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Shock Compression of Condensed Matter, Chicago
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Shock Compression of MgO: The Melt Transition

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NNSA National Nuclear Security Administration

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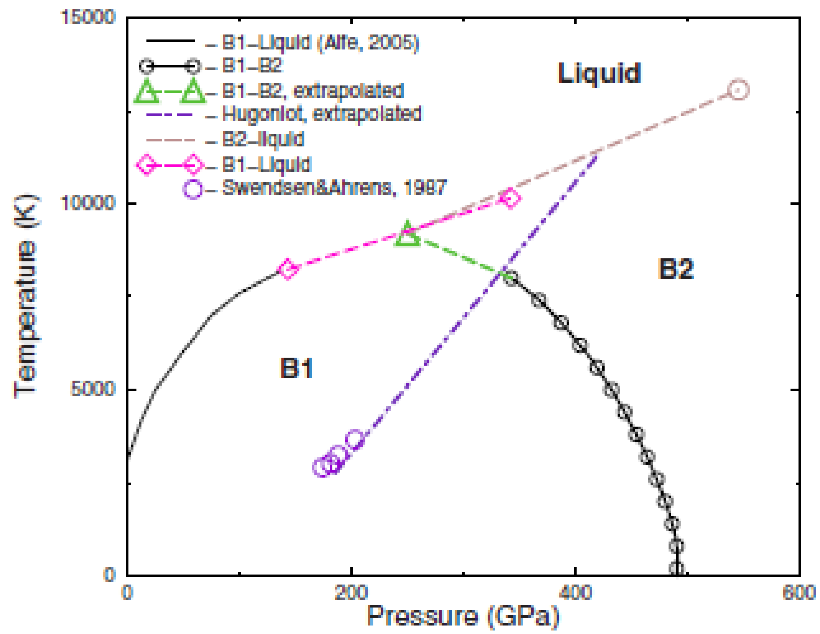
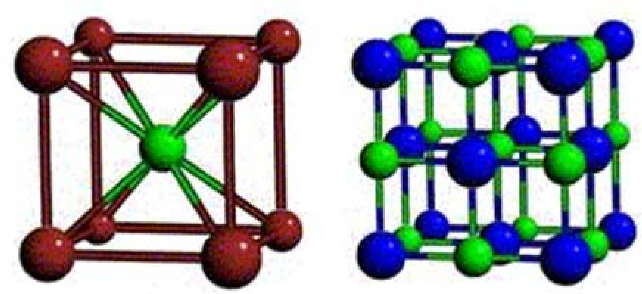
MgO Background

- MgO is abundantly found the Earth's mantle and likely other terrestrial exo-planets
- Understanding the high P-T behavior of MgO is important for modeling Earth's interior
- Static pressure data show no phase transition up to 227 Gpa at ambient temperature
- Hugoniot data (starting at ambient temperature) to ~ 200 GPa – no phase transition
- Pre-heat Hugoniot measurements (Fat'yanov et al SCCM 2009) show no indications of melt to 203 GPa and 6.5 kK
- Belonoshko et al predict a B1-B2 phase transition near 350 GPa and melt near 5 Mbar and 12kK.



Belonoshko *et al.*, Phys. Rev. B **81**, 054110 (2010)



CsCl NaCl

Objectives

- Use Sandia's Z – accelerator to shock compress MgO, measuring the Hugoniot to 10 Mbar
- Experimental determine the proposed solid-solid phase transition
- Determine melt on the Hugoniot
- Apply Density Functional Theory methods to corroborate experimental findings

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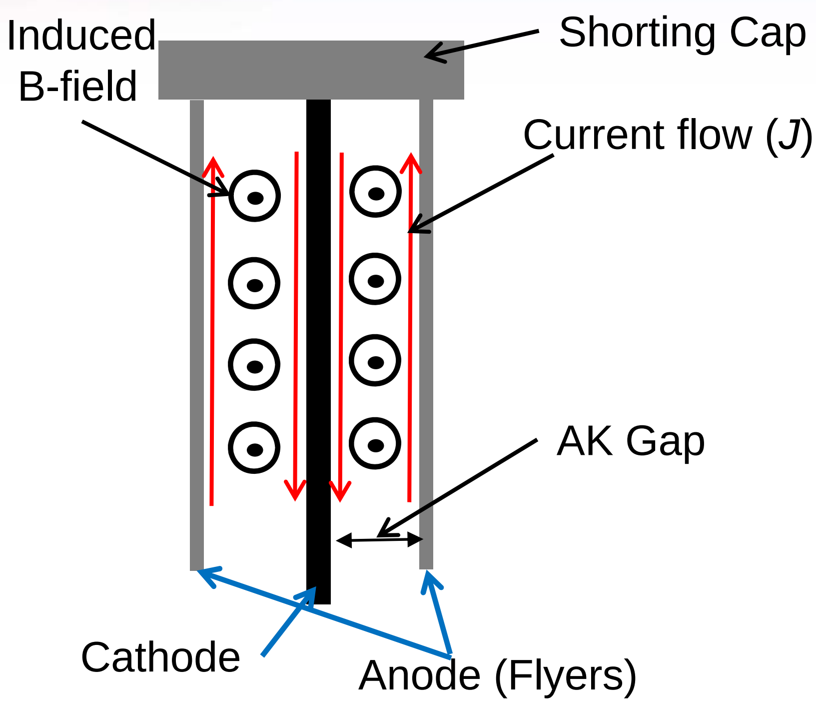
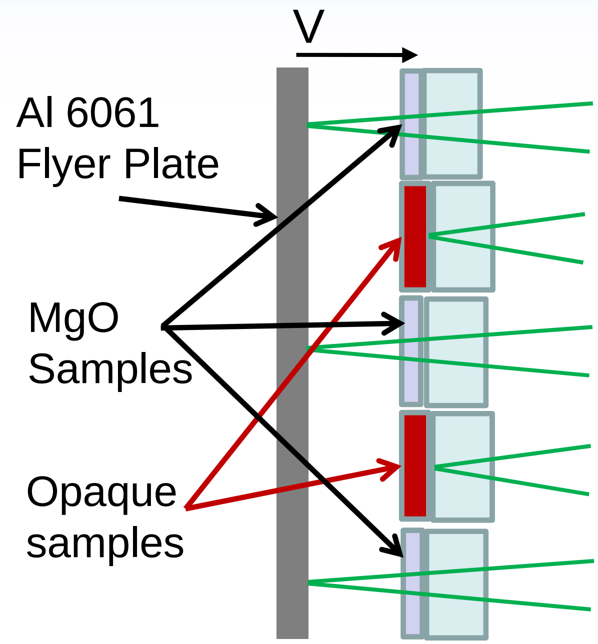
Experimental Approach





- Current pulse loops through shorting cap inducing a *B* – field.
- Resulting *J x B* force accelerates anodes (flyers) outward up to 40 km/s
- Asymmetric AK Gaps result in two different flyer velocities (two Hugoniot points per experiment

- Multiple samples per experiment
- MgO windows are transparent and are backed by quartz windows
- VISAR used to measure flyer velocity
- Multiple VPFs per sample – reduces uncertainty

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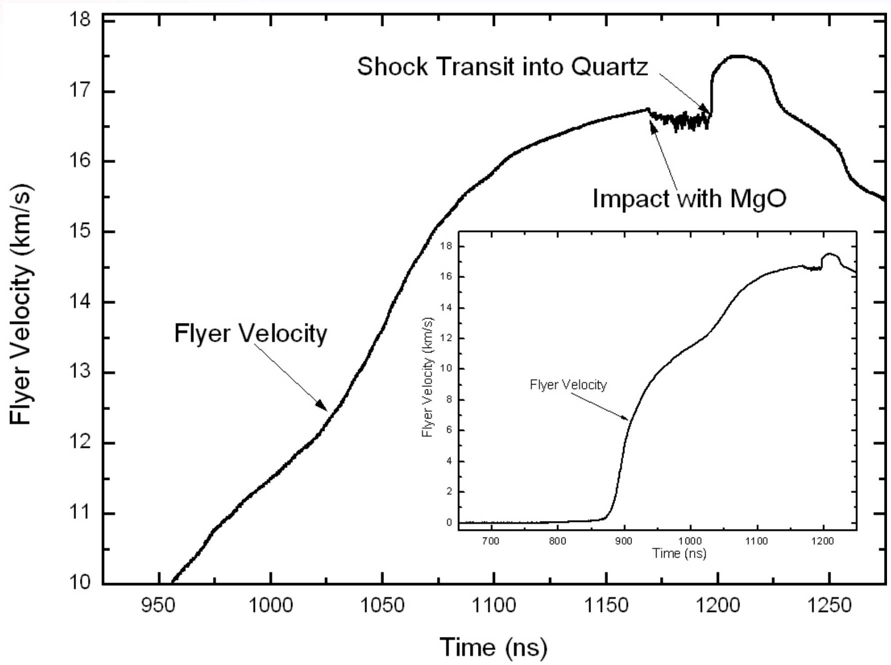
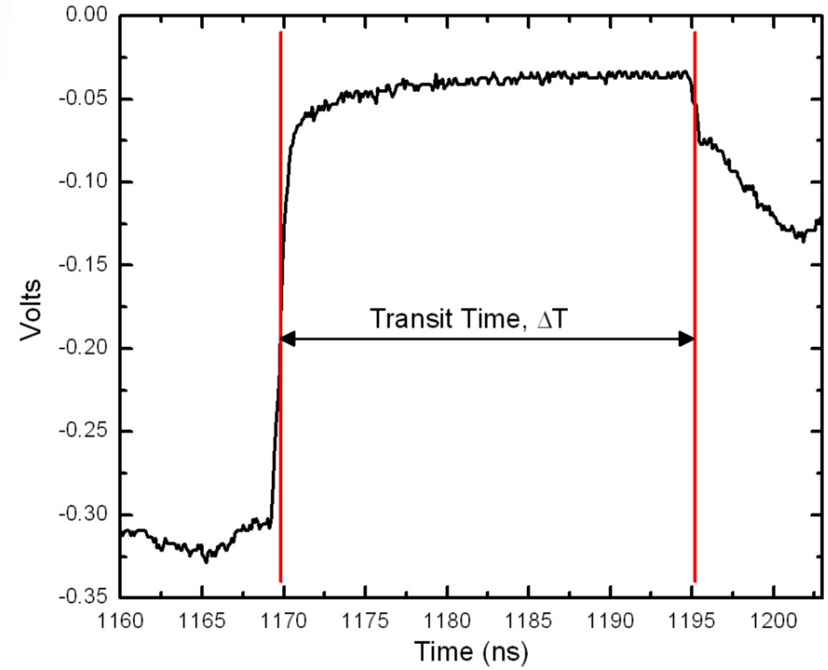
Experimental Measurements





- VISAR tracks flyer plate velocity up to impact
- Shock front in MgO not reflective – Loss of contrast in VISAR signal
- Clear impact and shock transit fiducials
- Transit time analysis to determine shock velocity
- Shock front in quartz reflective – release state for MgO can be determined (not discussed here)

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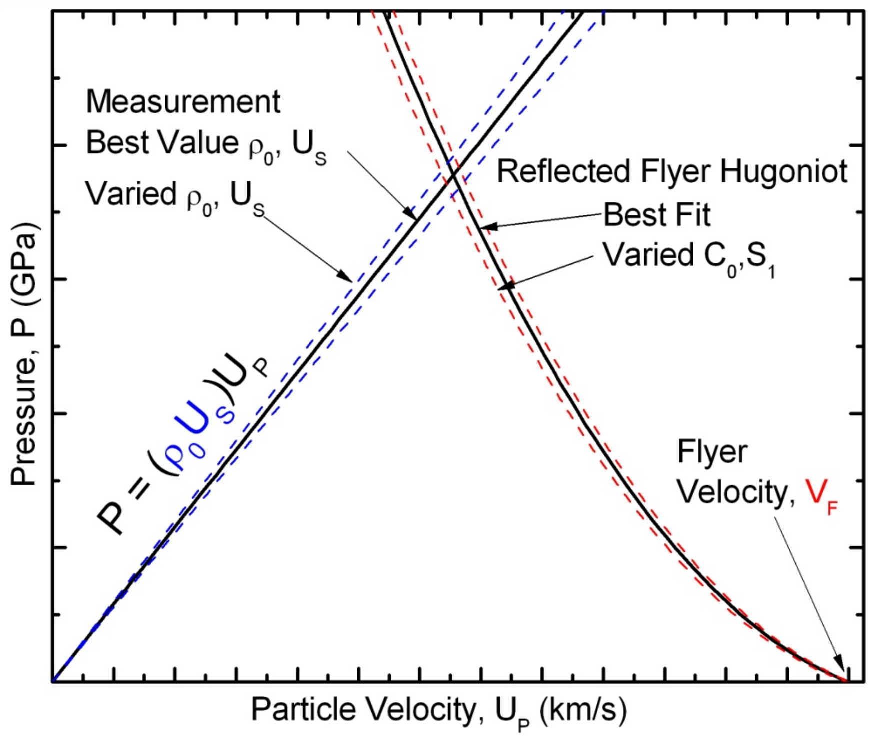
Monte Carlo (MC) Impedance Matching

- Uncertainty exists in experimental measurements and the aluminum Hugoniot
- Creates a region of uncertainty that the target U_P and P can exist
- MC method varies experimental measured values (U_S, V_F, ρ_0) within uncertainty using uncorrelated random numbers
- Al Hugoniot fit parameters varied using correlated random numbers.
- Impedance calculation performed 10^6 times to build a large sample for statistical analysis
- Data reported as the average of the resulting calculations with error of 1 – standard deviation



Monte Carlo techniques allow for calculation of uncertainties and error propagation of the aluminum standard into the resulting MgO data.

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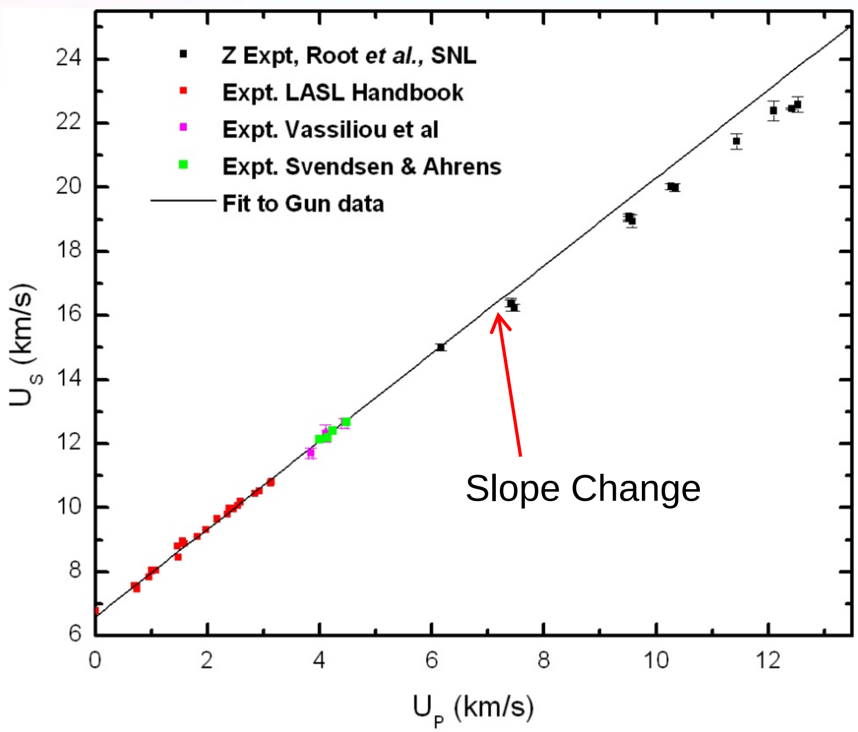
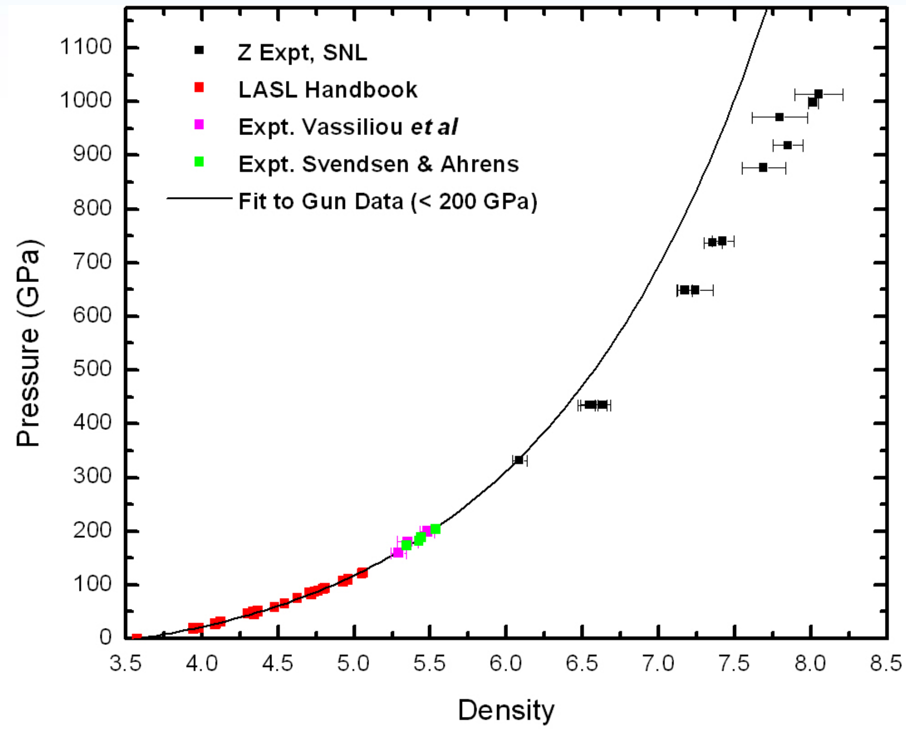
Experimental Data





- No reflective shock front below 10 Mbar, but very slight reflectivity at 10 Mbar
- Up to 330 GPa, the Hugoniot point lies on the extrapolation of the gun data fit
- Slope change in $U_S - U_P$ starting at 440 Gpa – suggests a phase transition
- No obvious changes at higher pressures that would suggest melt

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Density Functional Theory

- Use DFT-MD to assess the state of MgO at high pressures

- DFT-MD simulations performed using VASP 5.1.40*
- Electronic states occupied according to Mermin's finite-temperature formulation
- Calculate energy and pressure for a given density and finite temperature
- Minimize the Hugoniot Condition:

$$2\left(E - E_{ref}\right) - \left(P + P_{ref}\right)\left(v_{ref} - v\right) = 0$$

  - Simulations start from the B1 and proposed B2 phase
  - 216 atoms per simulation (B1 phase); 250 atoms (B2 phase)
  - AM05 (Armiento-Mattsson) exchange correlation functional
  - VASP PAW potentials for $Mg(2p^6 3s^2)$ and $O(2s^2 p^4)$

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

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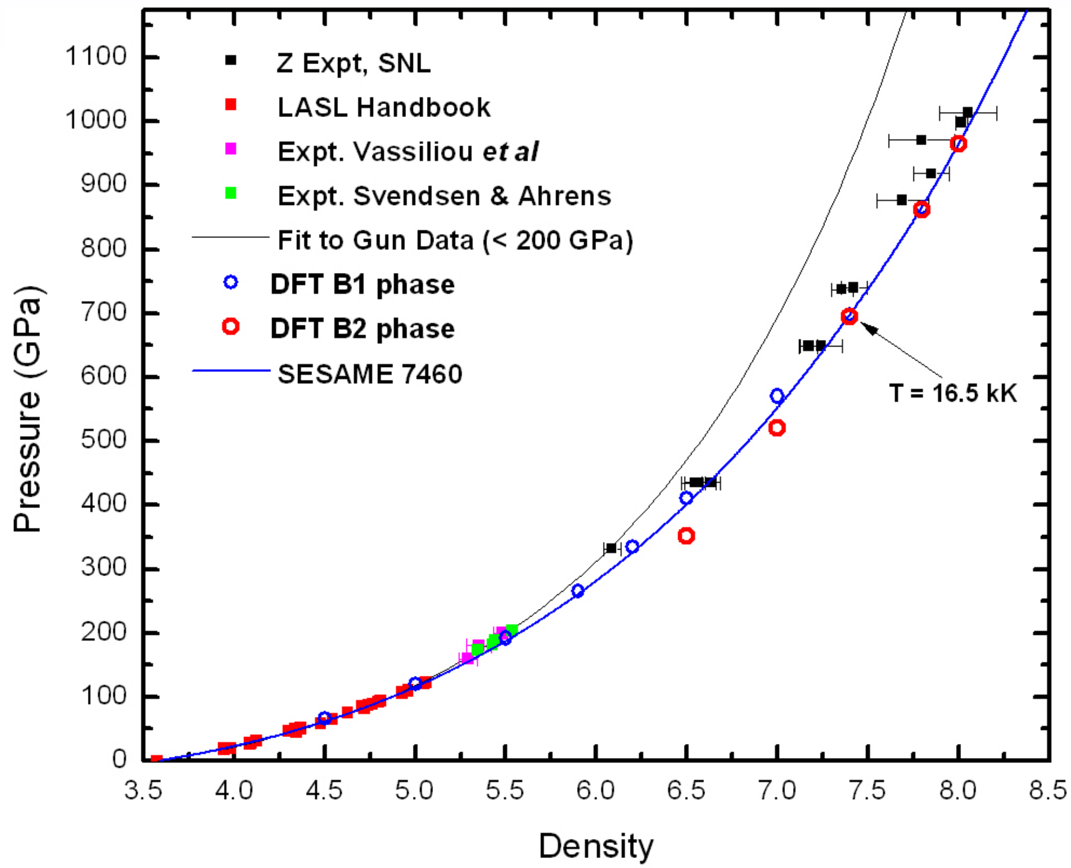
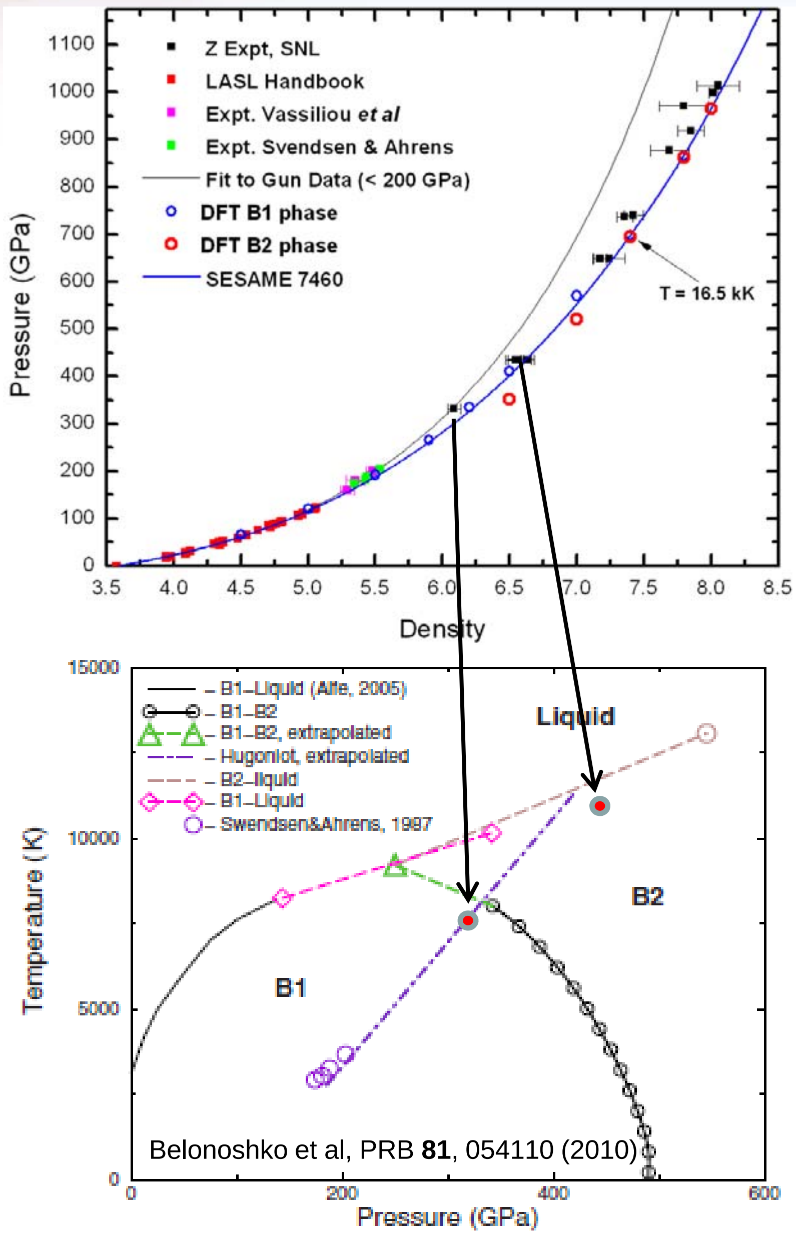
DFT Results and Comparison

- B1-phase DFT results show good agreement with gun data to 200 Gpa
- Simulations from the B2 phase show significantly lower Hugoniot pressure states than B1 phase
- The B1 and B2 initial phase simulations converge at 700 GPa and 16.5 kK – where MgO melt is complete
- SESAME 7460 agrees well with high pressure Hugoniot data and DFT results



DFT Simulations – Kyle Cochrane

Summary



- MgO Hugoniot extended to 10 Mbar
- Shock front is not reflective below 10 Mbar
- Slope change in Hugoniot suggests phase transition between 330 and 440 Gpa
- No significant changes in Hugoniot data between 4.4 Mbar and 10 Mbar
- DFT simulations indicate that melt on the Hugoniot is complete by 7 Mbar and 16.5 kK in both B1 and B2 phases

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