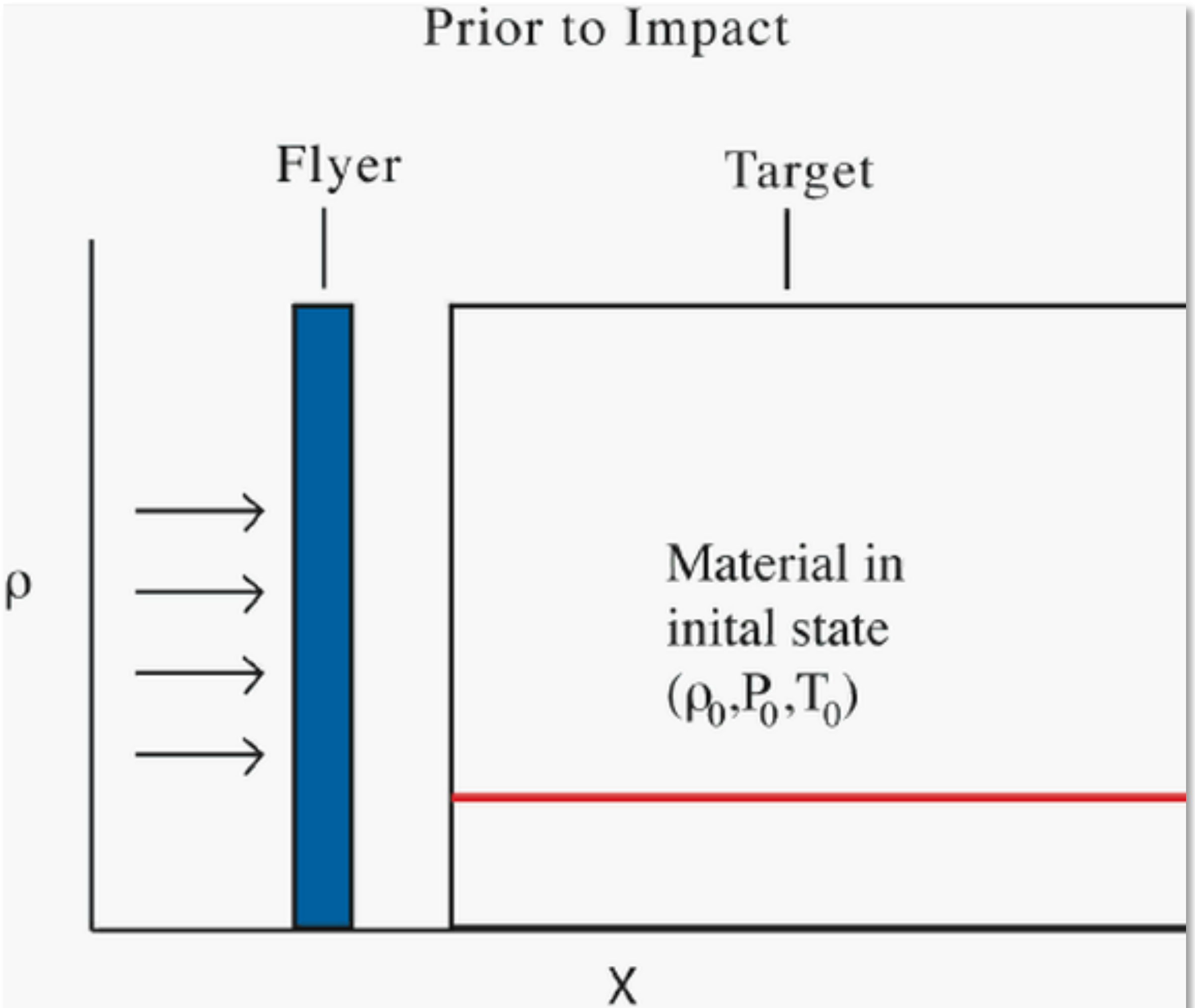
The "Hugoniot" (set of final states which can be achieved by a single shock) is typically represented in the (P,V), (u_s,u_p), or (P,u_p) planes:

$$\frac{P_1 - P_0}{V_1 - V_0} = -(\rho_0 u_s)^2$$

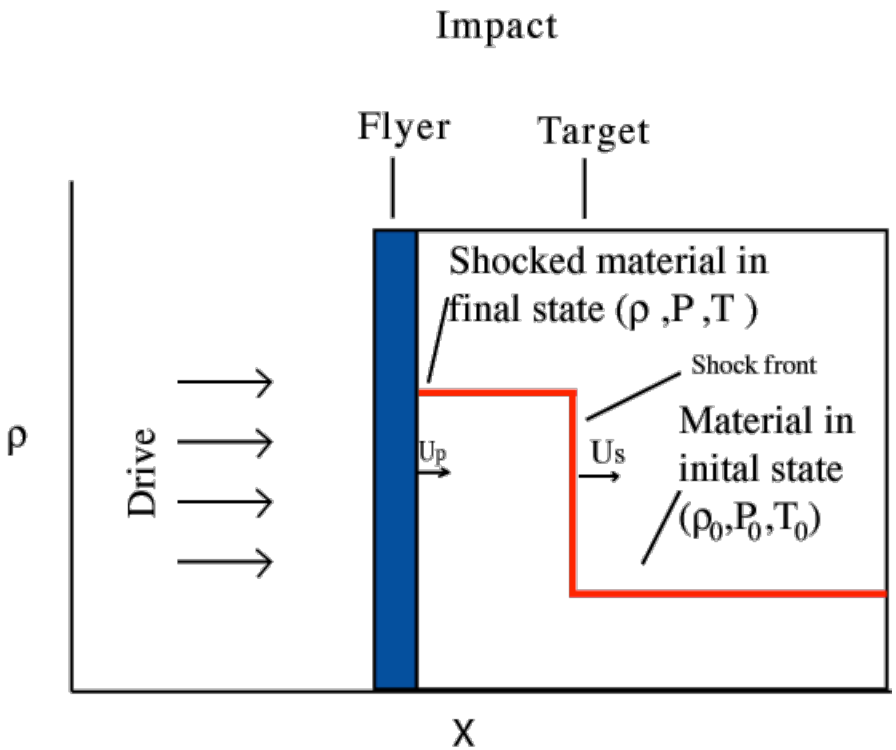


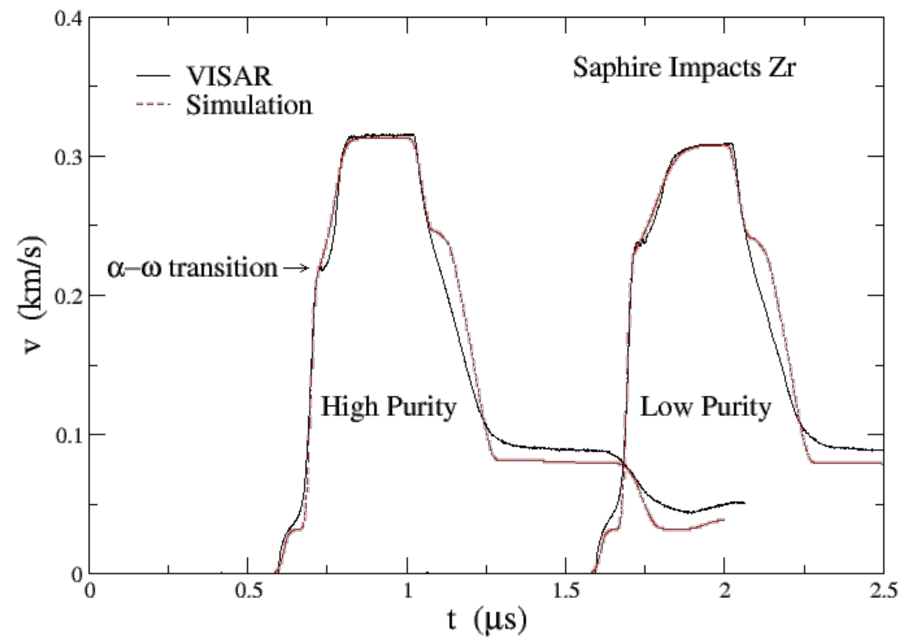


Shock Physics 101



Shock Physics 101





Experimental Equipment

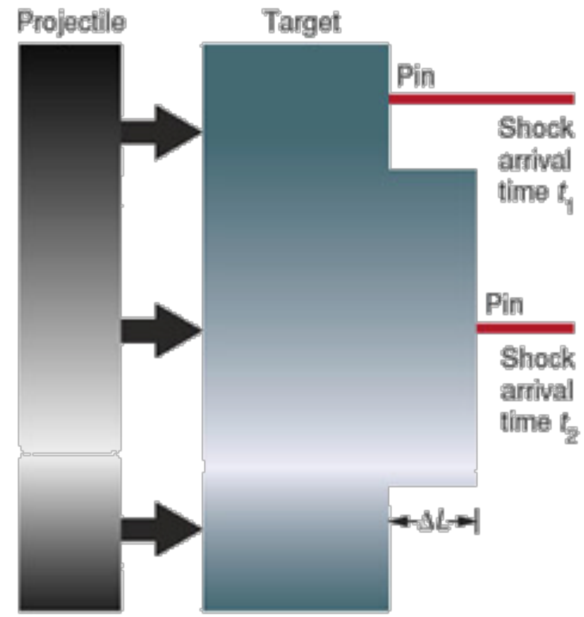
Used to Determine EOS Data

Static Experiments

- Diamond Anvil

Dynamic Experiments

- Pulse Power (Sandia Z, Atlas)
- Gas Gun (single, multi-stage)
- HE driven
- Laser

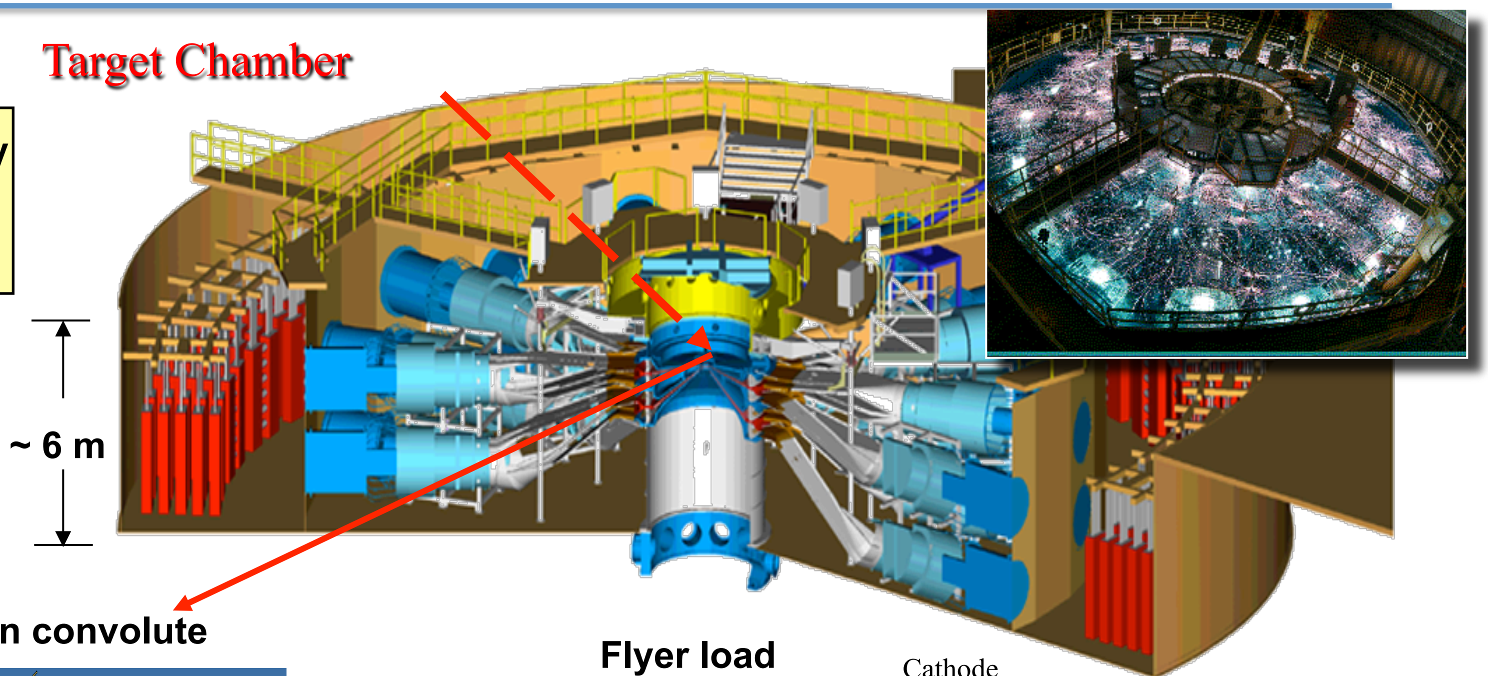


Other Experiments

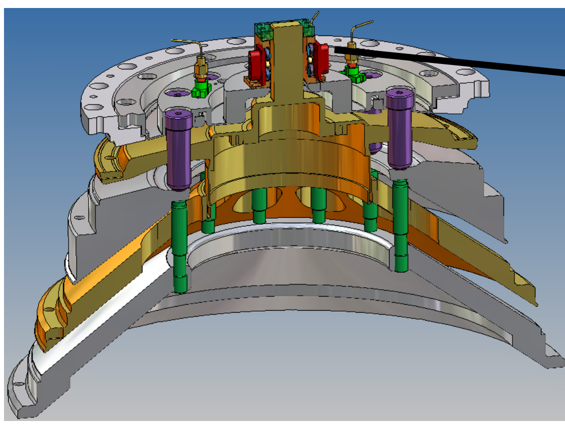
- RUS (resonant ultrasound spectroscopy)
- Calorimetry

Sandia Z accelerator

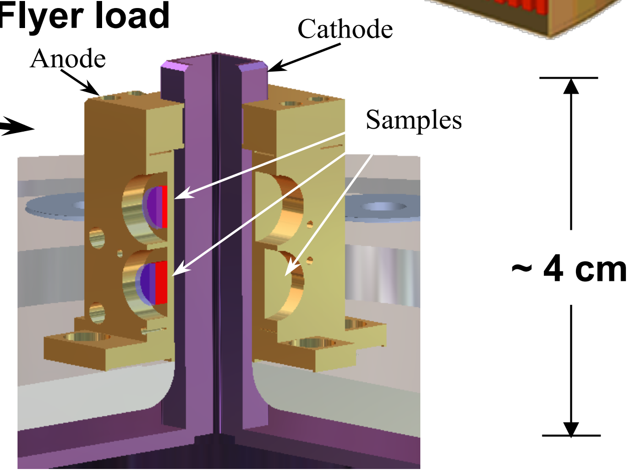
11.5 MJ stored energy
~22 MA peak current
~200 ns rise time

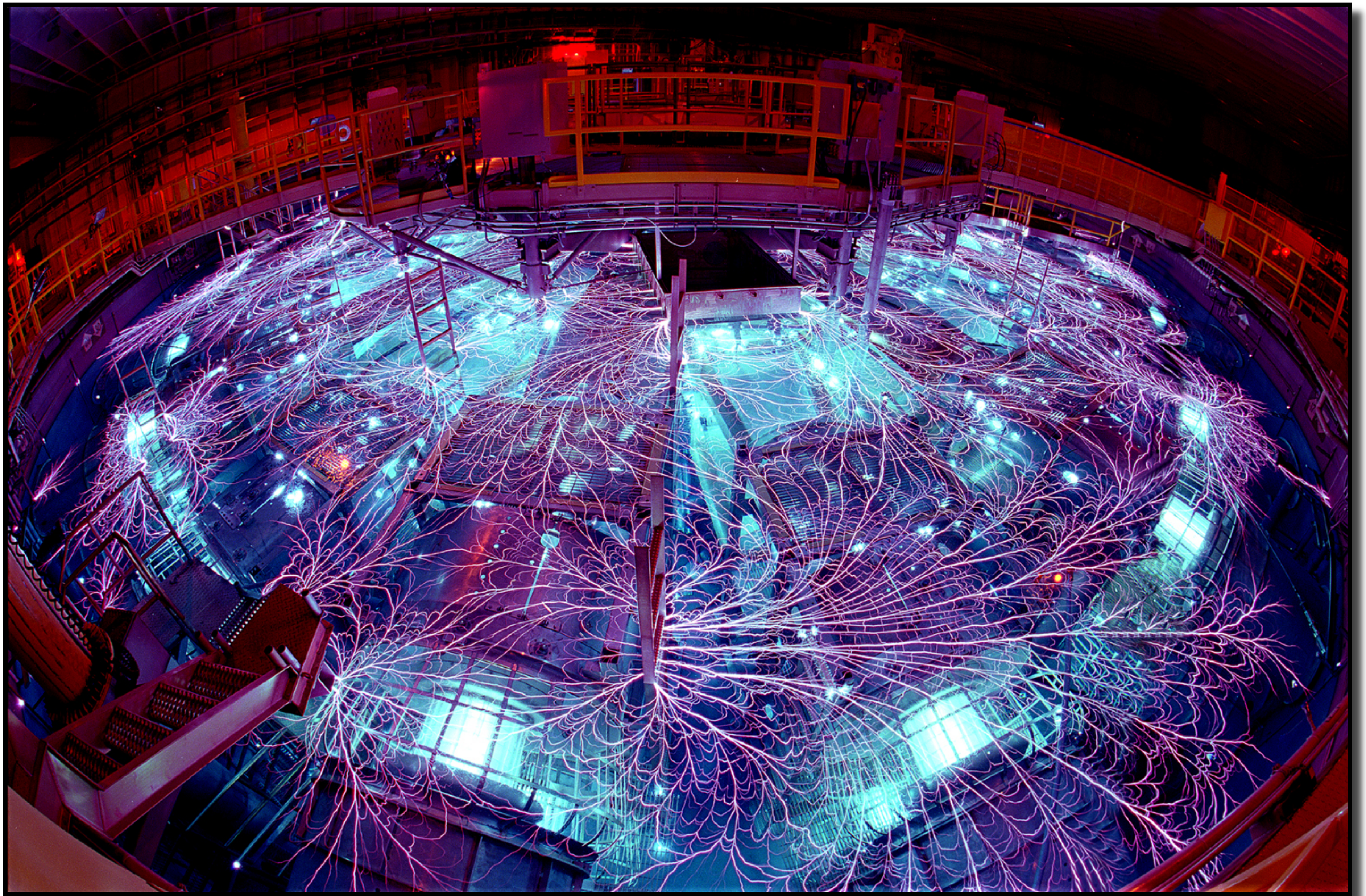


Flyer load on convolute



Flyer load





Los Alamos
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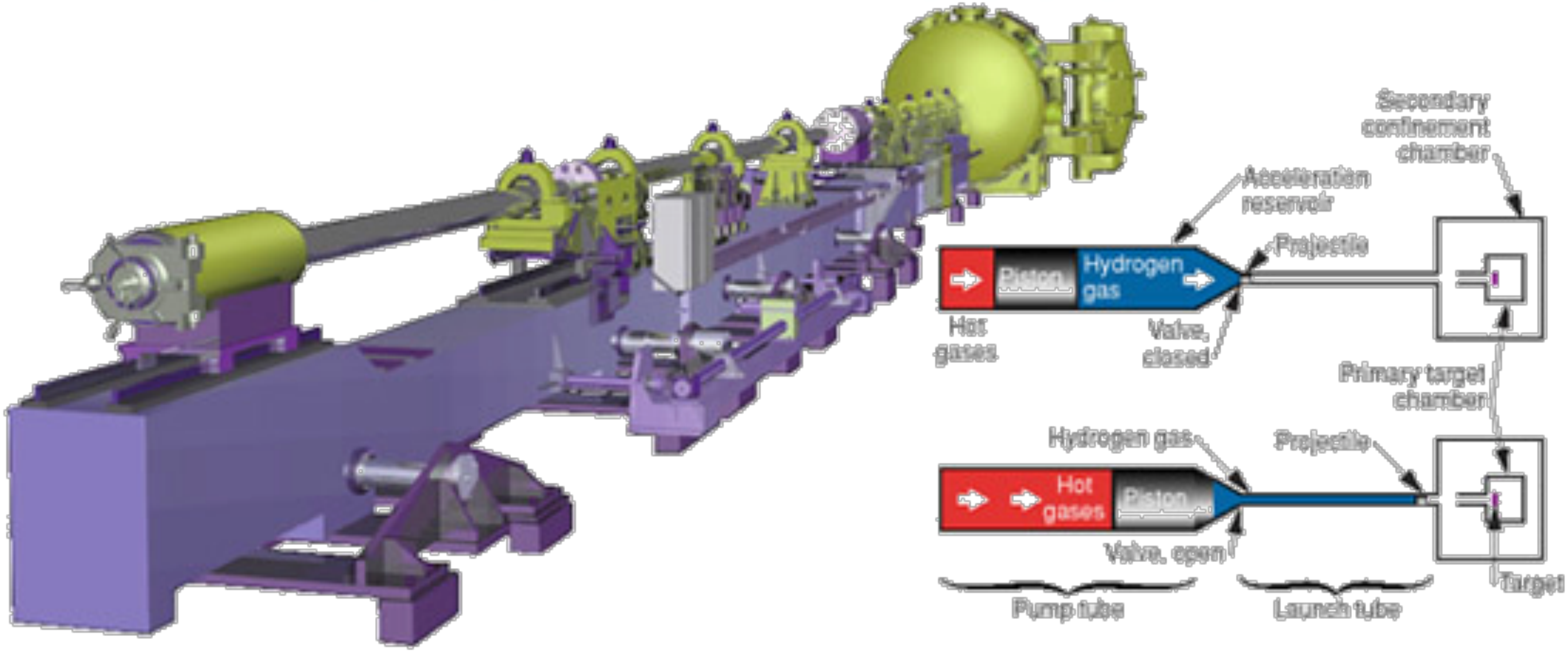
Physics and Chemistry of Materials

NNSA

LA-UR-14-****

Gas Gun

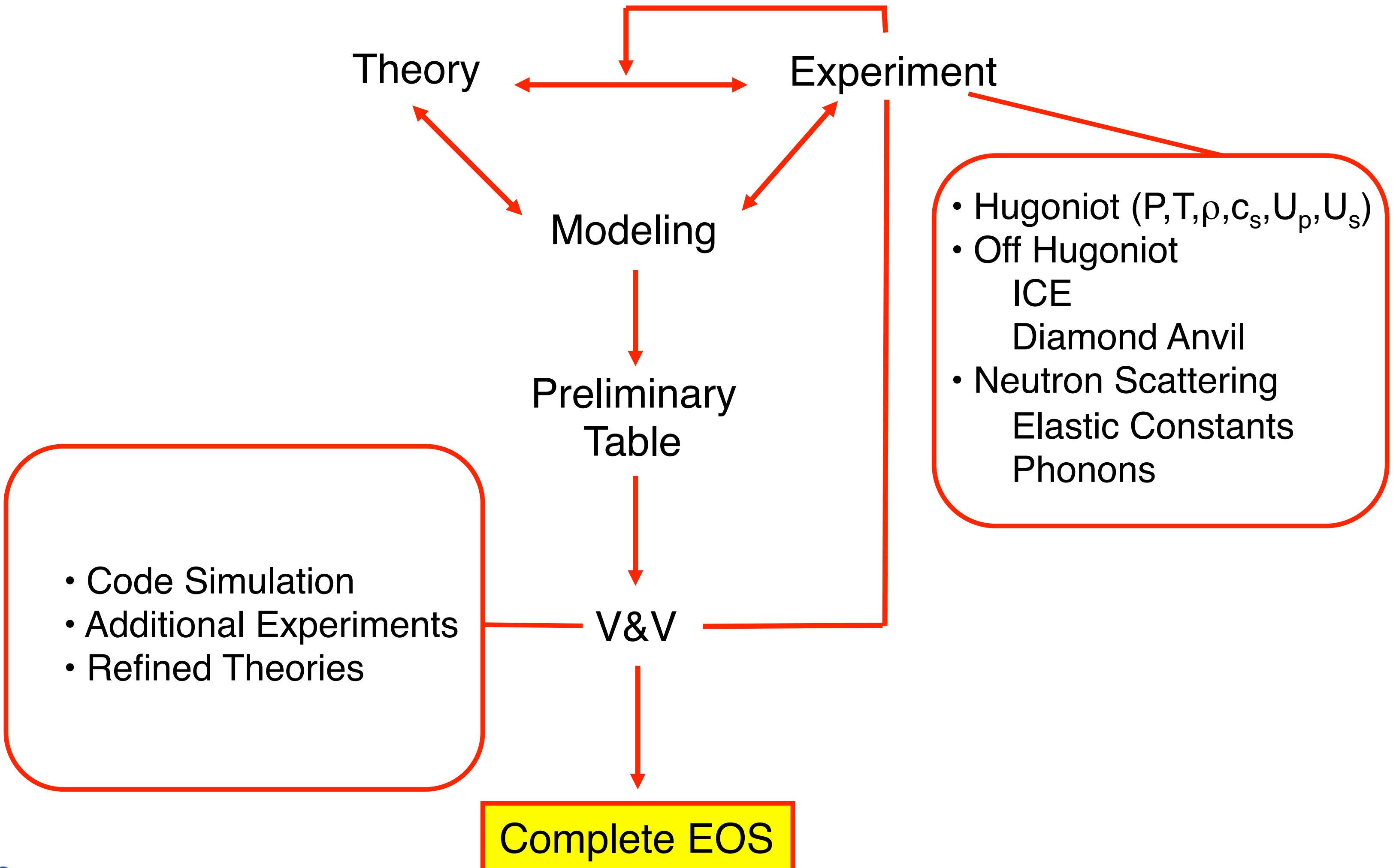
Joint Actinide Shock Physics Experimental Research Two-stage light gas gun



A schematic showing how a two-stage gas gun operates. In the first stage, hot gases from the powder propellant drive a piston, which compresses the Hydrogen gas in the pump tube. In the second stage, the high-pressure gas ruptures the valve, accelerating the projectile down the launch tube toward the target.

Equation of State

Standard Approach to Making an EOS



Germanium Multiphase Equation of State

Results published:

Crockett, S.D. ; Lorenzi-Venneri, G.D. ; Kress, J.D. ; Rudin, S.P.

Journal of Physics: Conference Series, 2014, Vol.500 (3), 032006

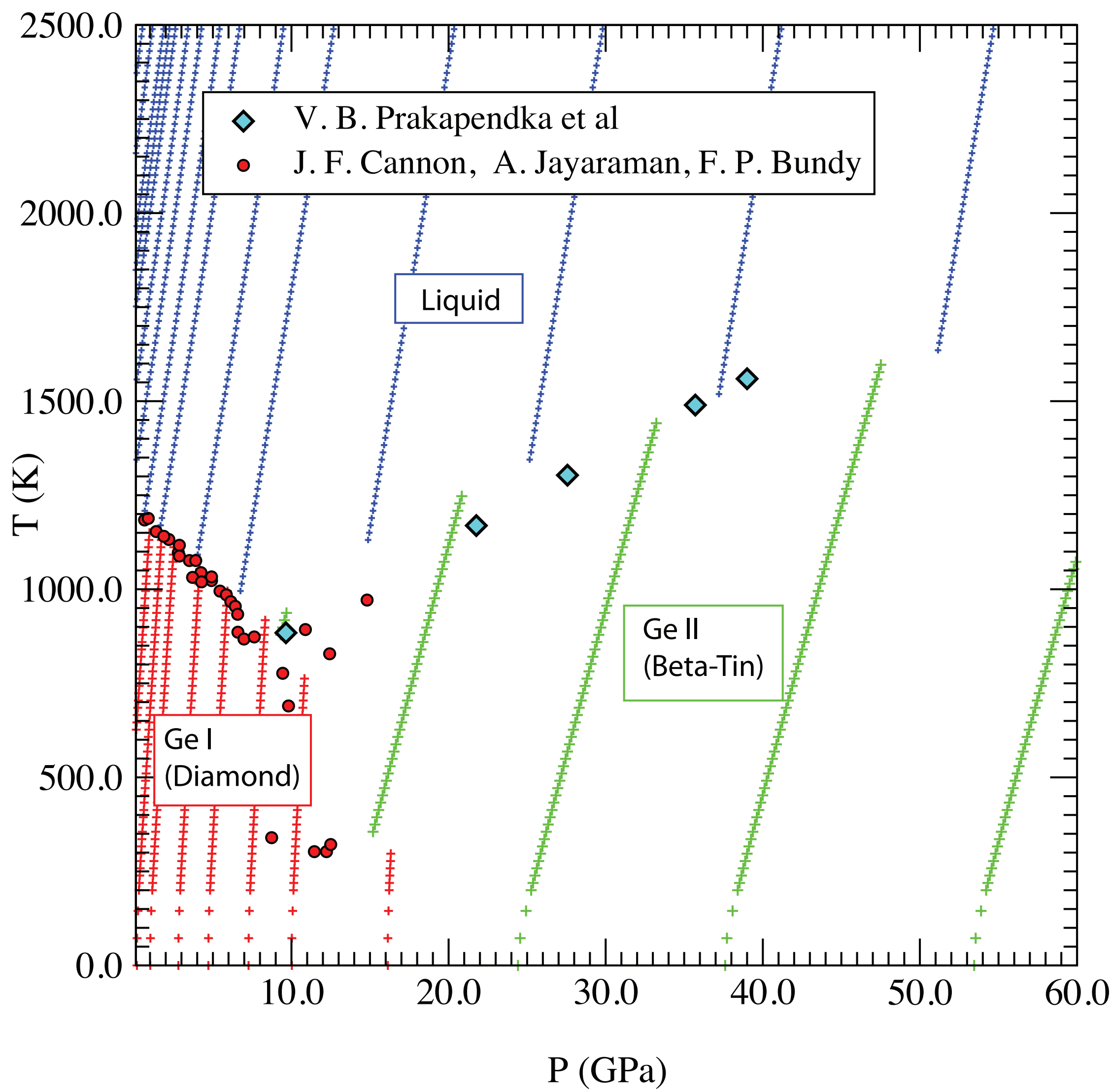
Germanium Phase Diagram

- Phases Included

  Ge I (diamond)
  Ge II (beta-tin)
  Liquid

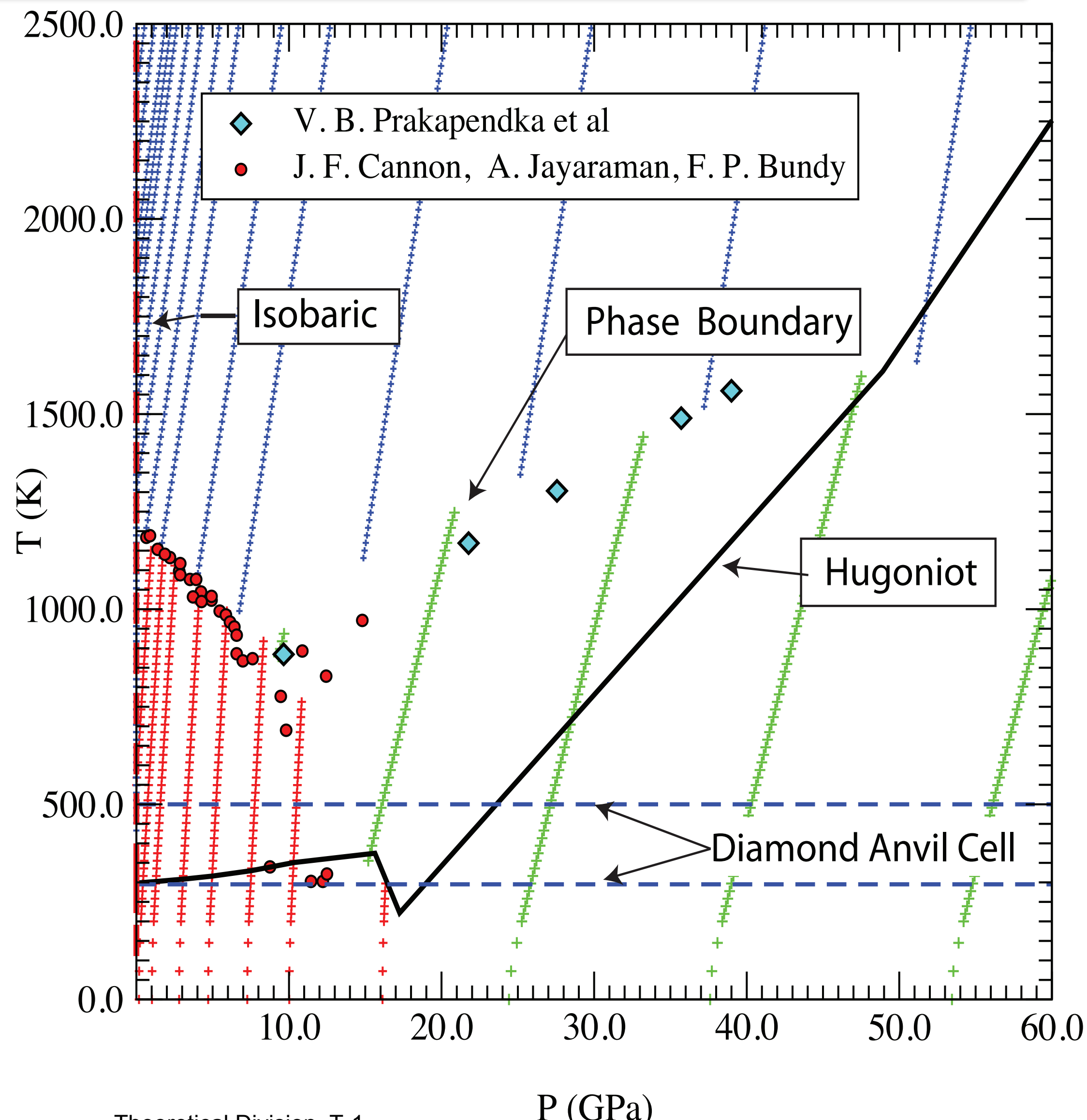
- To be continued .....

  Ge III
  Several high pressure

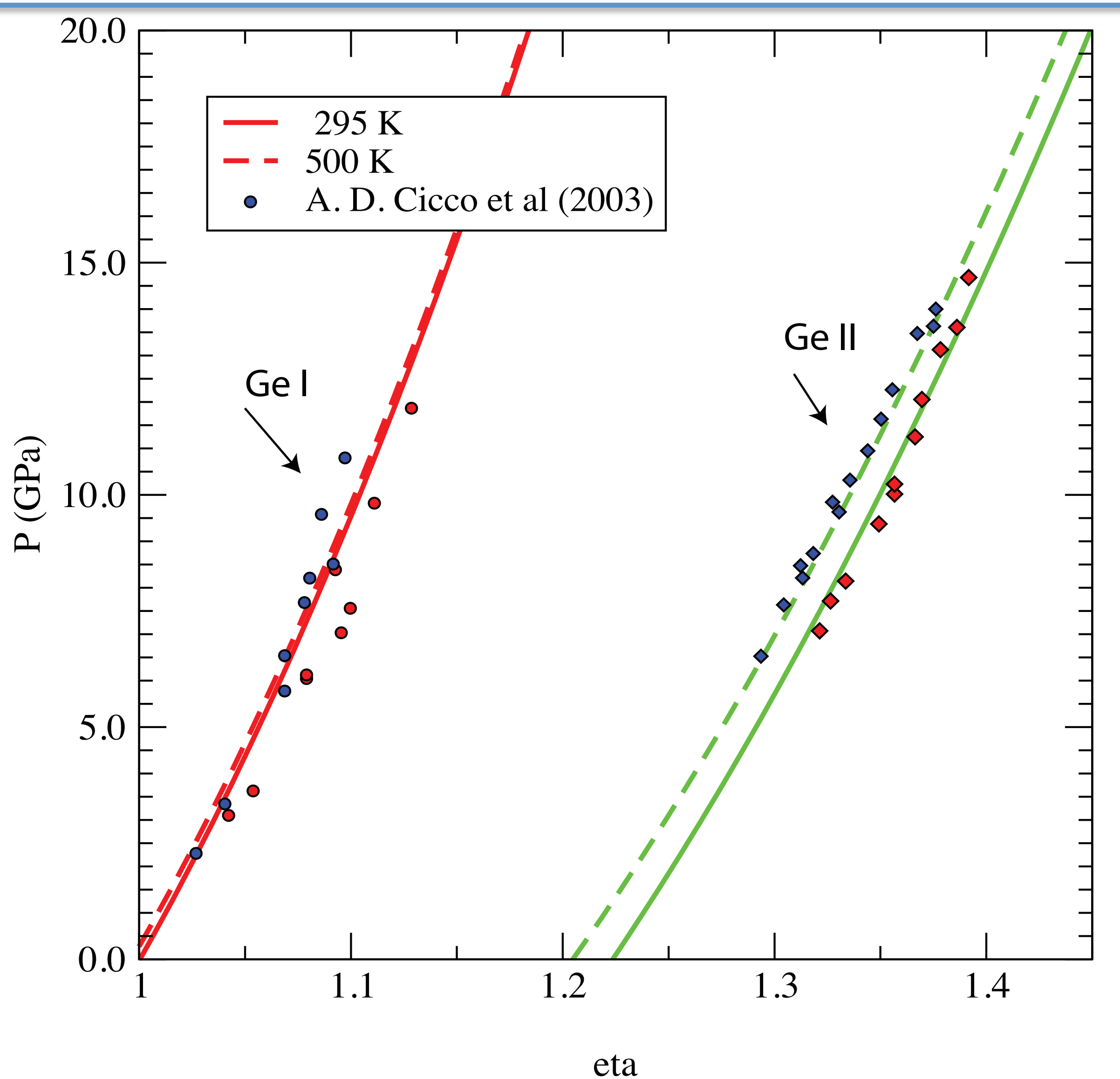


Essential Data

- Isobaric
  - High temperature
  - Energy differences between phases
- Hugoniot
  - Compression response
  - Phase boundaries
    - Change in density
- DAC
  - Compression response
  - Phase boundaries
    - Change in density
- Other Phase Information
  - Slopes help determine ratio of thermodynamic parameters

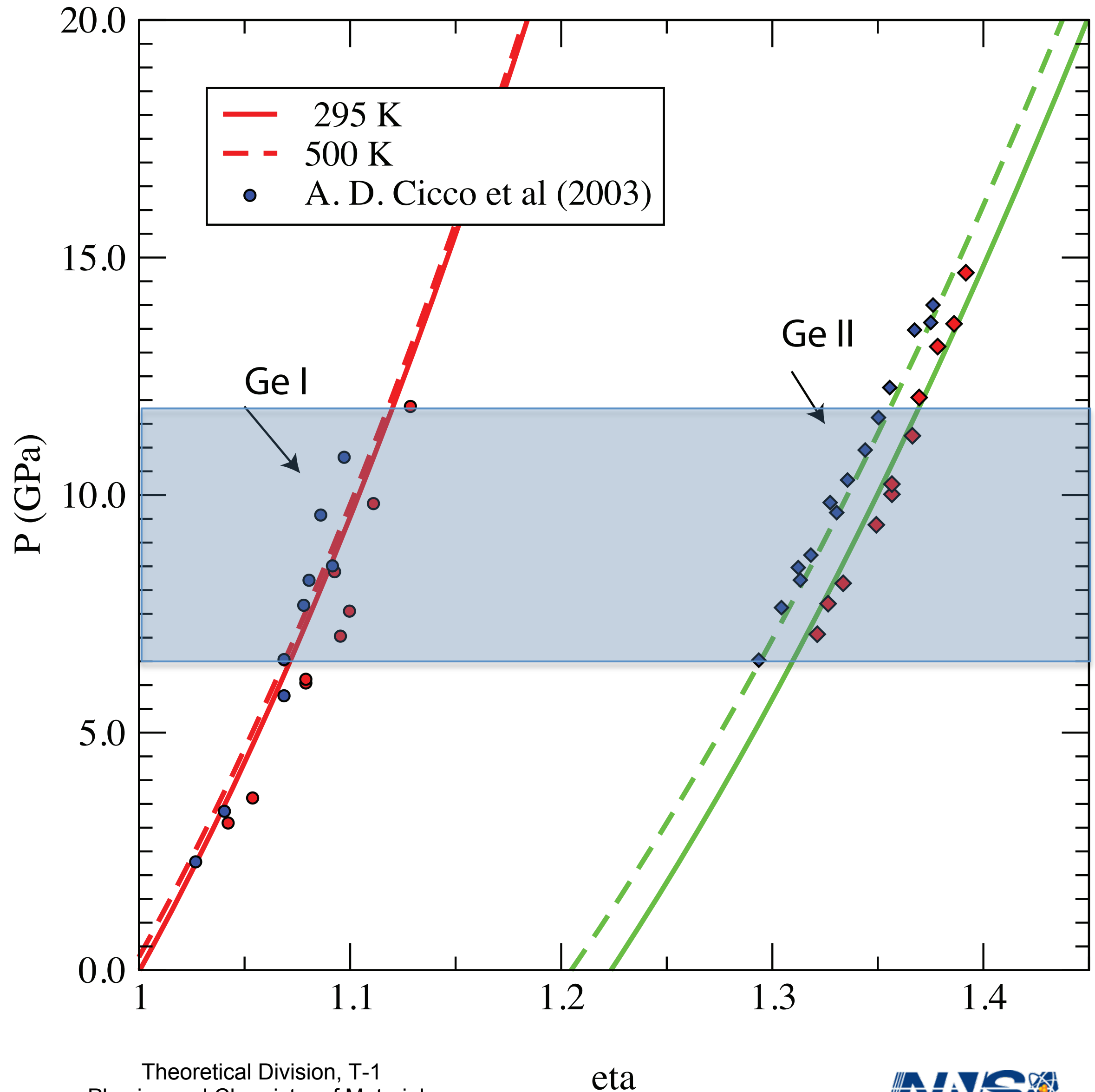


Diamond Anvil Data



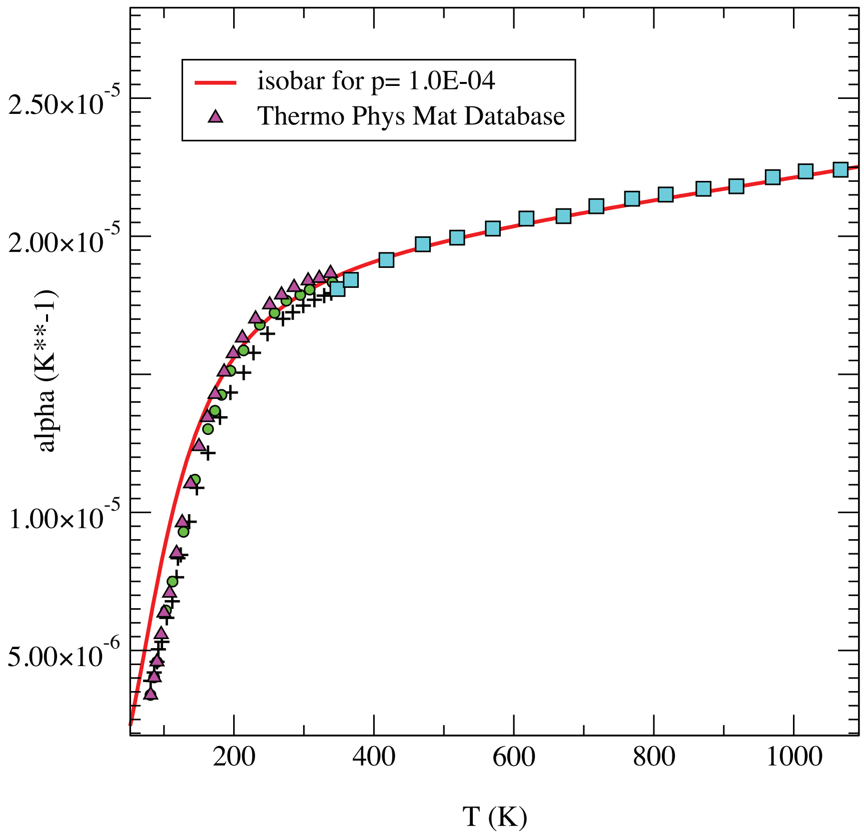
Diamond Anvil Data

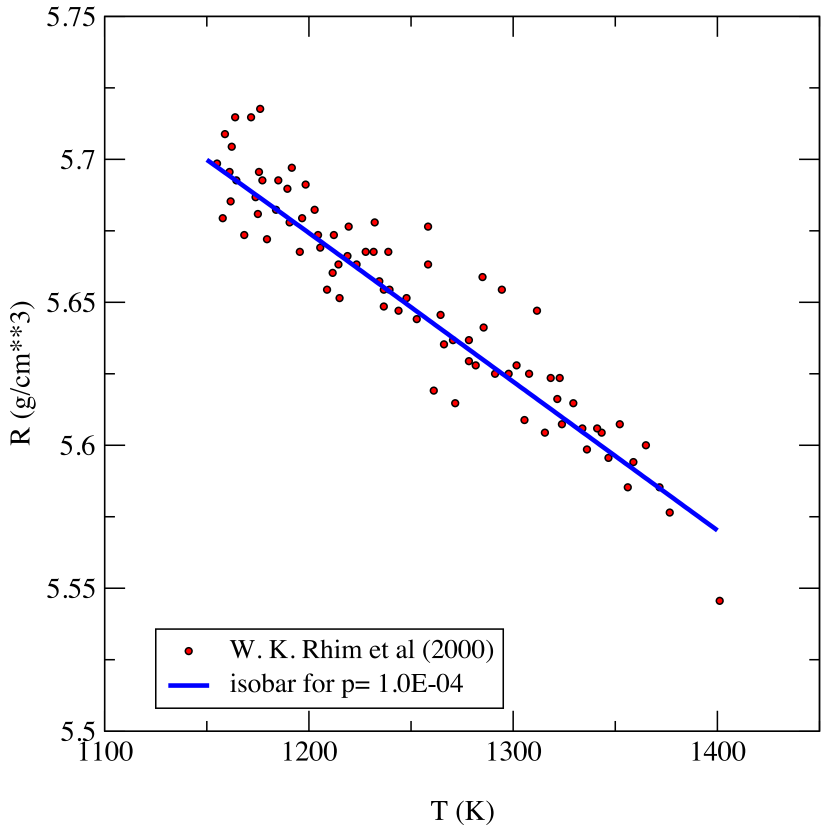
Large range of pressures where both phases can exist



Thermal Expansion for Alpha and Liquid

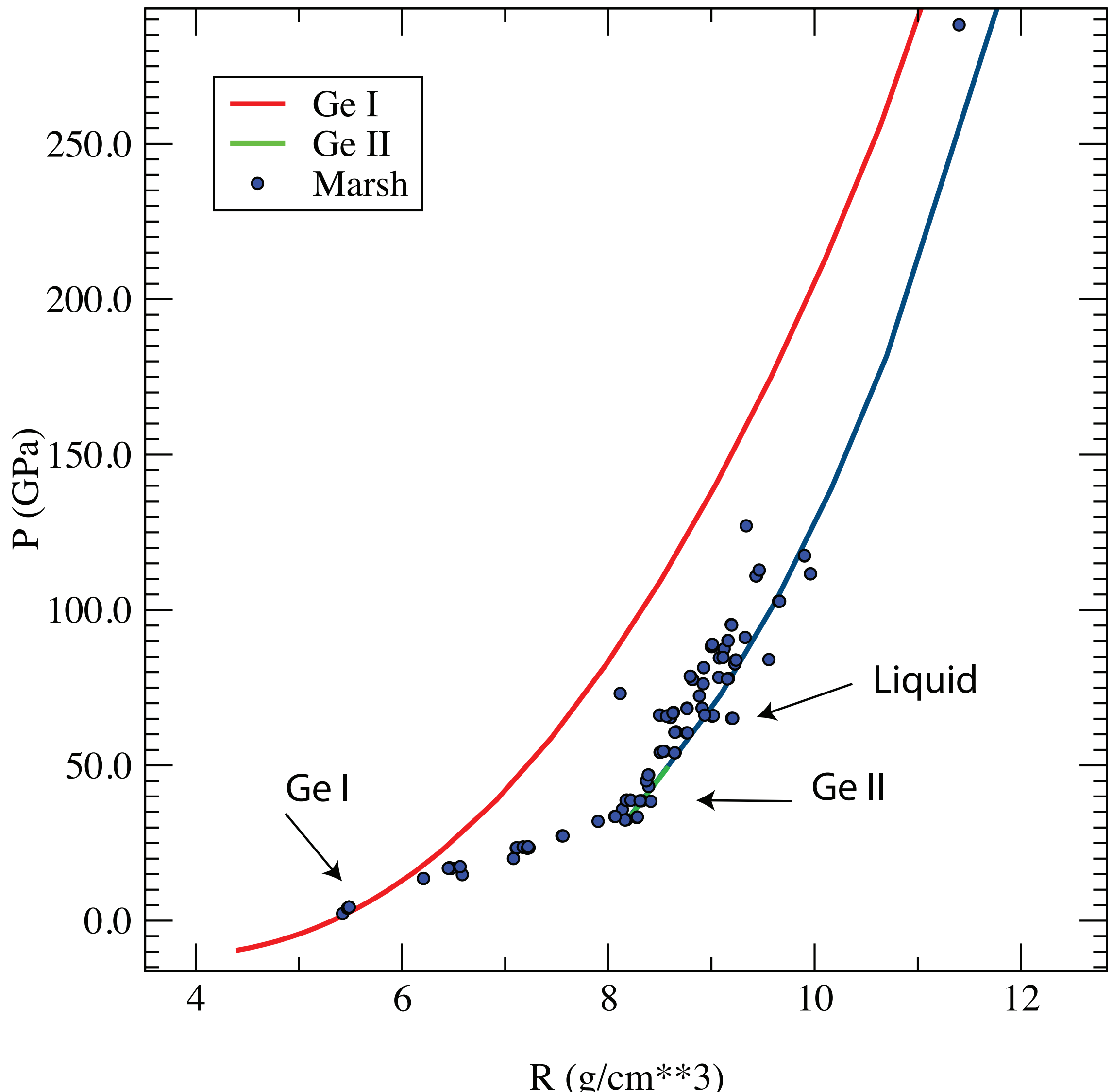
Huge constraint to gamma





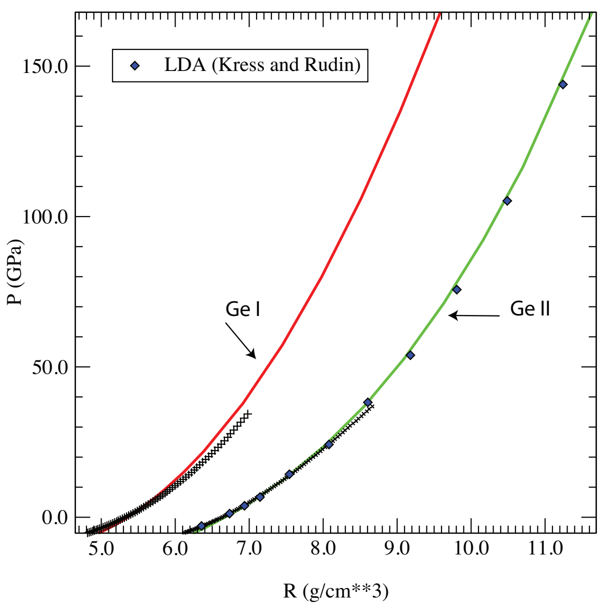
Hugoniot

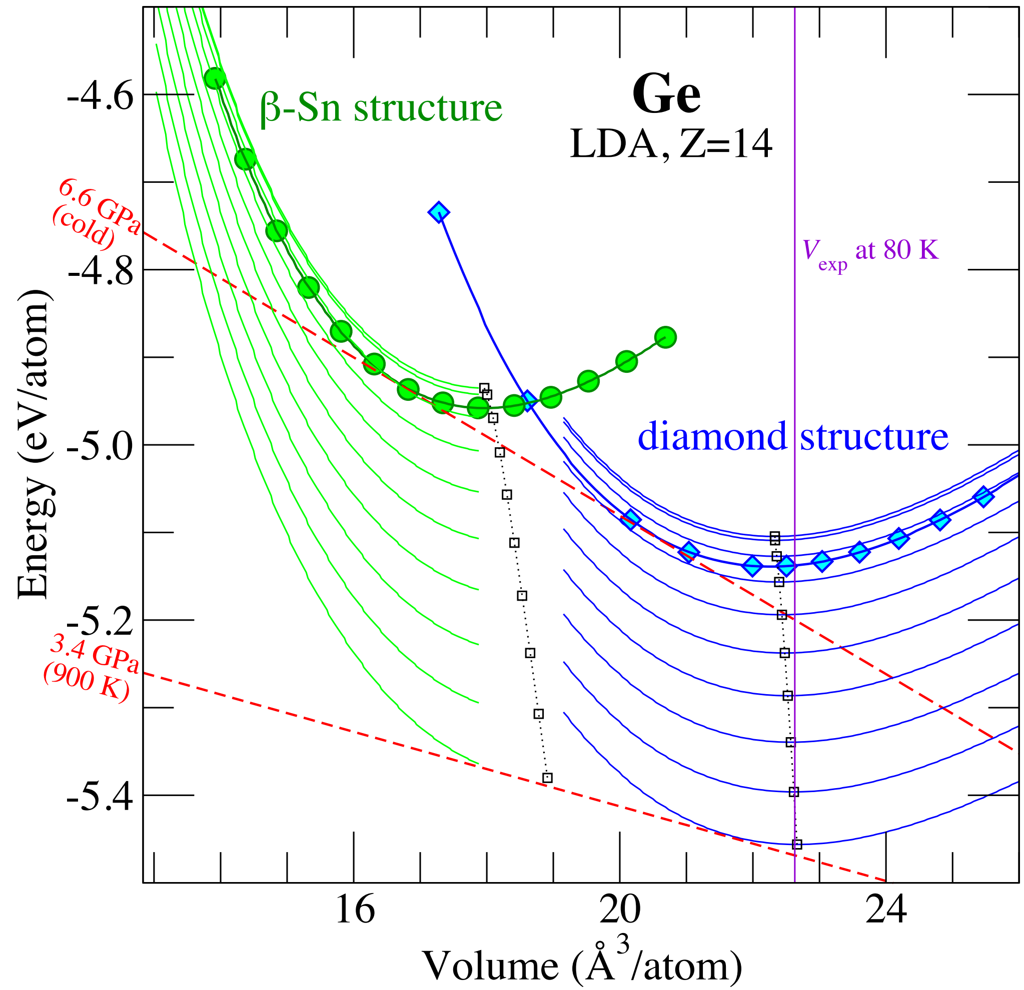
The scatter in the Hugoniot data required us to use other methods to further constrain the EOS



DFT cold curves

The scatter in the Hugoniot data required us to use other methods to further constrain the EOS

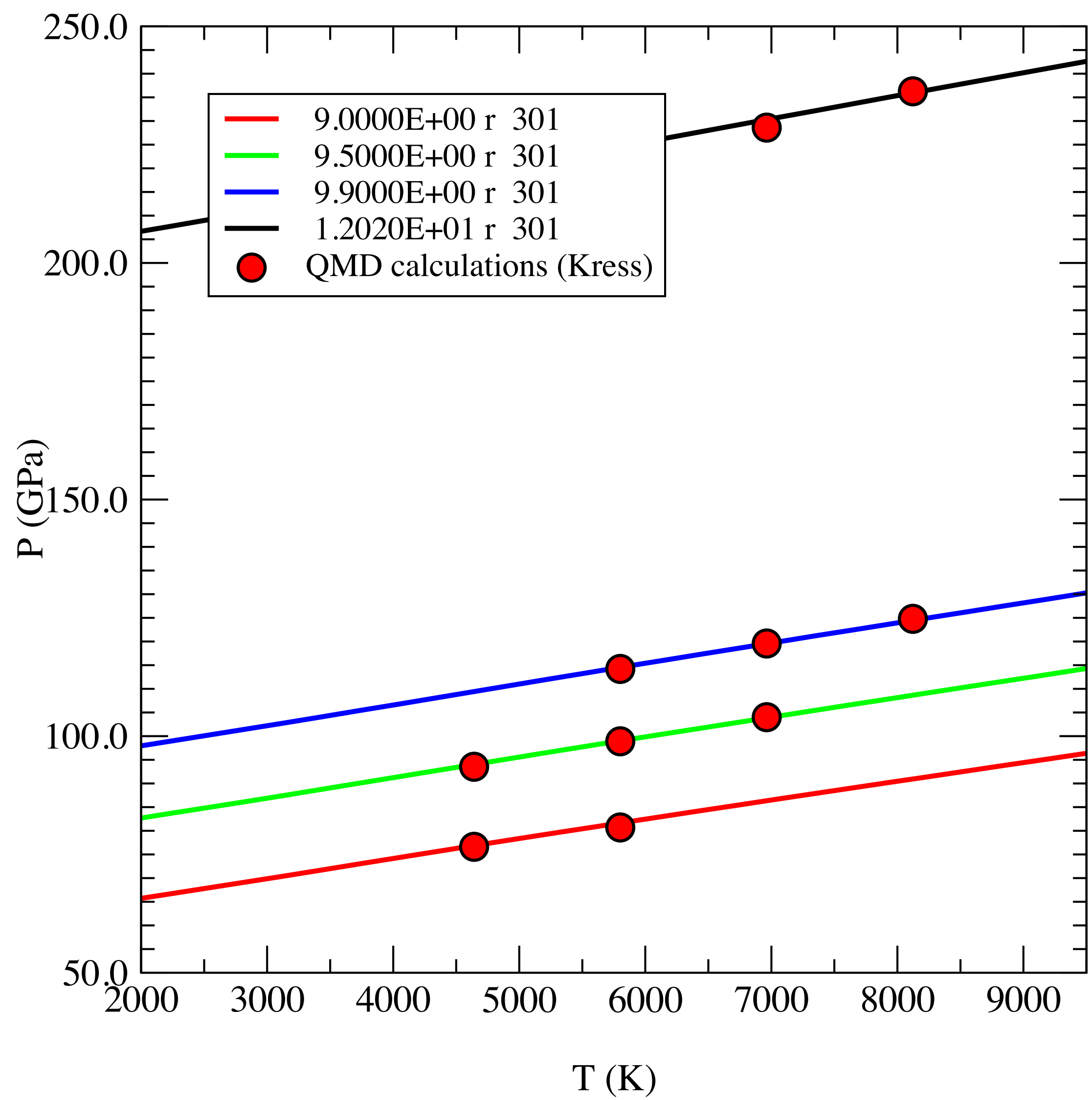




QMD for the Fluid

Isochores using LDA

- We can reproduce the same thermal dependency and compression behavior QMD predicts



Quantum Molecular Dynamics

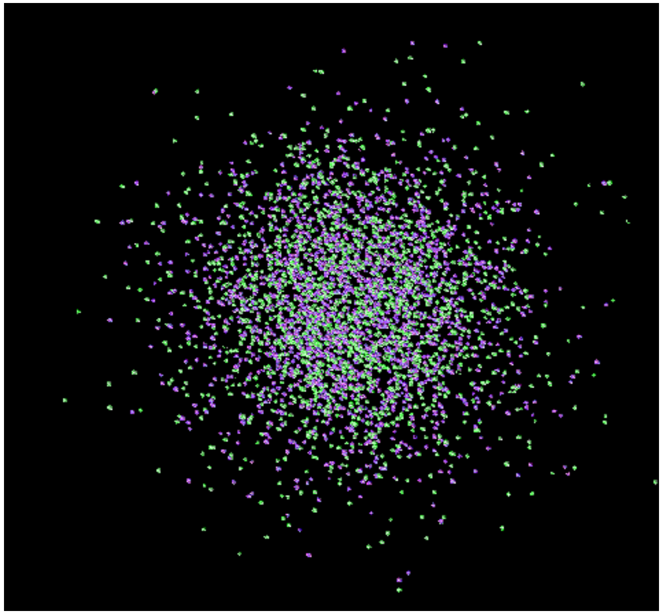
- 3D Periodic Cell of N atoms
- Born-Oppenheimer separation
- Electrons treated quantum mechanically

$$[-\frac{1}{2}\nabla^2 + U(\mathbf{r},\mathbf{R})]\Psi(\mathbf{r},\mathbf{R}) = \epsilon_i \Psi(\mathbf{r},\mathbf{R})$$

$$F_{elec}(\mathbf{R}) = \frac{\partial U(\Psi(\mathbf{r},\mathbf{R}))}{\partial \mathbf{R}}$$

- Ions follow classical dynamics

$$m\frac{\partial^2 \mathbf{R}(t)}{\partial t^2} = [F_{\rm ion}(\mathbf{R},t) + F_{\rm elec}(\mathbf{R};t)]$$



Quantum Molecular Dynamics

Consistent Set of Properties: $\{A_i, Z_i\} \rightarrow \{R_i, P_i, \Psi(r_i; R_i)\}$

- Static: EOS, pressure, internal energy
- Dynamical: Diffusion, ion thermal conductivity, viscosity
- Optical: Electrical conductivity, absorption, opacity, reflectivity
- Constituency: Species concentration
- Mixtures: Arise in a natural way since all intra- and inter-particle interactions are represented

Conclusion

- Equation of State modeling requires many different pieces of experimental and theoretical data.
- Shock physics plays an important role in probing different regions of thermodynamic phase space.
- Our basic models correlate the collection of information quite well.
- The complexity of the phase boundaries would naturally propose interesting experiments
  - Shock melt and release to study refreezing
  - Shock and release to study kinetics of solid-solid phase transitions

Supporting Slides

Mie-Grüneisen model … general derivation

$$\gamma = \frac{1}{\rho}\left(\frac{\partial P}{\partial E}\right)_{\rho}$$

If $\gamma=\gamma(\rho)$, then

$$P_a - P_b = \rho\gamma(E_a - E_b)$$

Let "a" equal the T=0 isotherm and "b" equal the Hugoniot

$$P_0 - P_H = \rho\gamma(E_0 - E_H)$$

"On Obtaining the Zero-Temperature Equation of State from Shock Data", B. Bennett, Los Alamos Report LA-9890-MS

Analytic Forms for a Cold Curve

Vinet

$$P = 3B_0\eta^{-\frac{2}{3}}\left(1-\eta^{\frac{1}{3}}\right)e^{\frac{3}{2}(B_0'-1)\left(1-\eta^{\frac{1}{3}}\right)}$$

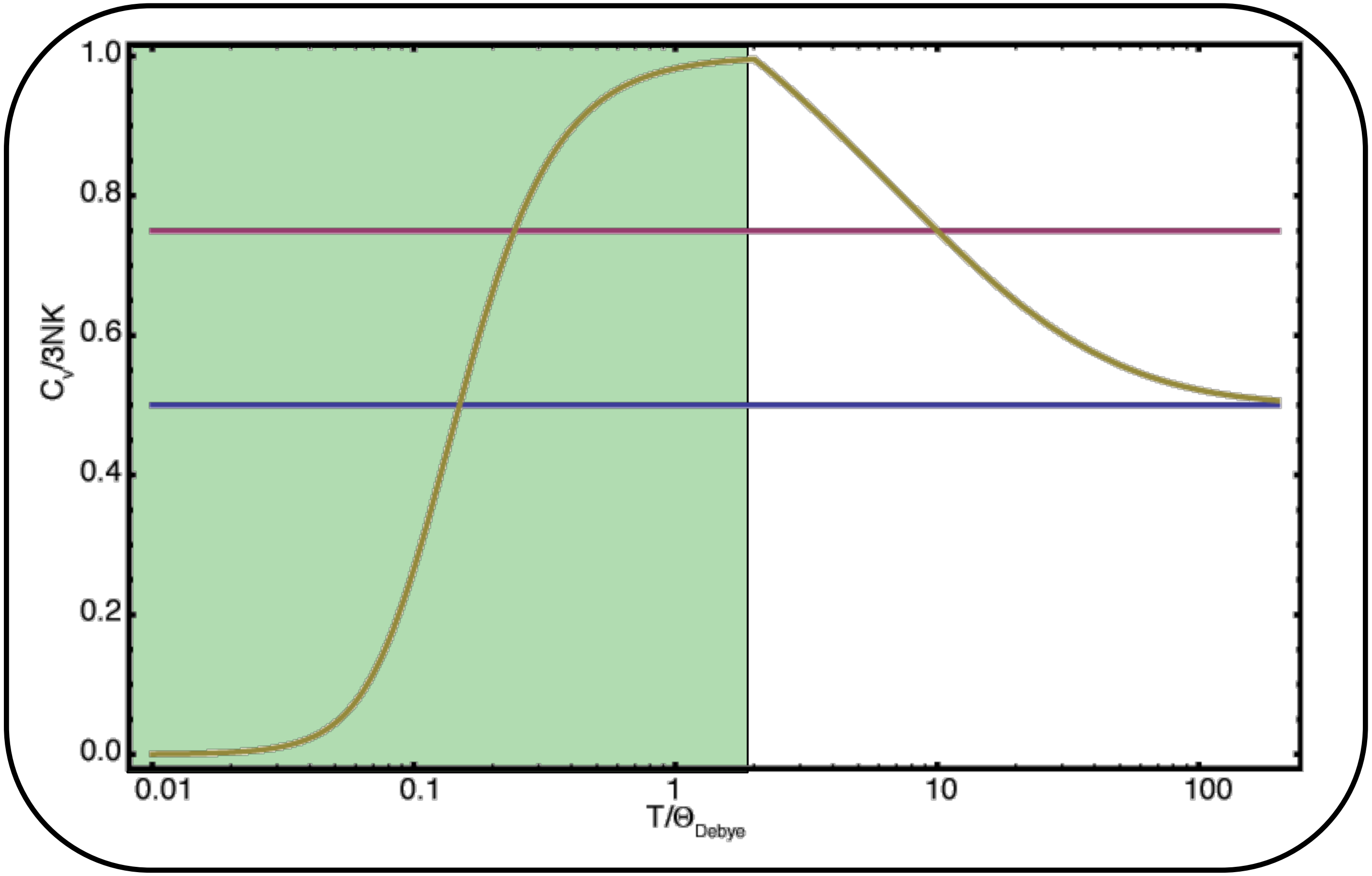
Birch-Murnaghan

$$\Phi = (\sqrt[3]{\eta}-1)\,a_1 + \frac{1}{2}\left(\eta^{2/3}-1\right)a_2 + \frac{1}{3}(\eta-1)a_3 + \frac{1}{4}\left(\eta^{4/3}-1\right)a_4 + \frac{1}{5}\left(\eta^{5/3}-1\right)a_5 + \frac{1}{6}\left(\eta^2-1\right)a_6$$

$$\Phi = E_0 + V_0\left(\frac{1}{384}C_4\left(\left(\frac{V_0}{V}\right)^{2/3}-1\right)^4 + \frac{9}{16}B_0(B_0'-4)\left(\left(\frac{V_0}{V}\right)^{2/3}-1\right)^3 + \frac{9}{8}B_0\left(\left(\frac{V_0}{V}\right)^{2/3}-1\right)^2\right)$$

Crystal, Liquid, Gas Nuclear Model

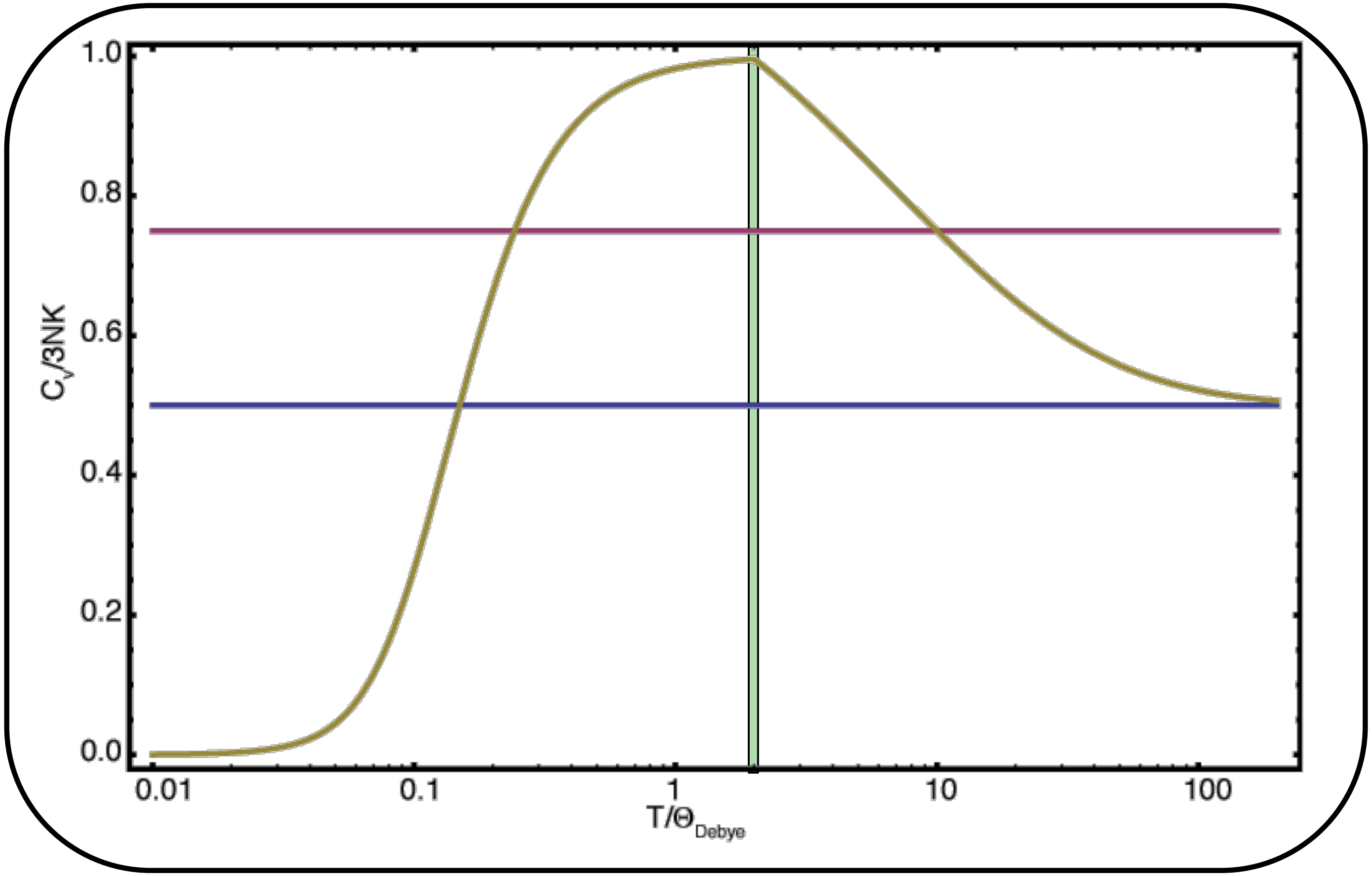
Solid (Debye Model)

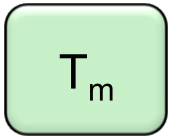


Solid Region

Crystal, Liquid, Gas Nuclear Model

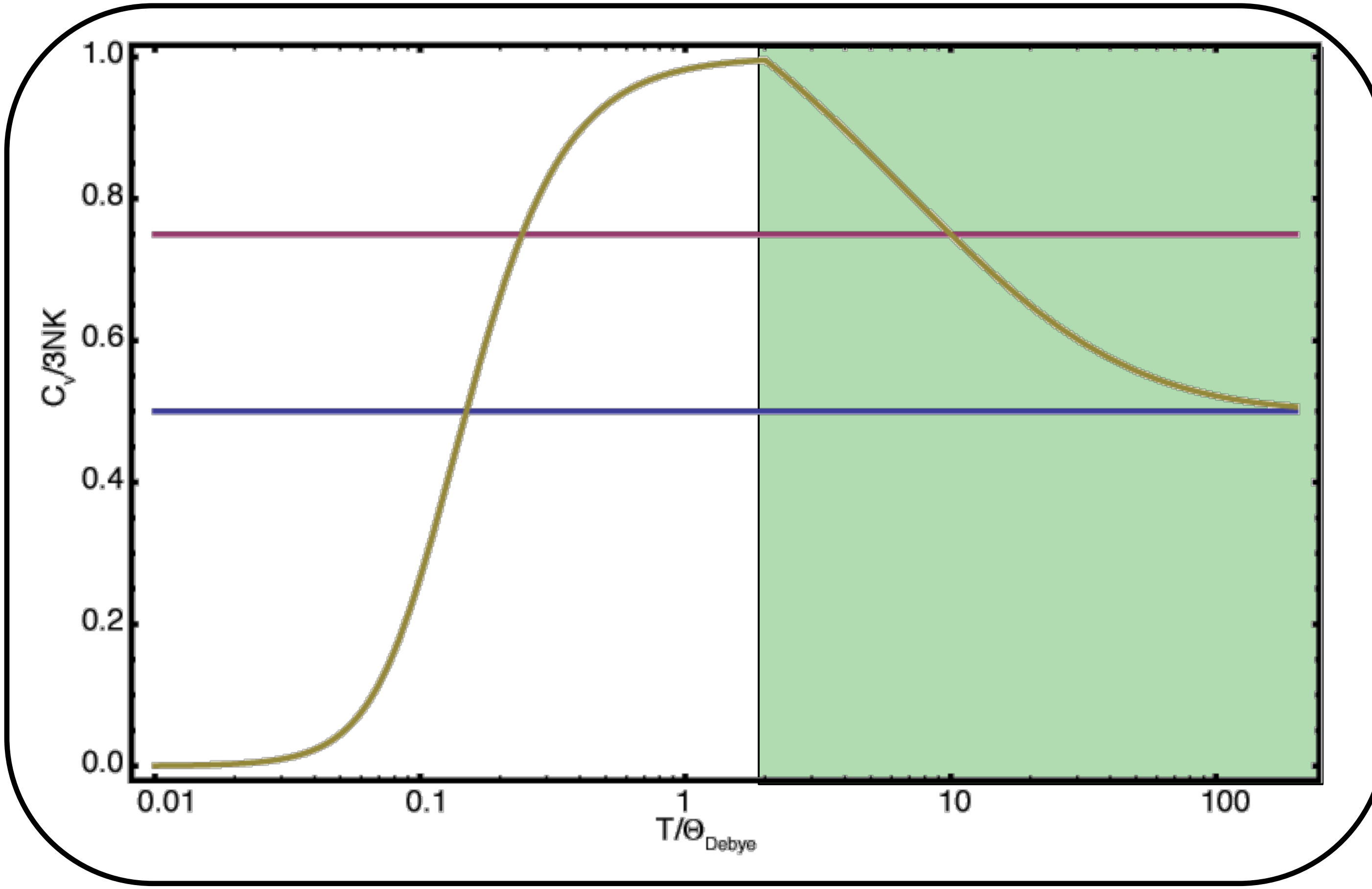
Melt





Crystal, Liquid, Gas Nuclear Model

Fluid



Liquid/Gas Region

Crystal, Liquid, Gas Nuclear Model

Grüneisen Gamma

$$\gamma = \gamma_\infty + c_1 \frac{1}{\eta} + c_2 \frac{1}{\eta^2}$$

$$\gamma = \gamma_{zero} + c_3 \eta + c_4 \eta^2$$

$$\eta = \frac{\rho}{\rho_0}$$

- Phonon Calculations (time intensive)
- A simple way to approximate the reference gamma is
  Γ= 2*Hugoniot Slope -1
- Thermal expansion data

- What should be the form of gamma when it has temperature dependence?

Phonon Frequency Calculations

Provided by Sven Rudin, Be phonon calculations