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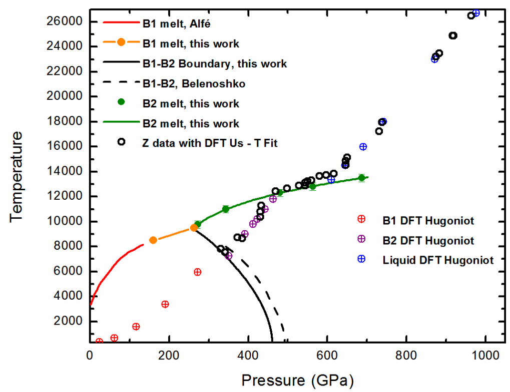

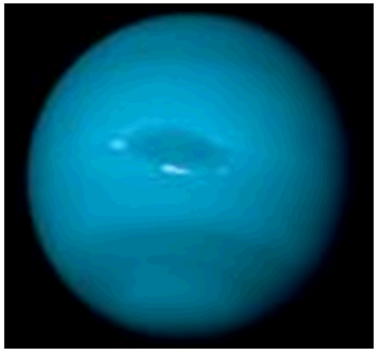

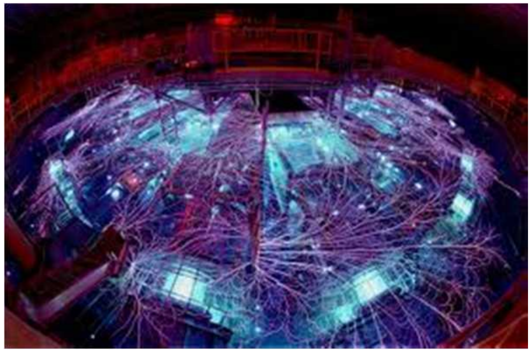

High Energy Density Physics at Sandia: Material Science at Mbar Regimes

Dawn G. Flicker, Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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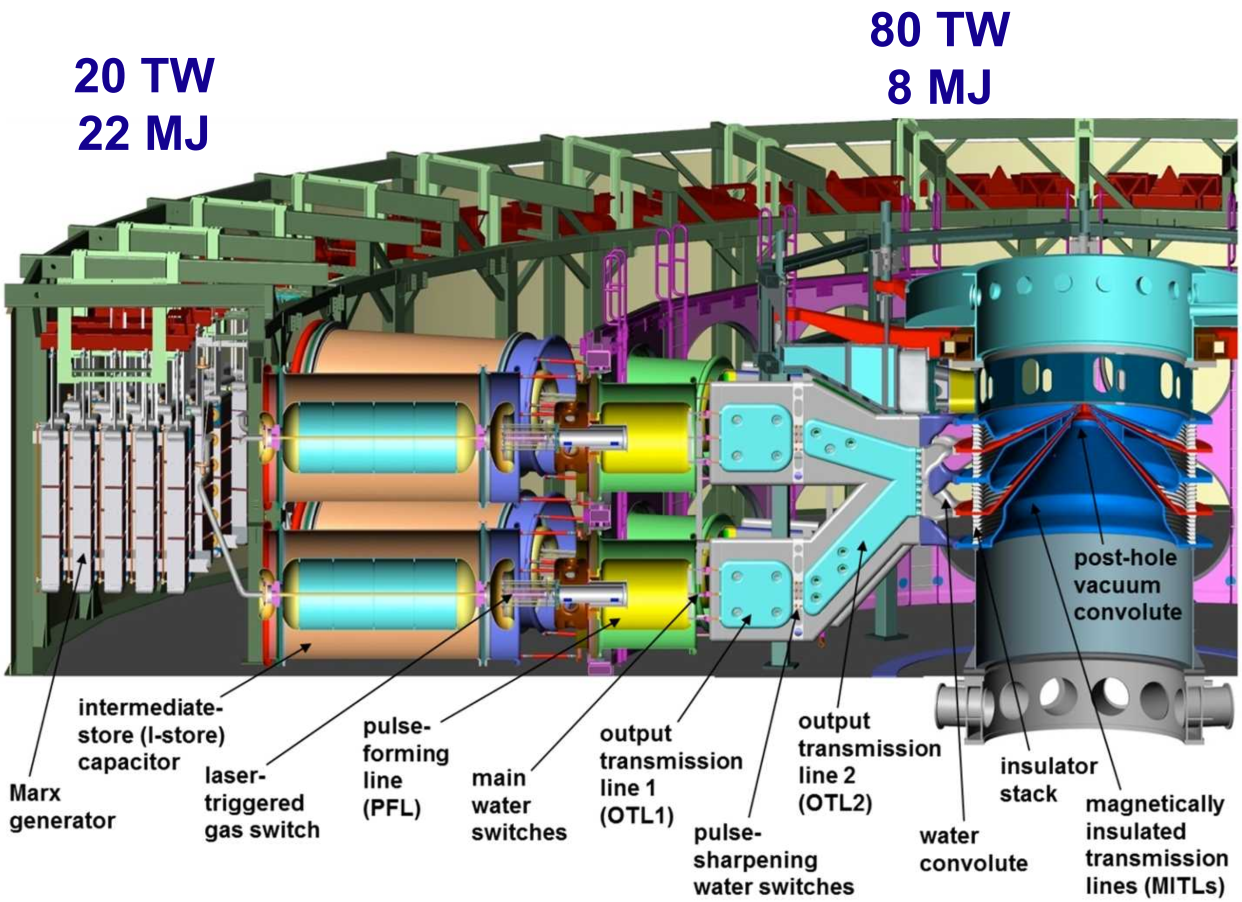
Outline:

- The Z facility and major programs
- Pulsed Power to probe material dynamics in extreme conditions
  - Diagnostics and techniques
  - Flyer experiments (Shock Hugoniot)
    - Gases
    - Compaction
    - Iron Vaporization
    - MgO
  - Ramp experiments: Quasi-Isentropic Compression Experiments (ICE)
    - Metals
    - Synthesis of nano-wires
  - Shock-Ramp experiments
    - Cu
    - D2 metalization
  - Strength Experiments
- The Z fundamental Science program and opportunities for collaboration

Lots of examples (teasers)!

Z compresses electrical energy in both space and time . . .

Charge for 3 minutes to reach 85 kV

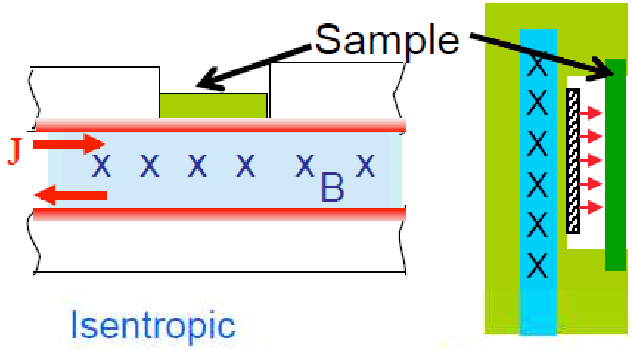


330 TWs & 2.5 MJ of x-ray output in a few ns

. . . and literally shakes the earth almost every day!

We use magnetic fields on Z in several ways to create High Energy Density matter for various physics applications

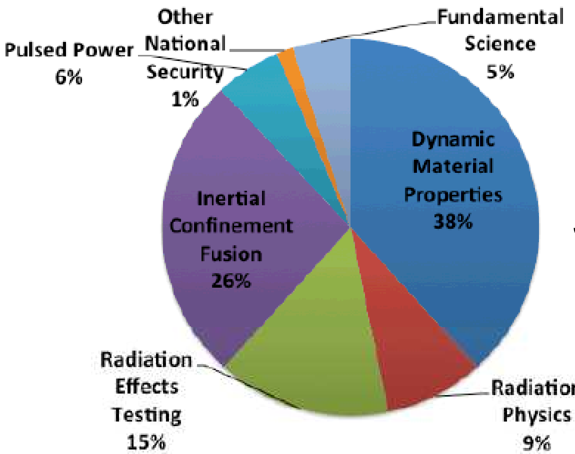
Dynamic Material Properties



Isentropic Compression

Flyer Plate

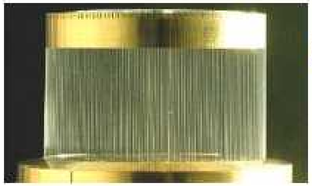
CY13 Z shot distribution

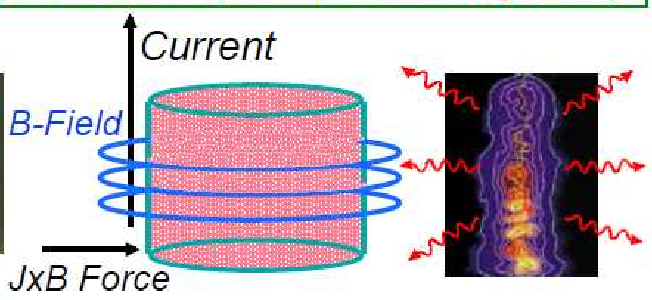


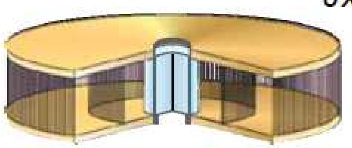
140-170 Shots/yr

Z-Pinch X-ray Sources (RES, Rad. Physics)

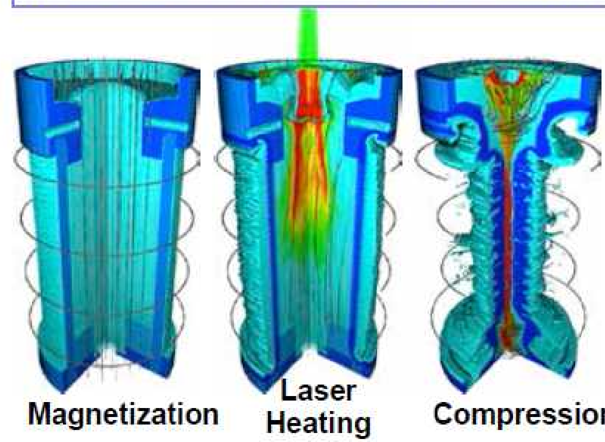
wire array







Inertial Confinement Fusion



Z Astrophysical Plasma Properties (ZAPP) collaboration uses the same x-ray source to simultaneously address 4 separate astrophysics topics

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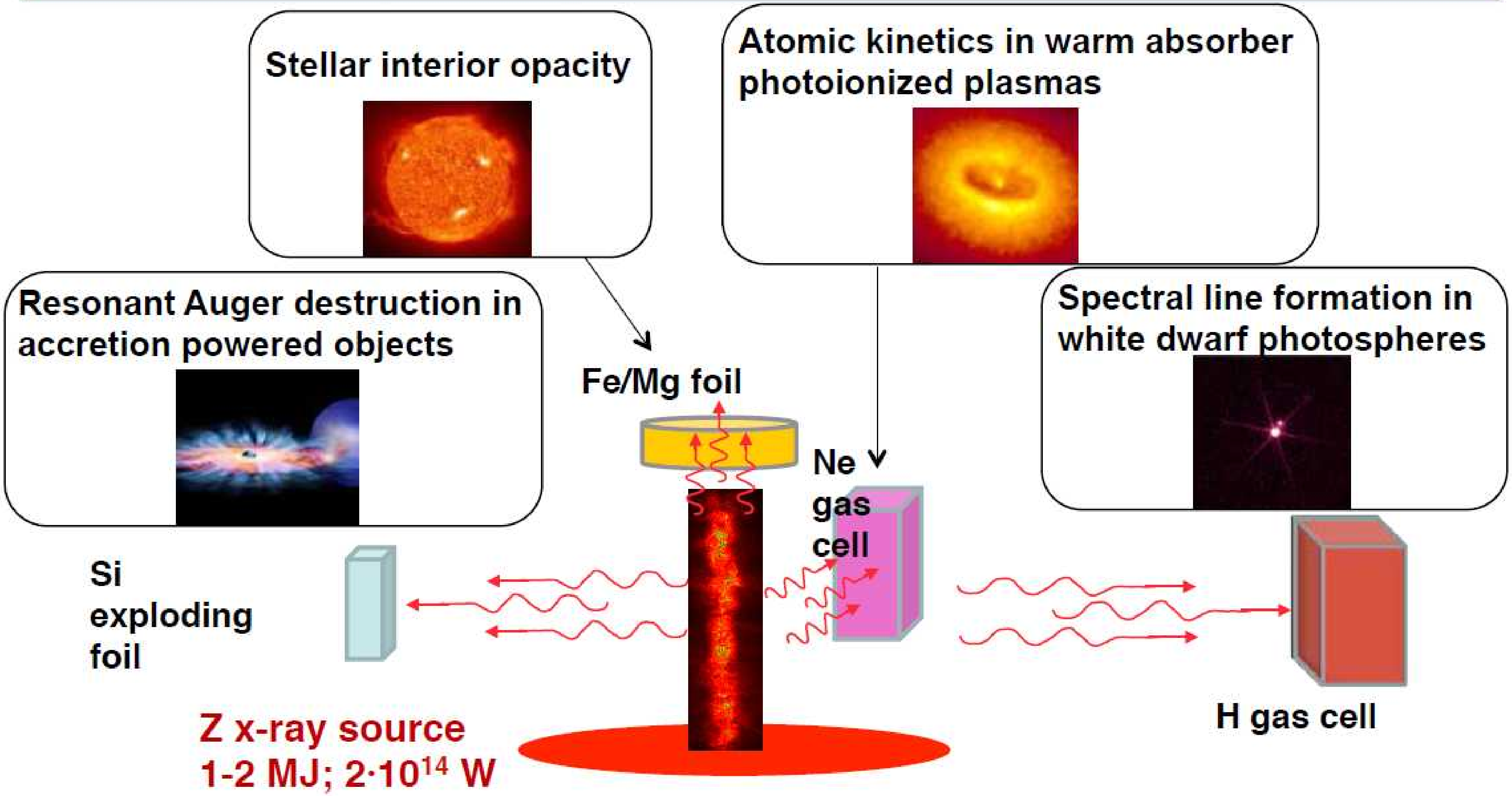

- Multiple samples are exposed to Z x-rays on each shot
- Highly efficient use of the facility

The Magnetized Liner Inertial Fusion (MagLIF) target design for Z leverages expertise from traditional ICF

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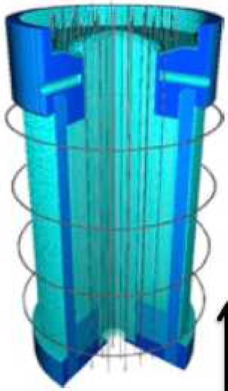
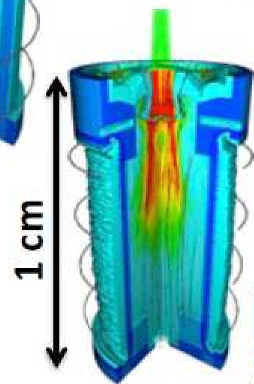


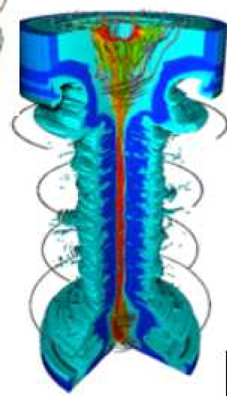
Axial Magnetic Field (10 T initially; 30 T available)

- Inhibits thermal losses from fuel to liner
- May help stabilize liner during compression
- Fusion products magnetized



Laser heated fuel (2 kJ initially; 6-10 kJ planned)

- Initial average fuel temperature 150-200 eV
- Reduces compression requirements (R_0/R_f ~ 25)
- Coupling of laser to plasma in an important science issue



Magnetic compression of fuel (~100 kJ into fuel)

- ~70-100 km/s, quasi-adiabatic fuel compression
- Low Aspect liners ($R/\Delta R$~6) are robust to hydrodynamic (MRT) instabilities
- Significantly lower pressure/density than ICF

Goal is to demonstrate scaling: $Y\ (B_{z0}, E_{laser}, I)$
DD equivalent of 100 kJ DT yield possible on Z

S.A. Slutz *et al.*, Phys Plasmas (2010); S.A. Slutz & R.A. Vesey, Phys Rev Lett (2012); A.B. Sefkow *et al.*, Phys Plasmas (2014).

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

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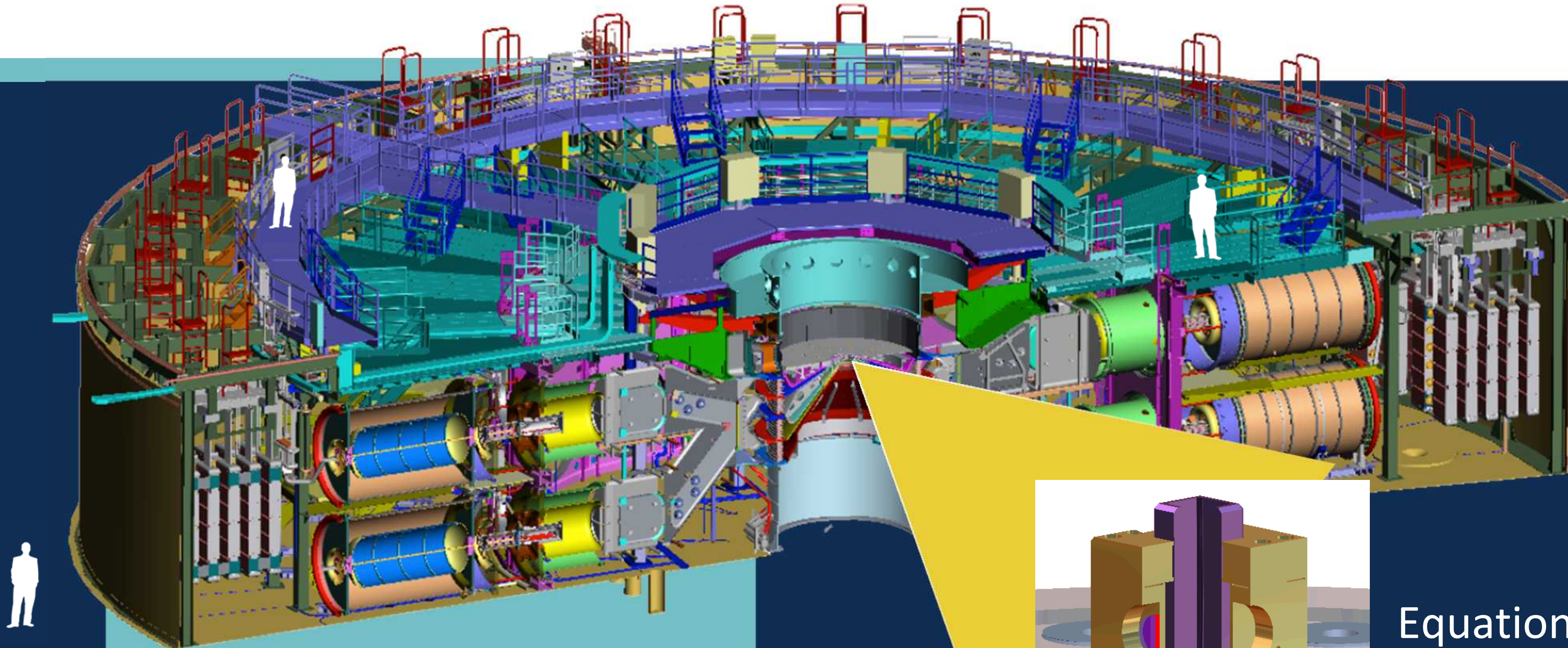
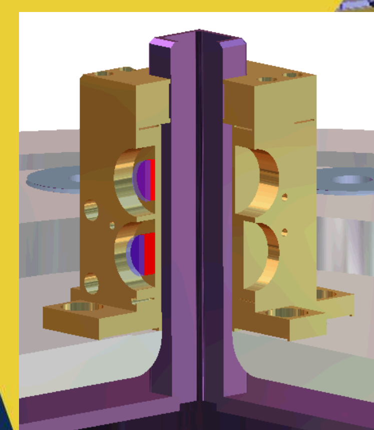


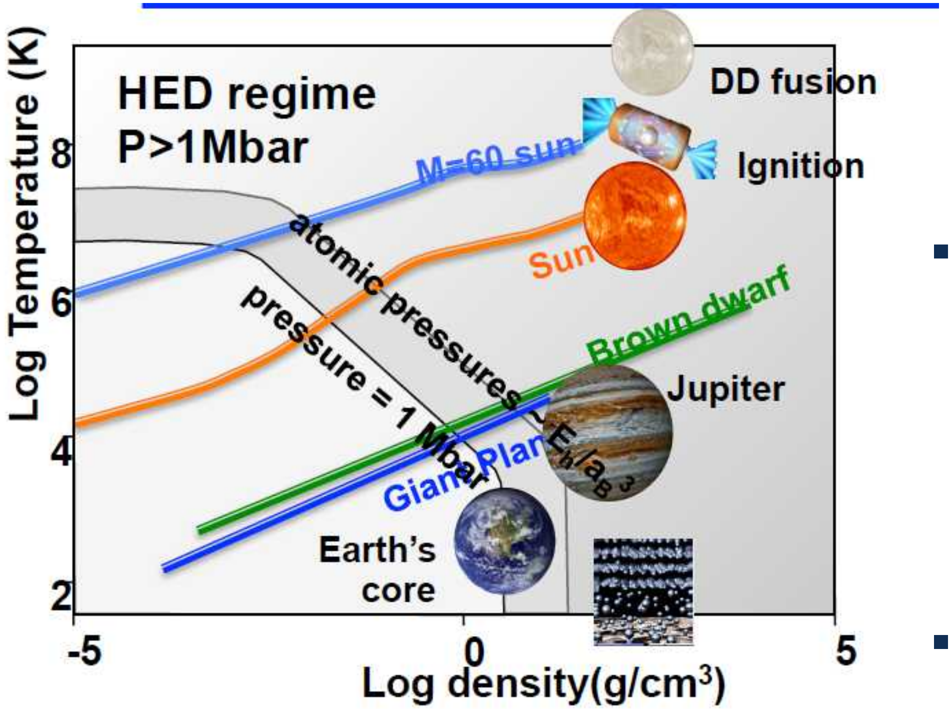
- Pulsed Power Technology
- Magnetically Driven Implosions
- Inertial Confinement Fusion
- Dynamic Materials



Equation of State

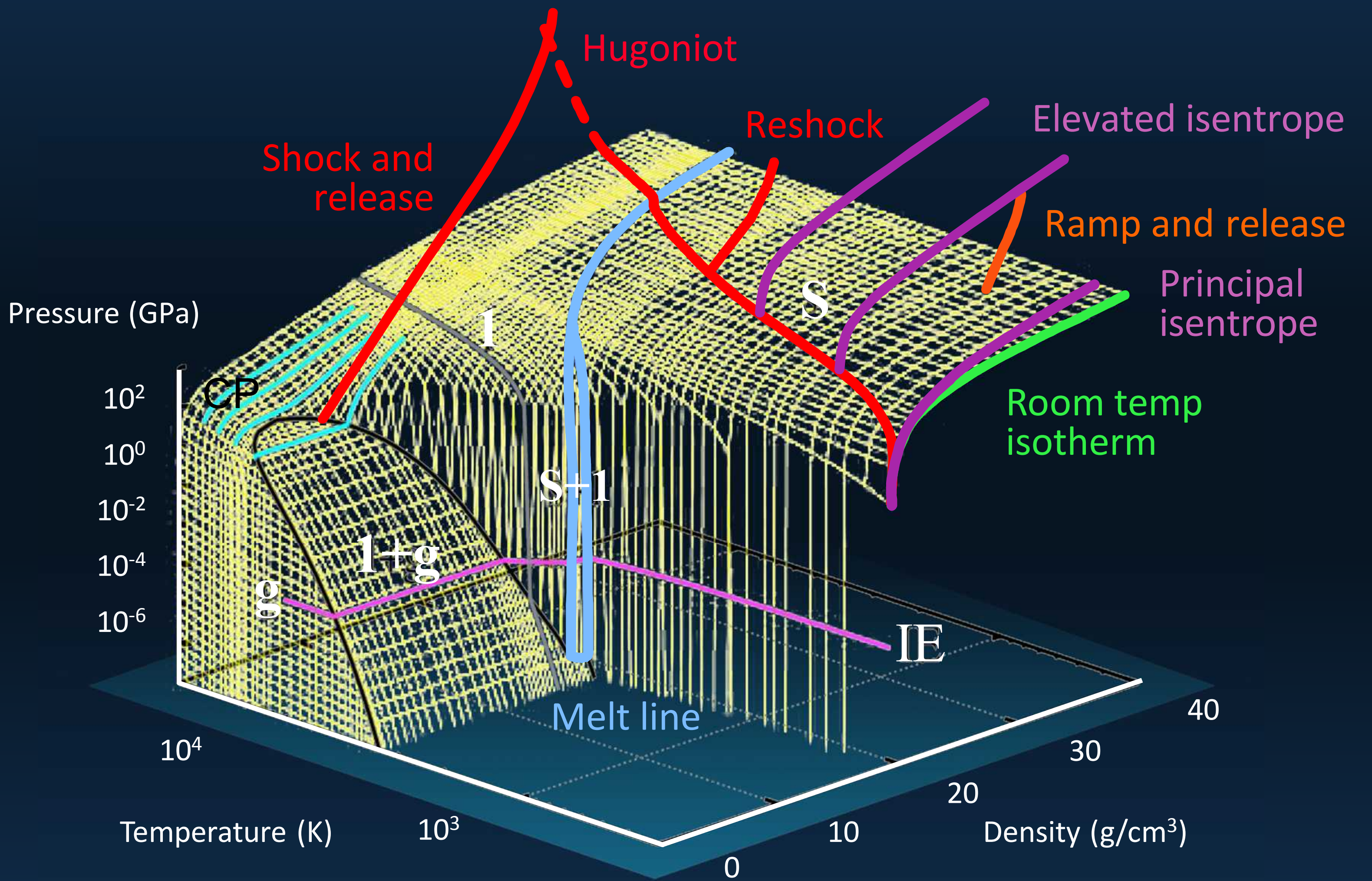
I ~ 26 MA, τ ~100-1000 ns
X-ray power > 250 TW
X-ray energy > 2 MJ

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

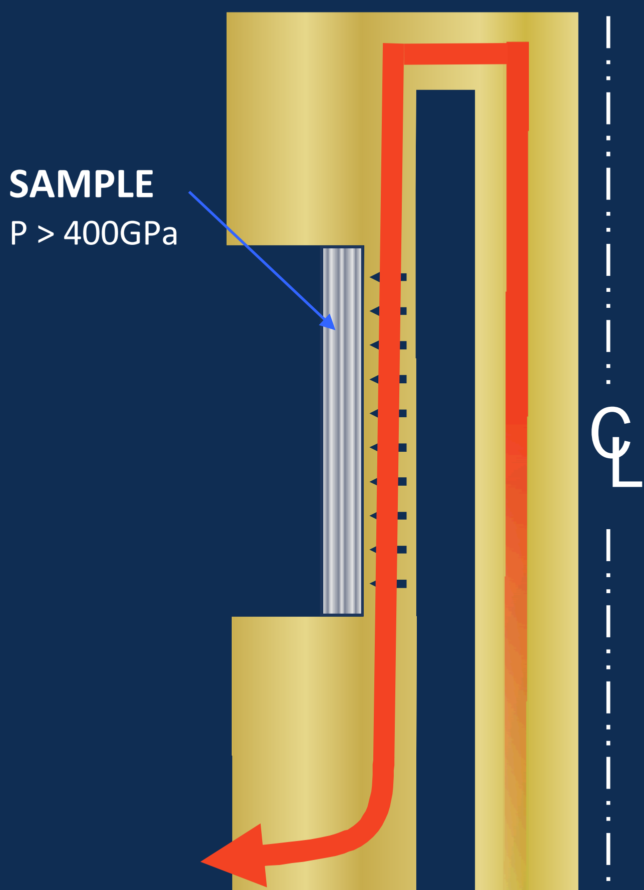


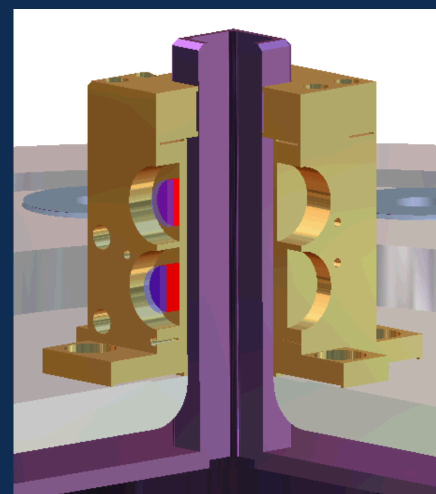
- Planetary science – Jupiter, Saturn, Uranus, Neptune, and exo planets [e.g. hot Neptunes]
  - Metallization of hydrogen/deuterium: SCIENCE 2015
- Planetary science – earths and super-earths
  - Silicates, MgO, and iron/iron alloys
  - Determining the vaporization threshold for iron – and implications for planetary formation, Nature Geoscience 2015
- Materials for Stockpile Stewardship, HED and inertial confinement fusion (ICF) and other applications
  - Investigating the periodic table from **A**luminum to **Z**irconium: a broad range of materials are of interest - a talk in itself

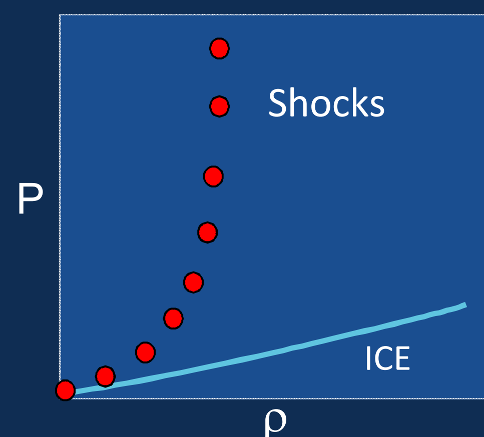
Dynamic compression experiments on Z can probe large regions of a material's equation-of-state surface

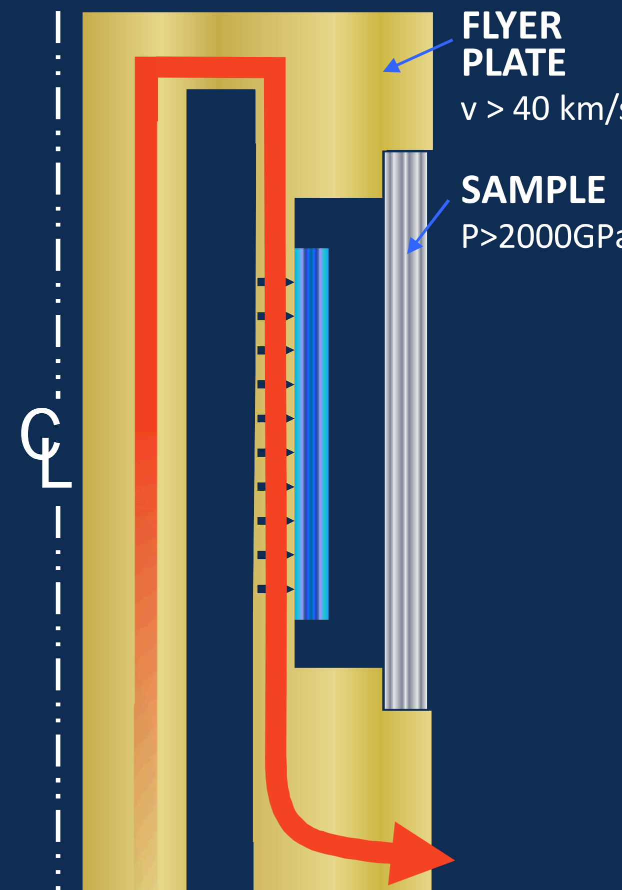


Isentropic compression and shock wave experiments map different regions of phase space





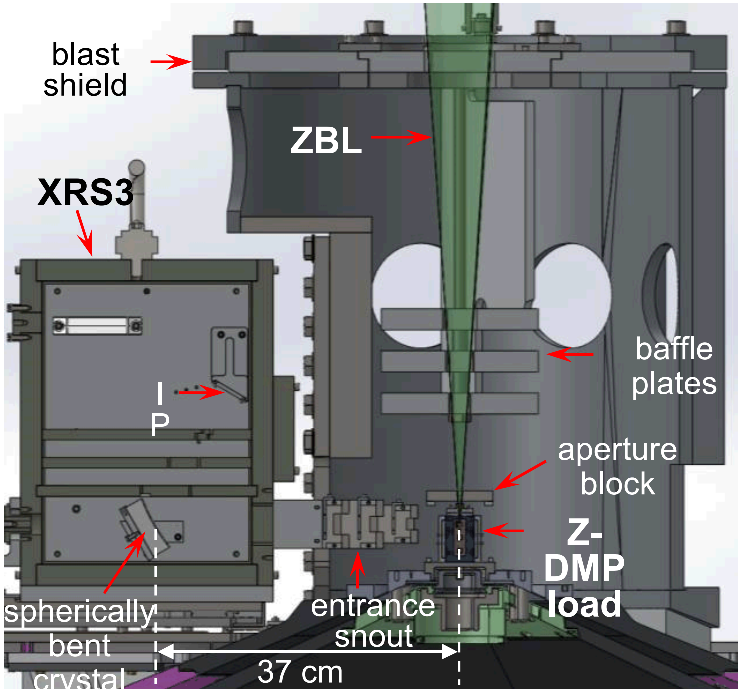




Isentropic Compression Experiments:
Gradual pressure rise in sample

Shock Hugoniot Experiments:
Shock wave in sample on impact

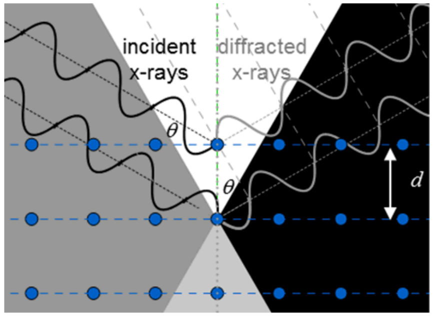
Existing and future diagnostics characterize materials in dynamic compression experiments (10-1000 ns durations)

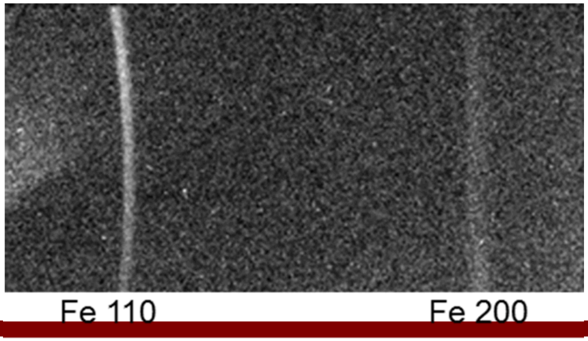


Xray Thomson scattering has been fielded
Still some challenges

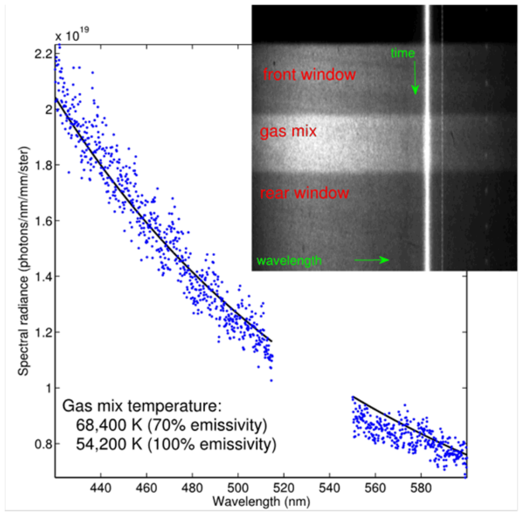
- Mechanical information
  - Measure velocity and derive pressure (stress) and density from conservation laws
  - Velocity profiles can also be compared directly with simulation
- Thermal information
  - Measure radiance (now) and/or reflectivity (in-progress)
  - Phase diagrams/kinetics and chemical reactions
- Other information
  - Microstructure (phase), which may not match equilibrium state
  - Transport properties (e.g., conductivity) in warm dense matter

Diffraction project for phase identification starting this year (Collaboration w/ UCSD on light source)

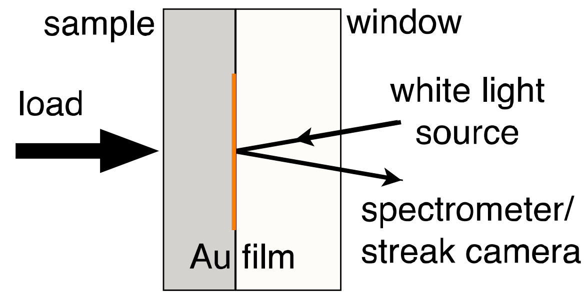


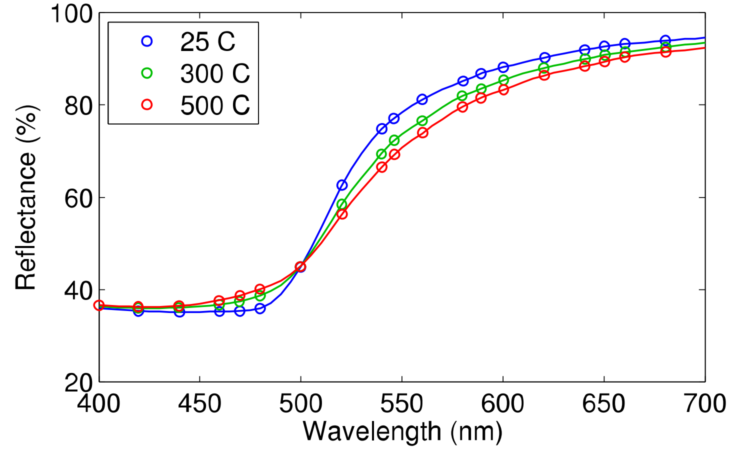


Temperature measurement on material experiments are critical and difficult!

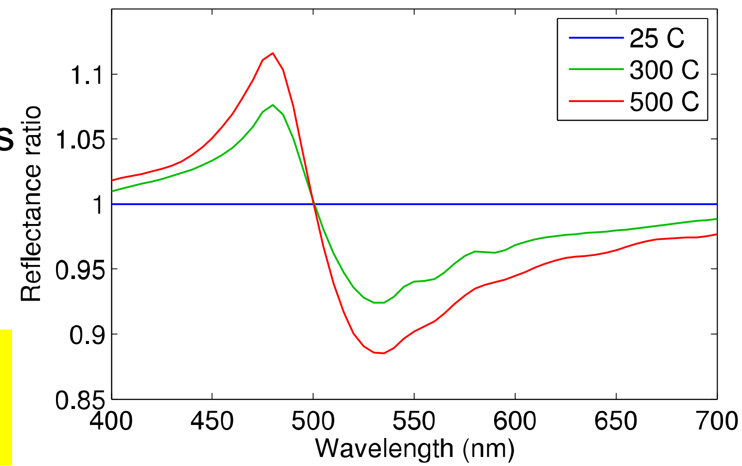


Absolute pyrometry for high T experiments recently implemented





Reflectance thermometry is better suited for ramp wave measurements (<1000 K) reflectance thermometry

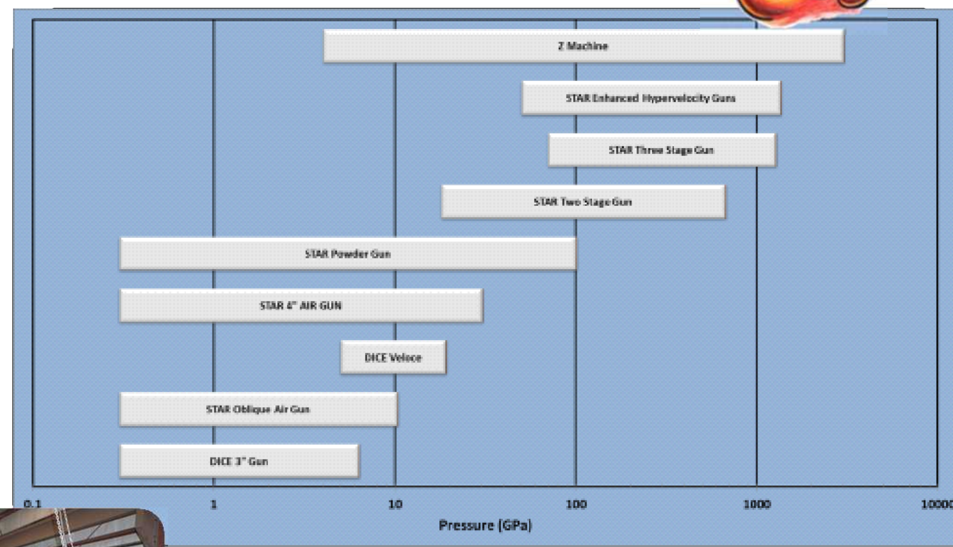


Diagnostics are excellent grounds for collaboration!

The STAR and DICE facilities enable high through-put lower cost experiments

Shock Thermodynamic Applied Research (STAR) facility
-Five guns (oblique to 3-stage)

Dynamic Integrated Compression Experimental (DICE) facility
-A 3" gun and a small pulse power machine (Veloce)



Oblique gun-
Direct shear measurements
@ 10 GPa

2/3 Stage 20-67mm Gun
Up to 12 km/s

Single Stage 89mm Powder Gun
100GPa impacts

Technique and diagnostic development / The right regimes for many applications!

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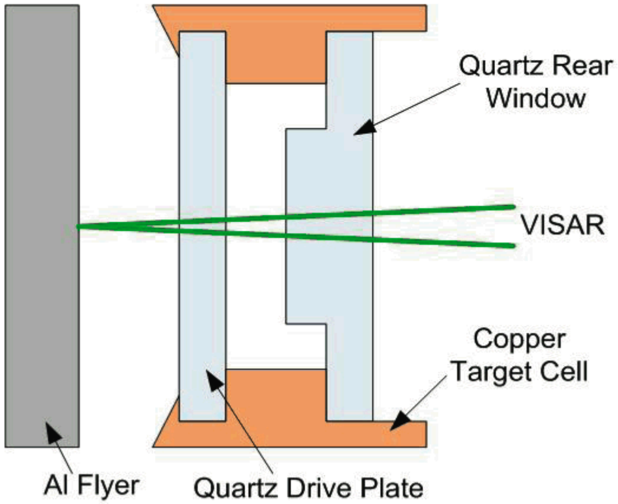
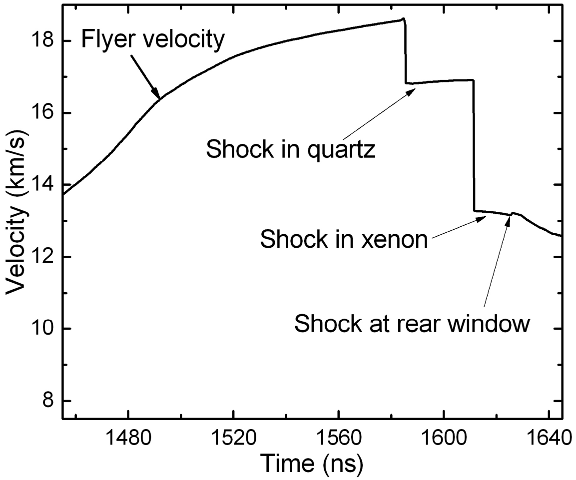
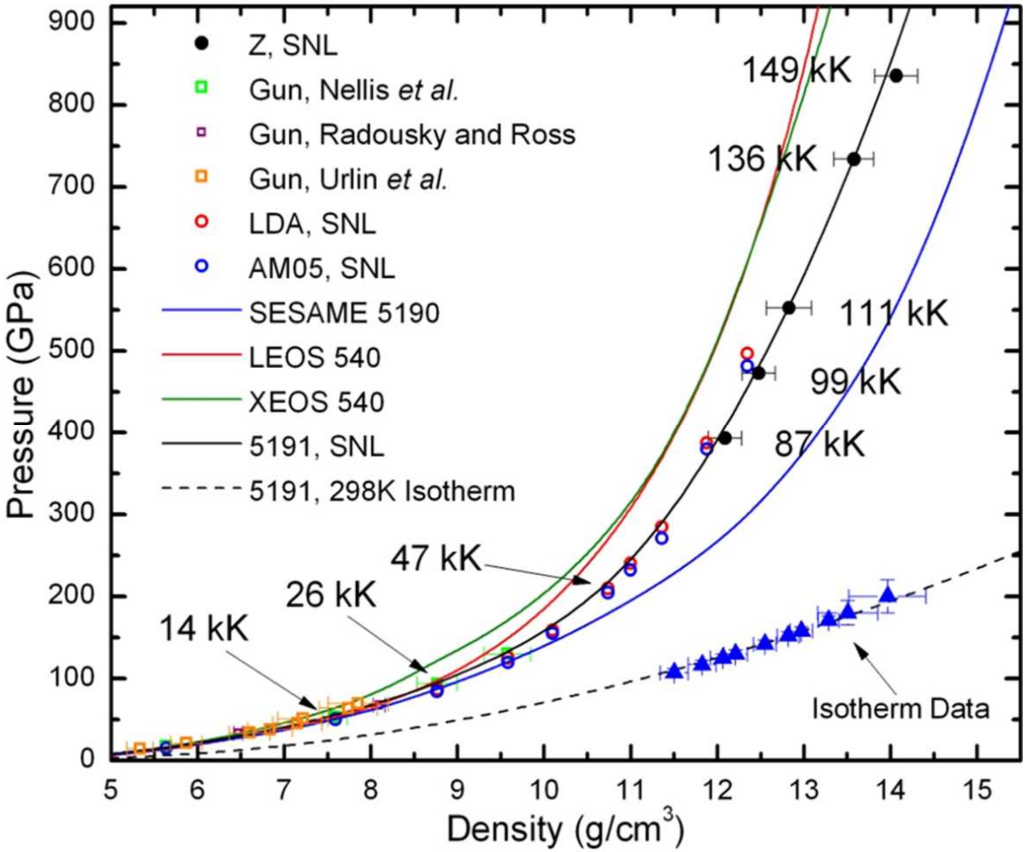
Lots of examples (teasers)!

Z flyer experiments and theory provided new understanding of high pressure Xenon



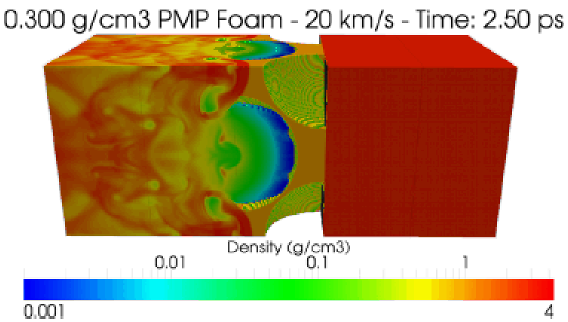


Shock velocities in transparent materials measured with sub-percent accuracy



Theory & data almost always diverge in previously unreachable regimes

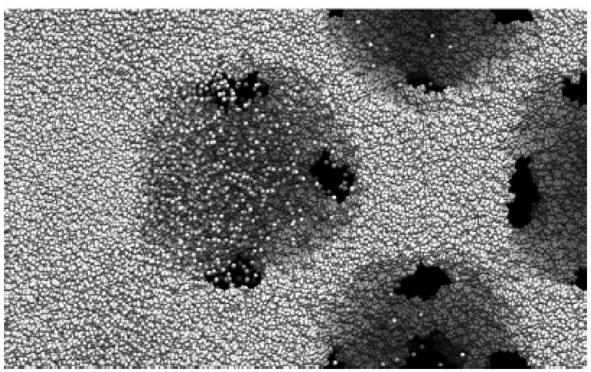
Theory and high pressure Z experiments study compaction at macro-, meso- and continuum scales



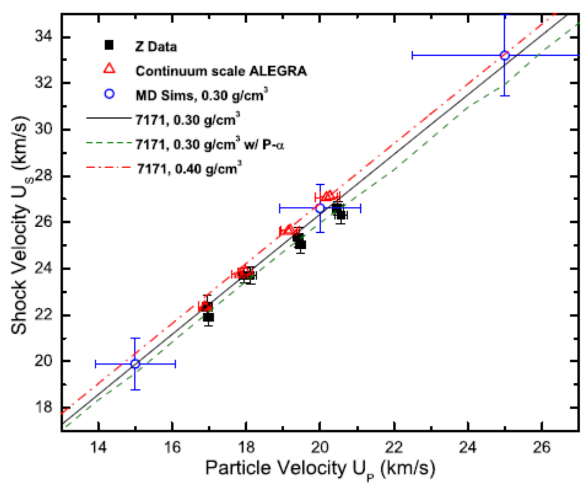
3D nm scale simulation

High pressure Z experiments (up to 200GPa) on PMP foams validated 3 different modeling approaches to conclude:

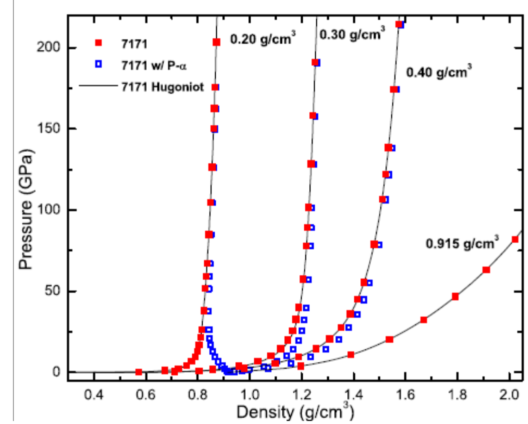
- MD : high temperatures due to hotspot formation in collapsing pores
- 3D nm-scale : ablation during pore collapse and significant variation behind the shock front
- P-α models (with higher than typical compaction pressures) represent continuum behavior well



Shock traversing a pore in the molecular dynamic simulation



Z data validates the different modeling approaches



P-α and standard PMP simulations

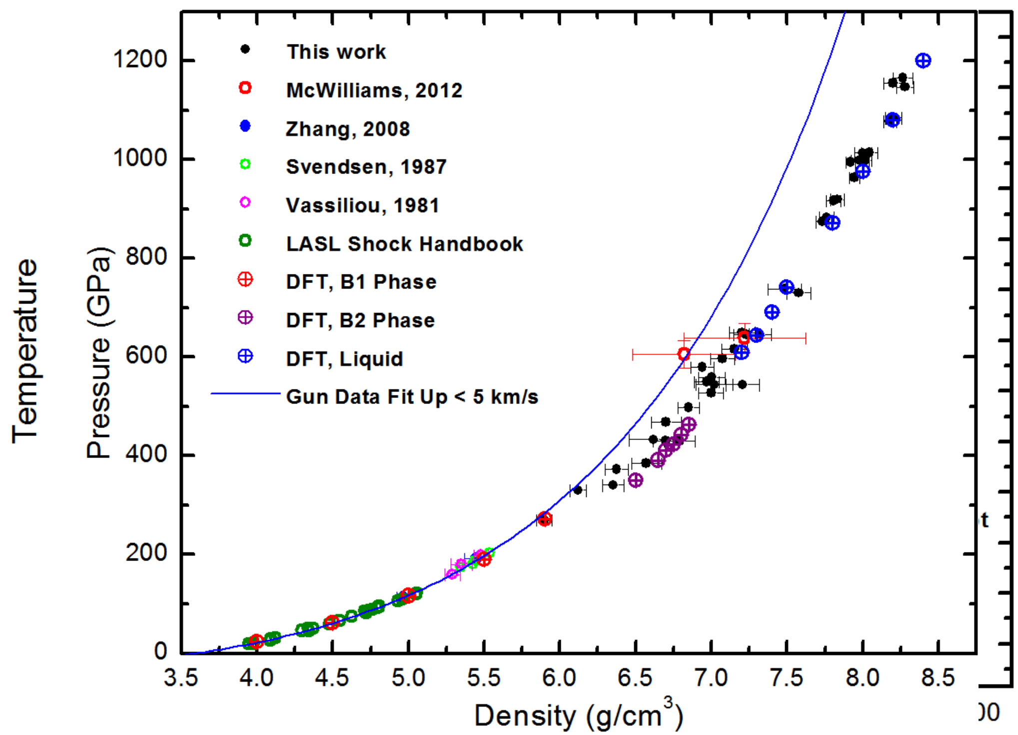
Root, et. al, “Shock compression of hydrocarbon foam to 200GPa: Experiments, atomistic simulations, and mesoscale hydrodynamic modeling”, J. Appl. Phys. 114, 103502 (2013);

New experimental techniques + theoretical tools allow definitive description of MgO phase space

- Accurately measured the MgO Hugoniot from 330 GPa to 1160 GPa
- MgO has a large coexistence region along the Hugoniot between B2 and liquid
  - Significant to planetary and moon formation
  - Shock pressures of >700 GPa needed to completely melt MgO
- Vastly expanding the domain of quantitative understanding for geomaterials

Root, et., al – to be published in PRL

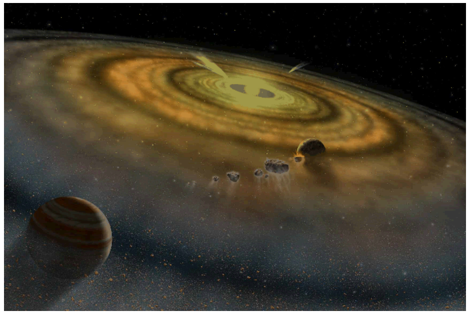
MgO: experiments and models



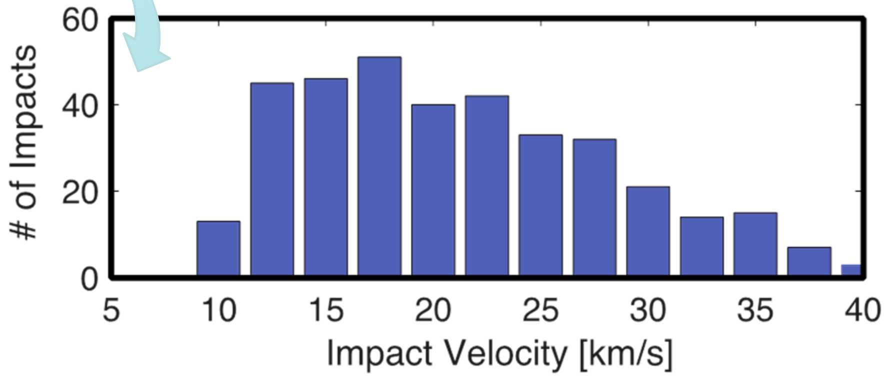
Pressure (GPa)

- Outstanding DFT agreement (for the MgO phases shown)
- Temperature inferred from DFT

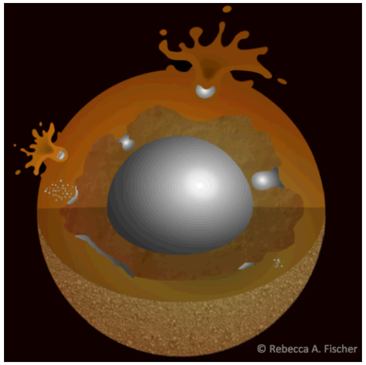
Z experiments provide material properties in HED conditions to address the moon formation mystery



When an iron meteor hits the earth,(in the future or during the formation of the solar system) does it plow into the ground as a bullet, splatter as a drop of rain, or vaporize into a cloud of iron to return to earth as iron rain?



Planetary dynamics suggests high impact velocities

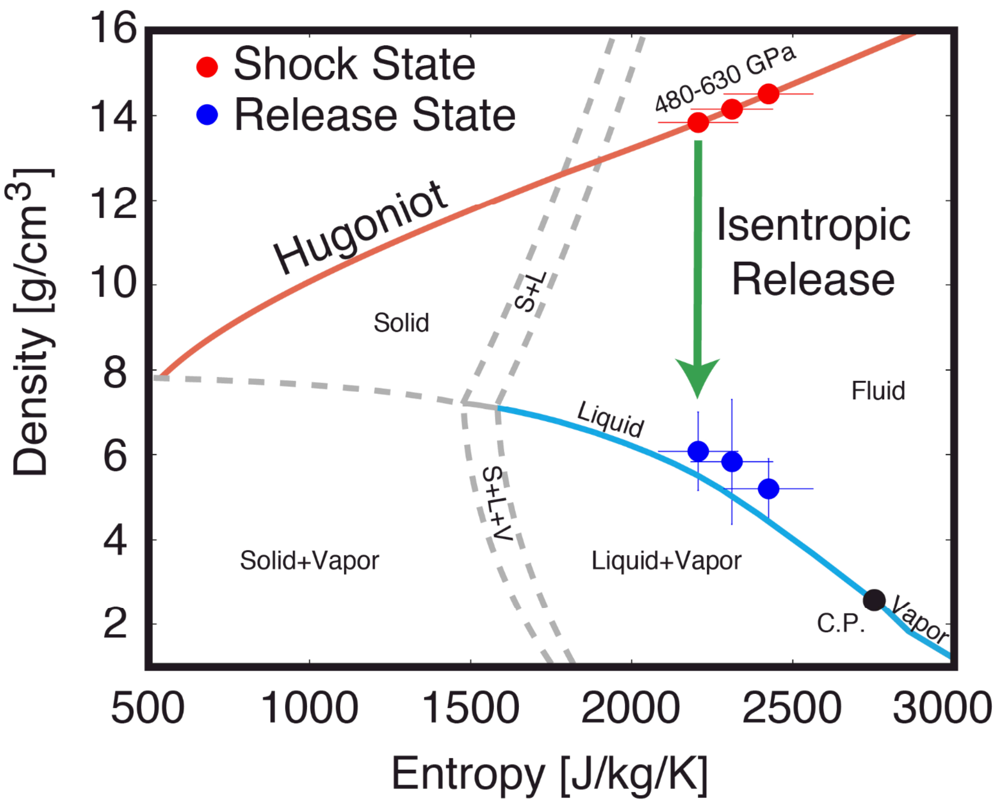


The models depend on the HED properties of iron (particularly vaporization)!

Geophysicists have shown fluid instabilities CAN NOT sufficiently mix the incoming iron cores to explain observed iron content in the mantel or the similarity in isotopics between the earth and the moon

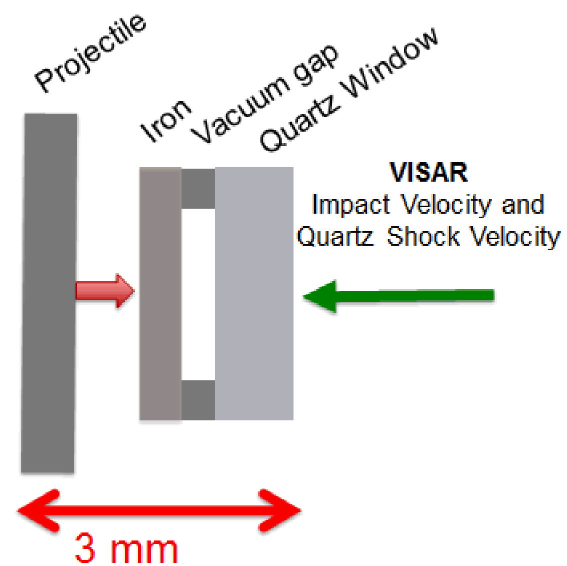
N-body simulations from Raymond et al. 2009

Z can study vaporization for states produced by planet forming impacts

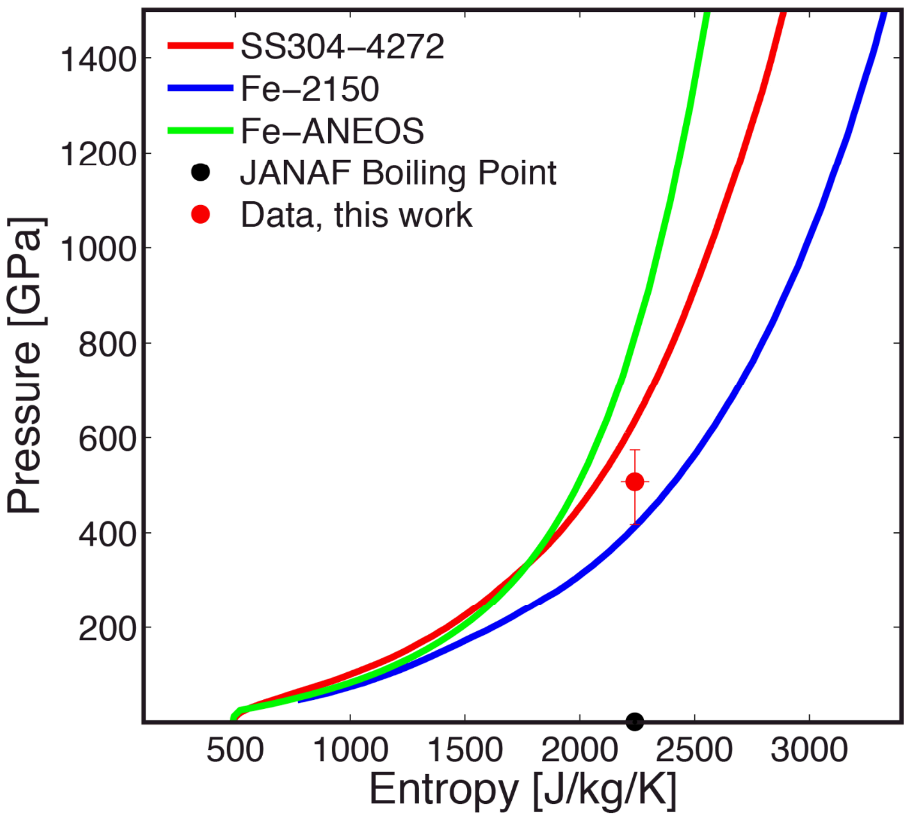


Iron Shock and Release Data

- Sandia Z facility can launch flyer plates at > 40 km/s
- We can directly simulate all impact conditions
- A shock-release approach was used to evaluate the liquid-vapor dome as a function of entropy



HED experiments: Iron vaporization occurs at lower pressures than previously assumed



- Vaporization is significantly easier than ANEOS , the most broadly used model for geophysics, suggests
- Iron cores will vaporize at 13 km/s impacts – The state of the earth and moon are now much easier to explain
- 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

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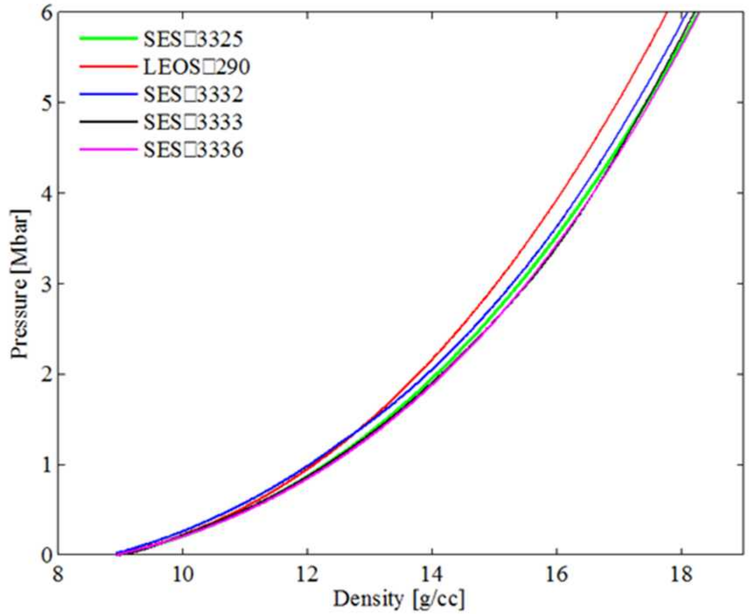
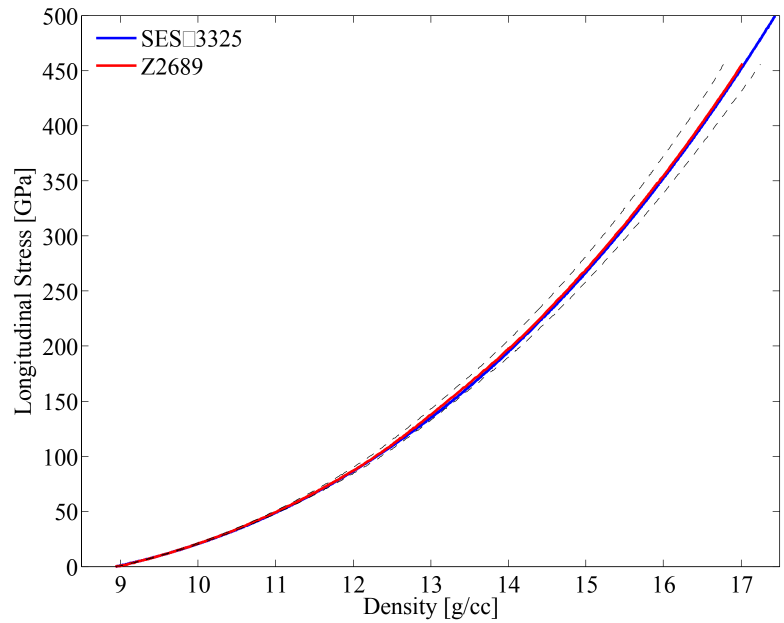
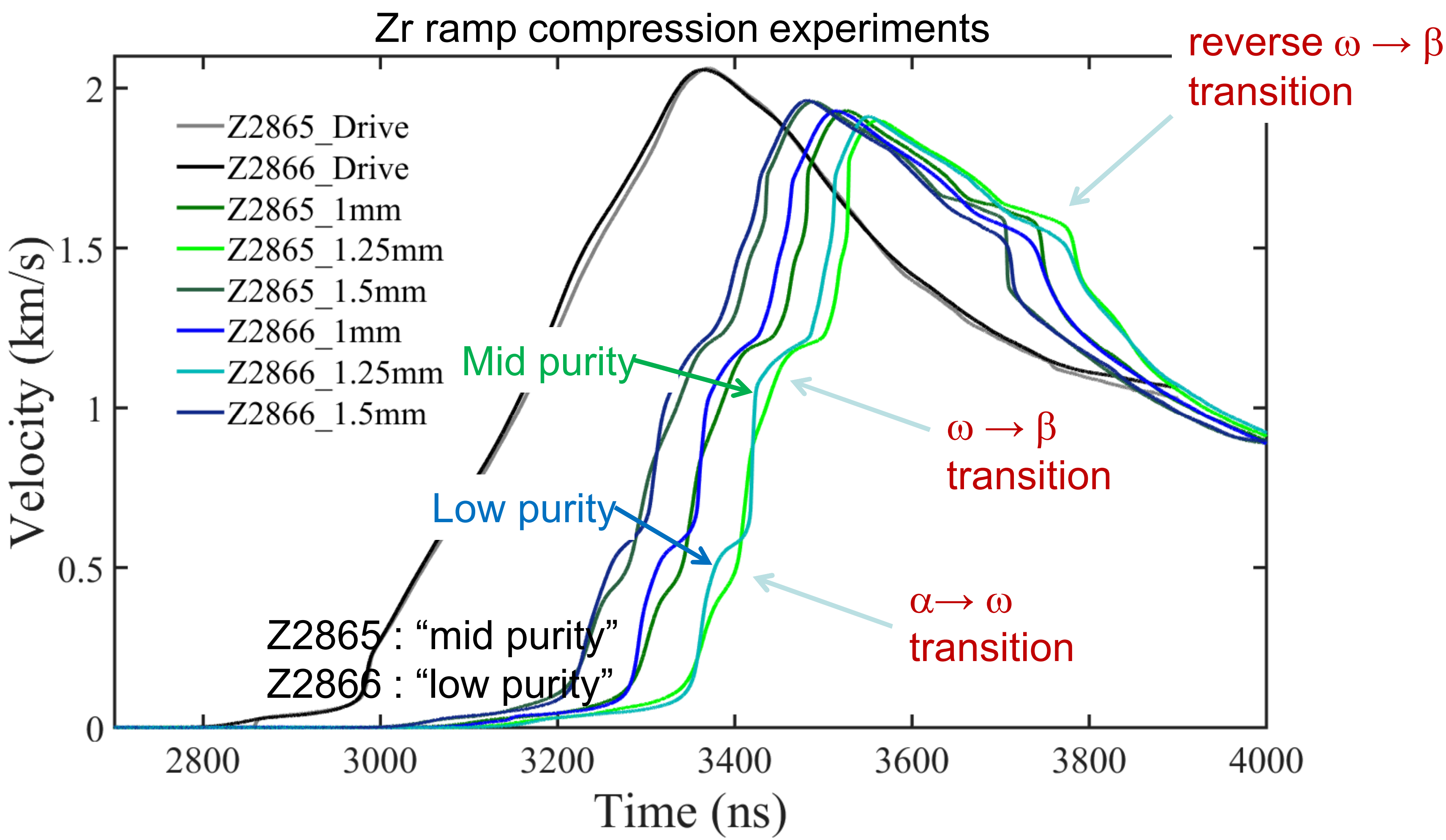
Ramp compression provides "low" temperature high pressure data





There was considerable variation in models for copper,
a simple, "standard" material important for NIF target designs
A Z experiment to 500GPa identified the best choice

Phase transitions are readily apparent in velocity measurements Contaminants in Zr affect phase change kinetics

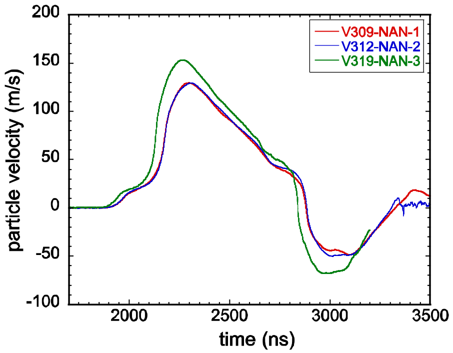


Synthesis of Nanostructured Materials through Magnetic Ramp Compression

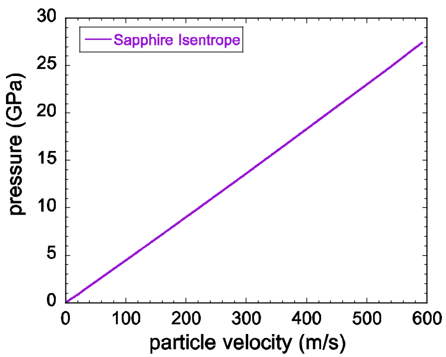
An external mechanical pressure overcomes balanced interparticle interactions, enables consolidation of ordered nanoparticle arrays to form new one-three dimensional nanostructured architectures.

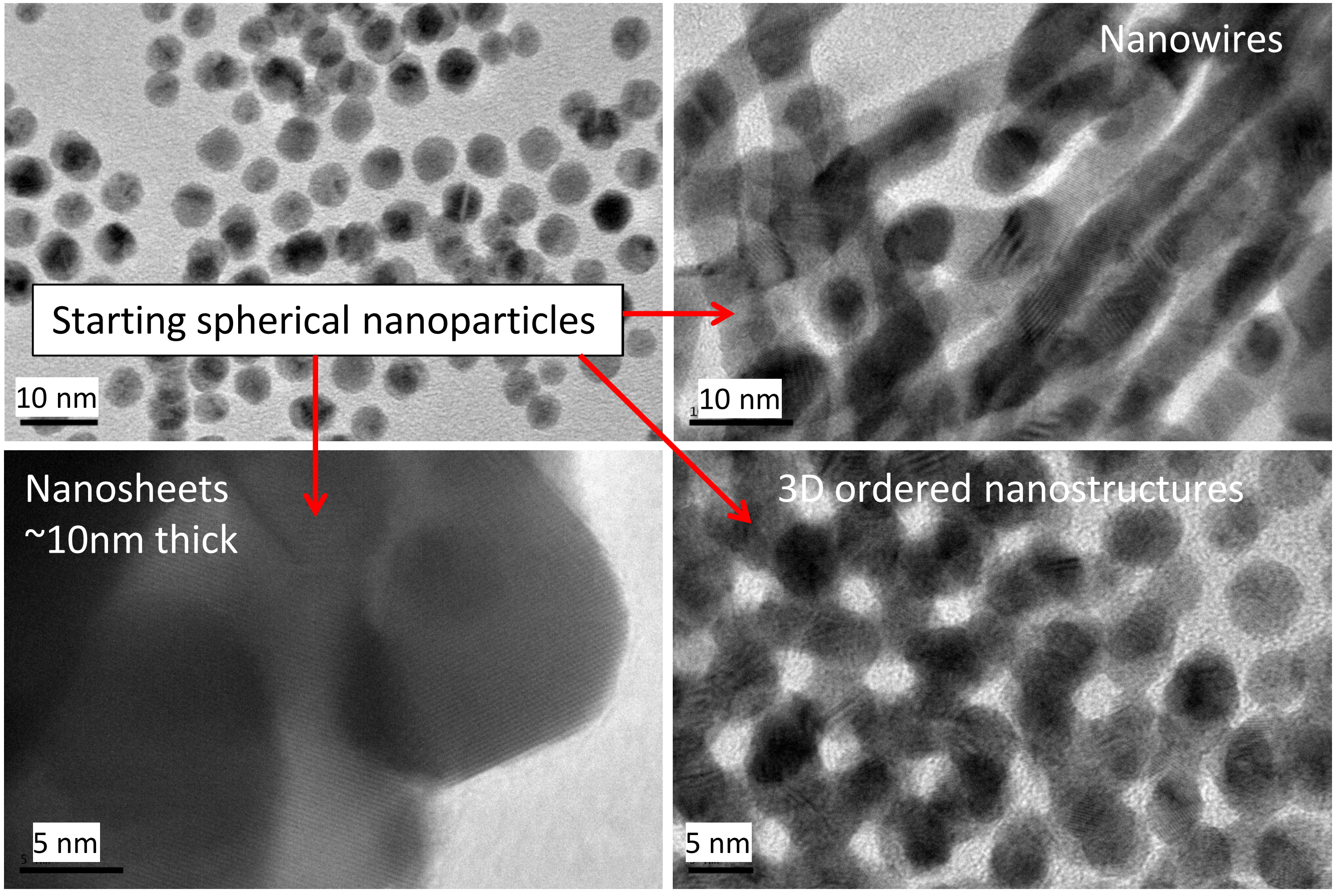
Li, B. *et al. Nature Commun*. 5:4179 doi: 10.1038/ncomms5179 (2014).

Peak velocity: v = 129 m/s - 153 m/s



Peak pressure: P = 5.8 GPa - 7.0 GPa





(Contact Hongyou Fan, hfan@sandia.gov, 505-272-7128)

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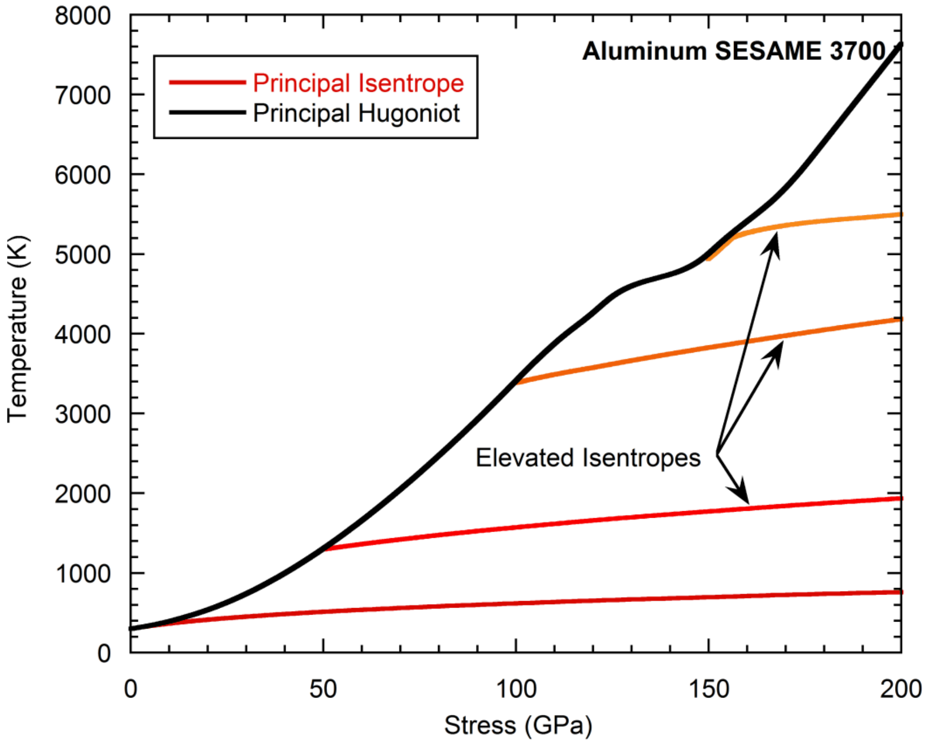
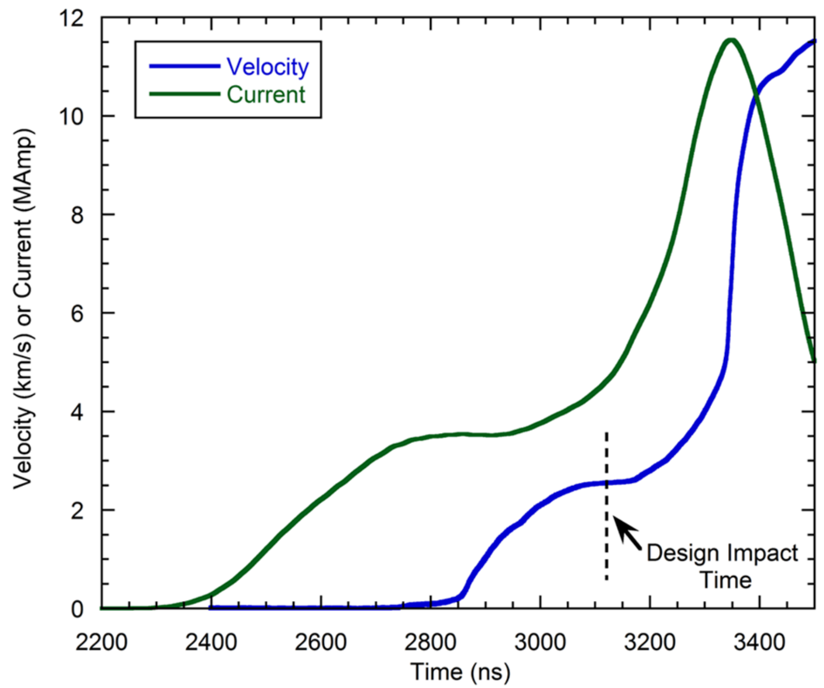
  - Shock-Ramp experiments
    - Cu
    - D2 metalization
  - Strength Experiments
- The Z fundamental Science program and opportunities for collaboration

Lots of examples (teasers)!

The Shock-Ramp technique probes between the principal Hugoniot and isentrope





Ramp compression from a Hugoniot state results in intermediate temperatures at high compression.

Flight gaps and pulseshape designed to enable impact at nearly constant velocity

This velocity plateau also generates a "hold" in the shock state

Liquid tin equation of state measured with the shock-ramp technique

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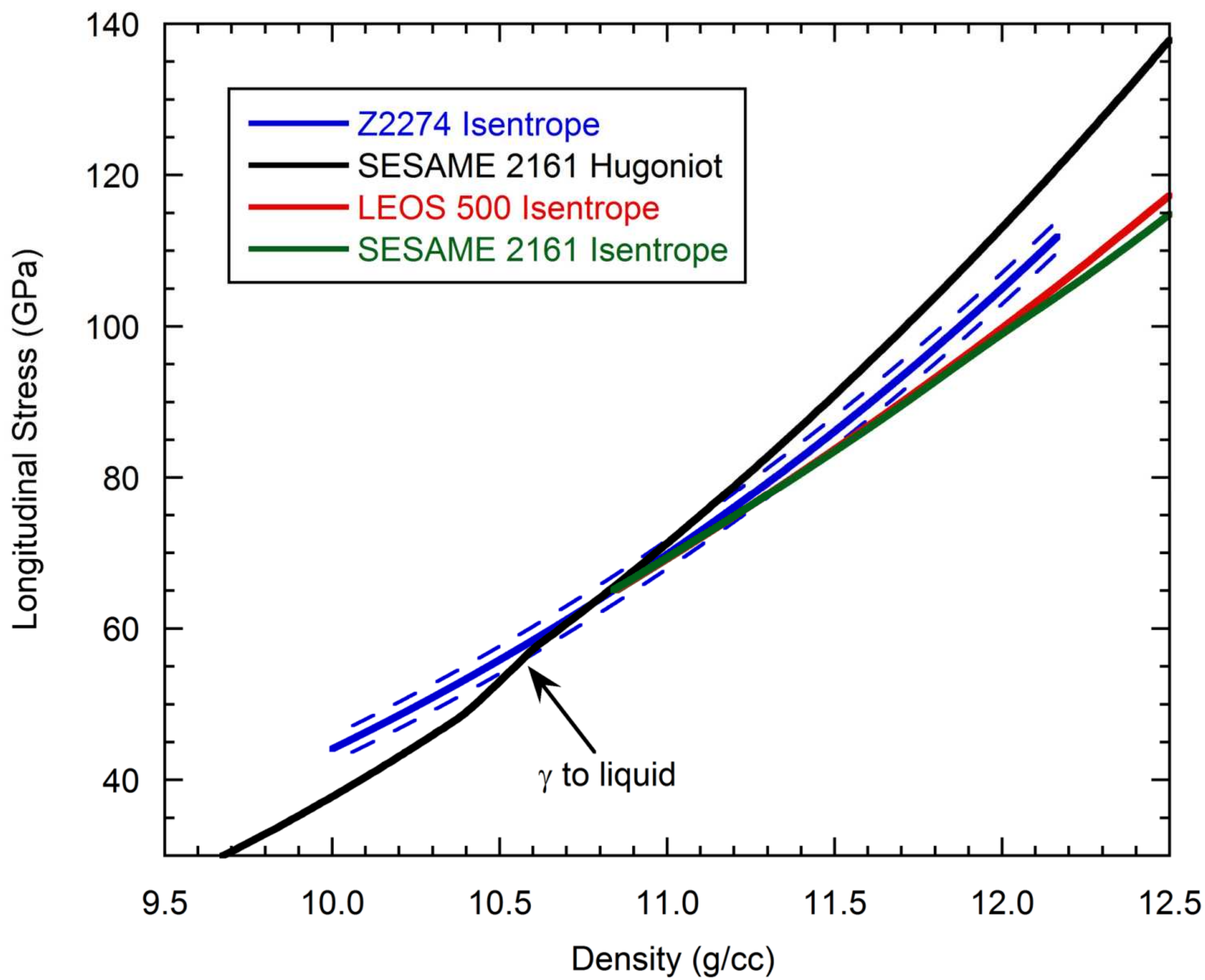
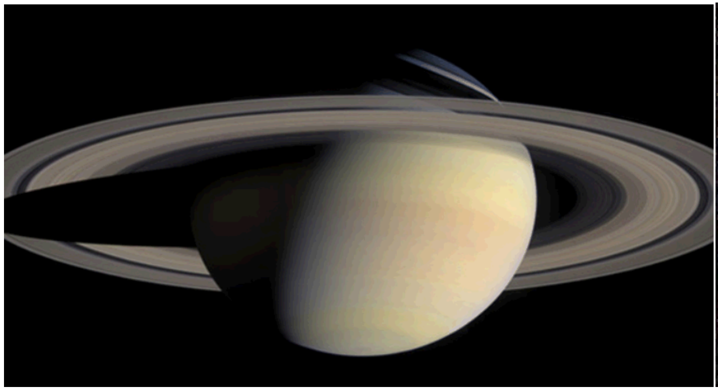
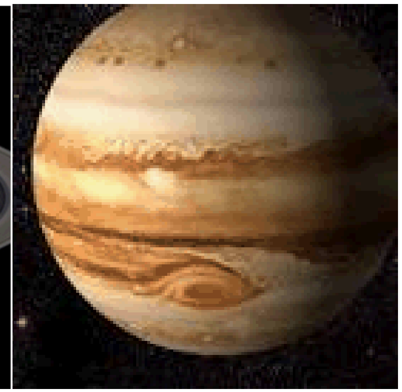
Liquid tin is stiffer than current EoS models



Observation of H2 metallization needed to address a planetary mystery

Why is Saturn hot?

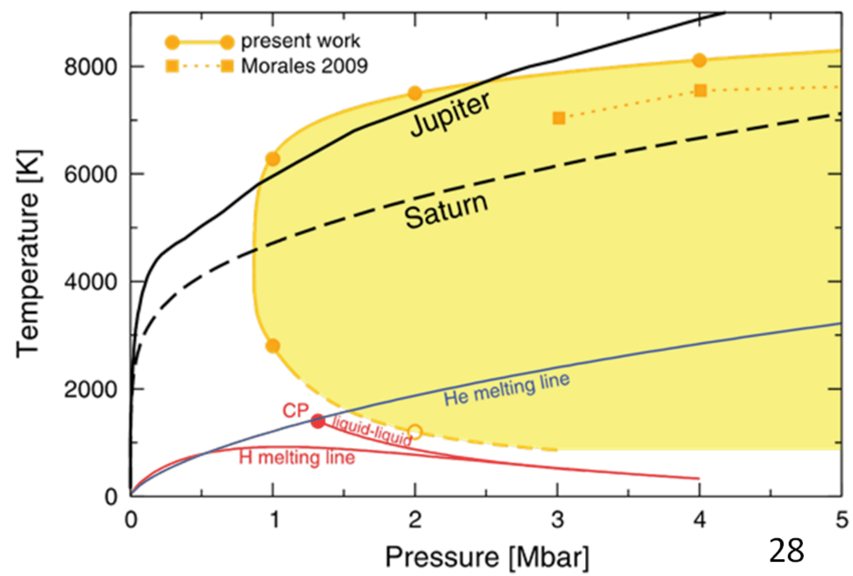




- Hydrogen metallization, as predicted by Wigner(1935) is linked to H-He demixing
- Formation of helium rain would generate heat
- But Jupiter would also have He rain and excess heat according to current models

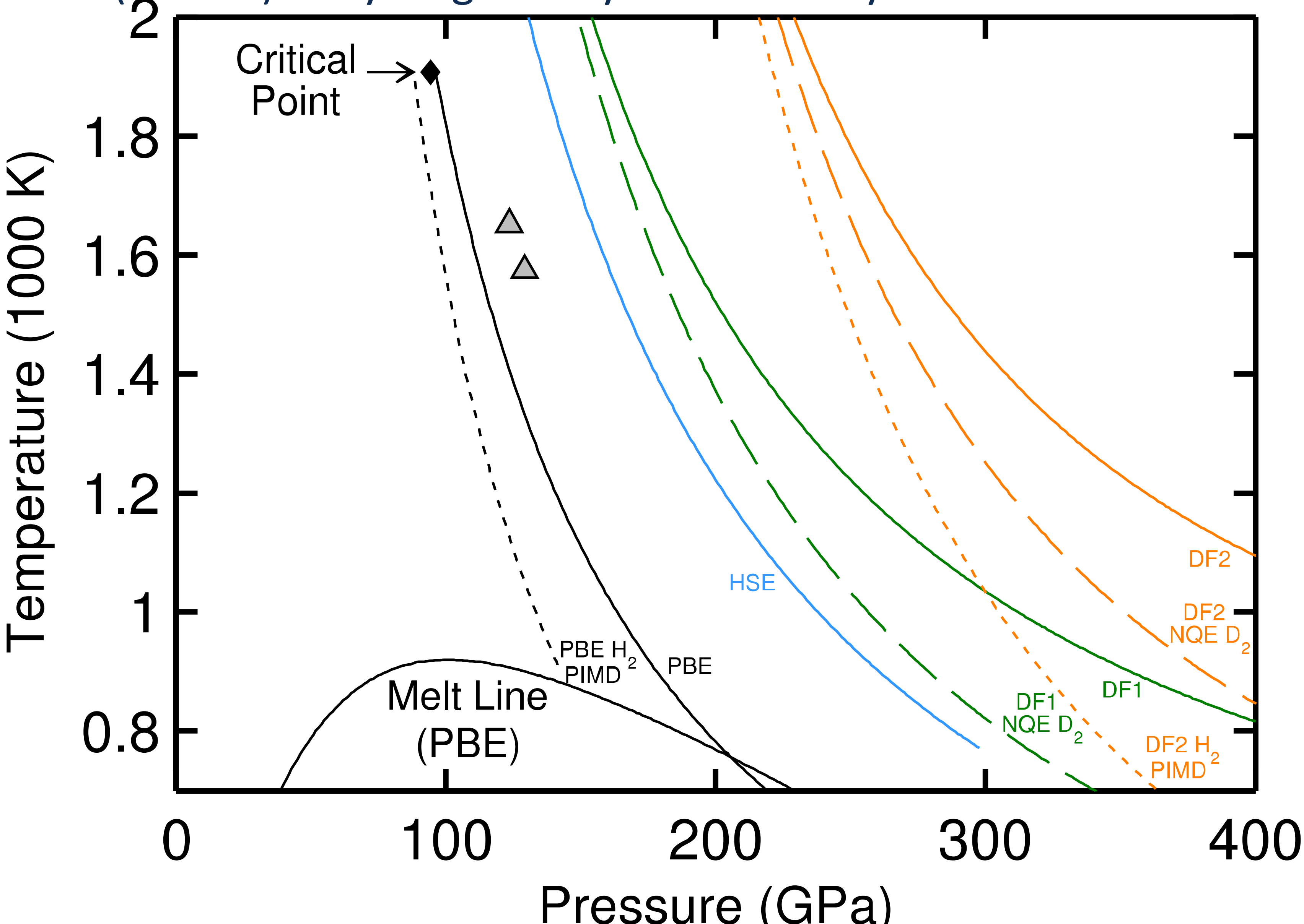
- Planets cool with age,
- Saturn's age is much hotter than would be expected if its age is in line with the rest of the solar system.
- Scientists believe that Saturn is two billion years older than its temperature indicates

Redmer & Knudson explored the D2 insulator to metal transition on Z



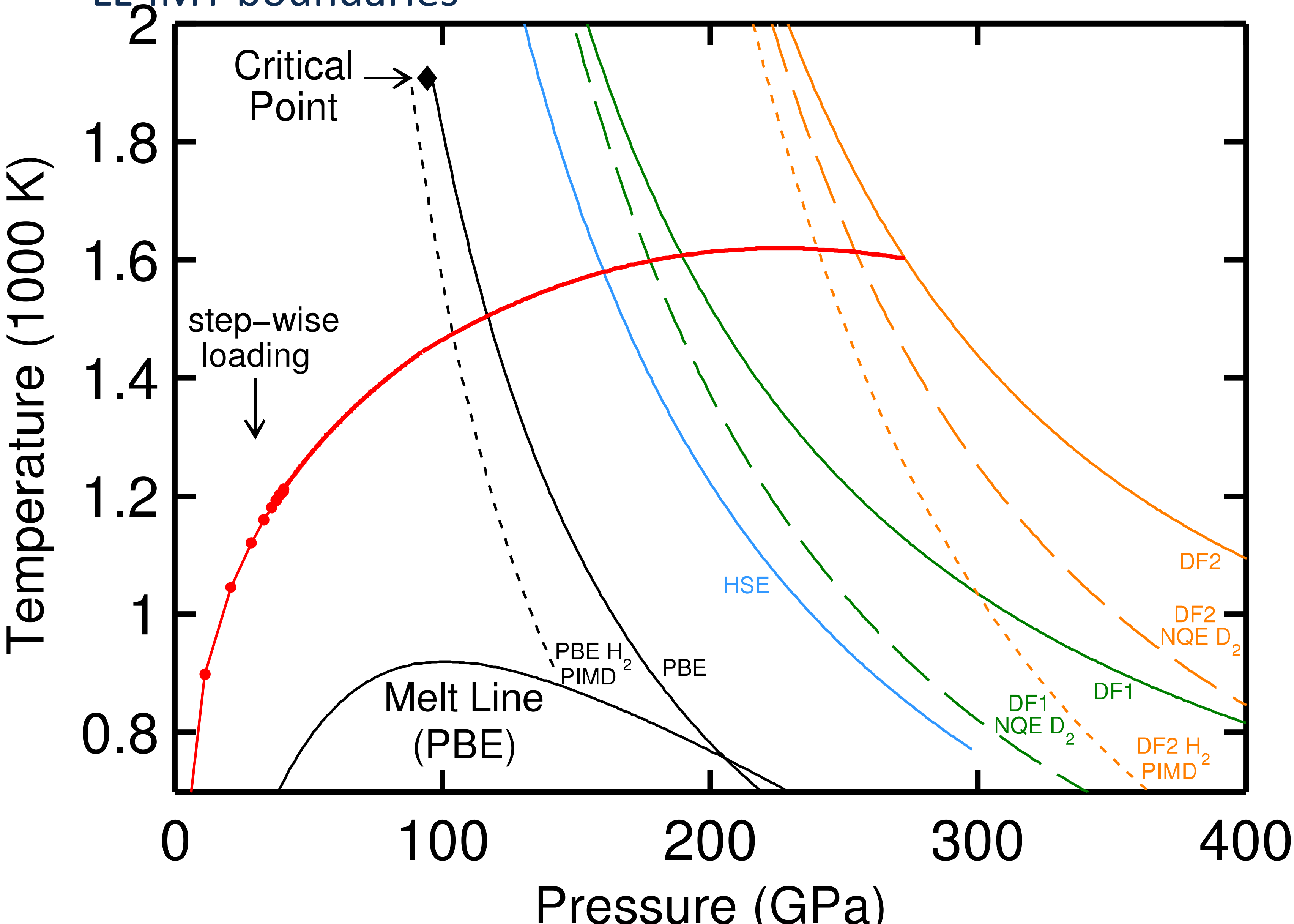
W. Lorenzen, B. Holst, and R. Redmer, Phys. Rev. B 84, 235109 (2011)

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

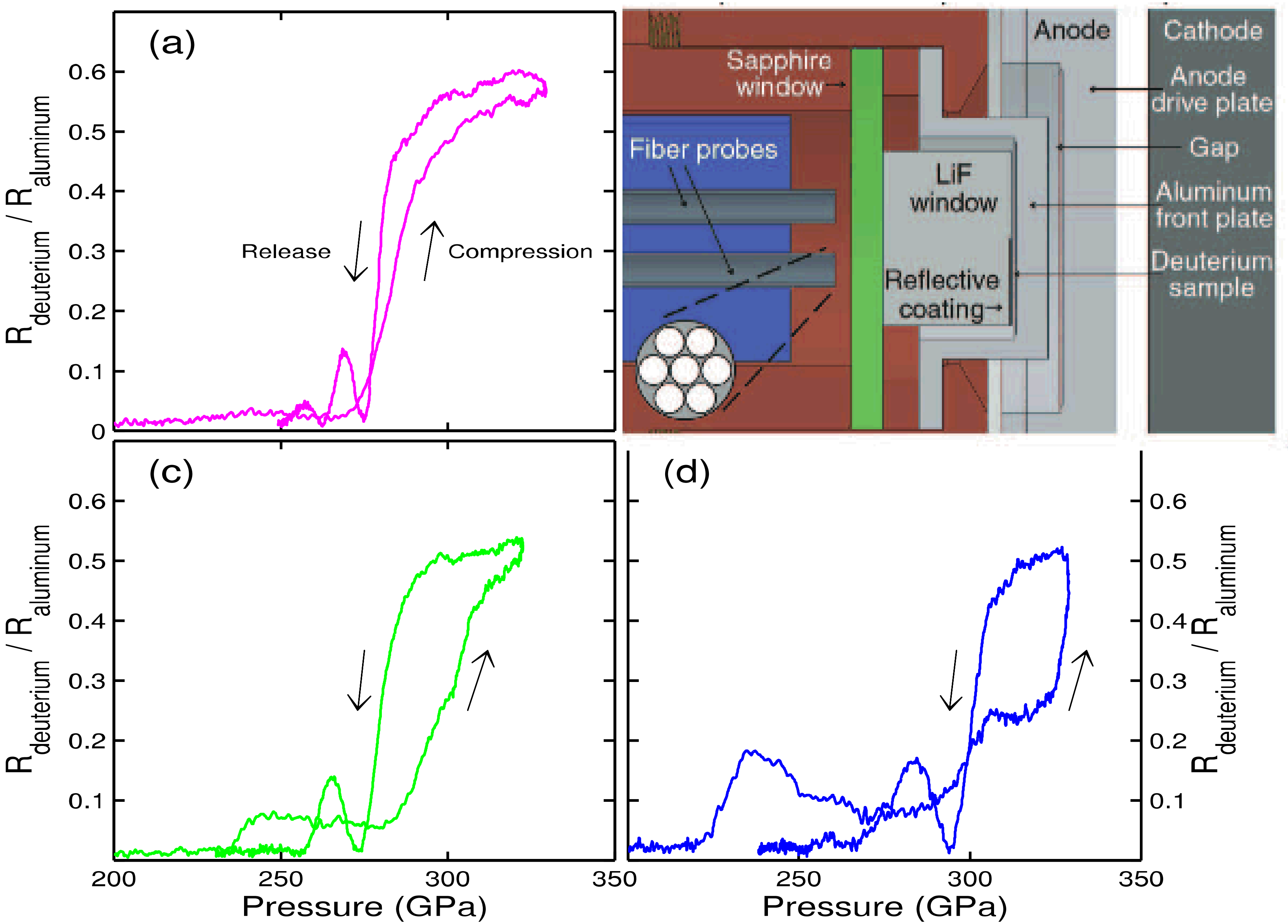


[illegible]atter (2014)

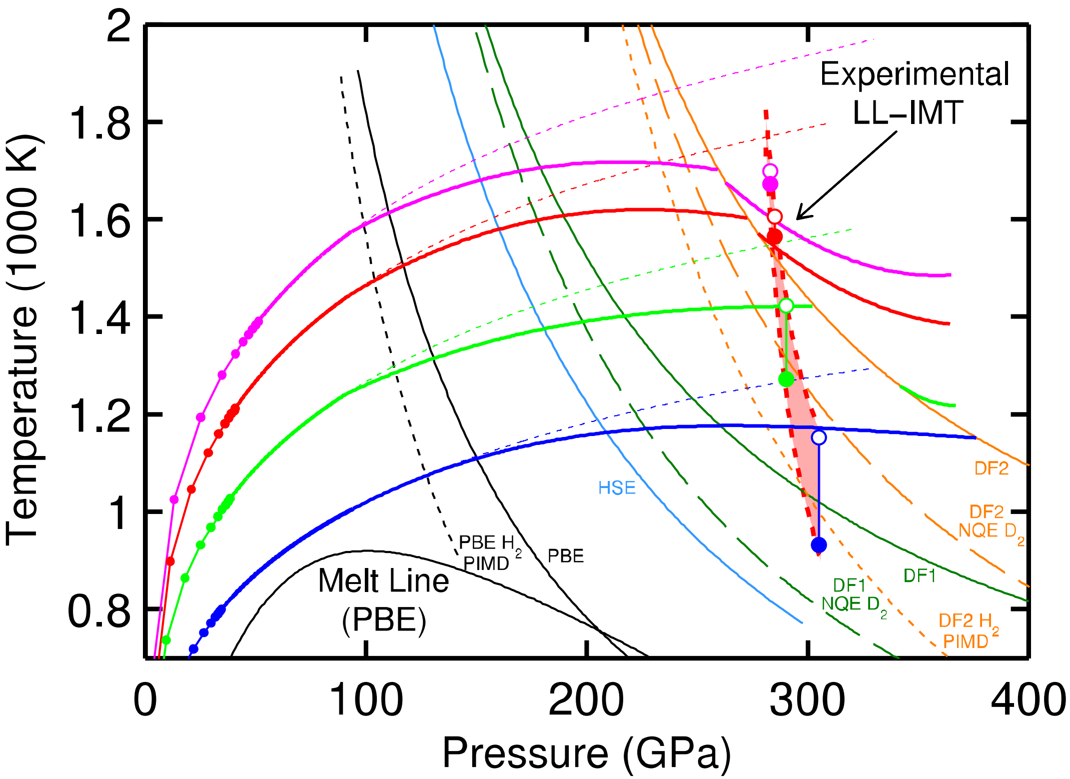
A shock – ramp experiment on Z traverses the proposed LL-IMT boundaries



The reflectivity is a sensitive diagnostics for metallization



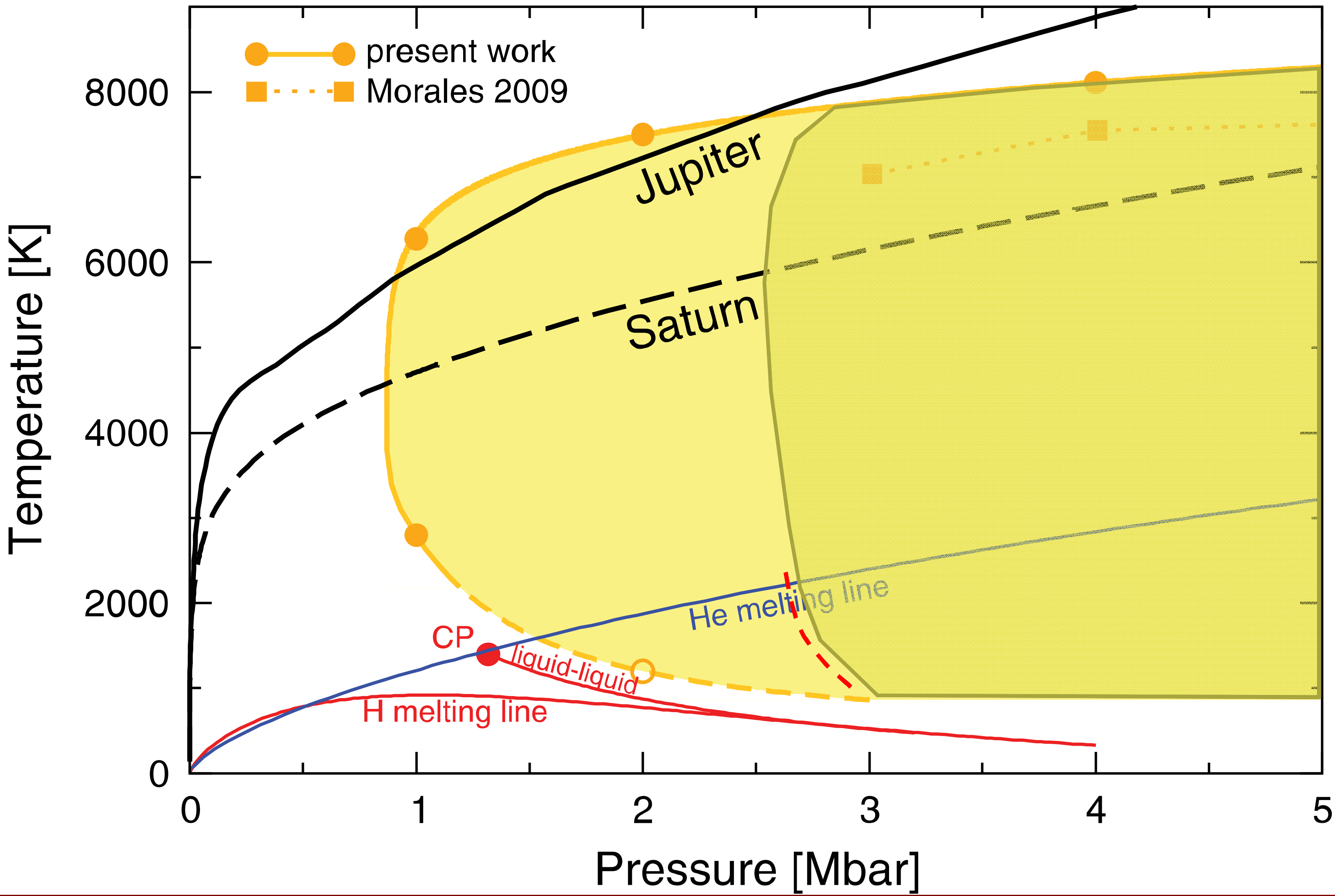
We have located the LL-IMT in deuterium to be at 300 GPa



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.

- *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

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)

Outline:

- The Z facility and major programs
- Pulsed Power to probe material dynamics in extreme conditions
  - Diagnostics and techniques
  - Flyer experiments (Shock Hugoniot)
    - Gases
    - Compaction
    - Iron Vaporization
    - MgO
  - Ramp experiments: Quasi-Isentropic Compression Experiments (ICE)
    - Metals
    - Synthesis of nano-wires
  - Shock-Ramp experiments
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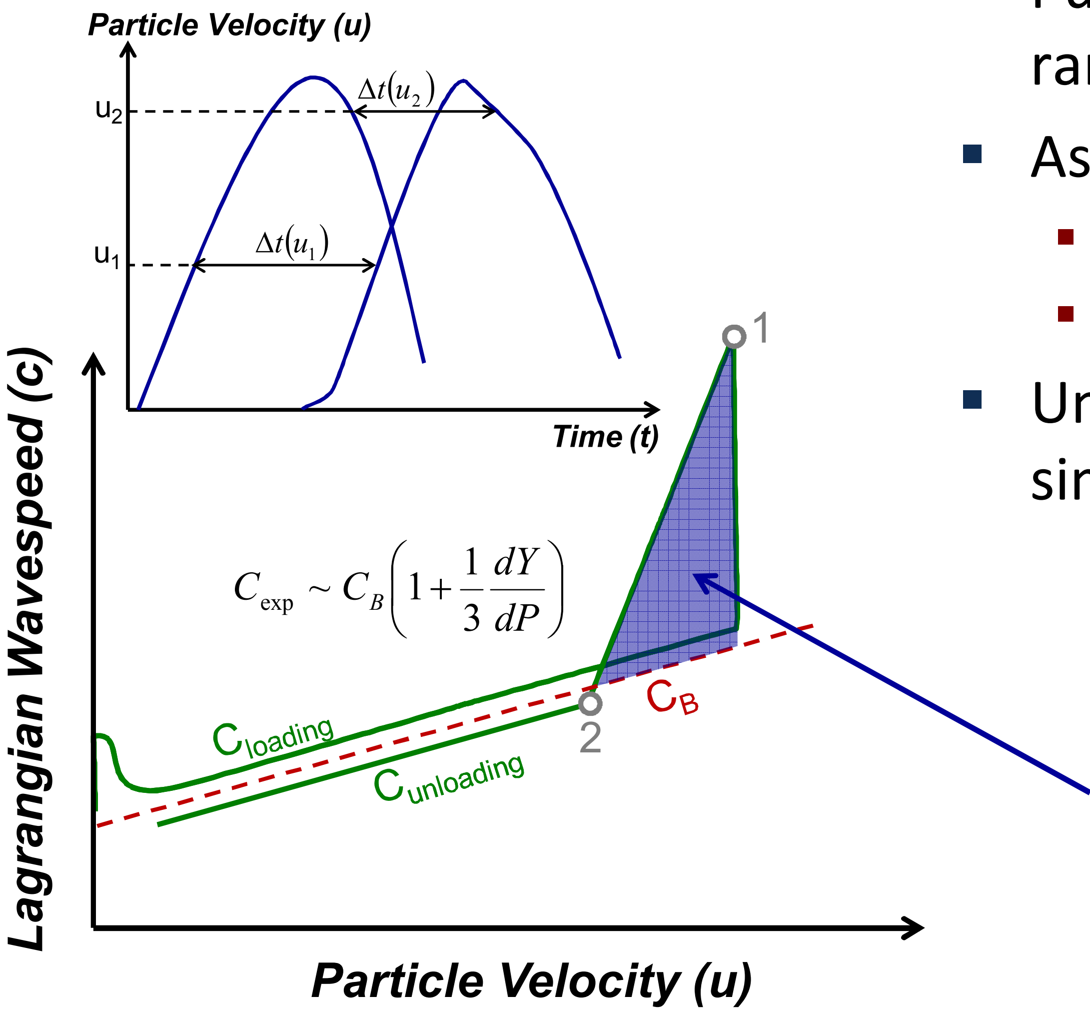
Lots of examples (teasers)!

Strength can be inferred from velocities in ramp-release experiments on Z using the self-consistent method



- Pulse shaping used to create ramp release loading
- Assumptions
  - Simple wave propagation
  - J2 plasticity (Von-Mises yield)
- Uniaxial strain results in simplified coupling:

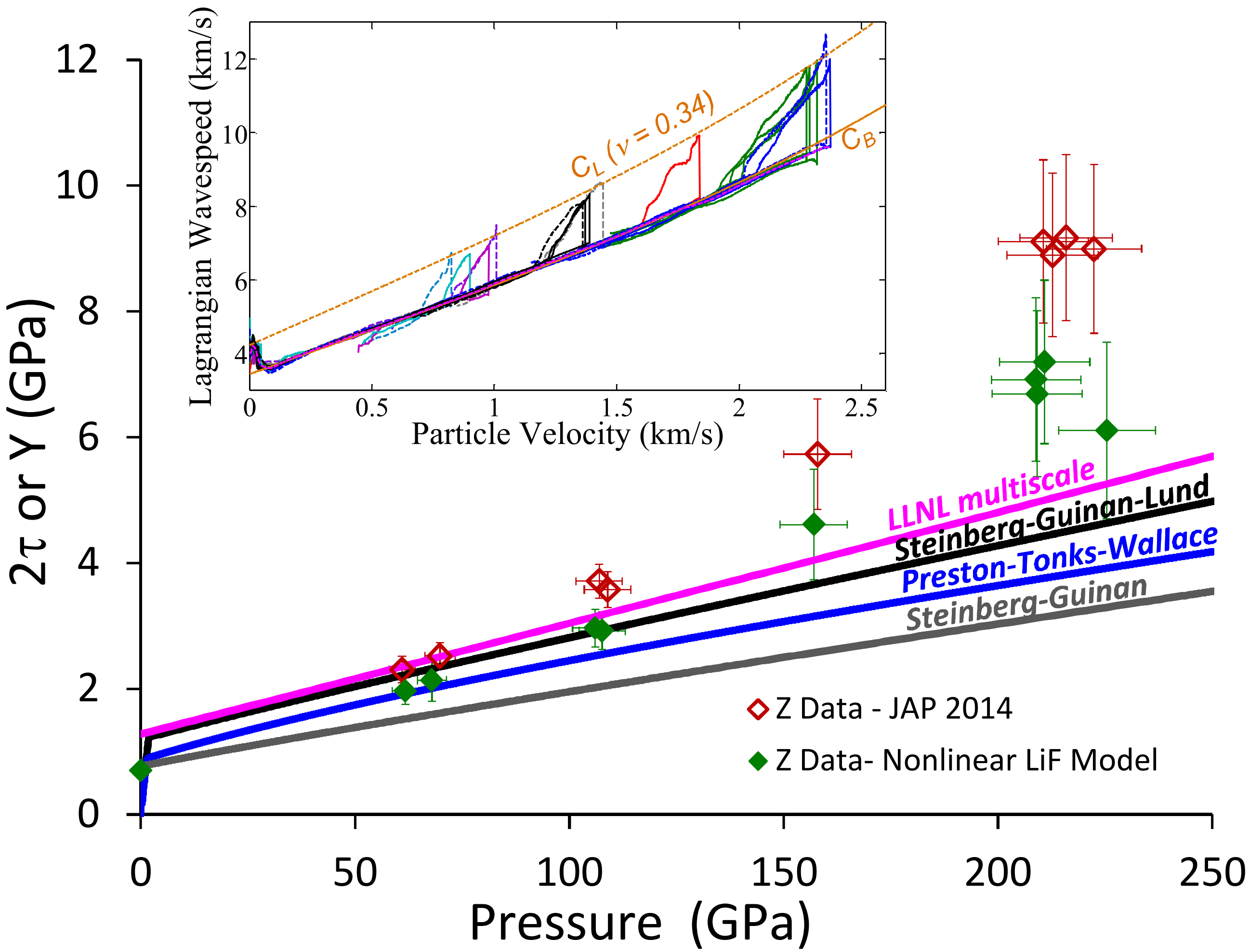
$$\sigma_x(\varepsilon) = P(\varepsilon) + \frac{4}{3}\tau(\varepsilon)$$

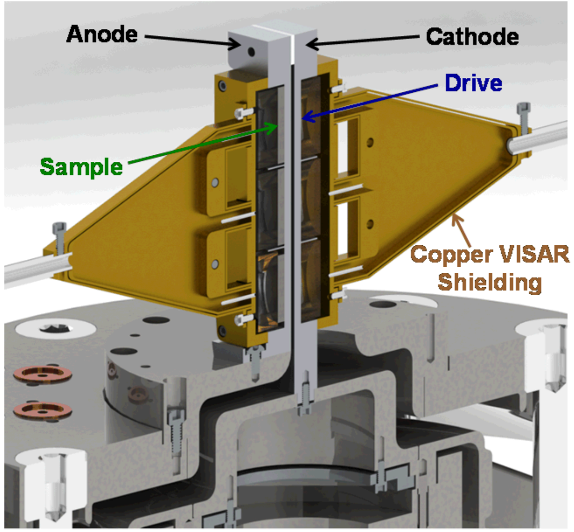
$$\frac{d\tau}{d\varepsilon} = \frac{3}{4}\rho_0\left[c_{exp}^2 - c_B^2\right]$$

$$\tau_2 - \tau_1 = \frac{3}{4}\rho_0\int_{u_1}^{u_2}\left[c_{exp}{}^2 - c_B^2\right]\frac{du}{c}$$

Brown, et. al, JAP 114, 223518 (2013); Asay and Chhabildas, 1981;

Z experiments on tantalum at strain rates of 10^5/s reveal higher than predicted shear stress near 200 GPa

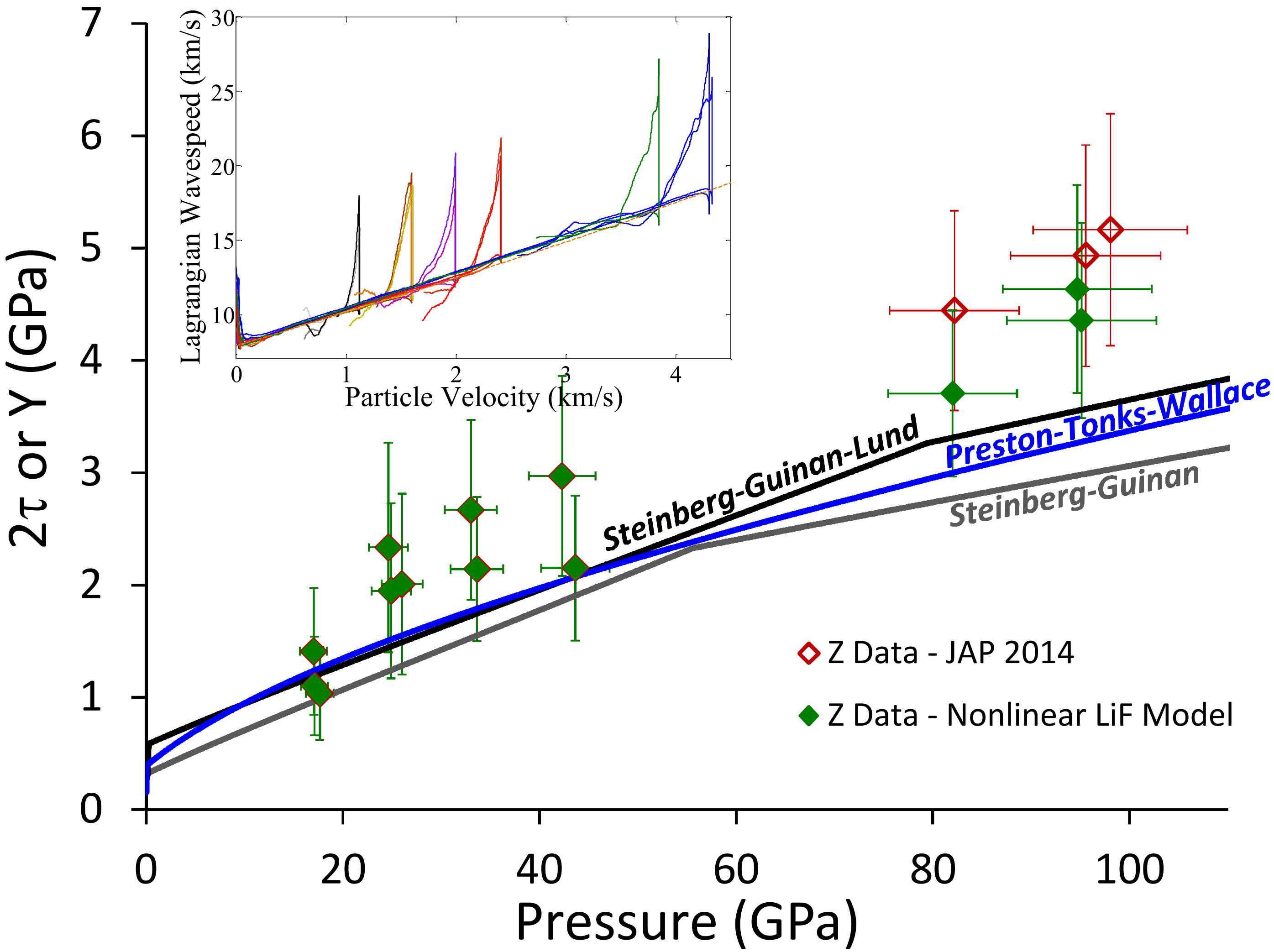




- LiF windows are used for both sample and drive measurements
  - It's important to correctly model its mechanical and optical properties

Brown et al., JAP 115, 043530, 2014

Z experiments on beryllium at strain rates of 10^5/s also show higher than predicted shear stress near 100 GPa



Brown et al., JAP 116, 033502, 2014

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Lots of examples (teasers)!

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

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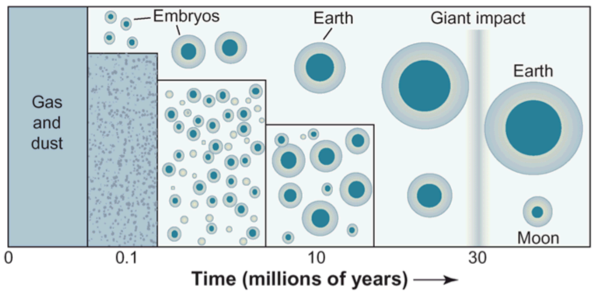
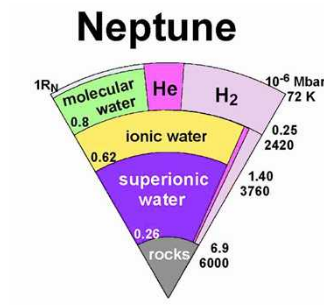
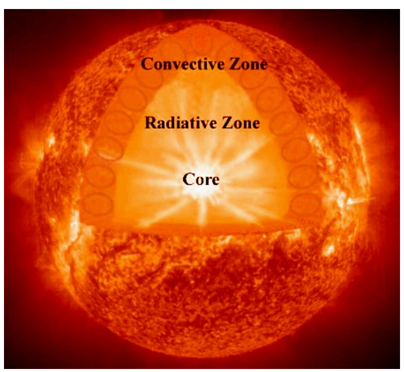


Earth and super earths
Properties of minerals and metals



Jovian Planets
Water and hydrogen



Stellar physics
Fe opacity and H spectra

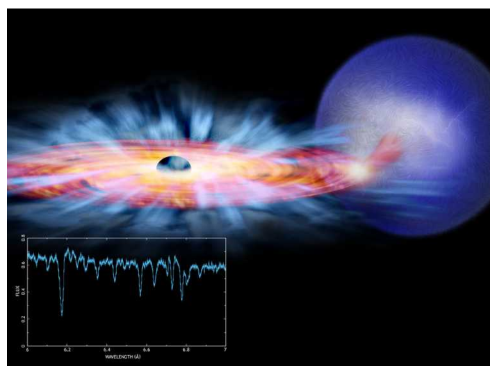


Photo-ionized plasmas
Range of ionization param. ξ

- 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

A high throughput megabar-class accelerator, THOR is under construction

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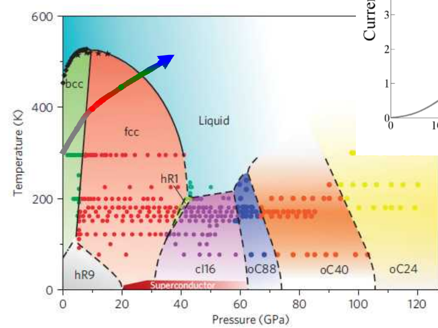
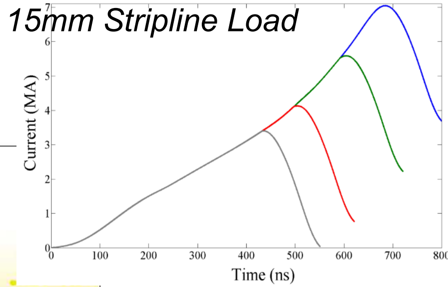
- Improved repetition rate allows systematic study of rate dependent phenomena
  - Phase transitions
  - Kinetics of melt and re-freeze under ramp compression
  - Strength, including phase transitions
  - Effect of ,eg, grain size and texture for phase-kinetics and strength
- Collaboration Focus

Peak Ramp Compression States in Li

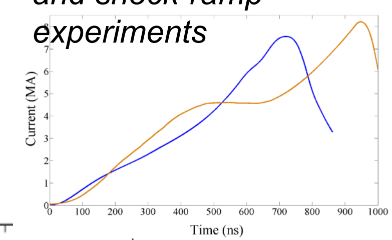


Design Currents for a 15mm Stripline Load

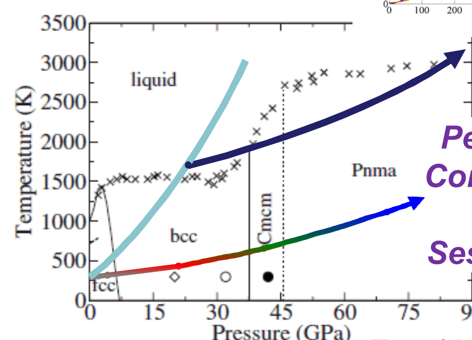


Guillaume, et al. , Nature Physics, 2011

Design Currents for ramp and shock-ramp experiments



Phase space accessible in Ca

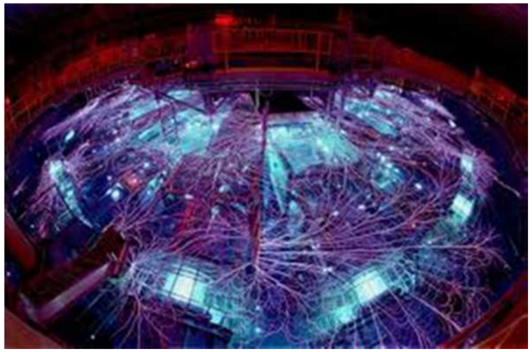


Shock-Ramp Example

Peak Ramp Compression States Sesame 2030 EOS

Teweldeberhan and Bonev, PRB, 2008

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 dynamic materials questions
- There are many opportunities to contribute to on-going programs
- 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

Deuterium equation of state is an active area of research

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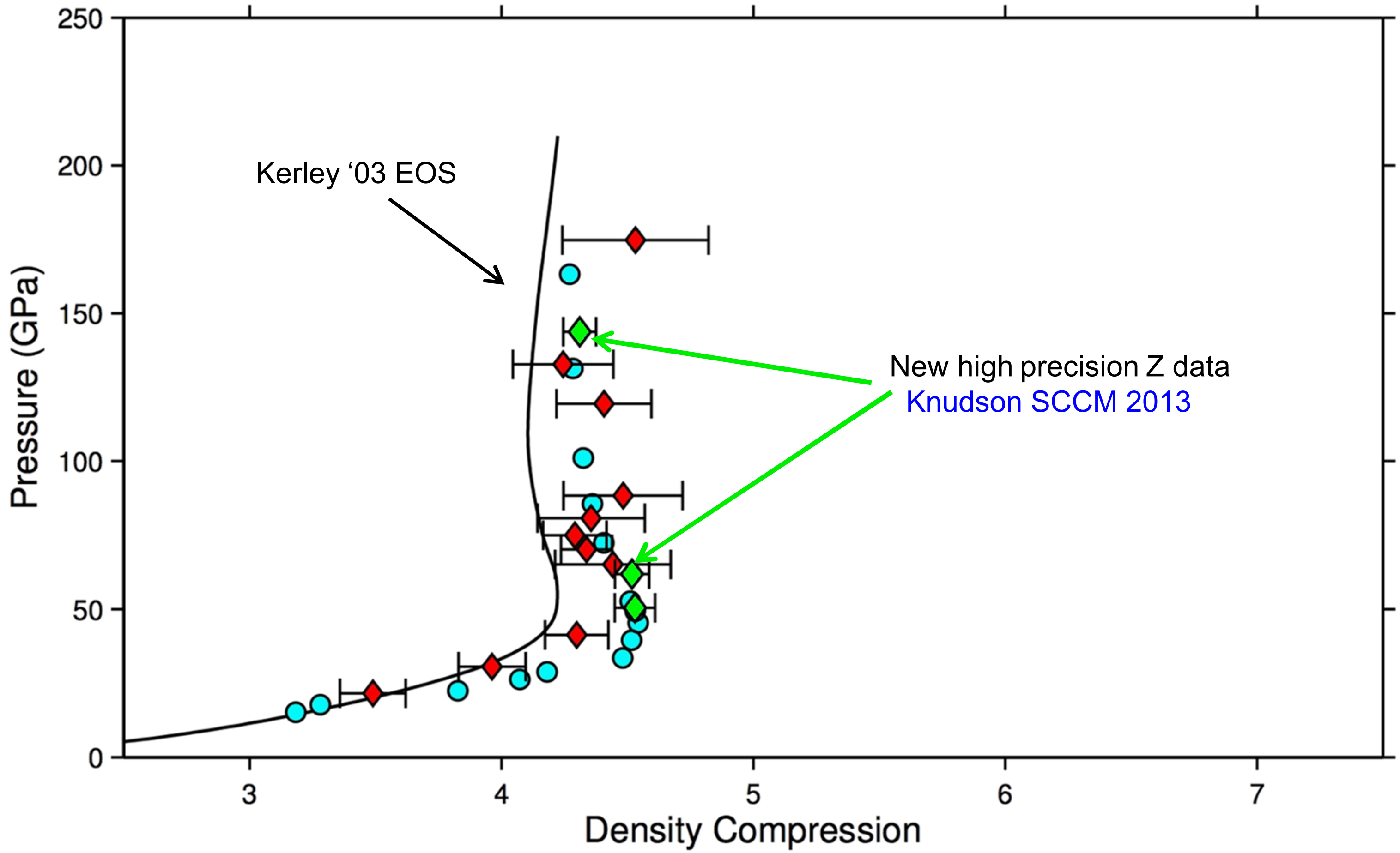

M. D. Knudson *et al.*, Phys. Rev. Lett. **87**, 225501 (2001)
M. P. Desjarlais, Phys. Rev. B **68**, 064204 (2003)

Newer AIMD based EOS, e.g. Holst *et al.*, PRB 2008; Caillabet *et al.*, PRB 2011; Morales *et al.*, HEDP 2012, are in good agreement with Z data

See McMahon *et al.*, Rev. Mod. Phys. **84**, 1607 (2012) for a recent review on H and He

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Experiment Design/Analysis

Marcus Knudson

Ray Lemke

Kyle Cochrane

Devon Dalton

Dustin Romero

Z operations team

Z Fundamental Science Program

Call for proposals in June 2015

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

QMD Calculations

Mike Desjarlais

Andreas Becker

Winfried Lorenzen

Ronald Redmer

Diagnostics

Charlie Meyer

Jeff Gluth

Devon Dalton

Anthony Romero

Dave Bliss

Alan Carlson

Planetary Modeling

Nadine Nettelmann

Andreas Becker

Ronald Redmer

Pulse Shaping

Ray Lemke

Jean-Paul Davis

Mark Savage

Ken Struve

Keith LeChien

Brian Stoltzfus

Dave Hinshelwood

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

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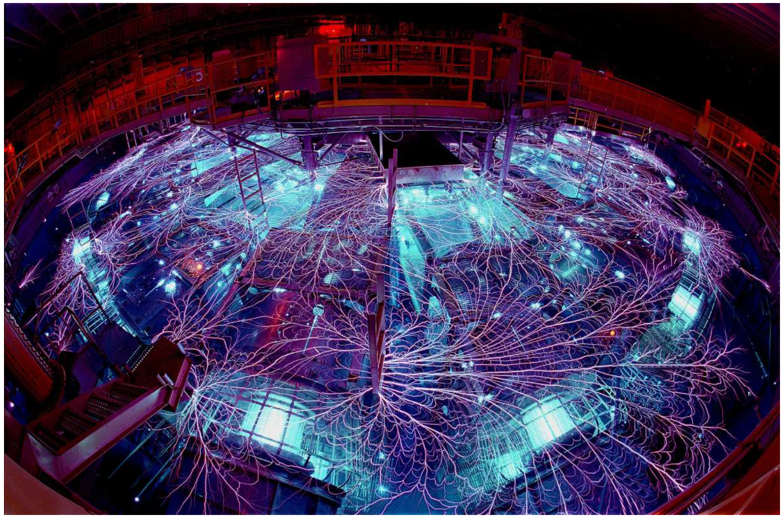

Backups

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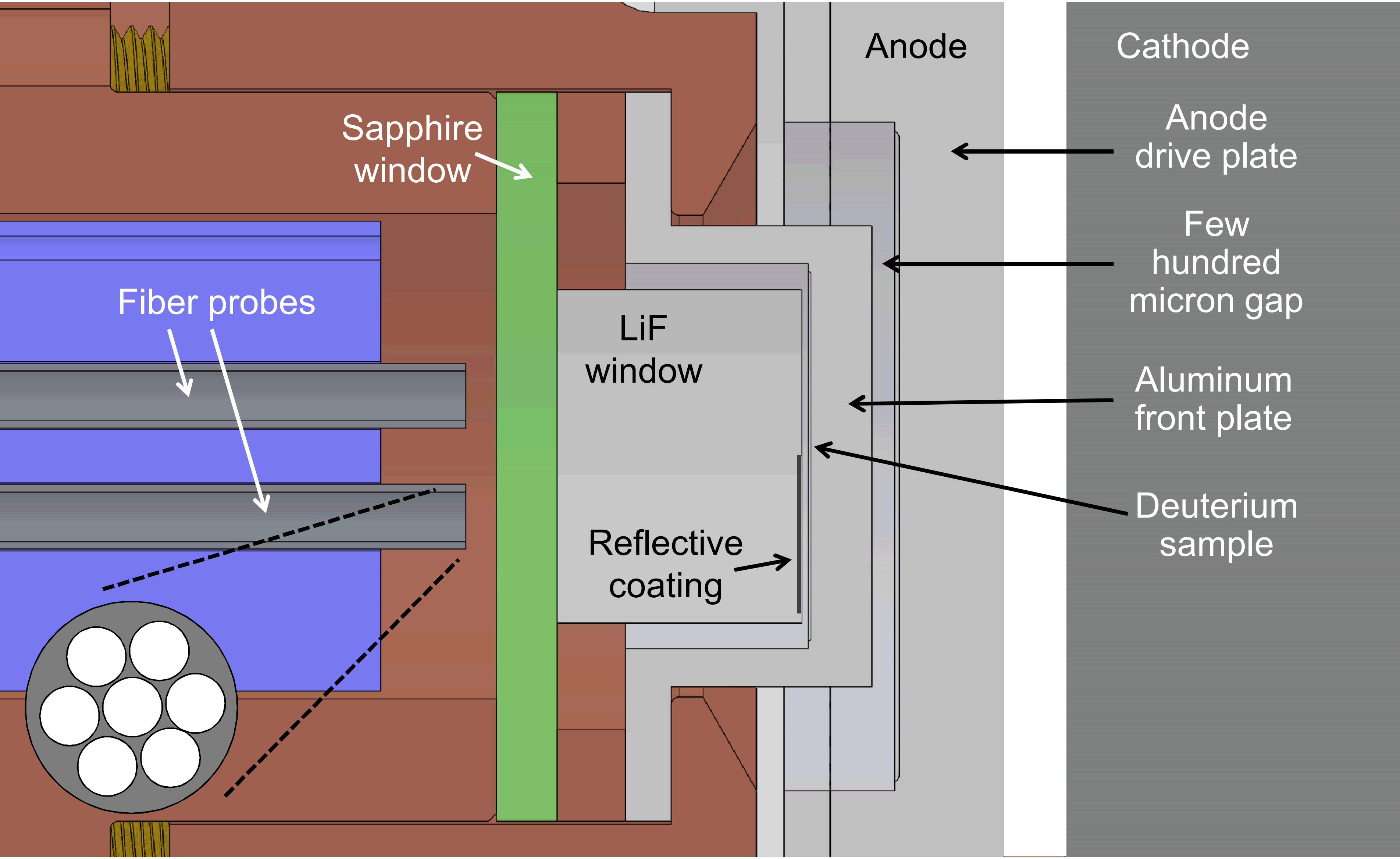
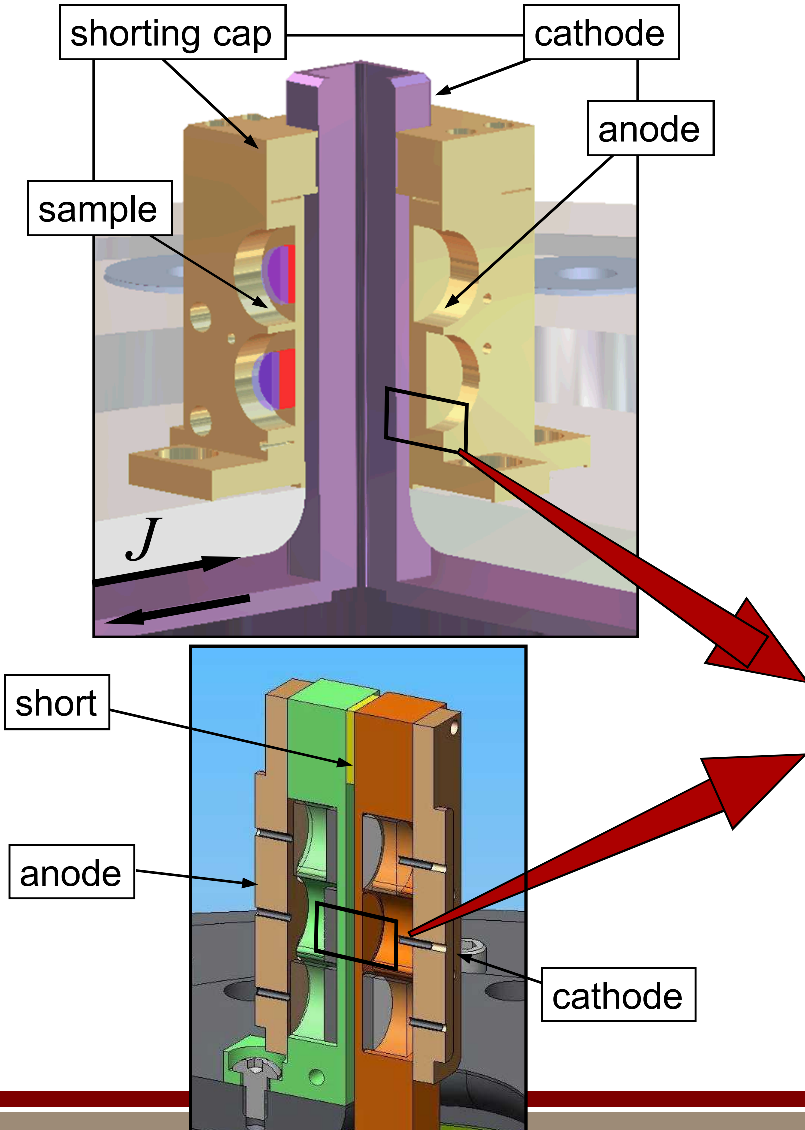
The experimental design allows for multiple diagnostics – tracking the shock-ramp compression of deuterium



Magnetic compression on Z produces smooth ramp loading to ultra-high pressures



- pulse of electric current through experimental load (shorted at one end) induces magnetic field
- *J´B* magnetic force transferred to electrode material