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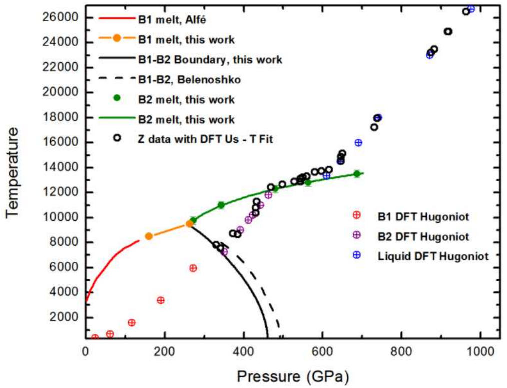

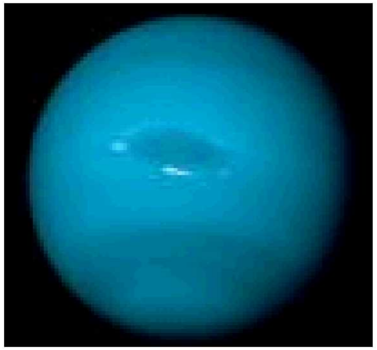

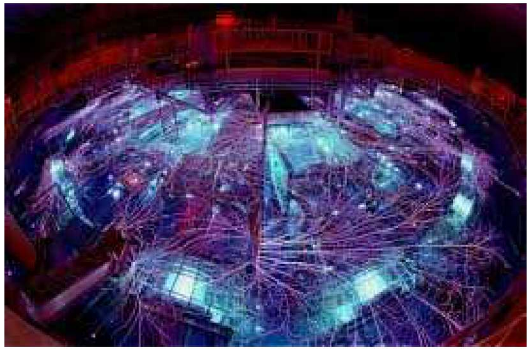

HED Material Physics at Sandia: Integrating Theory and Experiments to Explore the Mbar Regime

Dawn G. Flicker, Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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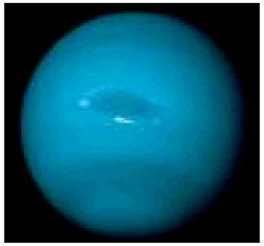
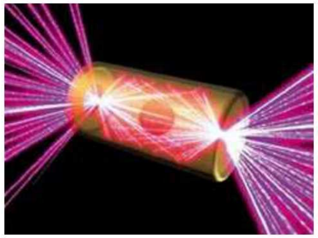
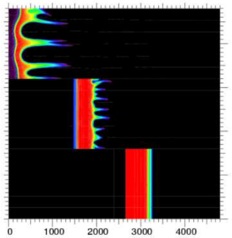
Properties of matter under HED (High Energy Density) conditions are important to many geophysical problems

- Planetary science – Jupiter, Saturn, Uranus, Neptune, and exo planets [e.g. hot Neptunes]
  - Water -2005-2012 (Presented here at Carnegie in May 2010 by Thomas Mattsson): 2 Phys Rev Lett and 2 Phys Rev B
  - Metallization of hydrogen/deuterium: SCIENCE 2015
- Planetary science – earths and super-earths
  - Silicates, MgO, and iron/iron alloys
  - Determining the vaporization threshold for iron – and implications for planetary formation, Nature Geoscience 2015
- Materials for Stockpile Stewardship, HED and inertial confinement fusion (ICF)
  - Investigating the periodic table from **A**luminum to **Z**irconium: a broad range of materials are of interest - a talk in itself
  - The programmatic work drives precision – *we rely on the data!*



We turn planetary science *quantitative* by high fidelity modeling and high-precision experiments





ICF concepts: laser driven hohlraum and MagLIF

There are many opportunities for and interest in collaboration!

Sandia's Z Machine is a unique platform for multi-mission research on high energy density (HED) environments

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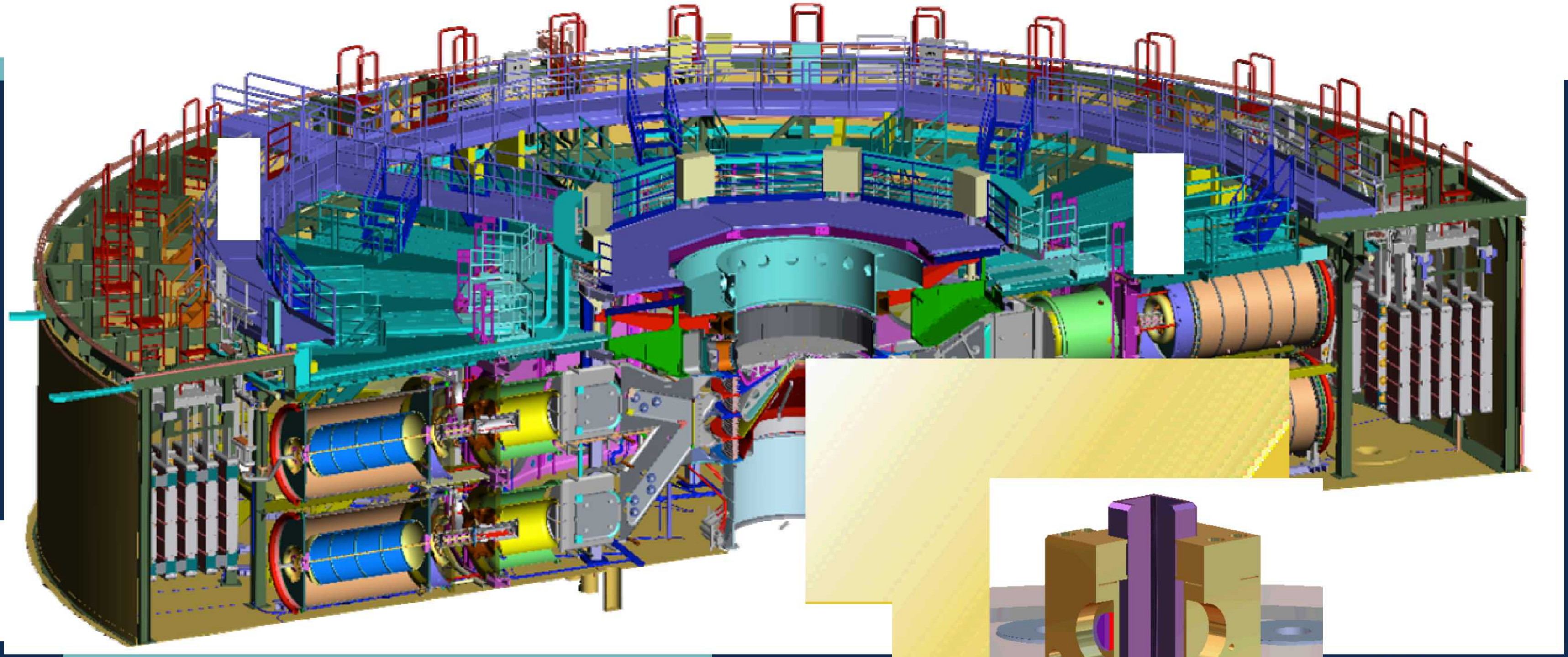
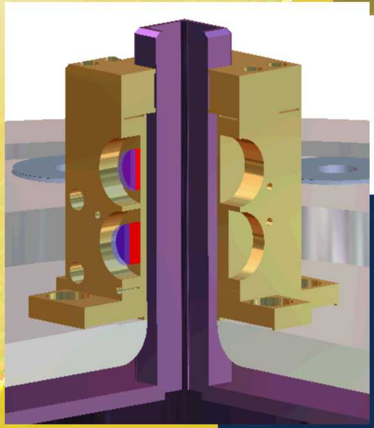




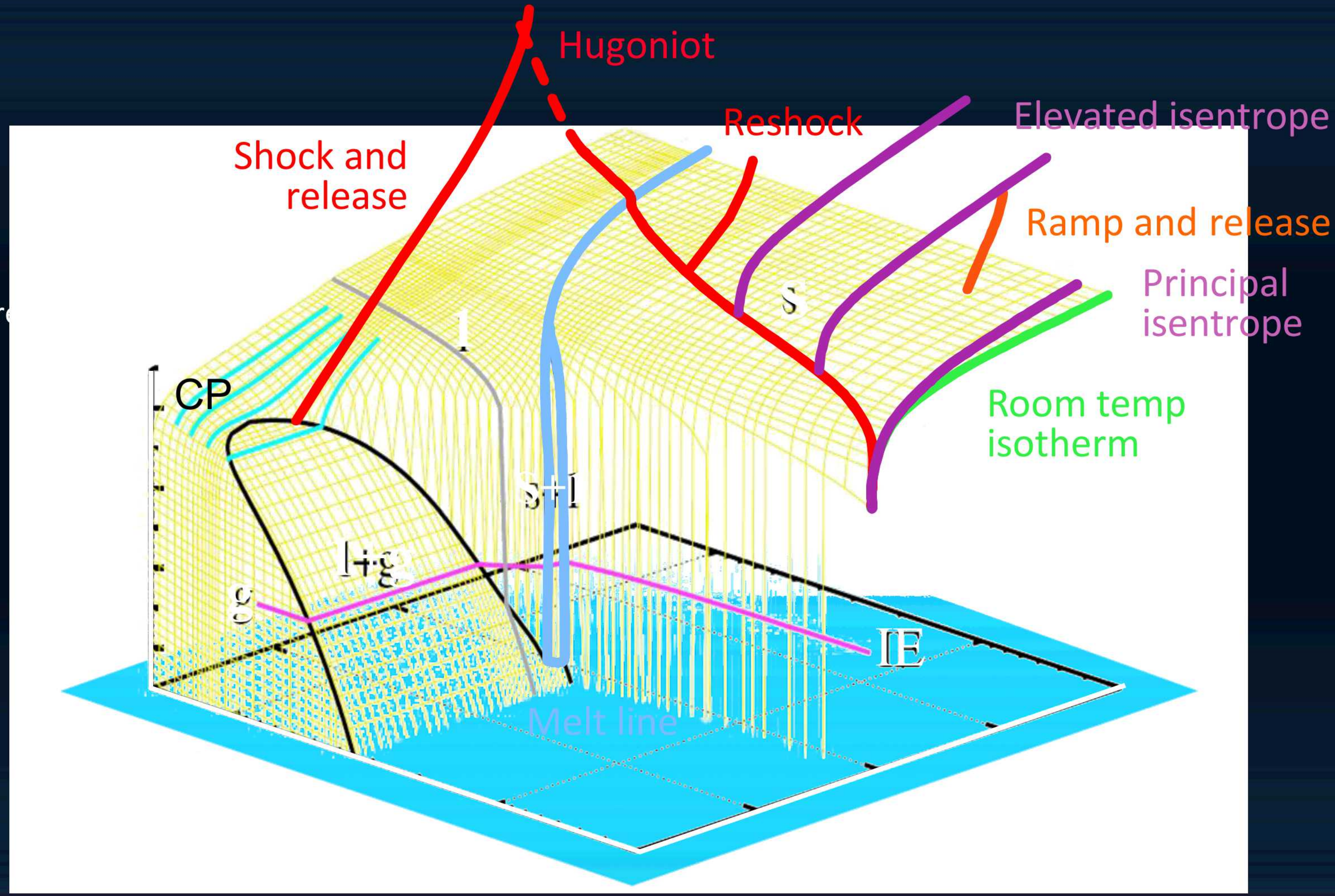
of State

- Pulsed Power Technology
- Magnetically Driven Implosions
- Inertial Confinement Fusion
- Dynamic Materials

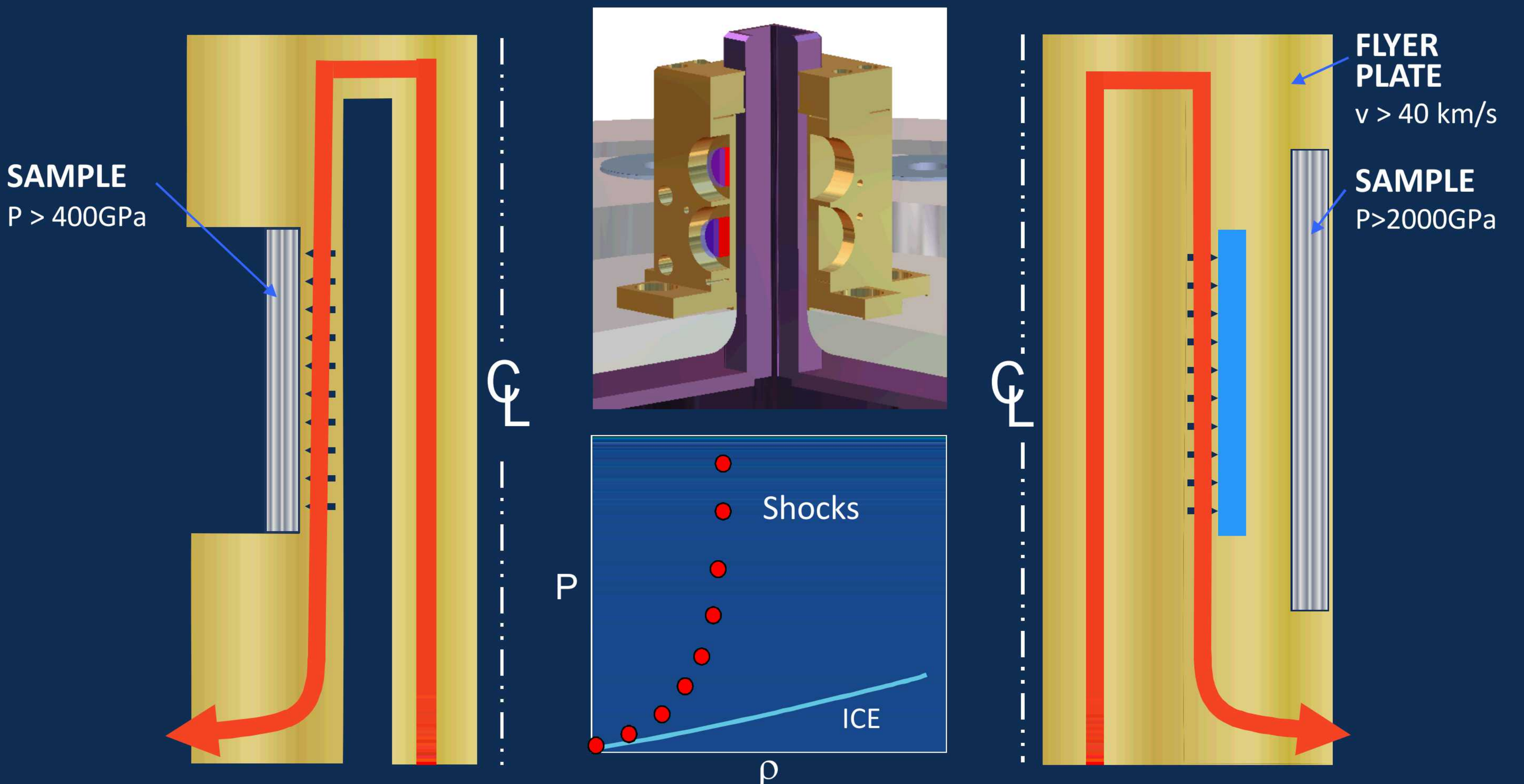
I ~ 26 MA, τ ~100-1000 ns
X-ray power > 250 TW
X-ray energy > 2 MJ

Dynamic compression experiments on Z can probe large regions of a material's equation-of-state surface

Pr



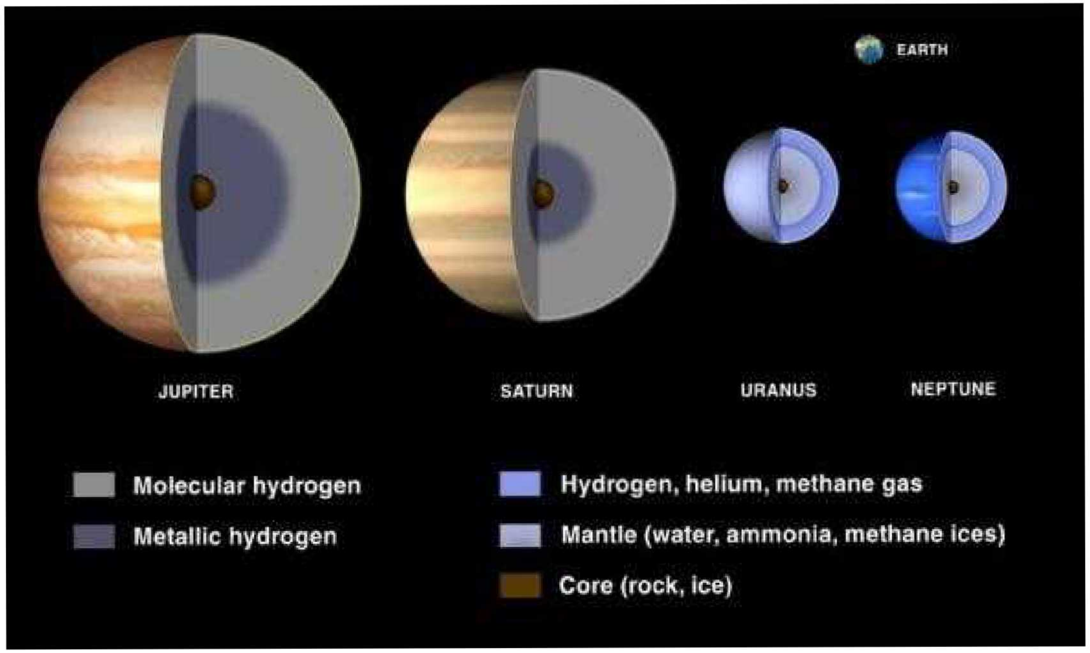
Isentropic compression and shock wave experiments map different regions of phase space



Isentropic Compression Experiments:
Gradual pressure rise in sample

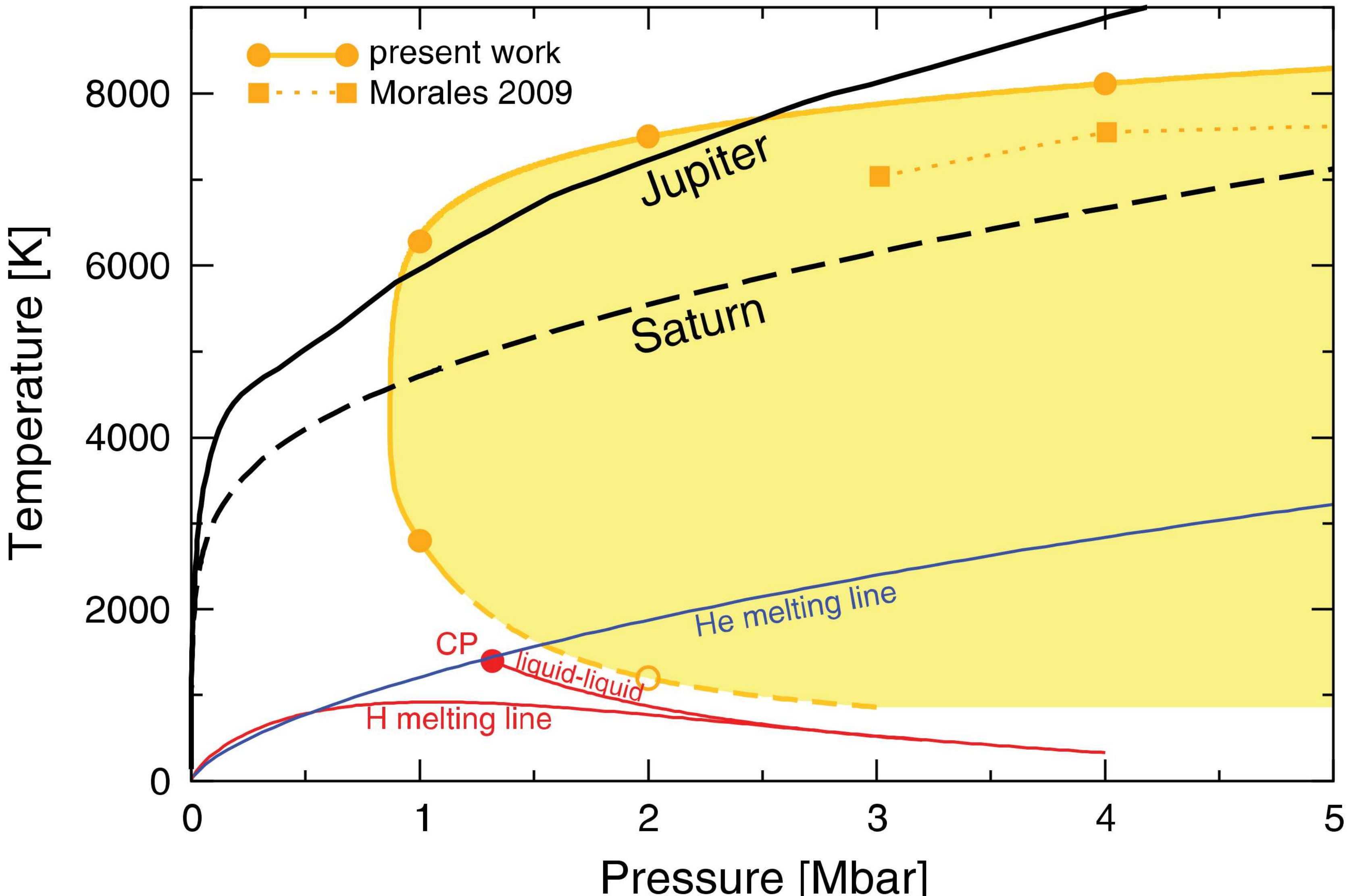
Shock Hugoniot Experiments:
Shock wave in sample on impact

Understanding the properties of hydrogen is crucial for understanding giant planets



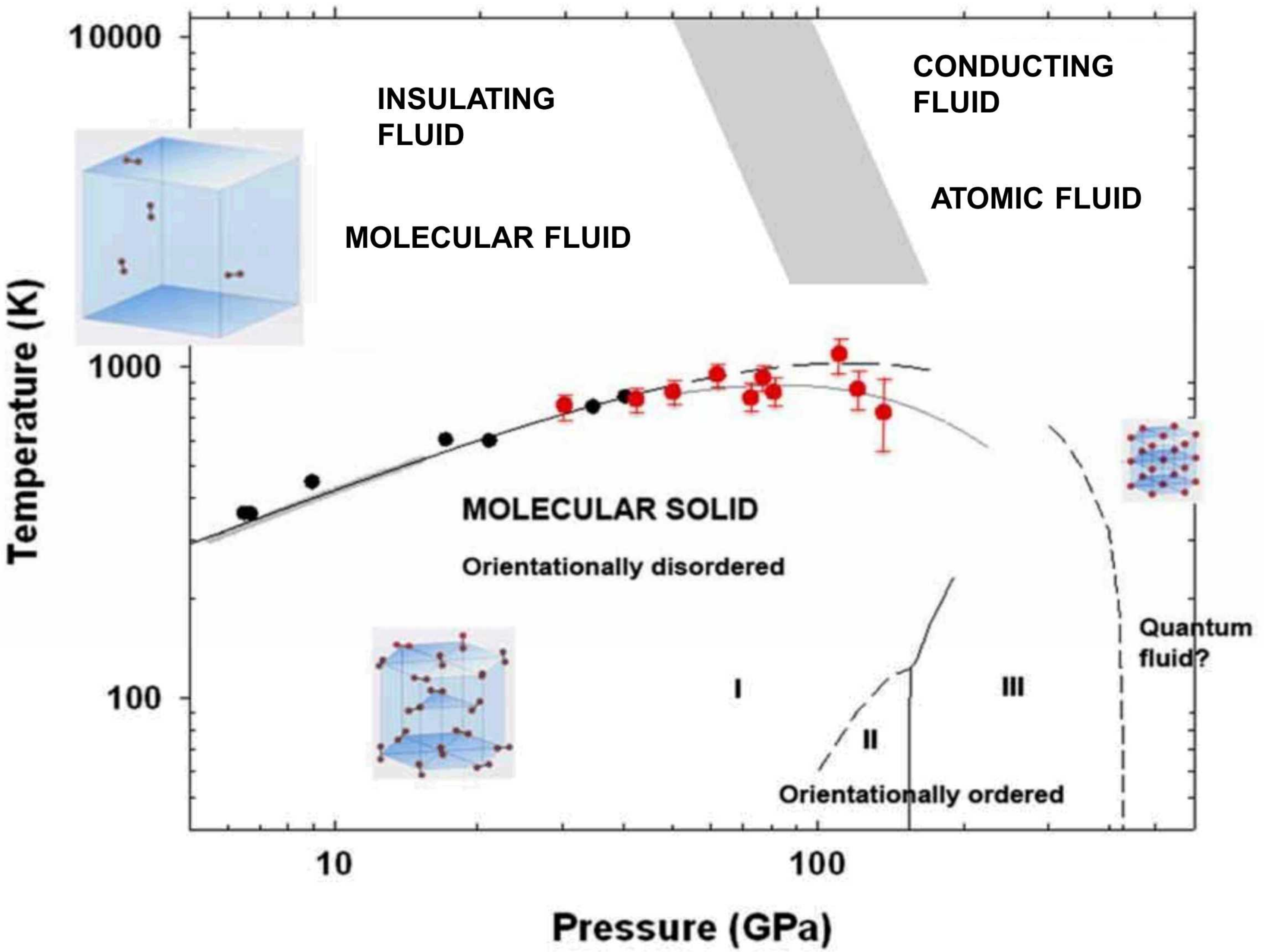
- Present structure
  - Layers of different composition while fulfilling observational constraints
- Evolution
  - Discrepancies in modeling the evolution of Jupiter and Saturn – the “Saturn age problem”
- Magnetic fields
  - Origin of multi-polar fields in Neptune and Uranus

H-He de-mixing appears to be precipitated at low T and P by metallization in hydrogen



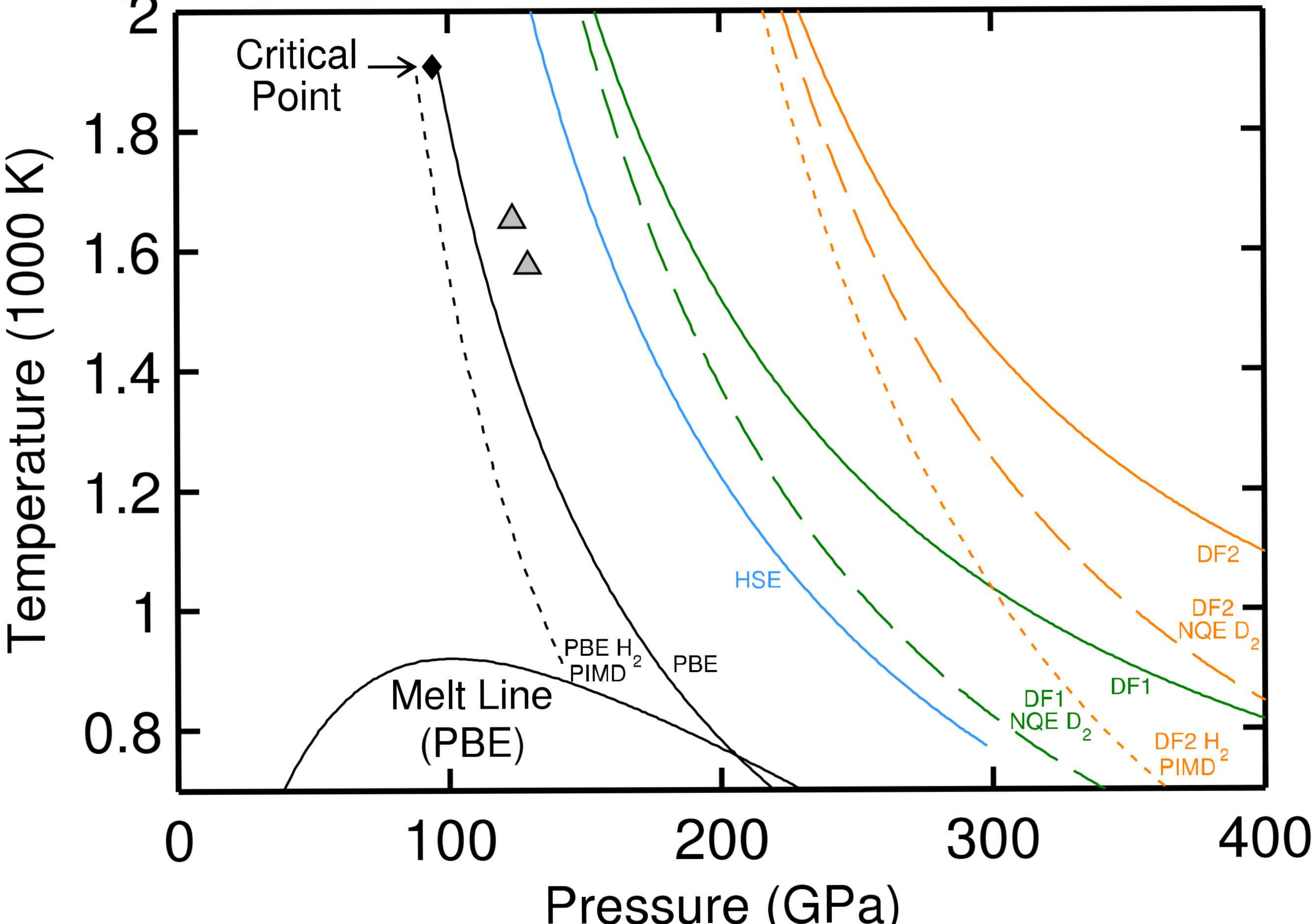
W. Lorenzen, B. Holst, and R. Redmer, Phys. Rev. B 84, 235109 (2011)

Hydrogen has an intriguing phase-diagram at high pressure with several unknown boundaries



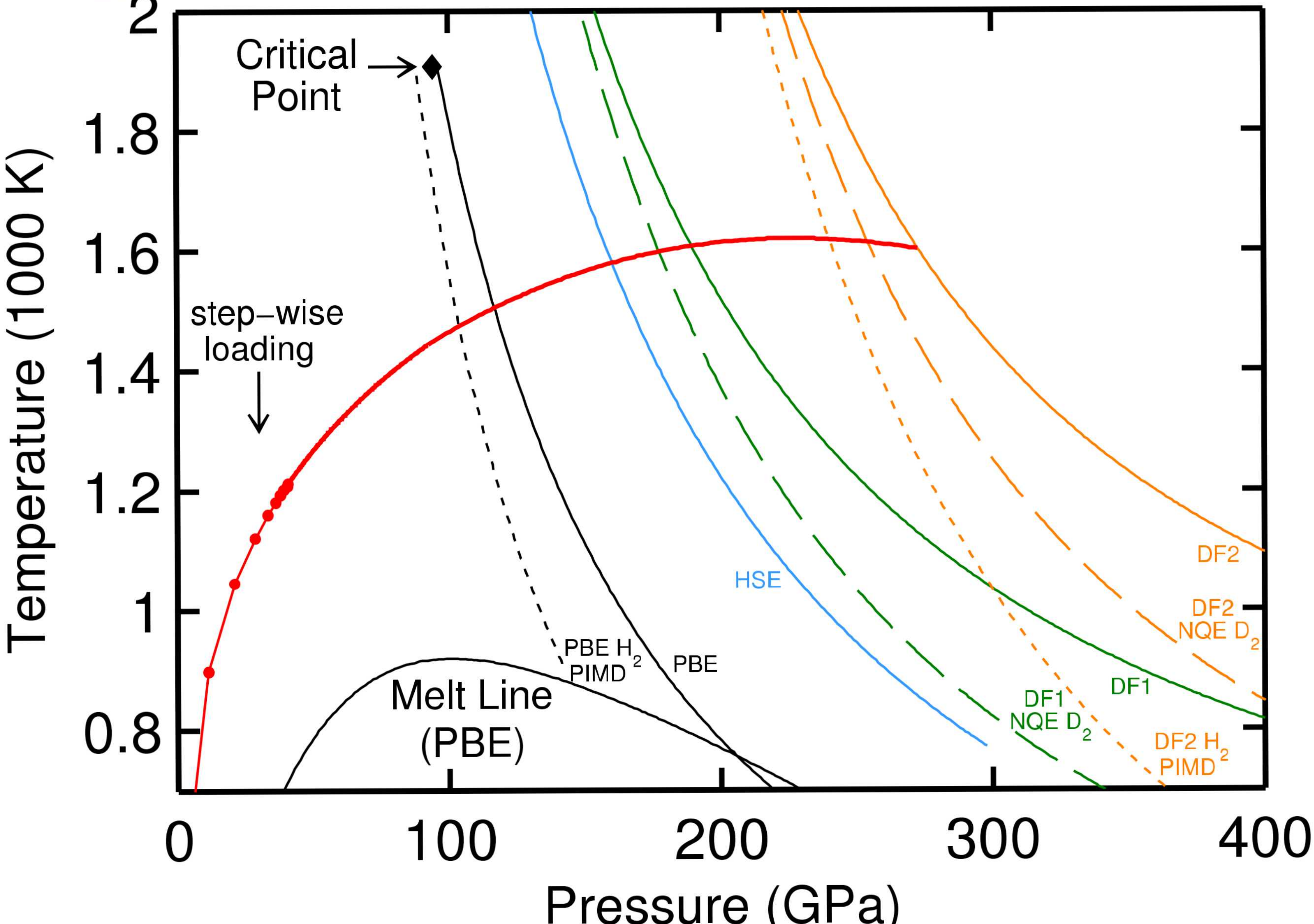
R.J. Hemley, High Press Res. 30, 581 (2010)

Predictions of the liquid-liquid insulator to metal transition (LL-IMT) in hydrogen vary considerably

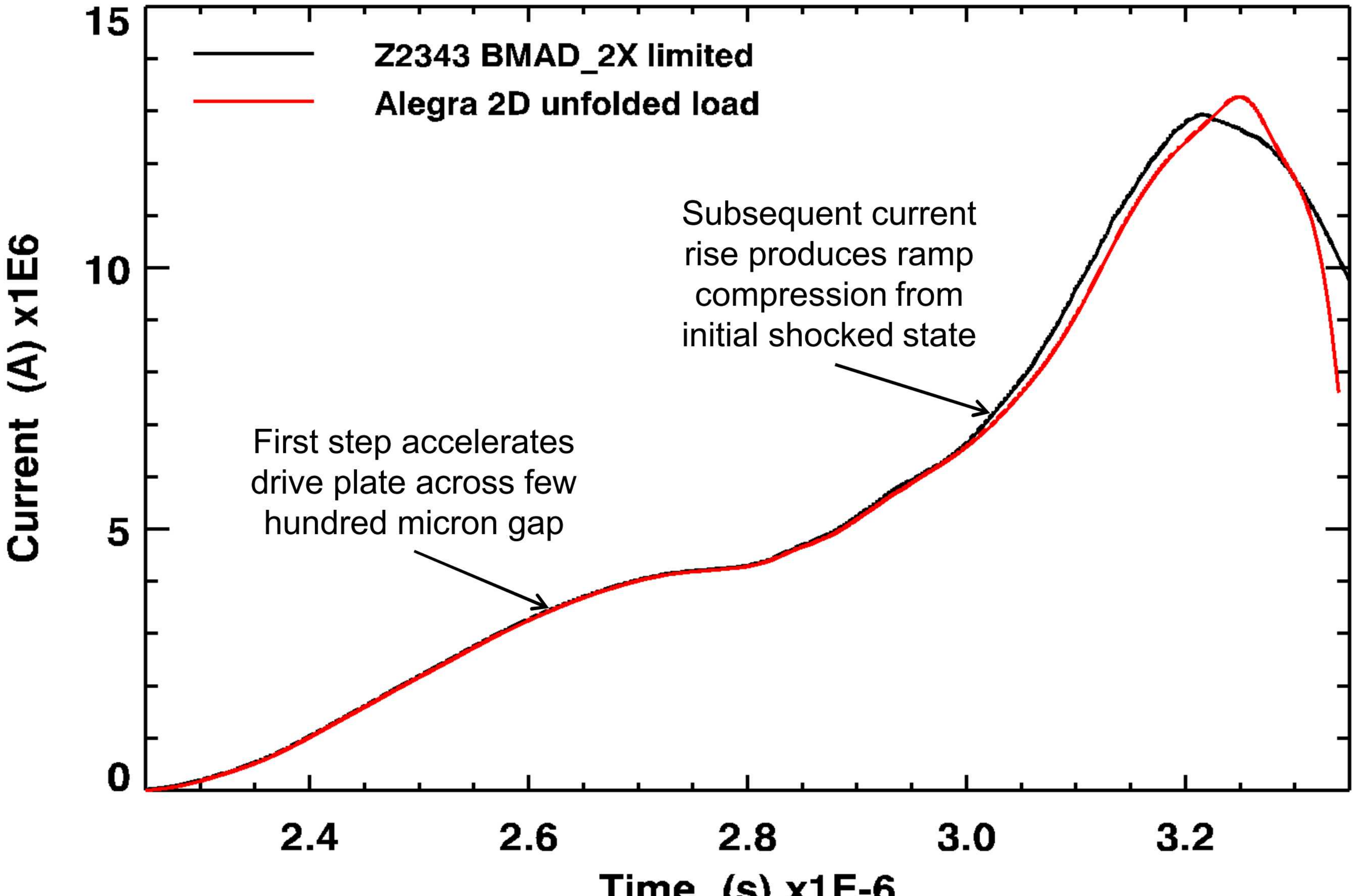


[illegible] atter (2014)

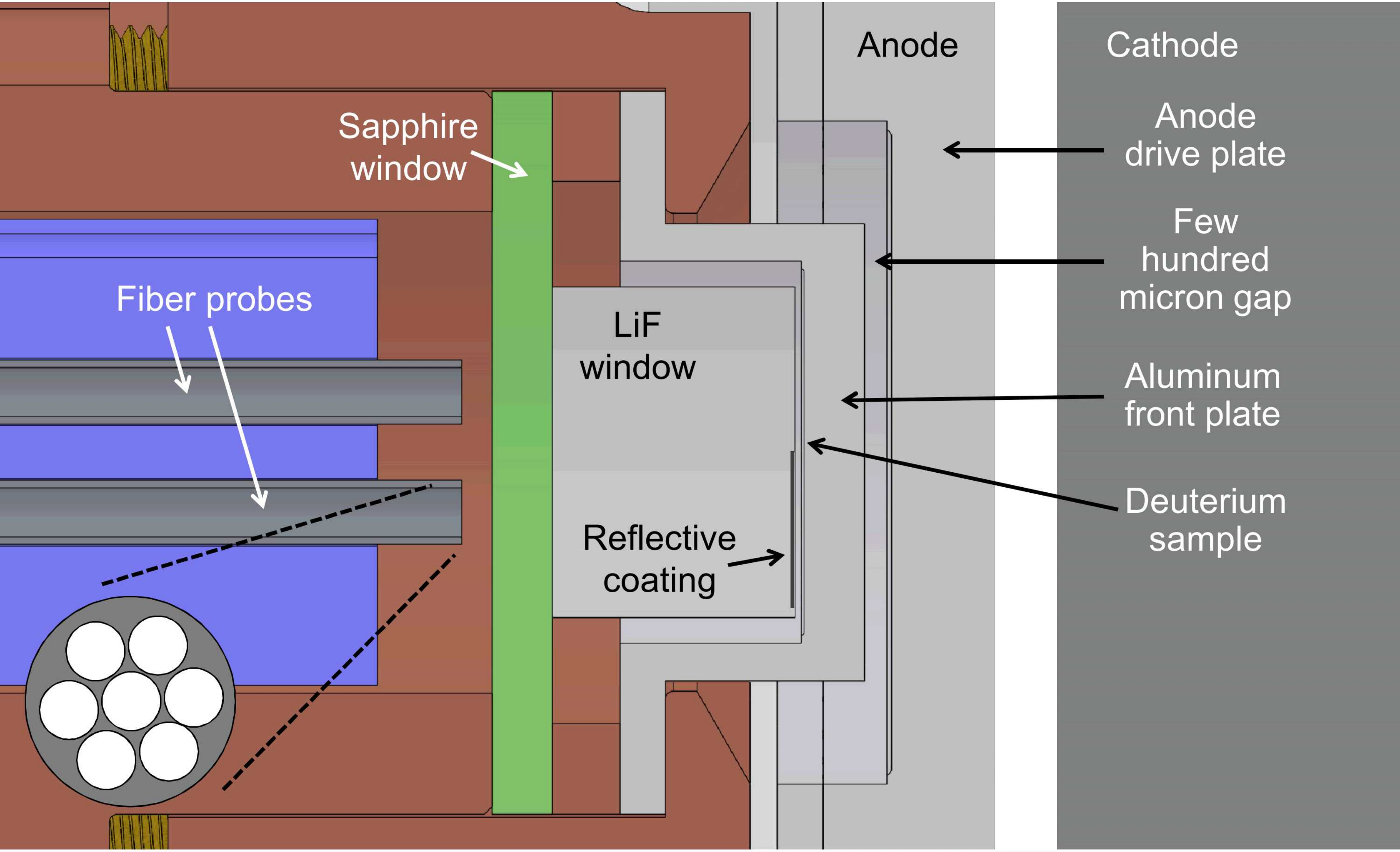
A shock – ramp experiment on Z traverses the proposed LL-IMT boundaries



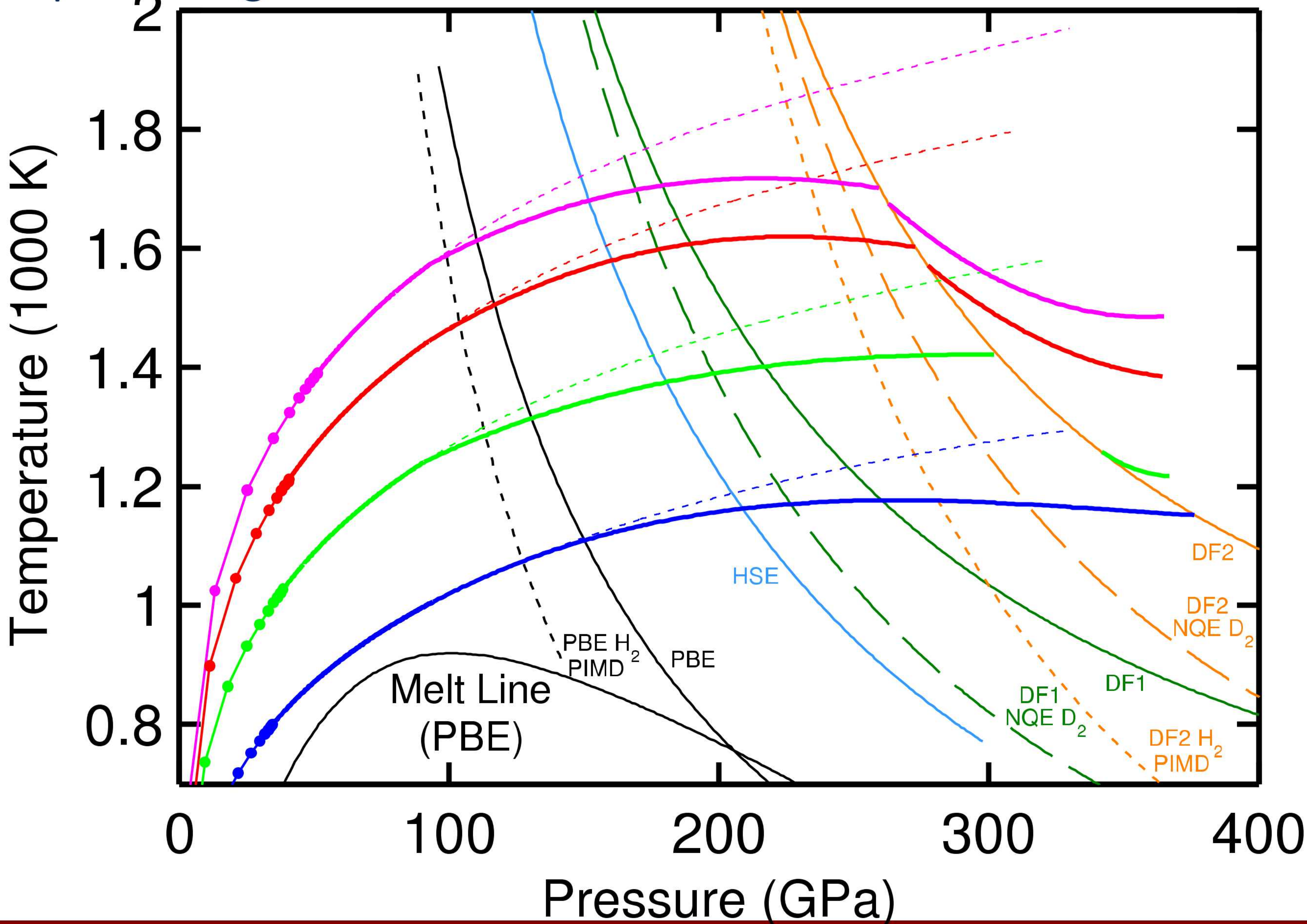
Two-step pulse shape enabled by dual Marx triggers provides the shock-ramp loading of the target



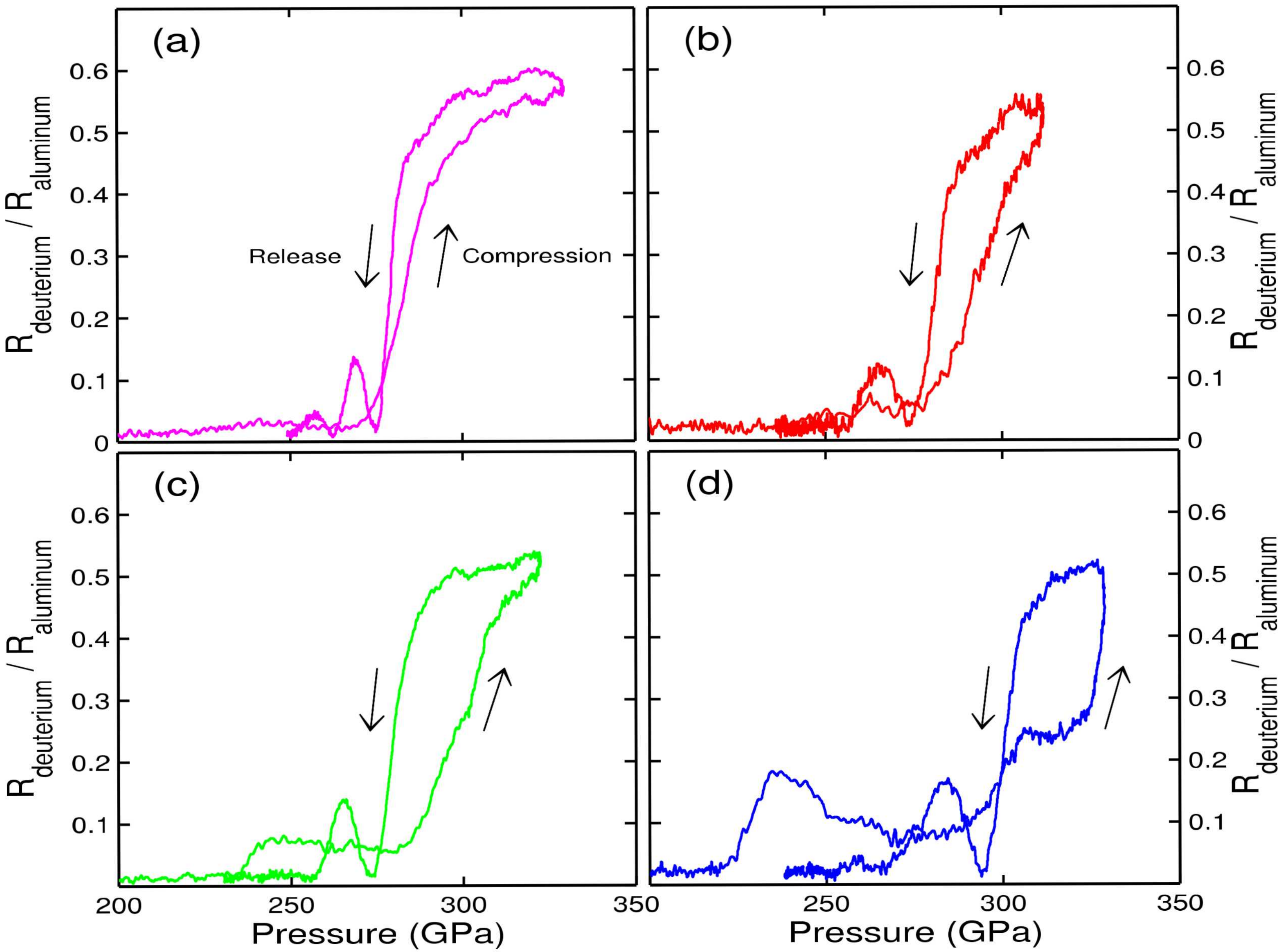
The experimental design allows for multiple diagnostics – tracking the shock-ramp compression of deuterium



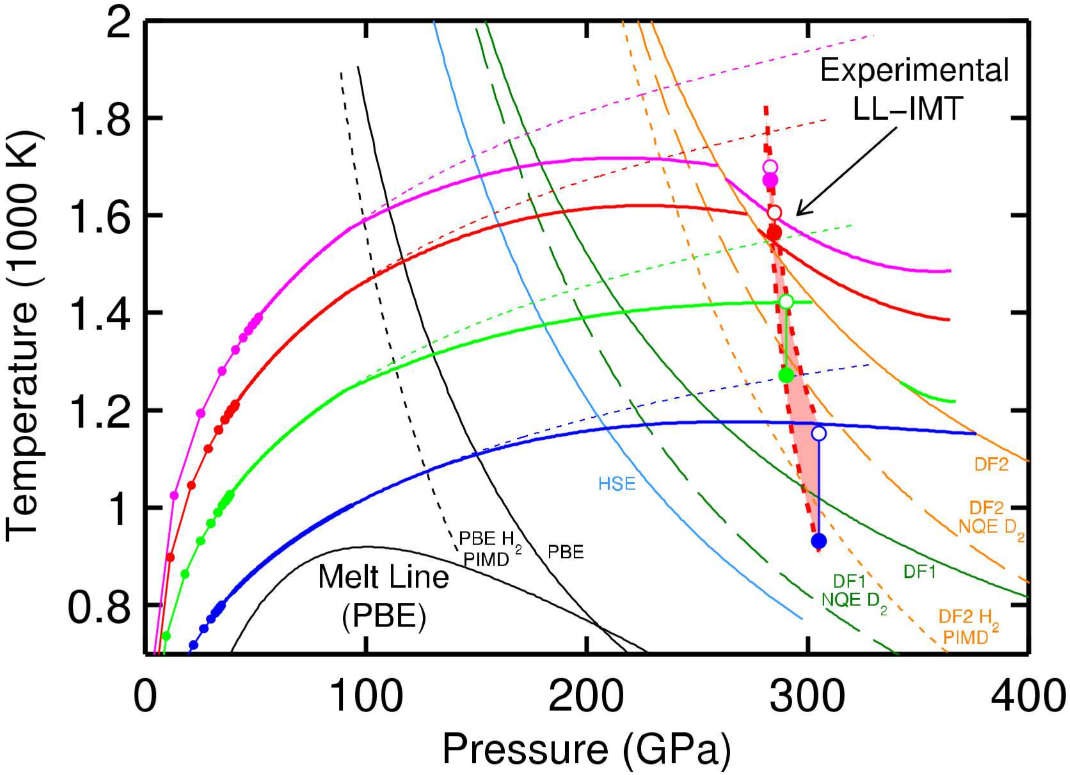
The experimental PT Paths span the important region of the phase diagram



The reflectivity is a sensitive diagnostics for metallization



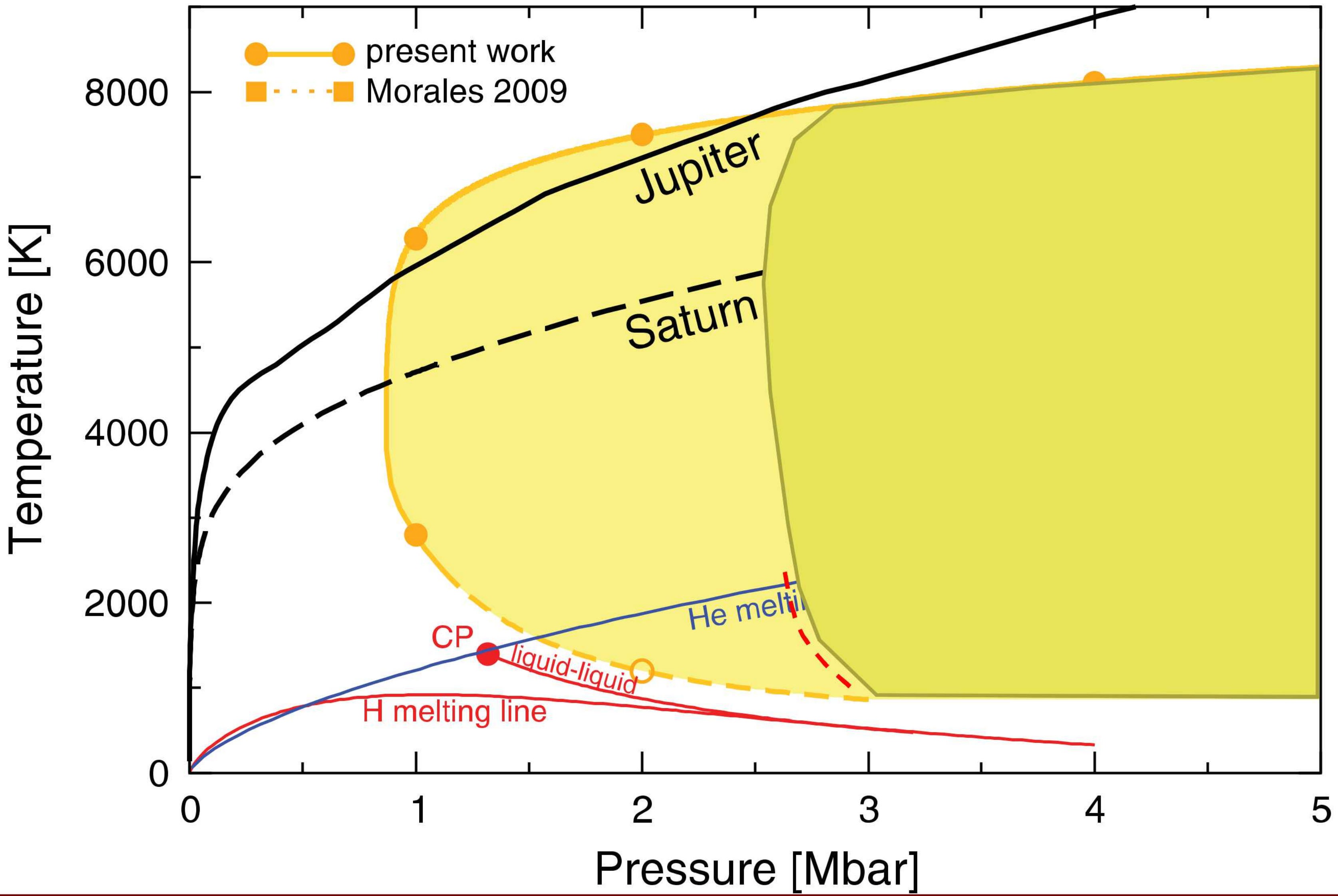
We have located the LL-IMT in deuterium to be at 300 GPa



- *Insensitivity to T suggests this is a ρ-driven transition*
  - ρ at the transition is inferred to be ~2-2.1 g/cc in deuterium
  - Qualitatively different transition than in shock experiments (T driven)
- Broad team with expertise in diagnostics, pulse-shaping, experimental design, and first-principles simulations
- A project within the Z Fundamental Science Program
  - Professor Ronald Redmer's group at University of Rostock

M.D. Knudson, M.P. Desjarlais, A. Becker, R.W. Lemke, K.R. Cochrane, M.E. Savage, D.E. Bliss, T.R. Mattsson, and R. Redmer, SCIENCE **348** 1455, 26 June 2015.

We expect the H-He demixing region to be shifted to higher pressure – possibly explaining the Jupiter/Saturn age discrepancy in evolution models

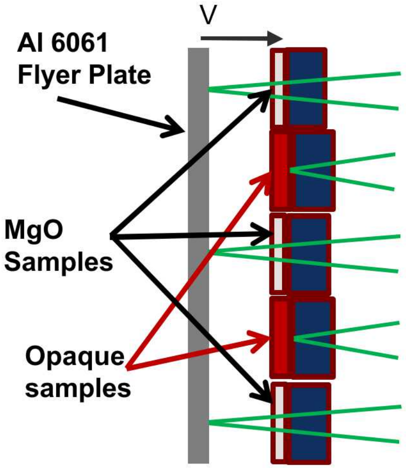


W. Lorenzen, B. Holst, and R. Redmer, Phys. Rev. B 84, 235109 (2011)

Two recent dynamic experiments offer new data

Steady shock from flyer plates

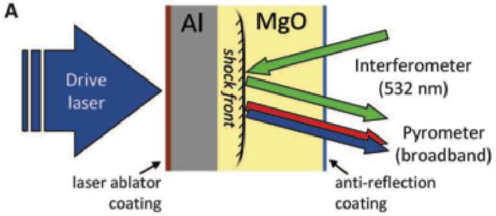
- Root et al.



- Measure u_s, reflectivity and u_p via impedance matching
- Longer transit times (~25 ns)
- Large number of shots to different final pressures (>30)

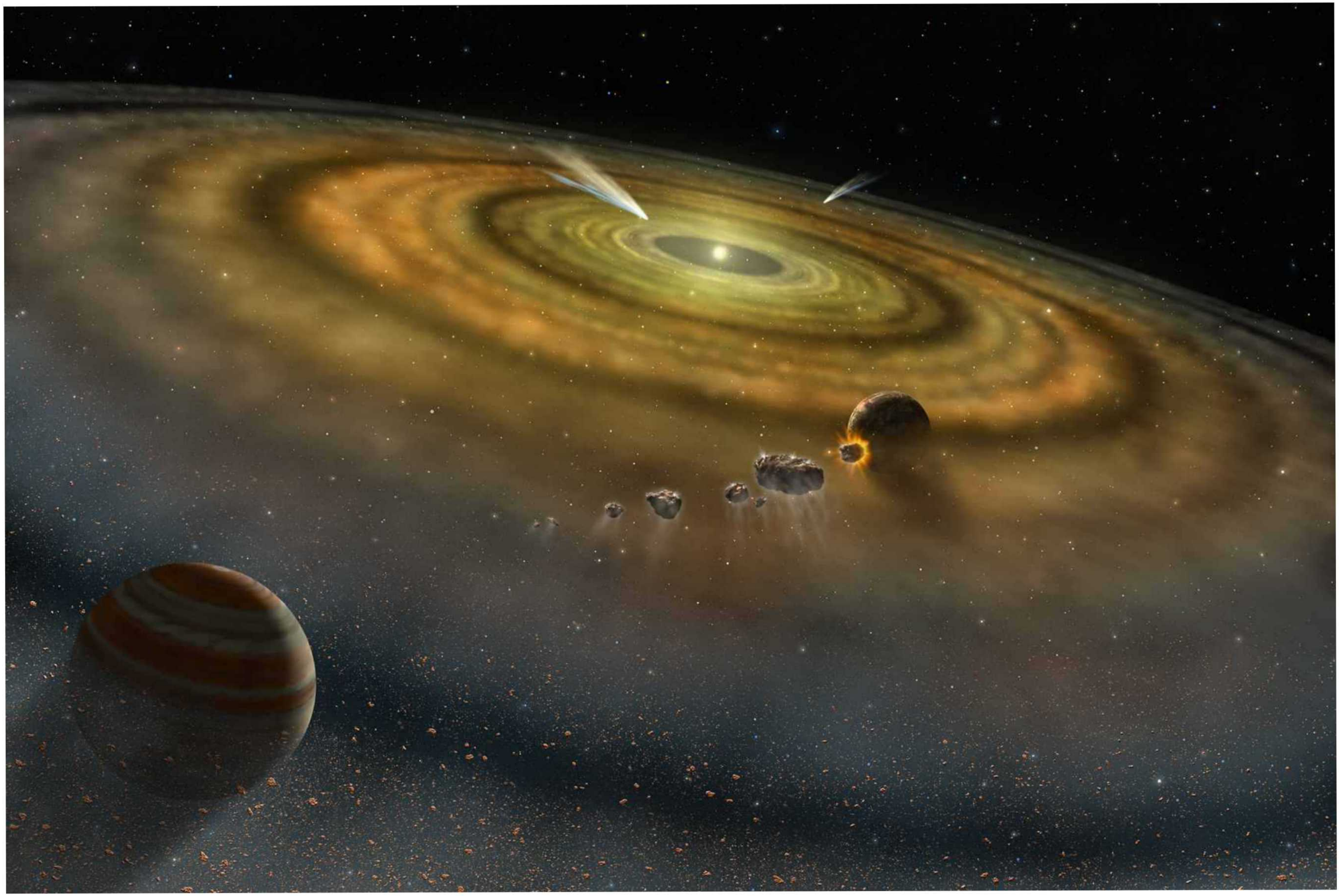
Laser driven decaying shock

- McWilliams et al. Science **338**, 1330 (2012)

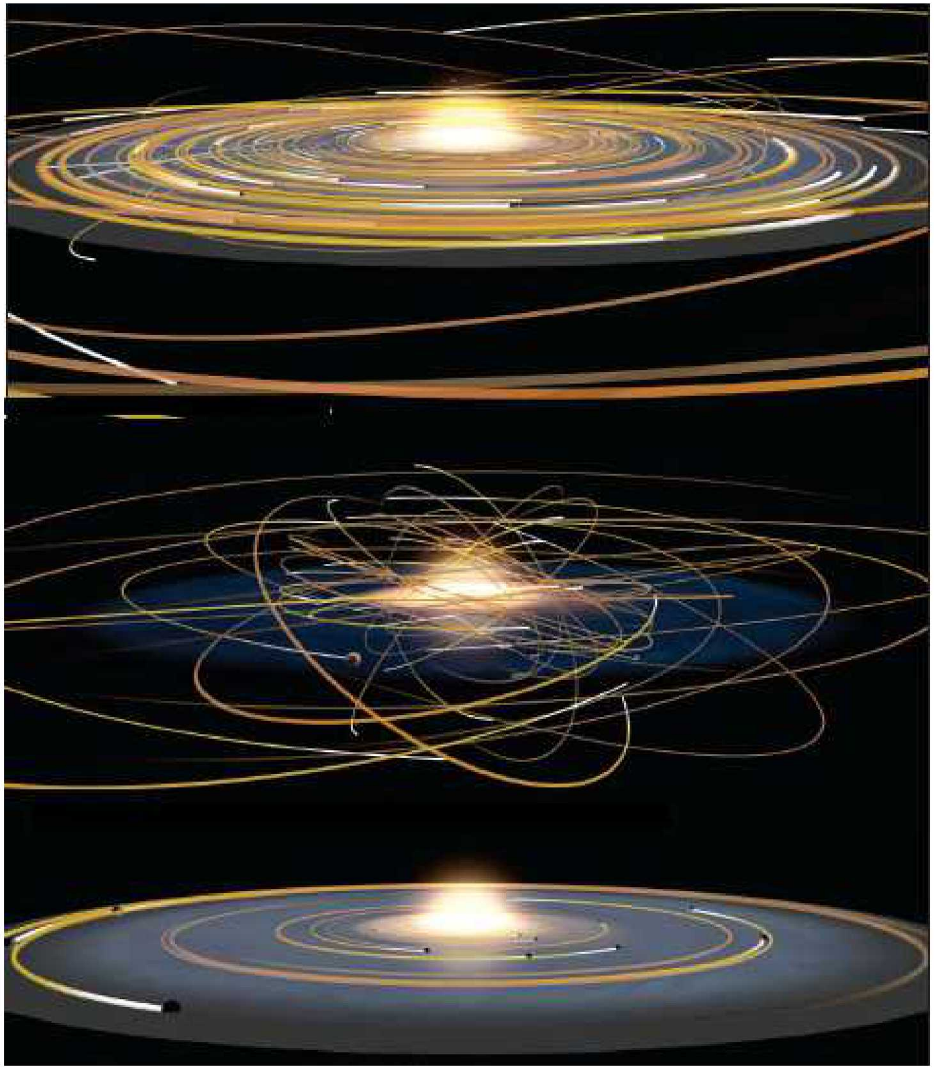


- Measure u_s, reflectivity and T as a function of time
- Potentially map entire Hugoniot in a single shot
- Must infer u_p from knowledge of Hugoniot
- Short time scales (transit through MgO lasts ~10 ns)

Planets form by a series of impacts – raising challenging questions on how material responds to strong shocks



Although impacts come in all speeds and sizes – we have focused on giant impacts



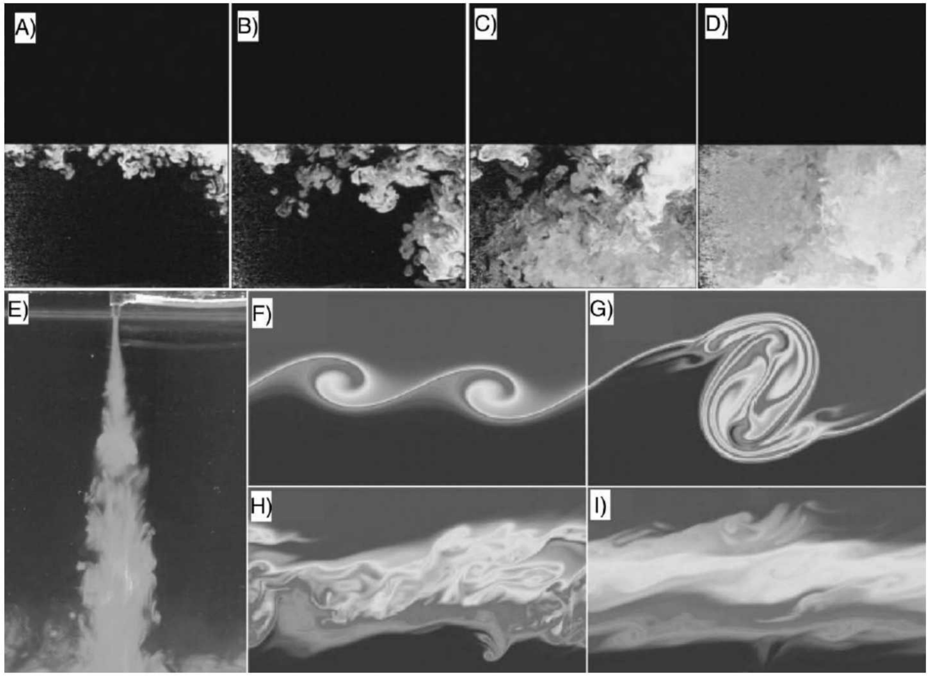
Dust particles impacting at fractions of miles per hour

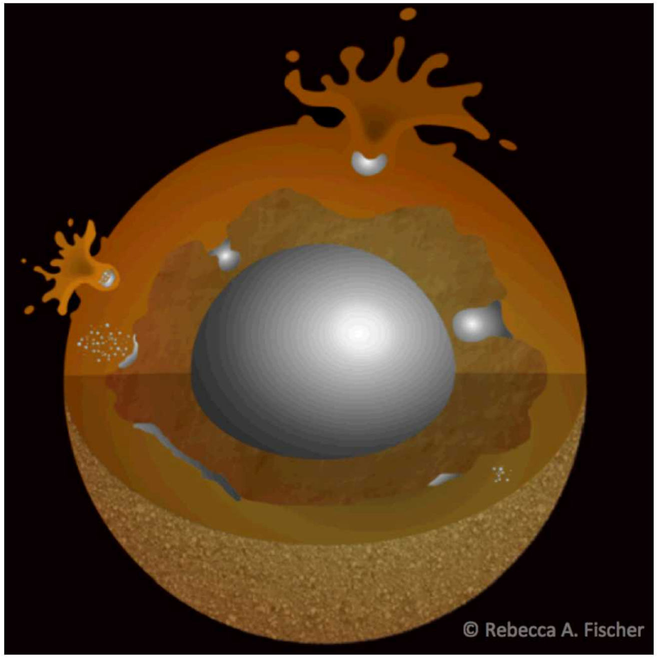
Boulders colliding at a few miles per hour

City sized planetesimal collisions

Moon sized giant impacts

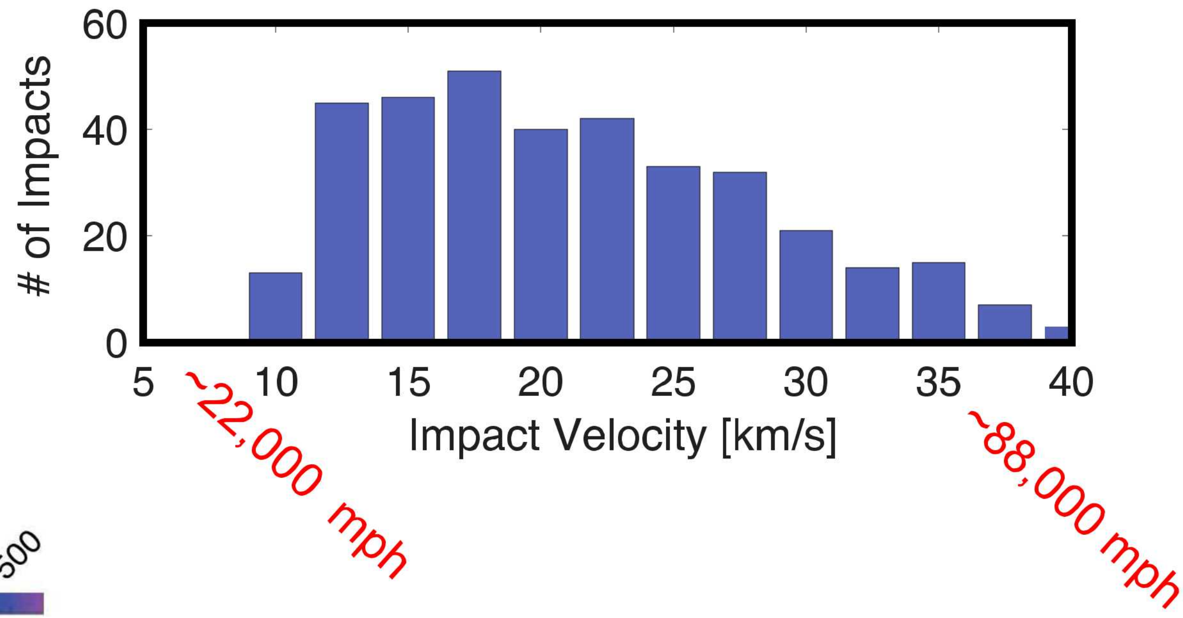
How well do the cores of impactors mix with the rocky part of the growing Earth?

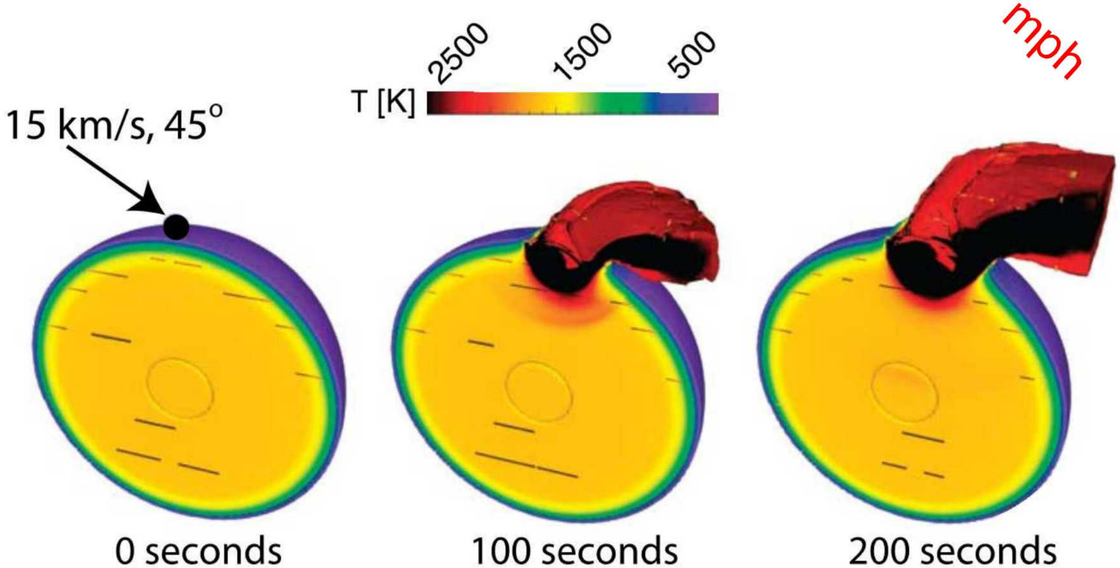




- Geophysicists have shown fluid instabilities CAN NOT sufficiently mix the incoming iron cores
- This points to an older core (100 Myr after the solar system formed)

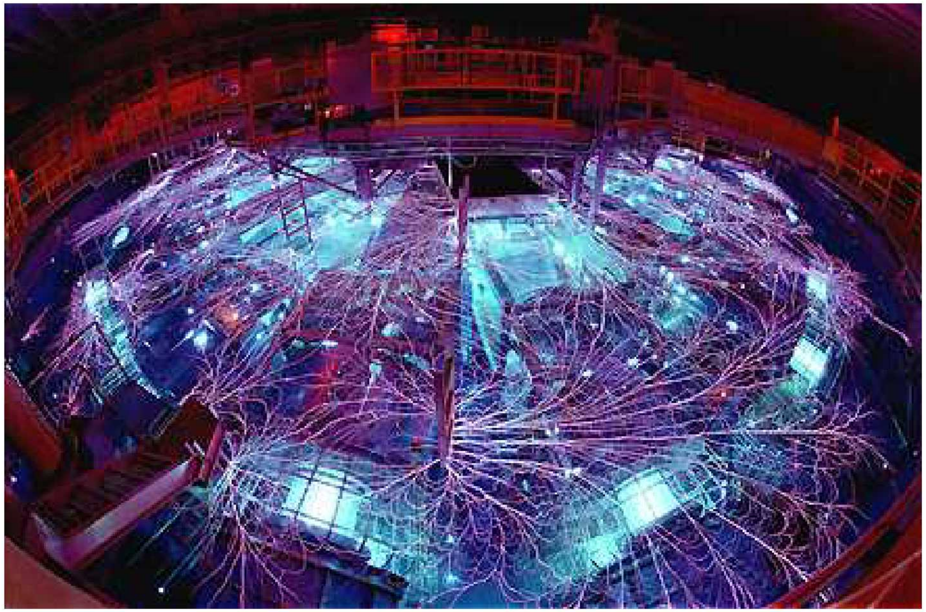
What happens to planetesimal cores during impacts?
Planetary dynamics studies suggest speeds are very high!



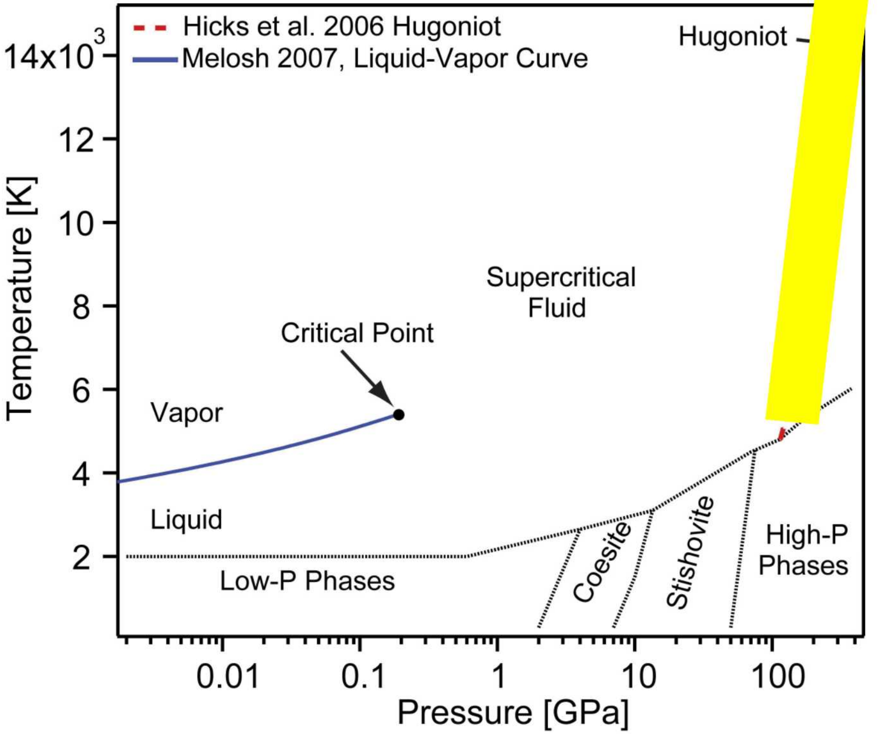


Only the NIF and Sandia Z Facility can reliably study the entire range of states

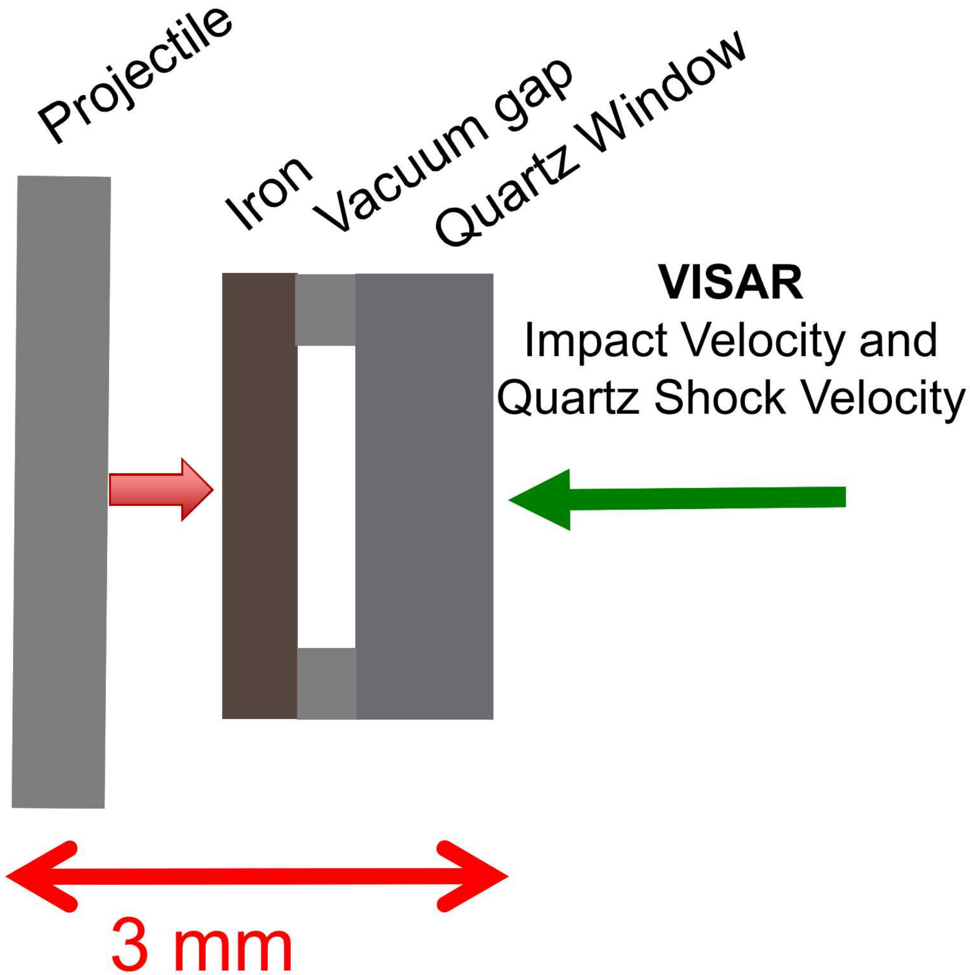
- Sandia Z facility can launch flyer plates at 100,000 mph
- We can directly simulate all impact conditions

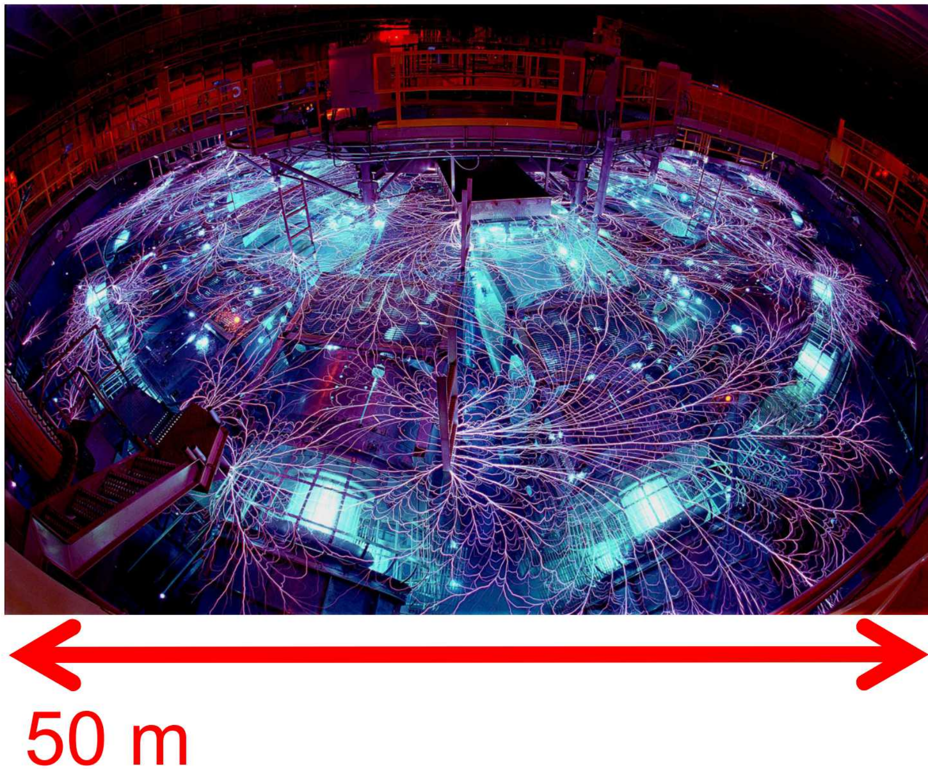


Sandia Z Facility

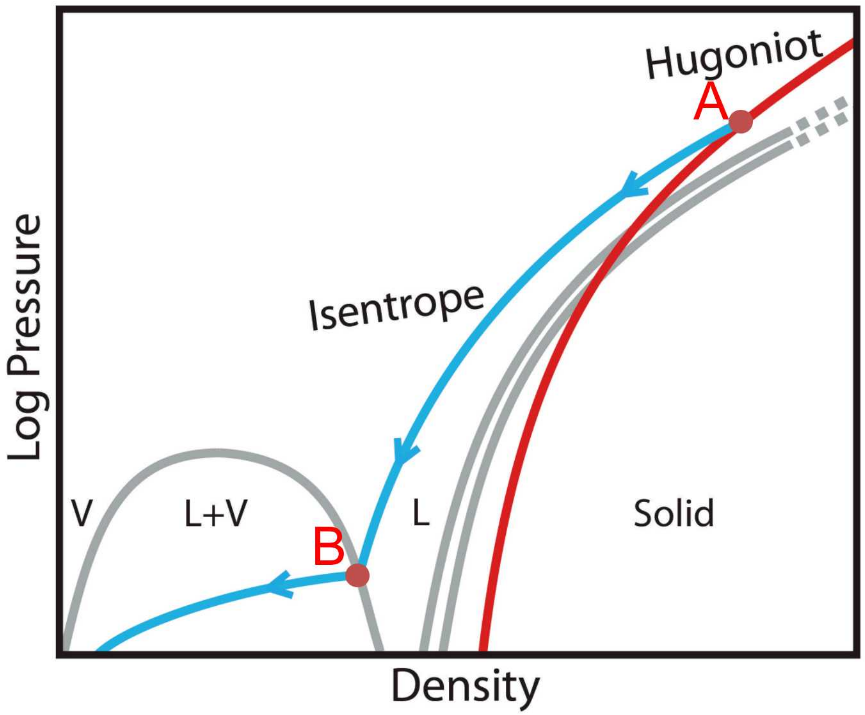


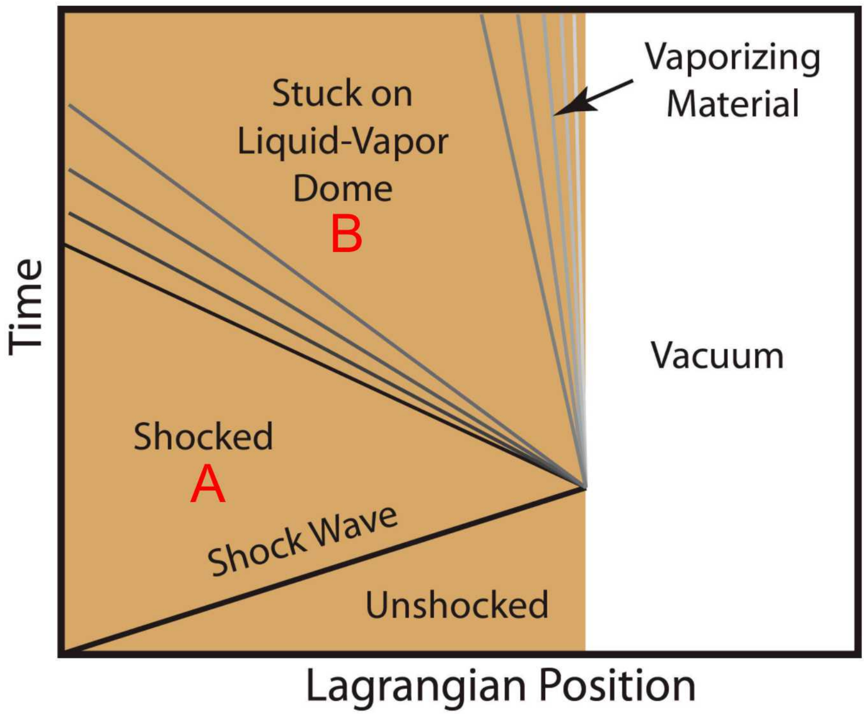
Impact Experiments at the Sandia Z Facility



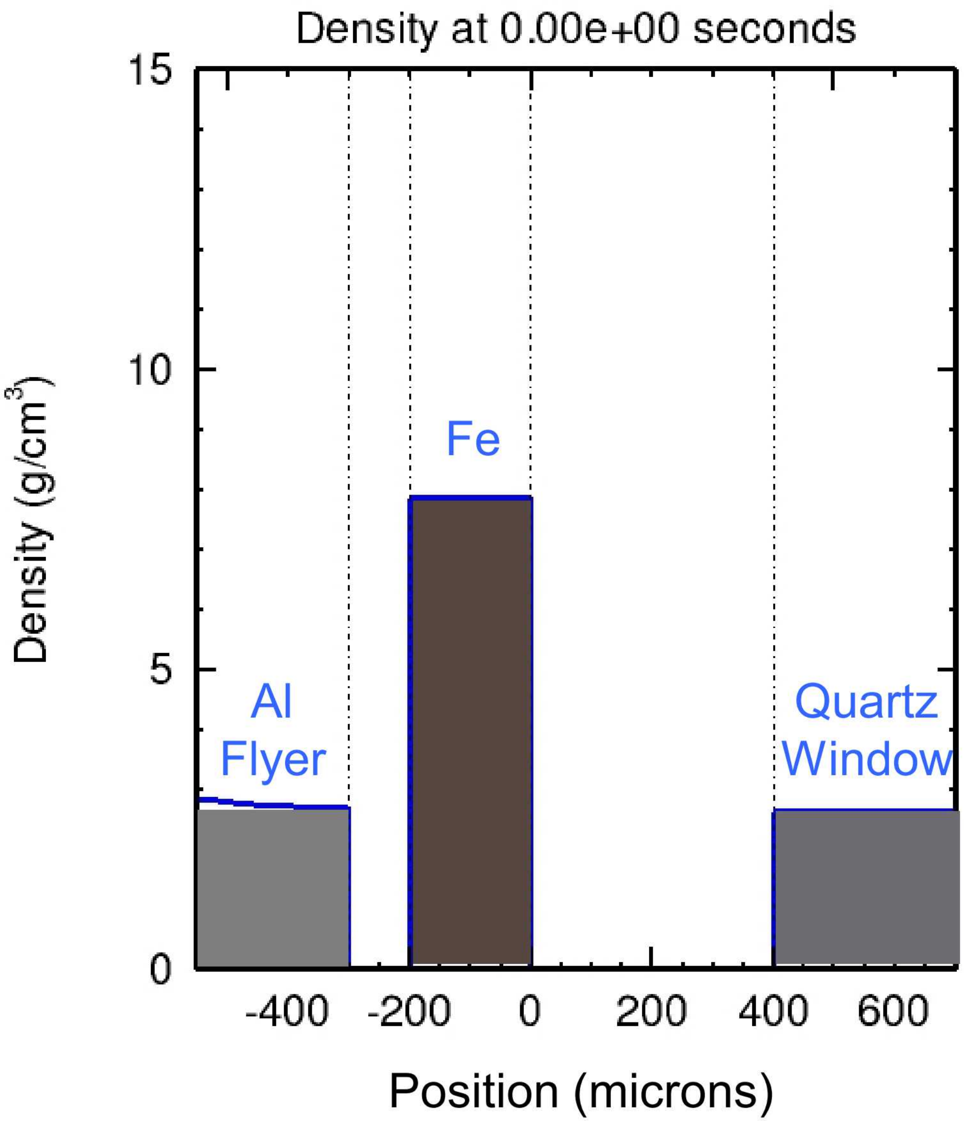


Measuring density on the liquid-vapor dome

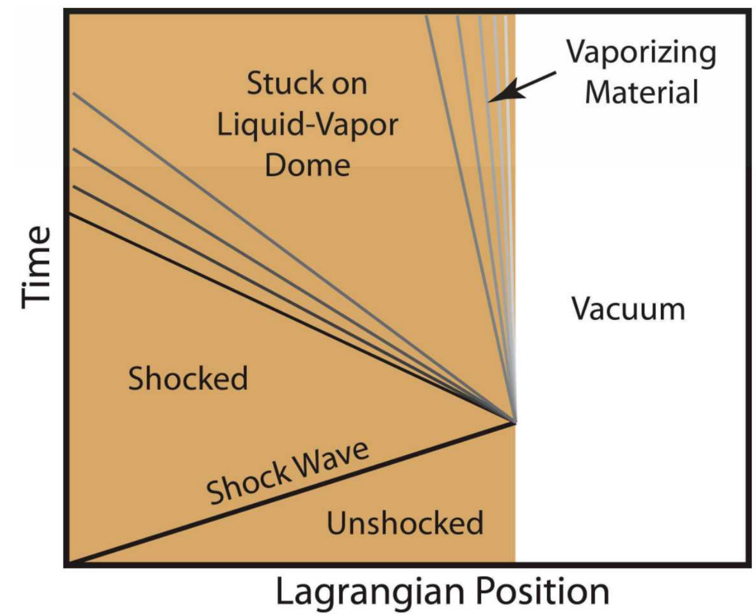




Using Z to launch an Fe liquid flyer plate

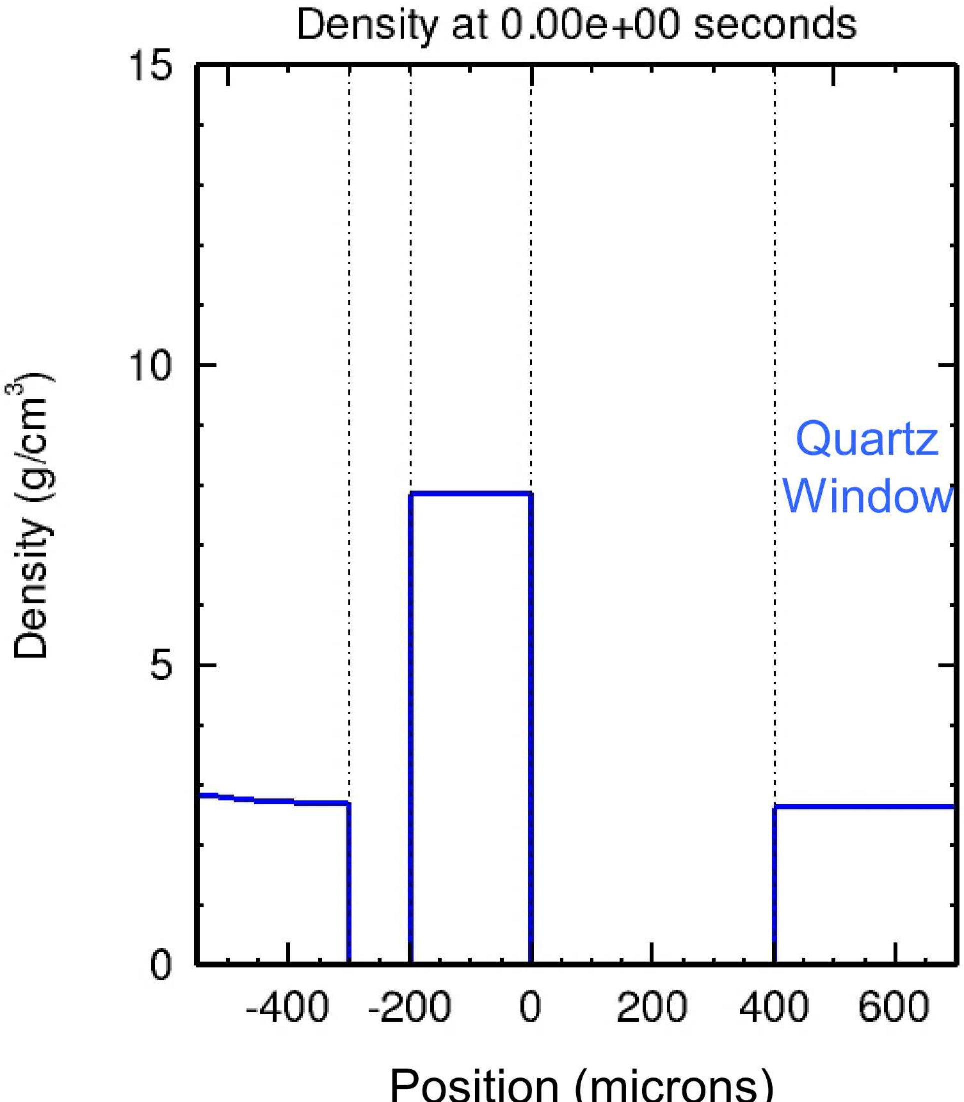


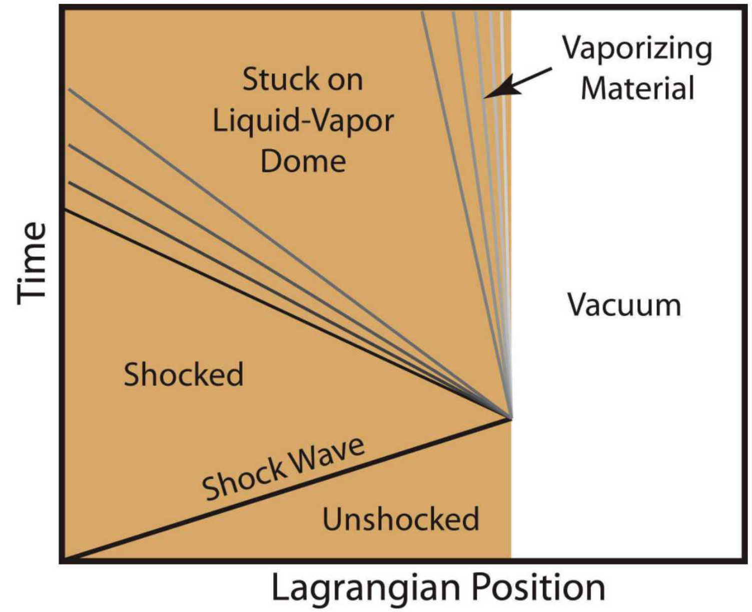
VISAR diagnostic: measures the shock velocity in the quartz window



1d CTH simulations

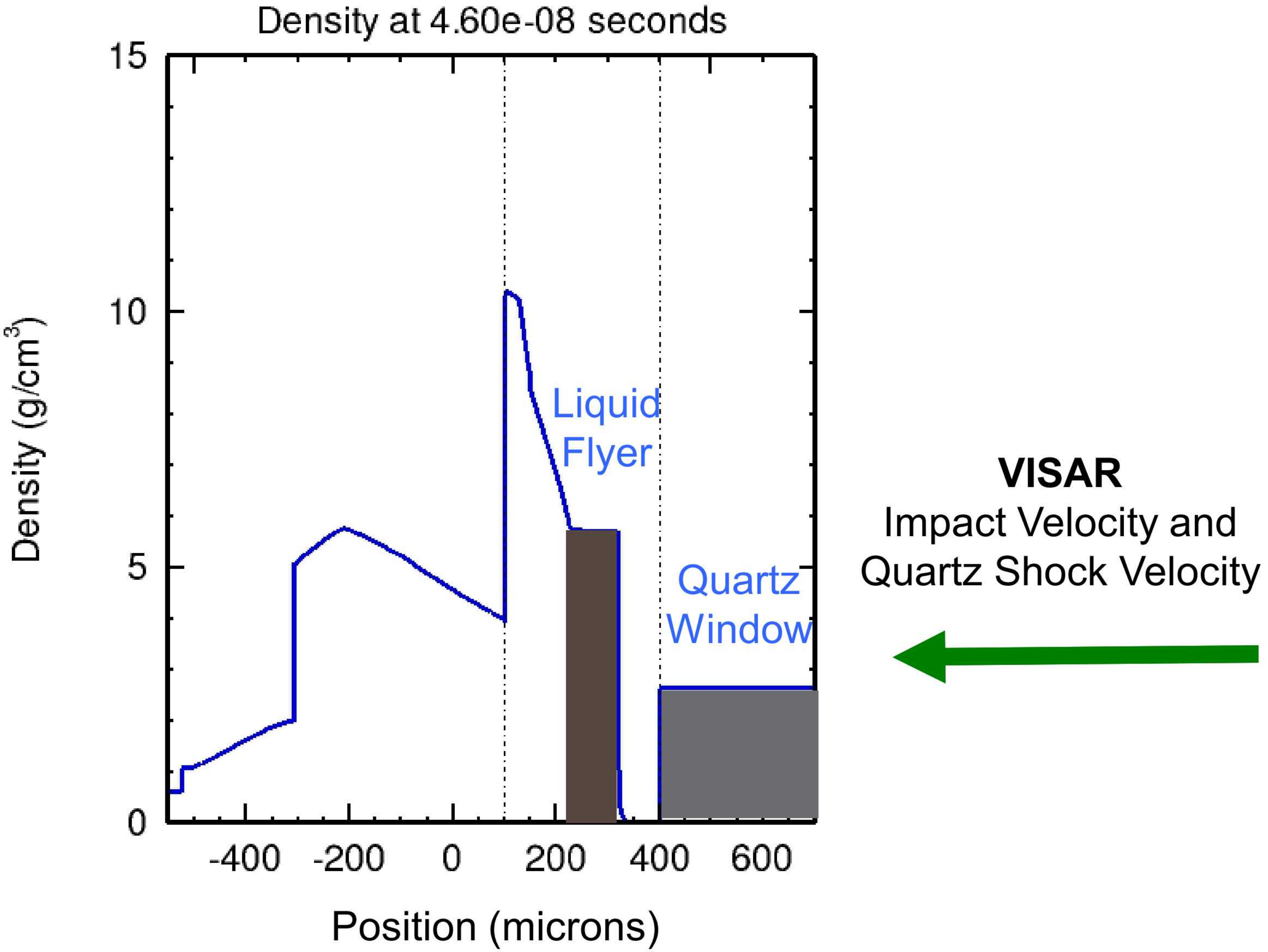
Using Z to launch an Fe liquid flyer plate





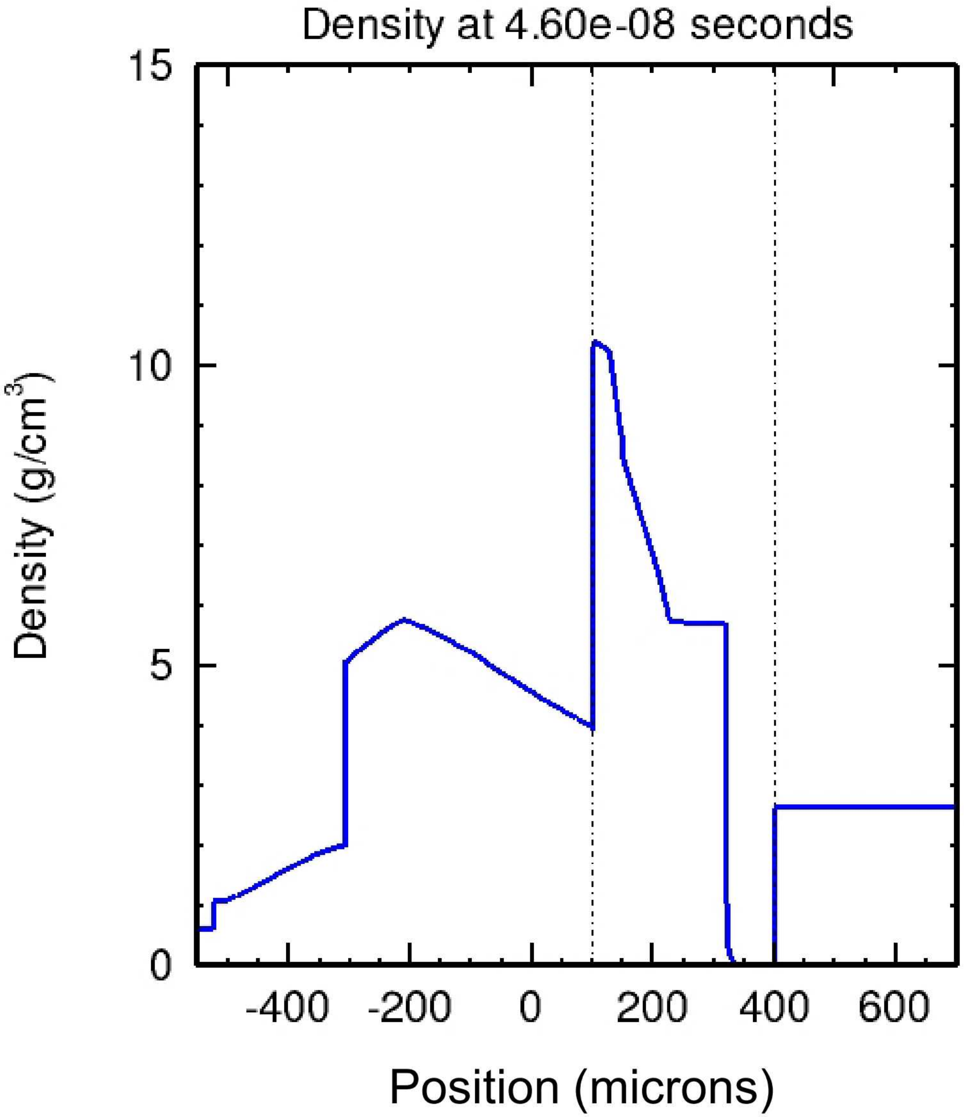
1d CTH simulations

Reverse Impact Experiment

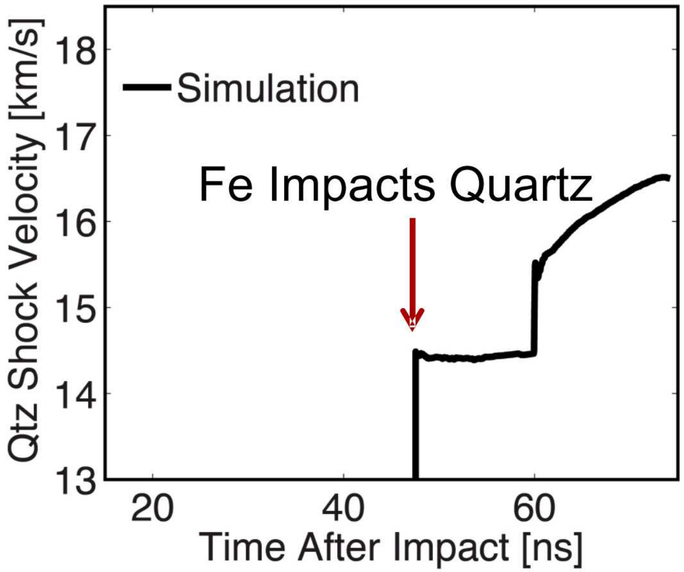


1d CTH simulations

Reverse Impact Experiment

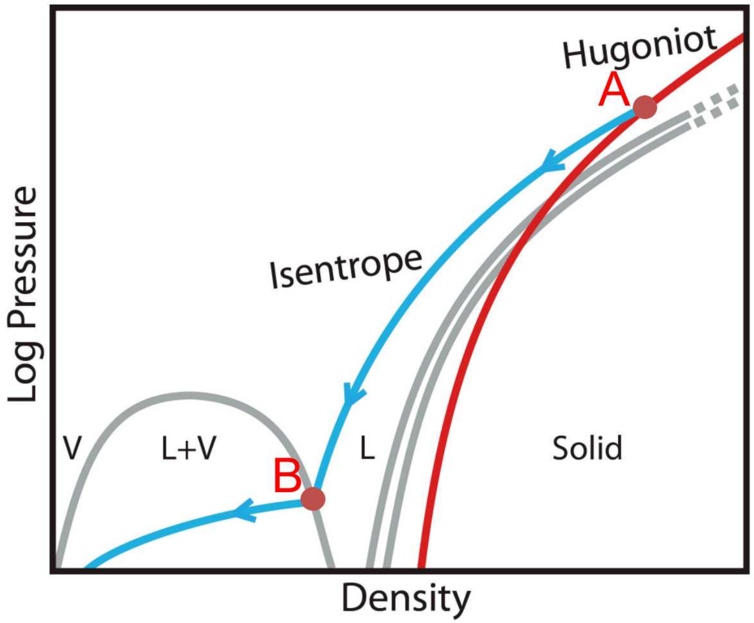


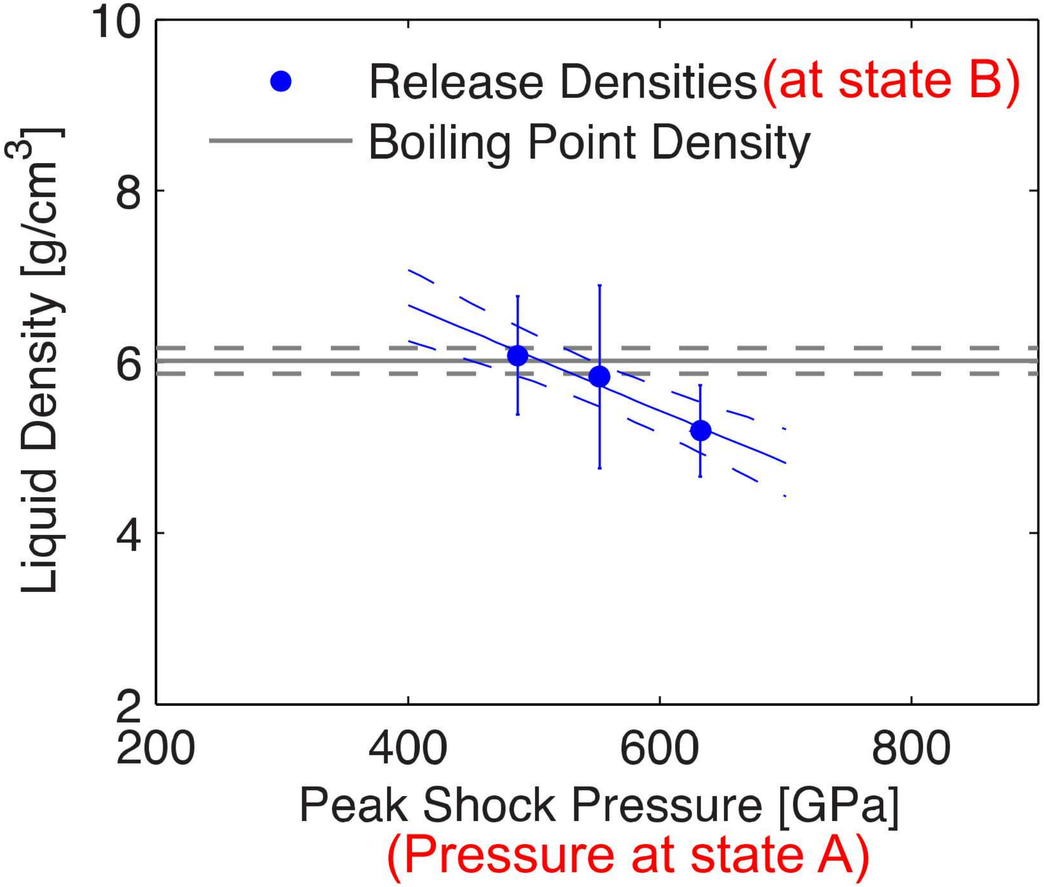
VISAR diagnostic: measures the shock velocity in the quartz window



1d CTH simulations

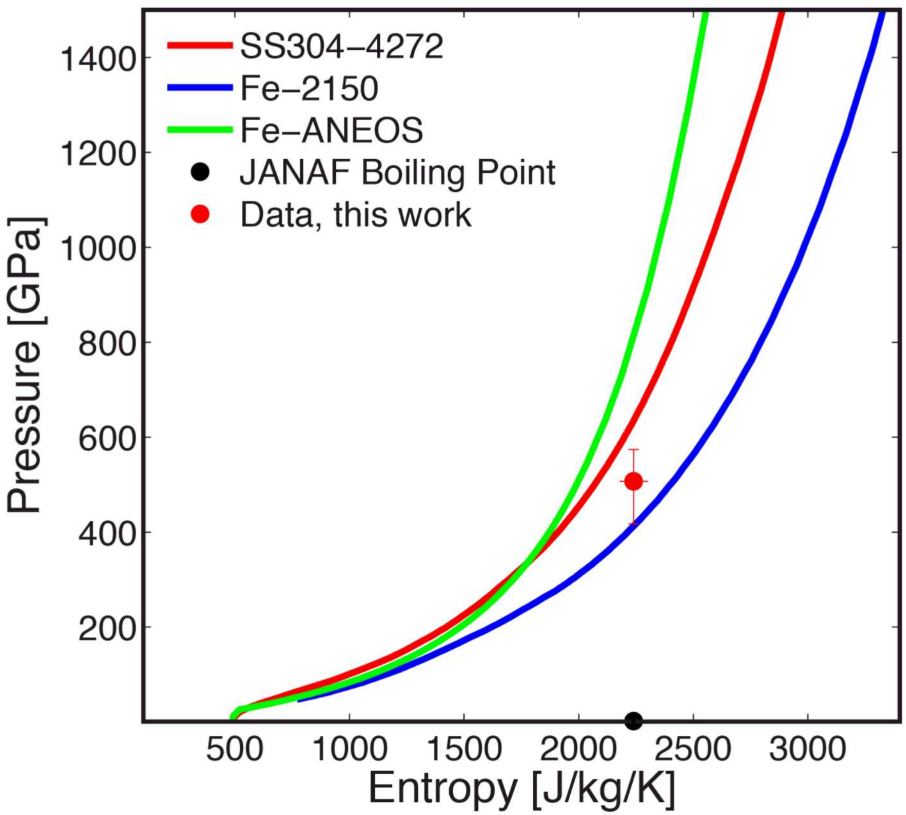
Iron Post-Shock Density Data Constrains Entropy on the Hugoniot





Post-shock densities tie the boiling point to the shock state
Entropy=2240(60) J/kg/K

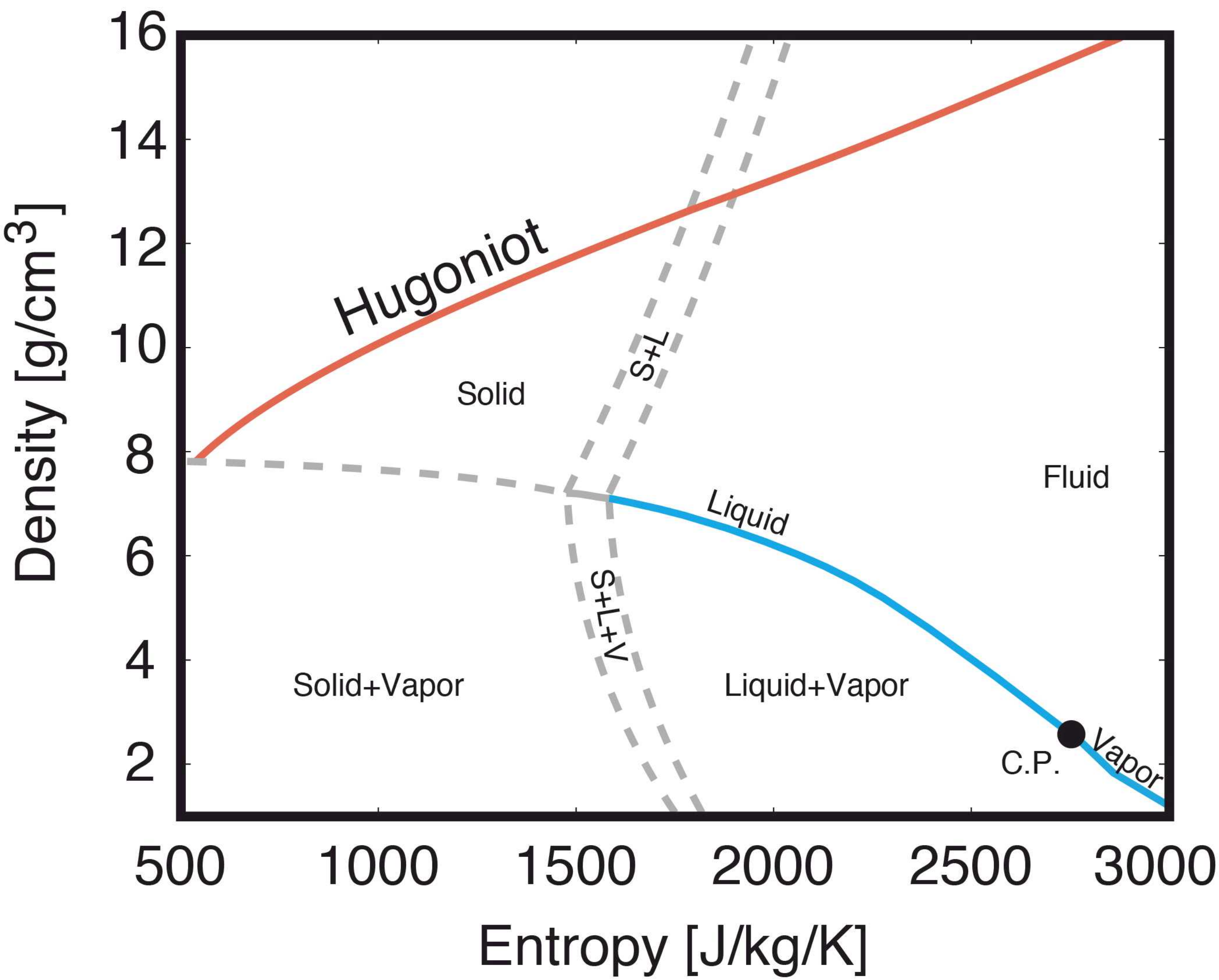
One of the first determinations of the thermal state of an opaque material on the Hugoniot



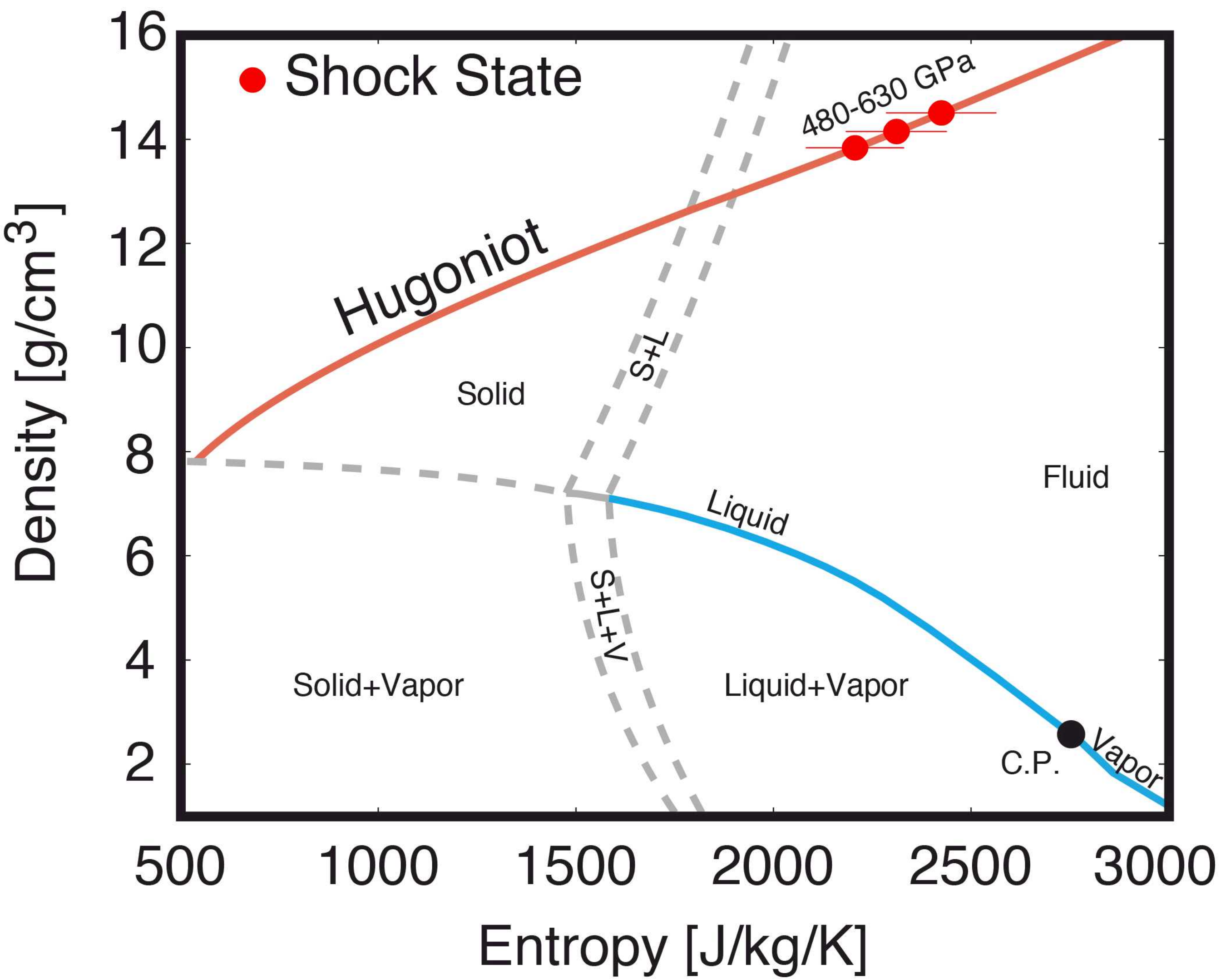
- *Vaporization is significantly easier than ANEOS suggests- the most broadly used model*
- A project within the Z Fundamental Science Program
  - Stein Jacobsen, Harvard
  - Sarah Stewart at UC Davis
  - Rick Kraus, LLNL

Impact vaporization of planetesimal cores in the late stages of planet formation, R.G. Kraus, S. Root, R.W. Lemke, S.T. Stewart, S.B. Jacobsen, and T.R. Mattsson, Nature Geoscience 2015 DOI: 10.1038/NGEO2369

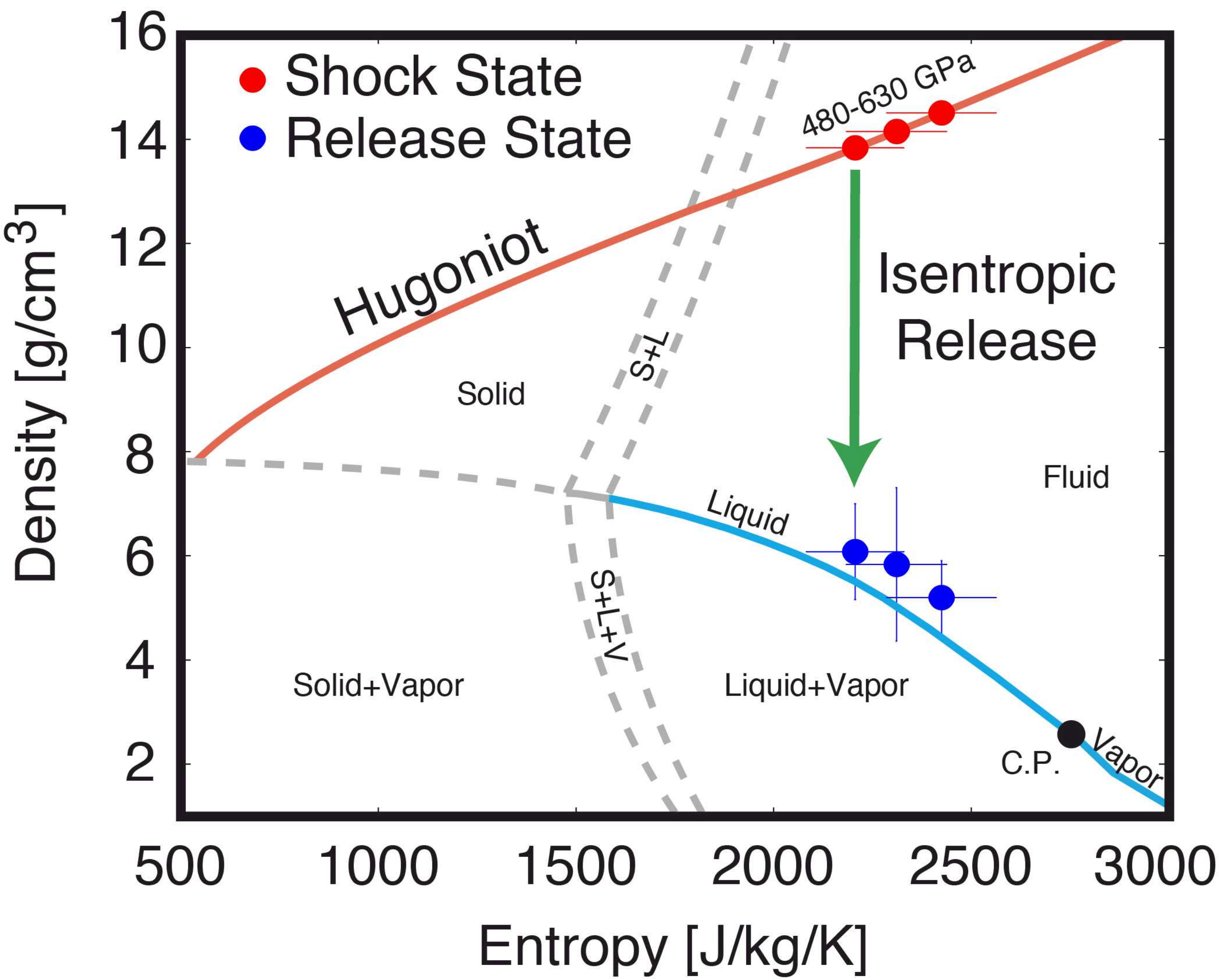
Iron Shock and Release Data



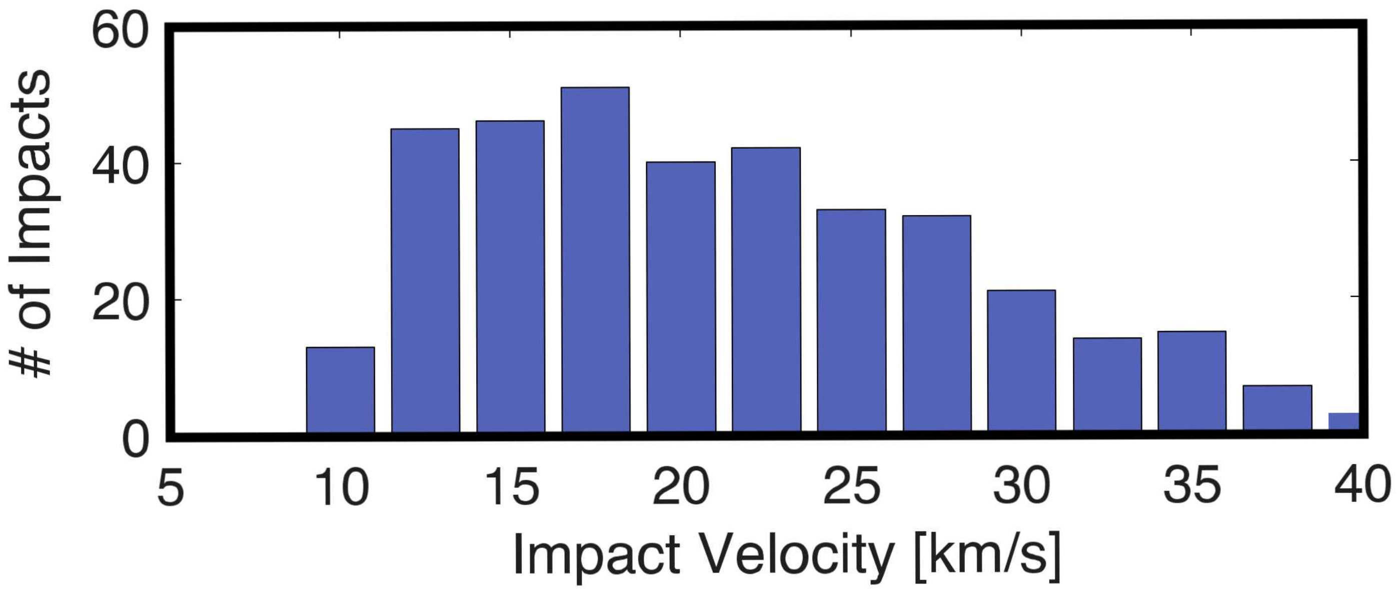
Iron Shock and Release Data



Iron Shock and Release Data



Planetesimals Will Vaporize at the End Stages of Accretion!



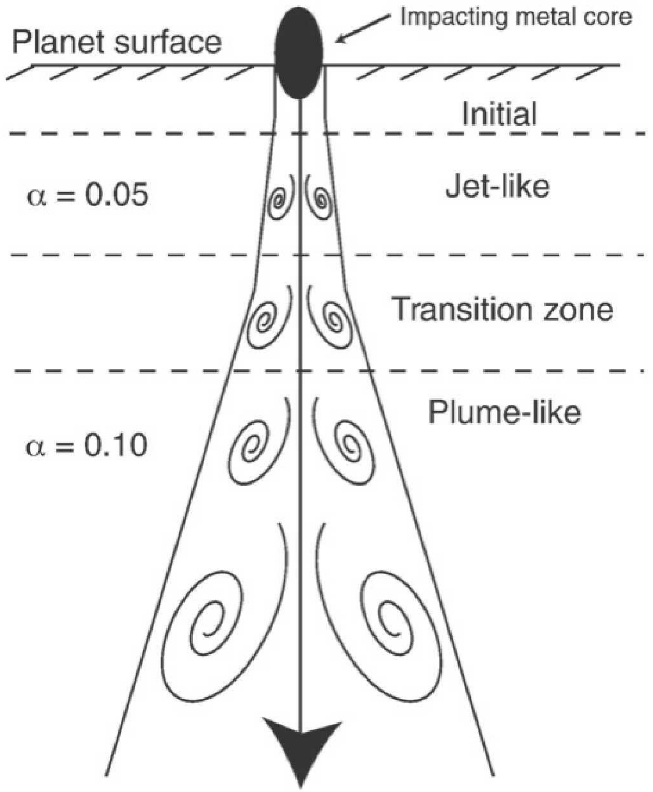
>7 km/s → Silica vaporize (Kraus et al. 2012)

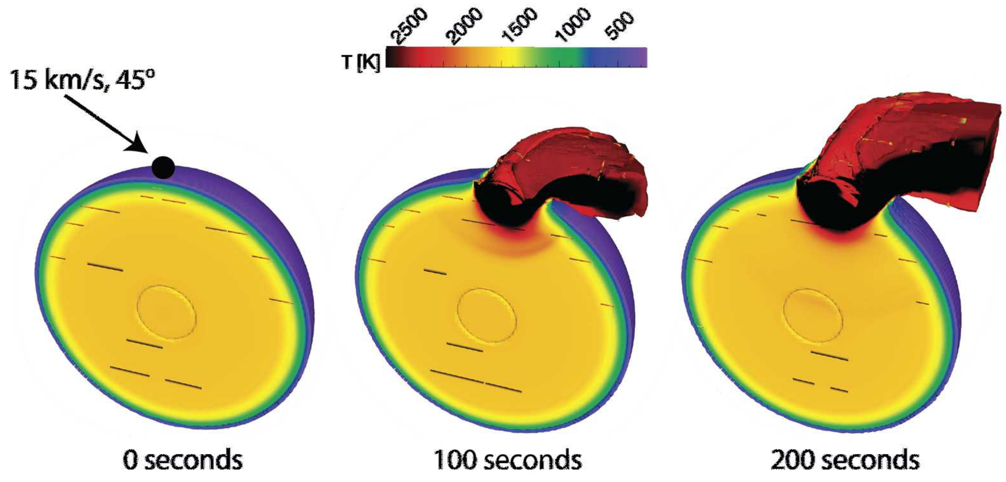
>13 km/s → Iron cores vaporize

N-body simulations from Raymond et al. 2009

New Physical Picture: Bulk Shock Vaporization

Iron Diapirs vs. Shock Vaporization

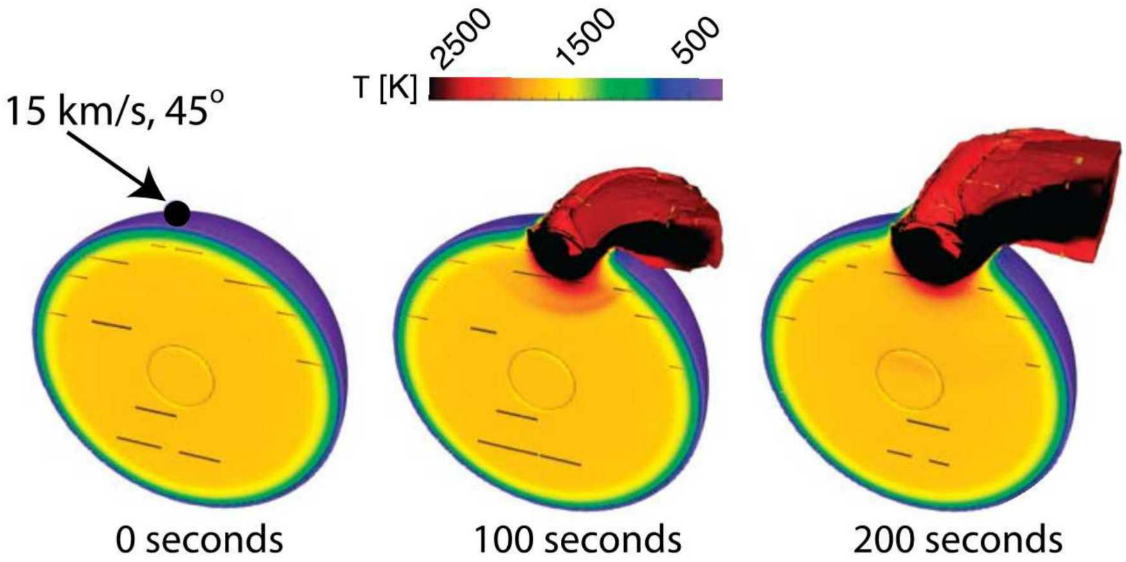




What happens to the vapor?

The Timing of Core Formation on Earth

Sandia National Laboratories



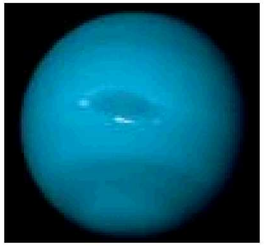
Planetesimals: Post-Impact

- Physical size: Think iron spherules
- Distribution: Global (e.g. spherule layers on Earth)
- Chemical Equilibration: Significant and Rapid!

Earth's Core Forms Early!

An invitation: What could you do with a few dynamic material experiments with us?

- Z experiments reach very high pressures
- There is flexibility to reach regions of phase space of interest
- Collaborations with academic groups have resulted in exciting discoveries
- There are opportunities for collaborations to generate data to address geophysical questions
- The Z Fundamental Science Program provides access to Z and Sandia experimentalists
- THOR will soon be a an option with lower pressures but higher availability
- We are interested in hosting students and in post-docs

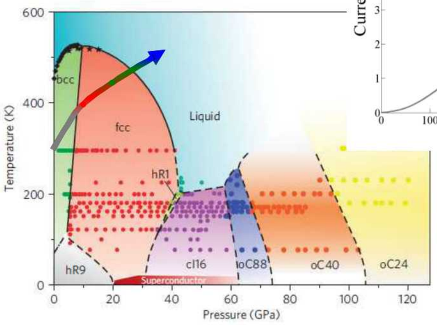


We turn planetary science *quantitative* by high fidelity modeling and high-precision experiments

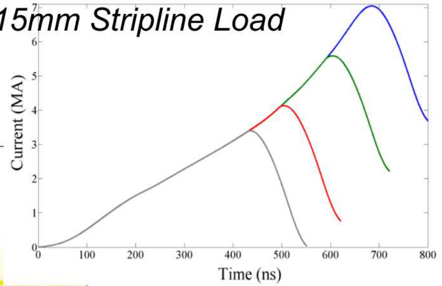
A high throughput megabar-class accelerator is under construction

- Improved repetition rate allows systematic study of rate dependent phenomena
  - Phase transitions
  - Kinetics of melt and re-freeze under ramp compression
  - Strength, including phase transitions
- We have developed experimental designs for phase-transition and strength experiments
- Systematic studies of materials, grain size and texture for phase-kinetics and strength
- Targeting late 2017 completion
  - Interesting possibility for DCS

Peak Ramp Compression States in Li

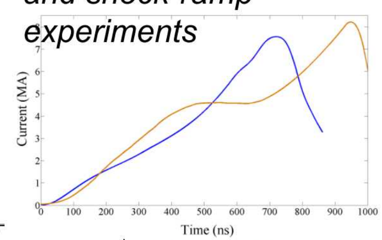


Design Currents for a 15mm Stripline Load

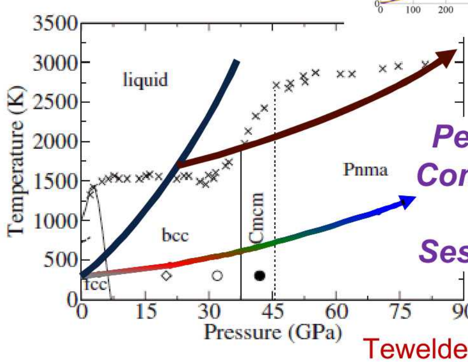


Guillaume, et al. , Nature Physics, 2011

Design Currents for ramp and shock-ramp experiments



Phase space accessible in Ca

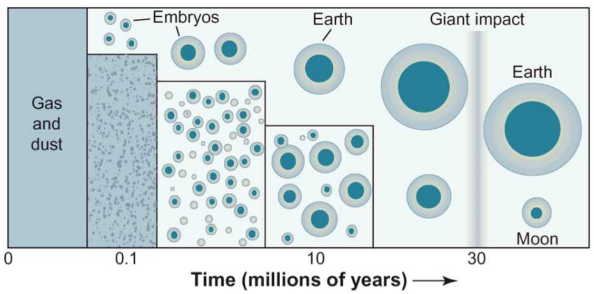


Shock-Ramp Example

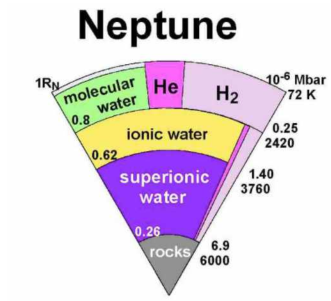
Peak Ramp Compression States Sesame 2030 EOS

Teweldeberhan and Bonev, PRB, 2008

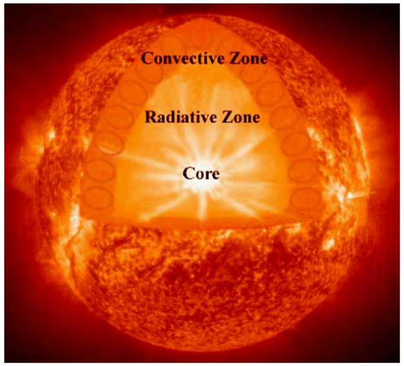
The Z Fundamental Science Program has created strategic partnerships with leading institutions



Earth and super earths
Properties of minerals and metals



Jovian Planets
Water and hydrogen



Stellar physics
Fe opacity and H spectra

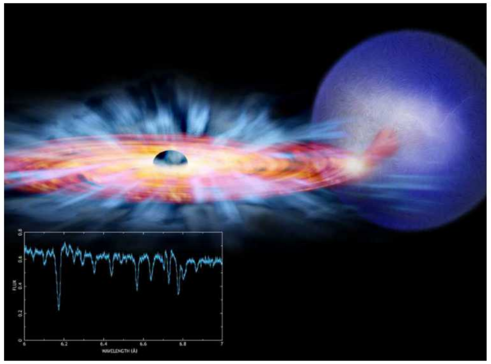


Photo-ionized plasmas
Range of ionization param. ξ

- Resources/shots on Z since 2010
  - 50+ dedicated ZFS + 50 ride-along
- Science with significant impact
  - Bailey et al, Nature (2015)
  - Kraus et al, Nature Geoscience (2015)
  - Knudson et al, SCIENCE (2015)
  - 1 PRL, 3 PoP, 1 PRA, 1 PRB, and 8 other peer-reviewed publications
- Students and postdocs
  - 4 M.Sc., 2 Ph.D.
  - 5 postdocs
- Workshops most years since 2009
- Call for proposals for CY16 and 17
  - Yingwei Fei, Chris Seagle
- Opportunities for collaboration and access to Z!
- Opportunities for ride-along experiments also exist

Backups

Acknowledgements

Sandia National Laboratories

Experiment Design/Analysis

Marcus Knudson

Ray Lemke

Kyle Cochrane

Devon Dalton

Dustin Romero

Diagnostics

Charlie Meyer

Jeff Gluth

Devon Dalton

Anthony Romero

Dave Bliss

Alan Carlson

Z operations team

QMD Calculations

Mike Desjarlais

Andreas Becker

Winfried Lorenzen

Ronald Redmer

Planetary Modeling

Nadine Nettelmann

Andreas Becker

Ronald Redmer

Z Fundamental Science Program

Call for proposals in June 2015

Workshop July 19-22, 2015 in Albuquerque, NM.

Pulse Shaping

Ray Lemke

Jean-Paul Davis

Mark Savage

Ken Struve

Keith LeChien

Brian Stoltzfus

Dave Hinshelwood

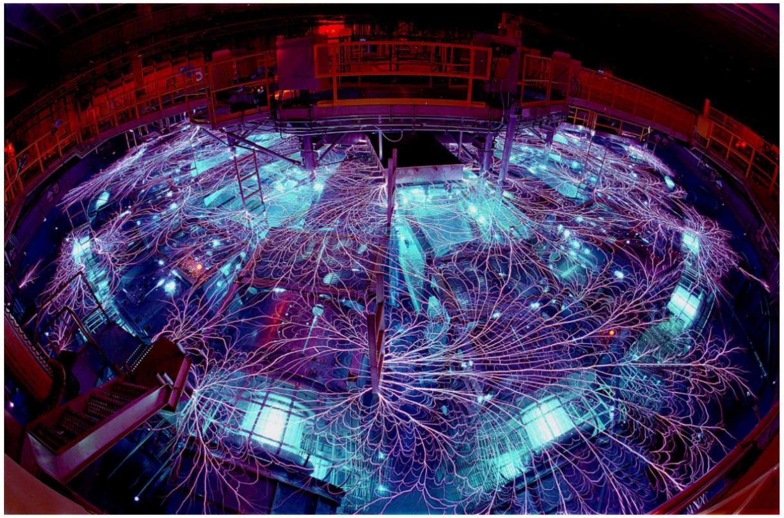
Acknowledgements

- Seth Root
- Kyle Cochrane
- Mike Desjarlais
- Dan Dolan
- Marcus Knudson
- Thomas Mattsson
- Z operations and target fabrication teams

Acknowledgements

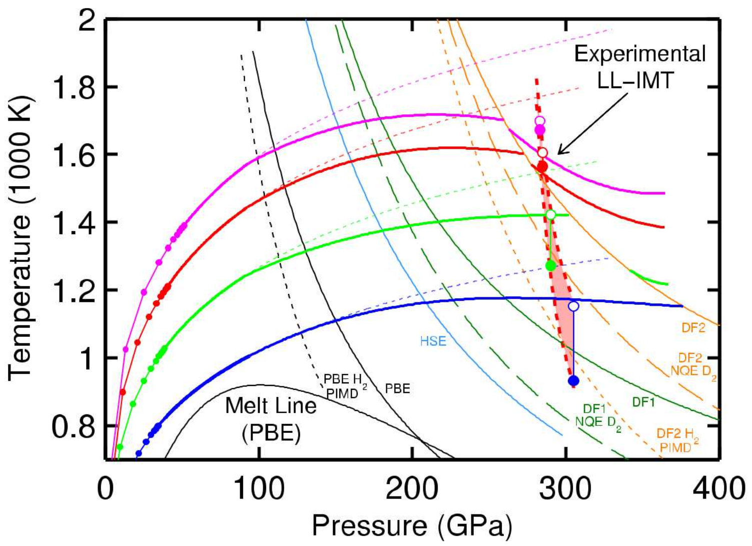
Research Team: Seth Root, Ray Lemke, Sarah Stewart, Stein Jacobsen, and Thomas Mattsson

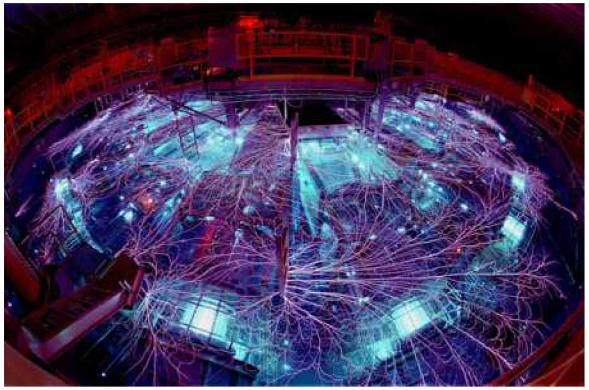
Financial Support: Sandia Z fundamental science program, NNSA HEDP program, NNSA SSGF program, LLNL Lawrence Fellowship



We have determined the location of the density-driven LL-IMT phase transition in hydrogen

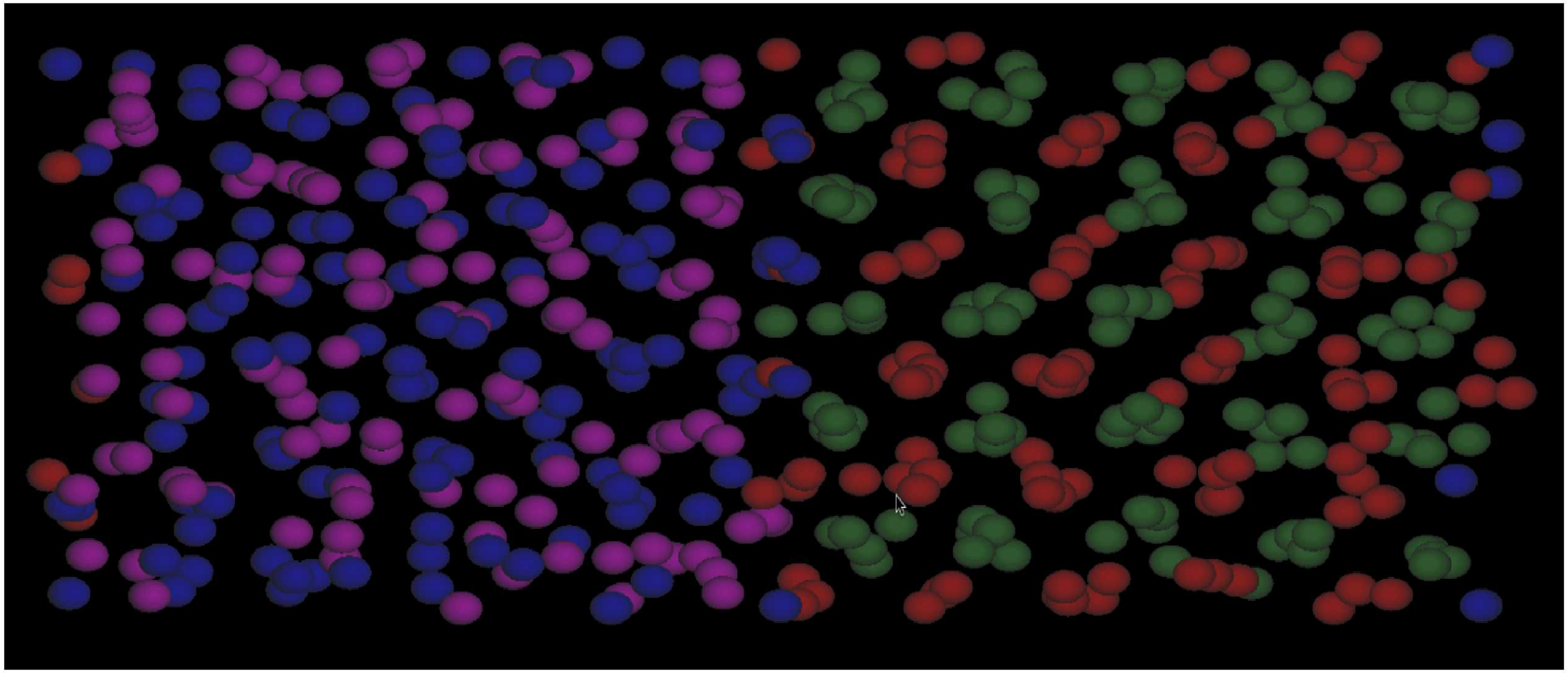
- Shock-ramp technique enables experimental access to the liquid-liquid, insulator-metal transition (LL-IMT) for hydrogen
  - The temperature is set by the initial shock
- Experiments above ~250 GPa show clear evidence of metallization of deuterium
  - Very abrupt increase in reflectivity to ~40-50%
  - Pressure is well above numerous first principles predictions
  - Implications for understanding Jupiter, Saturn, and thousands of exoplanets
- Insensitivity to T suggests this is a ρ-driven transition
  - ρ at the transition is inferred to be ~2-2.1 g/cc in deuterium
  - Qualitatively different transition than in shock experiments (T driven)





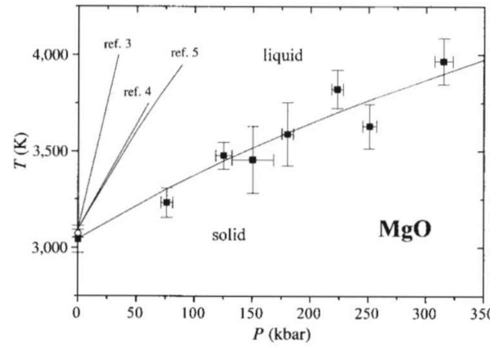
Directly calculate Solid-Melt Boundaries

- For melting boundary use two phase coexistence simulations
- Place solid and liquid in contact with each other
- Run at different temperatures and watch phase boundary
- Relative heat capacities and enthalpy of melting determine range of coexistence

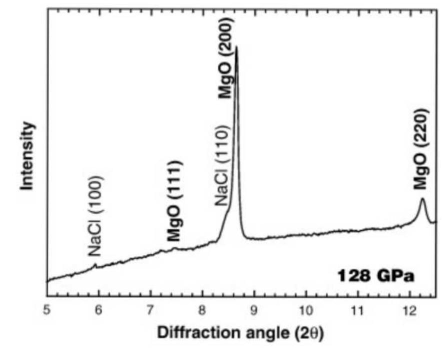


State of experiments prior to 2012

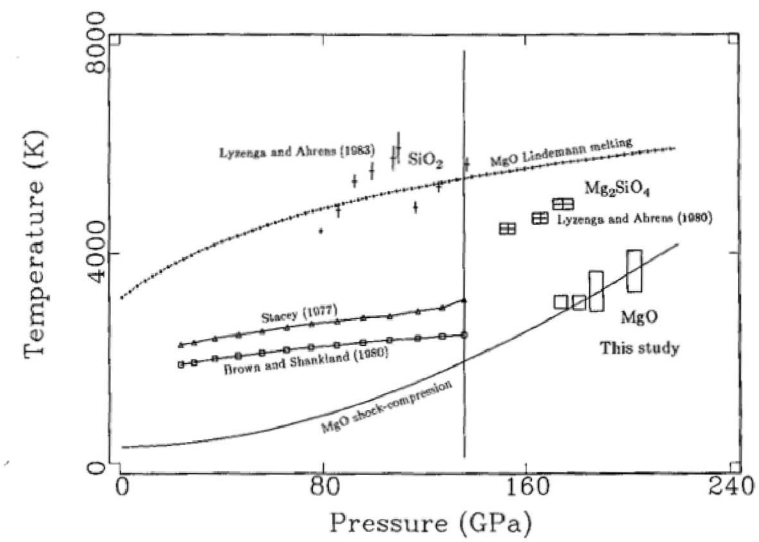
- Diamond anvil cell measurements of melt
- Diamond anvil cell XRD, Brillouin spectroscopy etc.
- Gas gun driven Hugoniot measurements of $u_s(u_p)$ and temperature
- Possibility of shock melting was unclear



Zerr and Boehler, Nature **371**, 506 (1994)



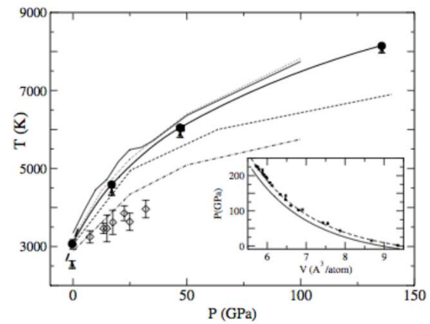
Murakami et al., EPL **277**, 123 (2009)



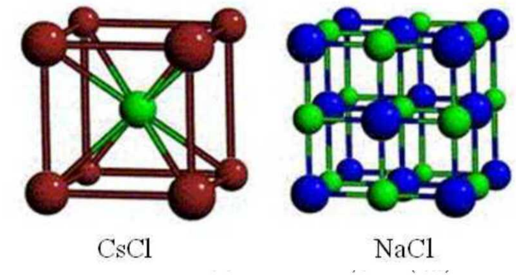
Svendsen and Ahrens, Geophys. J. R. astr. Soc. **91**, 667 (1987)

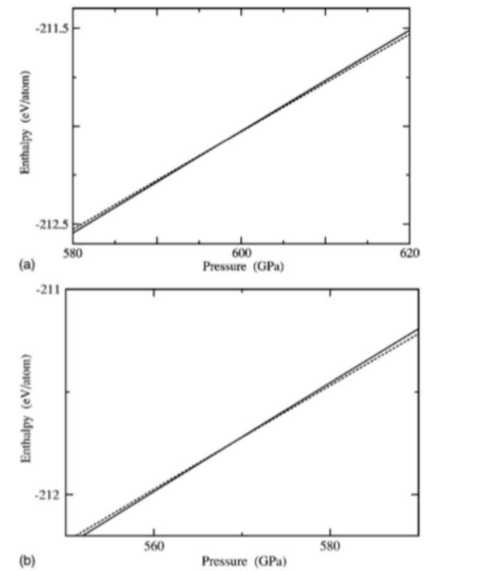
State of theory prior to 2012

- DFT and QMC predicted solid-solid phase transition at ~ 570-600 GPa
- Melt curve as a function of pressure from DFT-MD
- Wide range phase diagram utilizing ab initio calculations

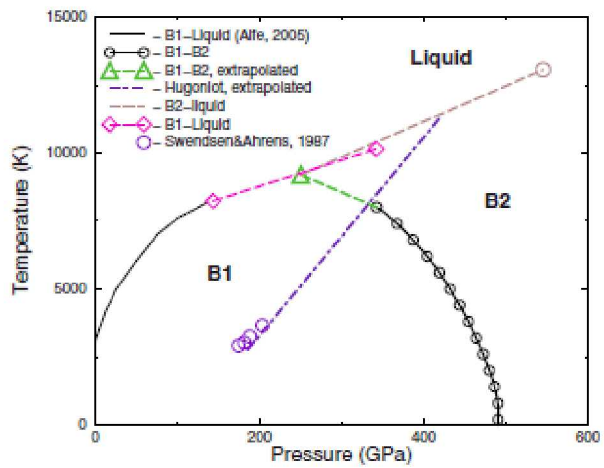


Alfe, PRL **94**, 235701 (2005)





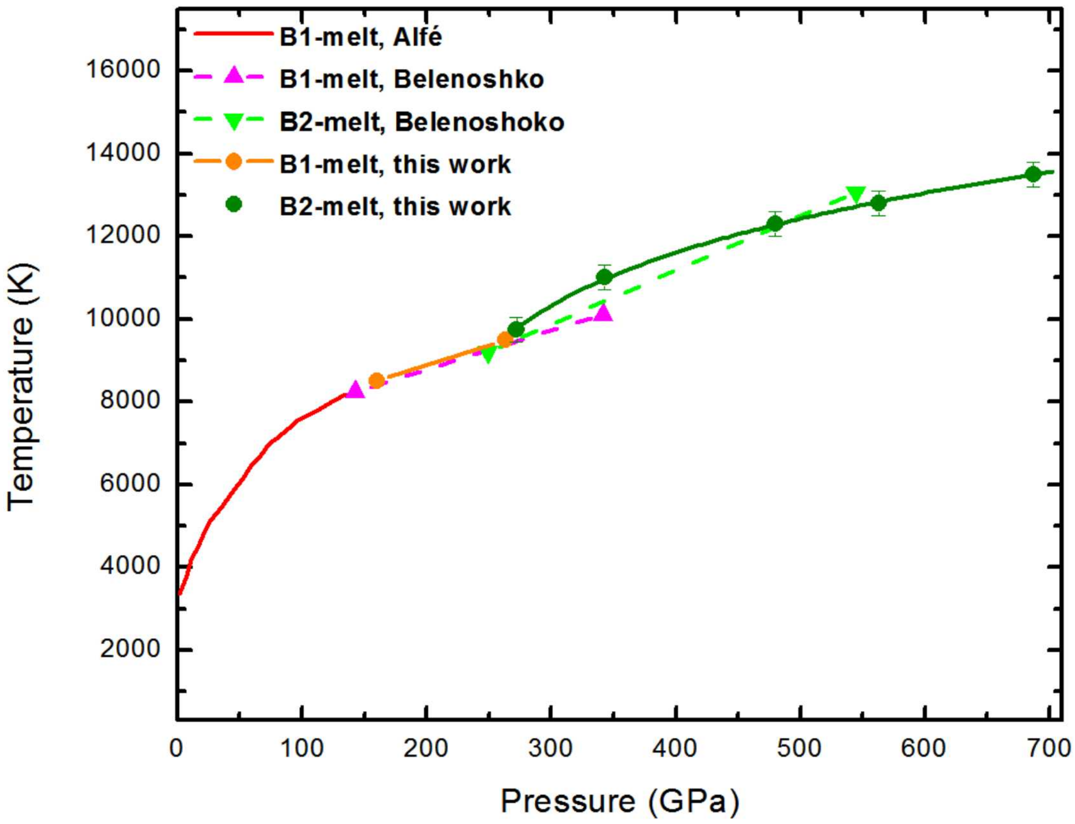
Alfe et al., PRB **72**, 014114 (2005)



Belonoshko *et al.*, PRB **81**, 054110 (2010)

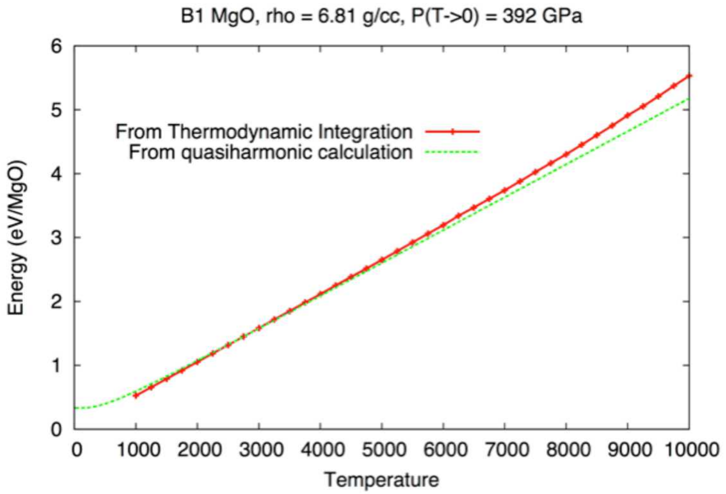
Directly calculate Solid-Melt Boundaries

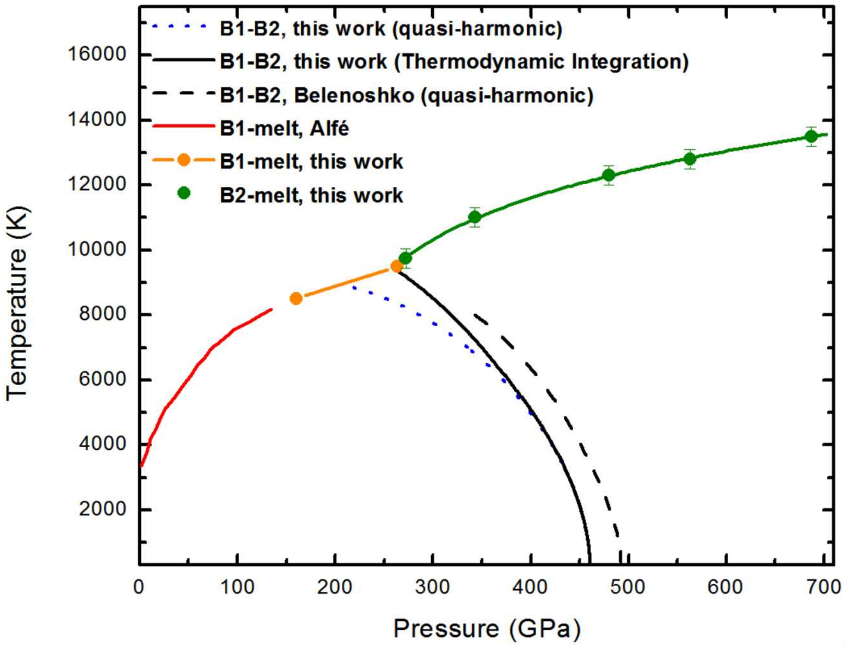
- For melting boundary use two phase coexistence simulations
- Place solid and liquid in contact with each other
- Run at different temperatures and watch phase boundary
- Relative heat capacities and enthalpy of melting determine range of phase coexistence
- Follow work of Belonoshko, but include quantum calculations of B2 phase melting



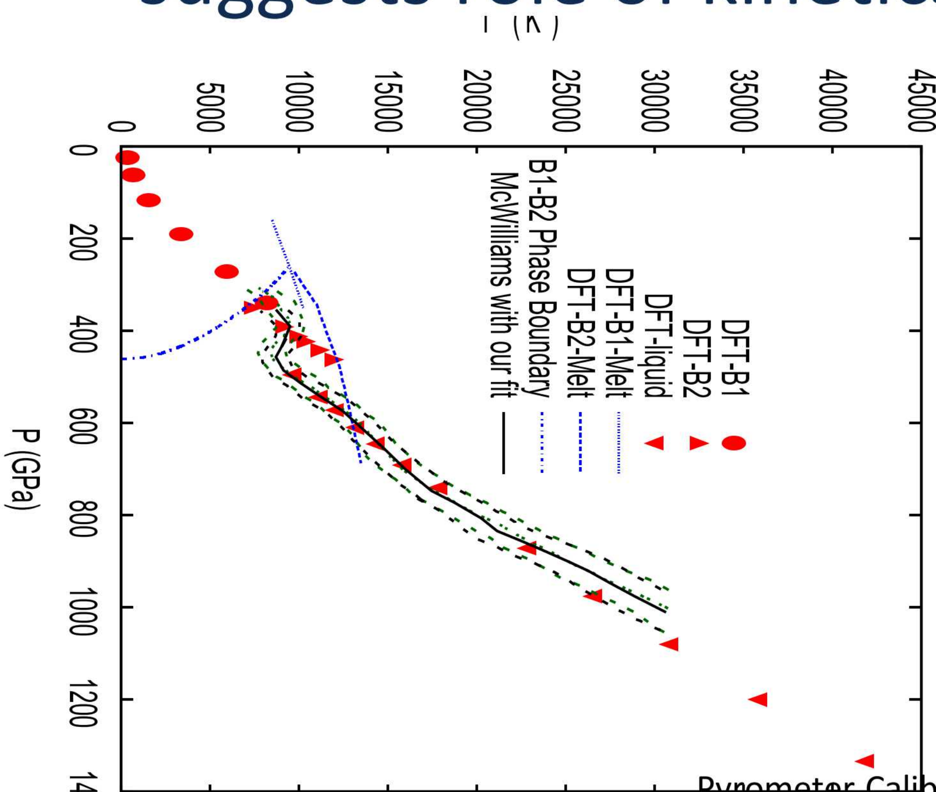
Calculation of solid-solid phase boundary

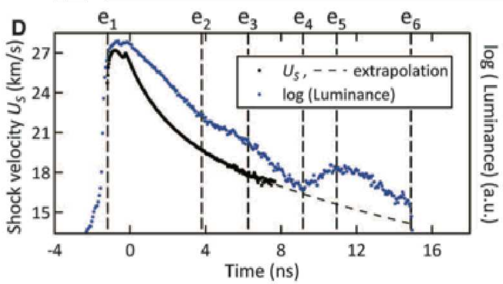
- At low temperatures, harmonic phonon approximation provides free energies
- Entropy can be calculated directly using analogy to finite temperature quantum harmonic oscillator
- Approximation breaks down for moderate temperatures
  - Effect is strongest in B1 phase
- Switch to thermodynamic integration using multiple DFT-MD calculations along each isochore
- Resulting phase boundary finds triple point between B1, B2 and liquid



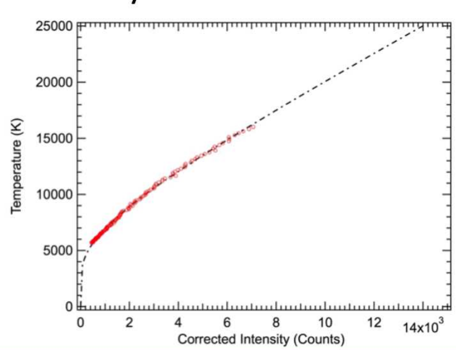


Comparison to McWilliams results suggests role of kinetics





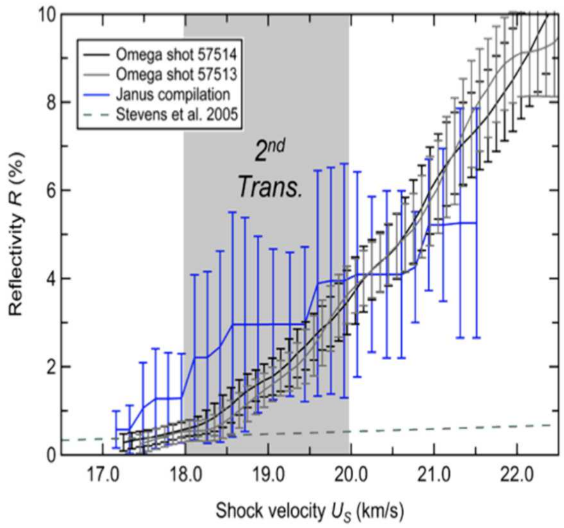
Pyrometer Calibration



- Excellent agreement at higher pressures in liquid phase
- Slight discrepancy with temperature at high pressure explained by calibration
- Disagreement occurring at B2 – Melt boundary
  - Decreased luminance due to scattering in two phase region?
  - Extrapolation of $u_s(t)$ for nonreflective shocks?
  - Metastable liquid observed in decaying shock front?

Reflectivity change provides additional evidence of melt boundary

- McWilliams and Root both measure reflectivity at 532nm as a consequence of their use of VISAR interferometry
- In each case, the reflectivity disappears for shock speeds less than ~18 km/s
- Explanation due to metal to insulator transition going from liquid to B2 phase



McWilliams et al. Science. **338**, 1330 (2012)

Confirm melting hypothesis by calculating reflectivity using QMD

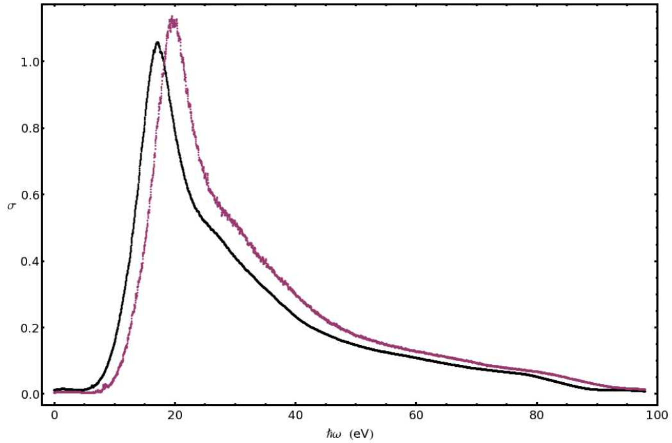
- Use Kubo-Greenwood formulation on snapshots from the B2 solid and liquid near the melt boundary

- Kramers-Kronig relation allows calculation of complex dielectric function

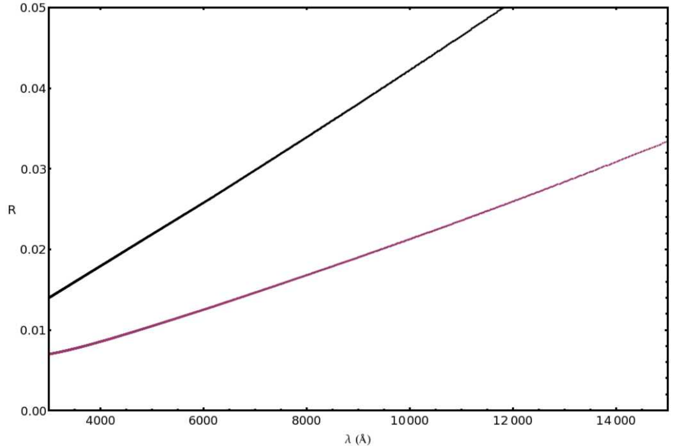
$$\sigma_2(\omega) = -\frac{2}{\pi} P \int \frac{\sigma_1(\nu)\omega}{(\nu^2 - \omega^2)} d\nu$$

- Use of HSE functional provides a better description of the gap and the reflectivities agree with experiment

Optical conductivity of solid



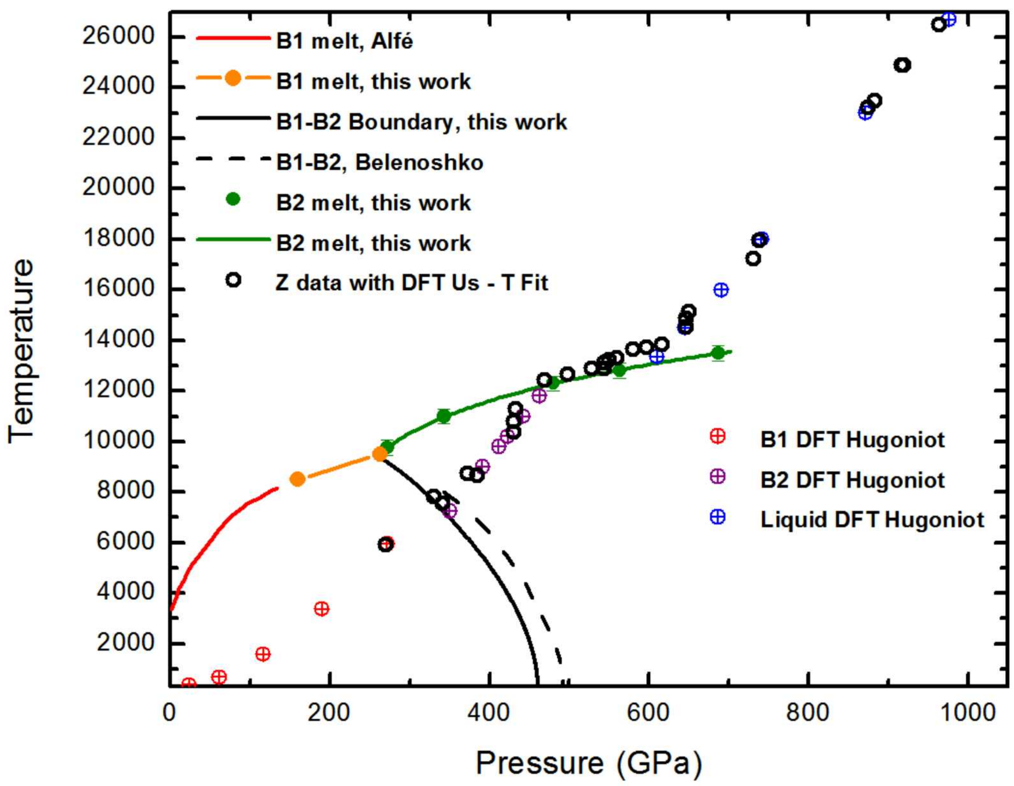
Reflectivity of liquid



Solid reflectivity at 532 nm: 0.02%
Liquid reflectivity at 532 nm: 1.1%

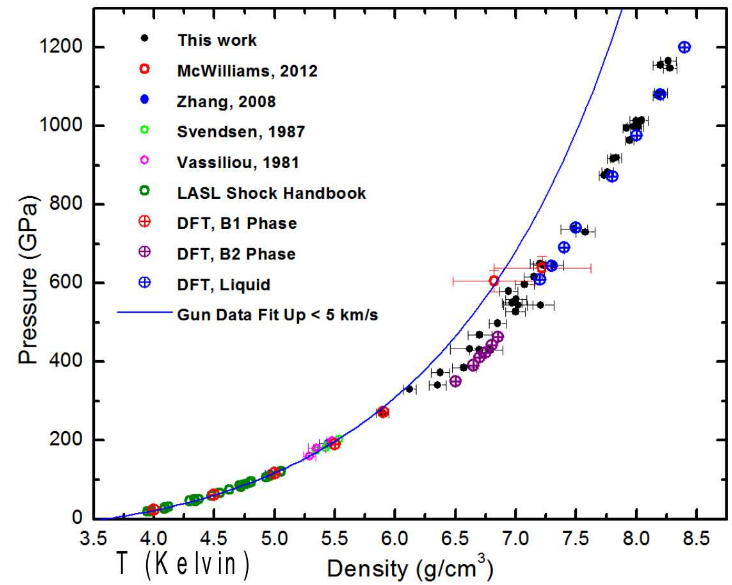
New experimental techniques combined with theoretical tools allow quantitative exploration of an unprecedented region of phase space for geomaterials

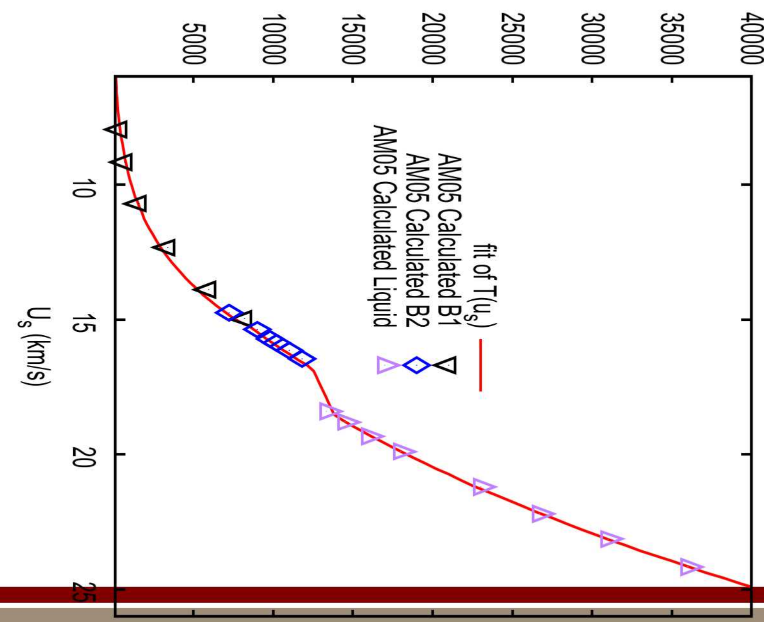
- Accurately measured the MgO Hugoniot from 330 GPa to 1160 GPa
  - Data starts at pressures and temperatures that had never been probed prior to 2012
- MgO has a large coexistence region along the Hugoniot between B2 and liquid
  - Significant to planetary and moon formation
  - Shock pressures of ~7 Mbar or greater needed to completely melt cold MgO
- Vastly expanding the domain of quantitative understanding for geomaterials



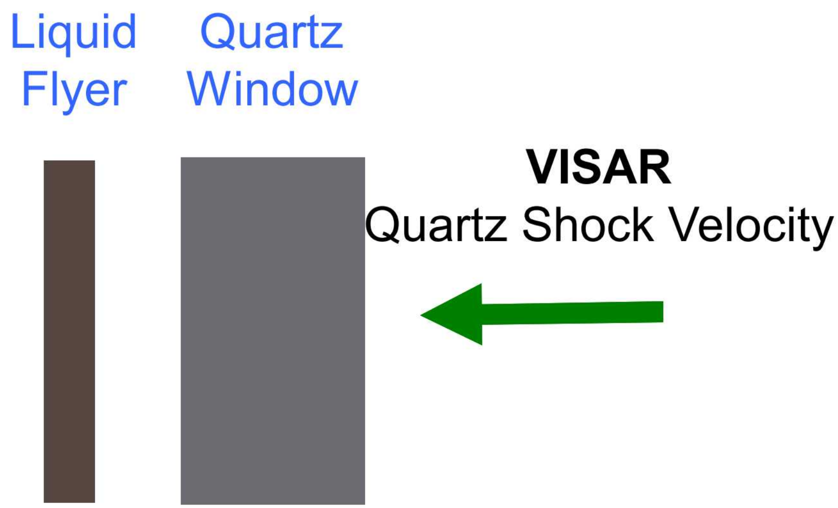
Use QMD to assign temperatures to the Sandia experiment

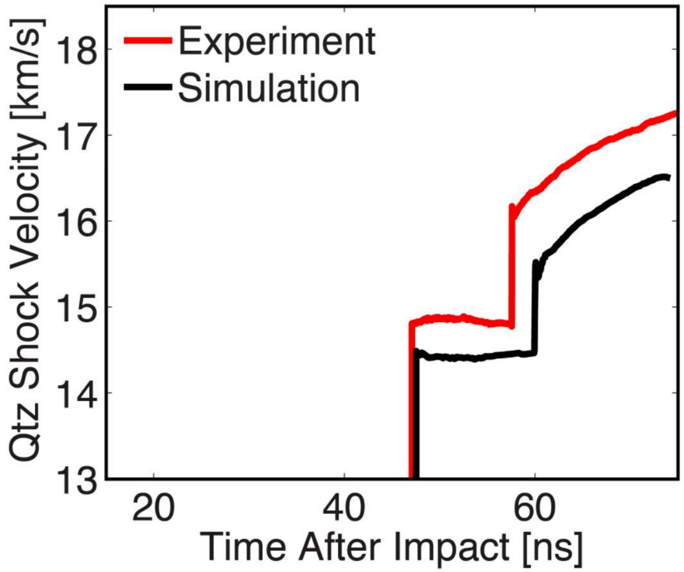
- No pyrometry is available for the Root et al data set
- Close agreement with QMD allows for possibility of using theoretical temperatures
- Construct $T(u_s)$ along the Hugoniot from QMD





Reverse Impact Experiment to Measure Flyer Density





Impedance Matching to Obtain Density