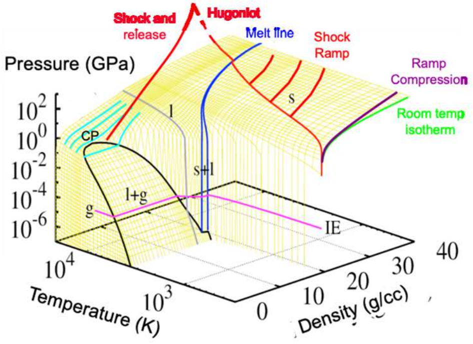
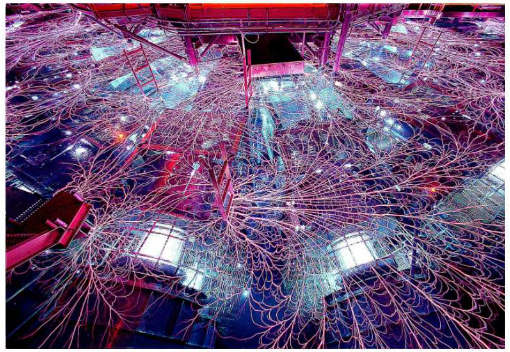
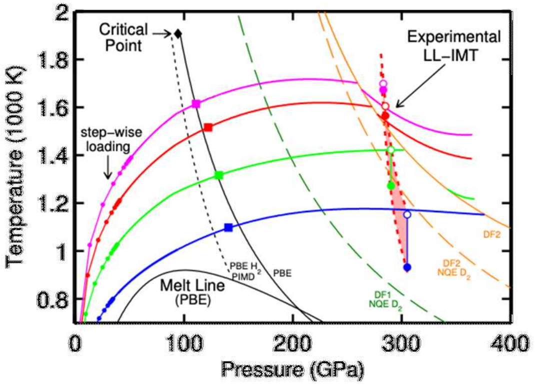
SAND2020-XXXX

SAND2020-0229C

Dynamic Materials Program at Z







PRESENTED BY

Marcus D Knudson

ZNetUS Workshop
6-8 January 2020 in La Jolla, CA, USA

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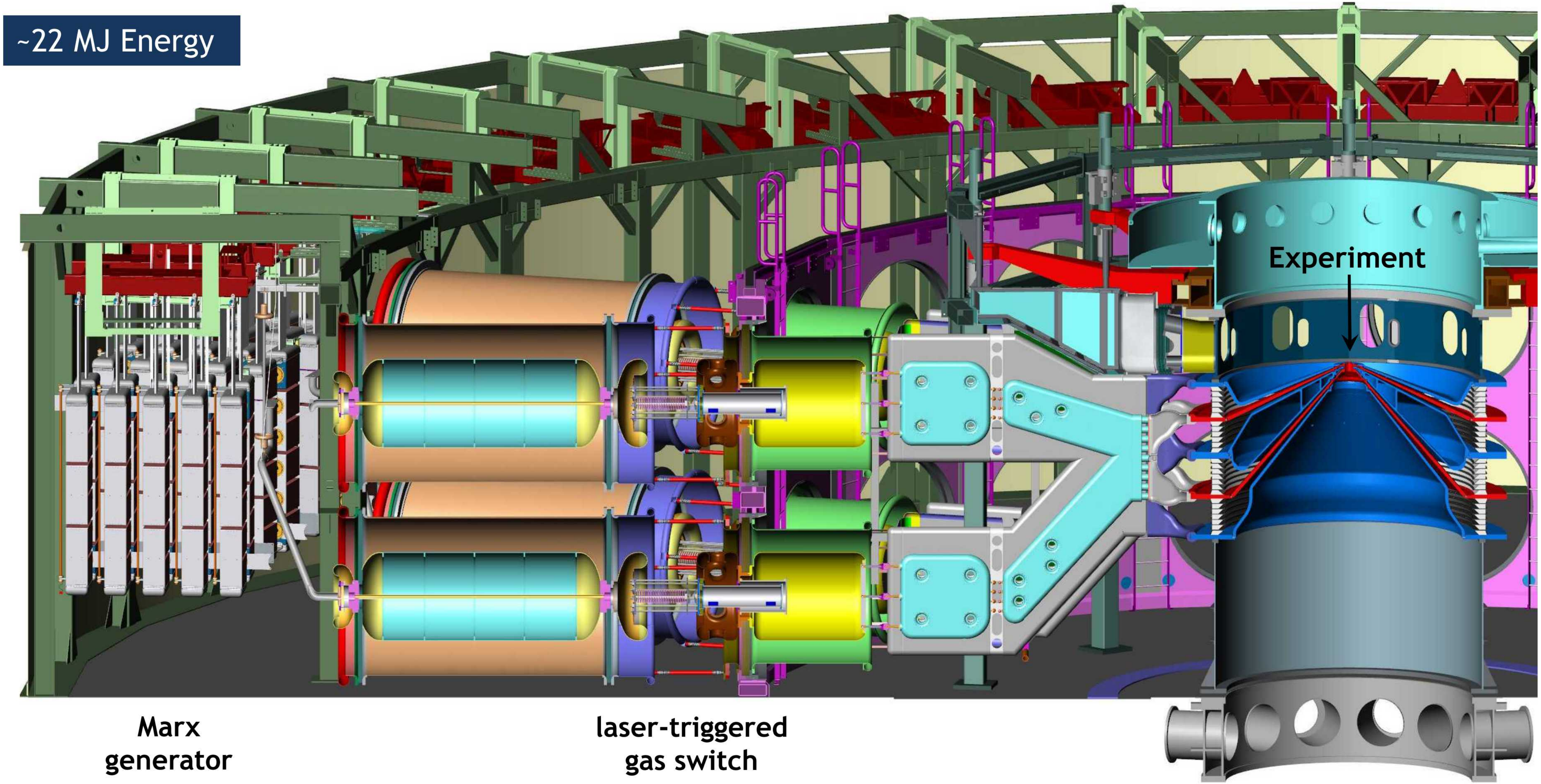
Pulsed Power

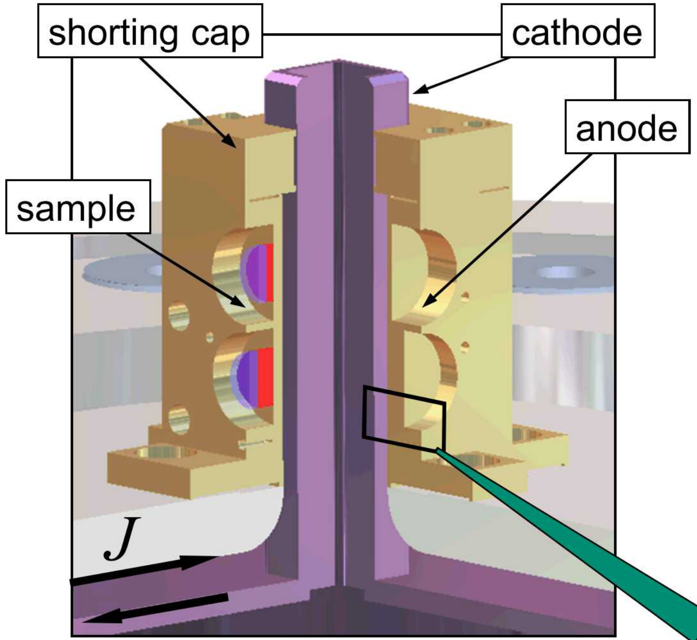
~22 MJ Energy

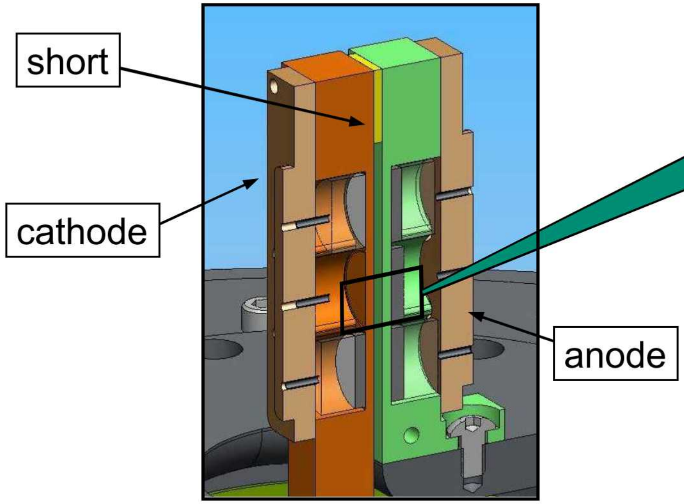


Marx generator

laser-triggered gas switch

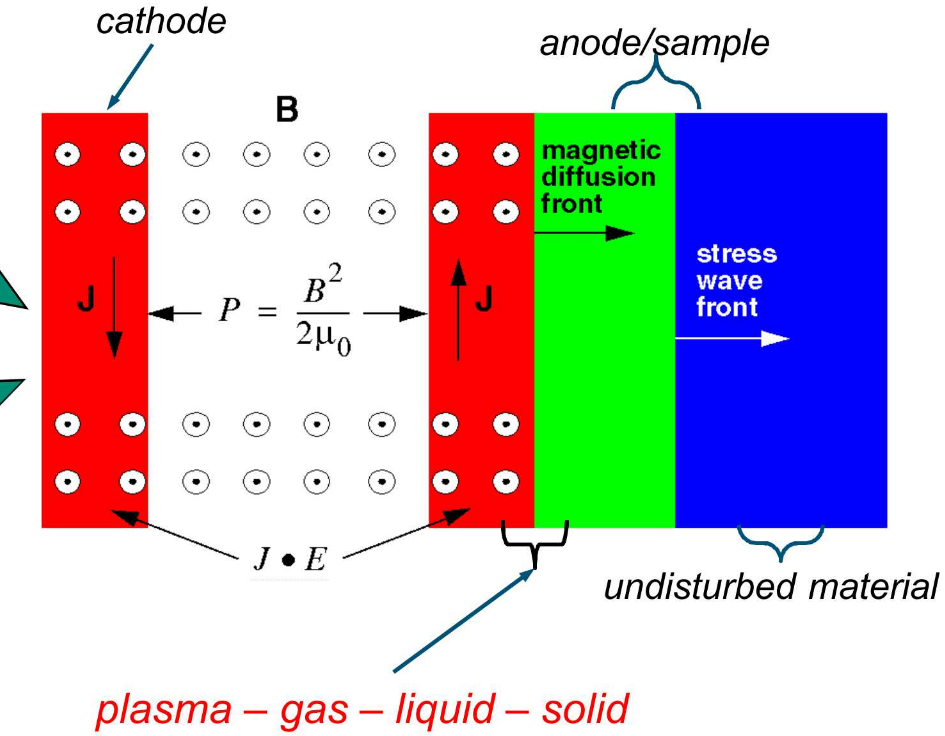
Pulsed Power

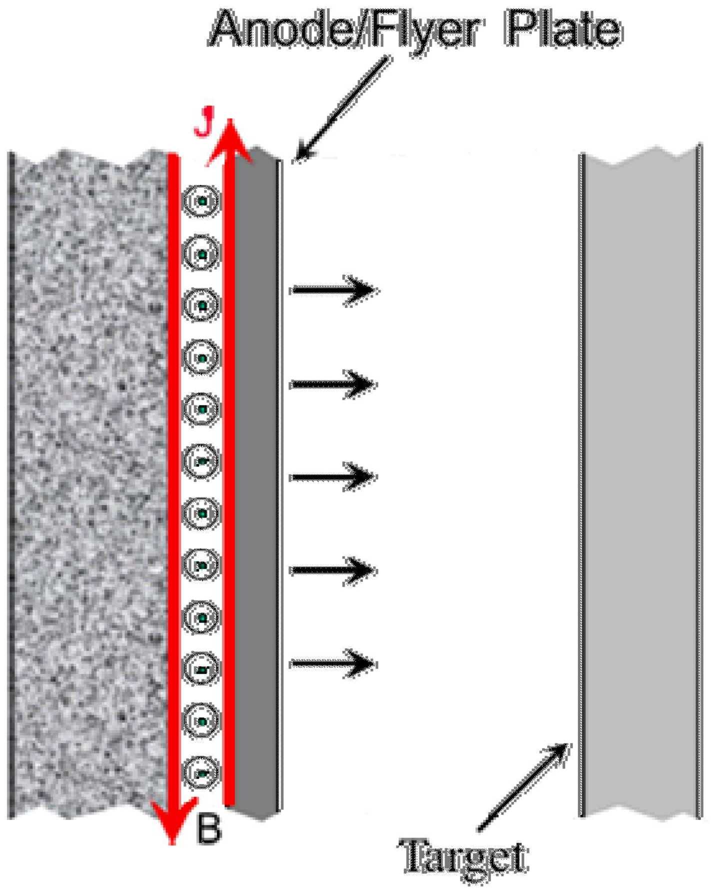




Pulse of electric current through rectangular coaxial electrodes (shorted at one end) induces magnetic field

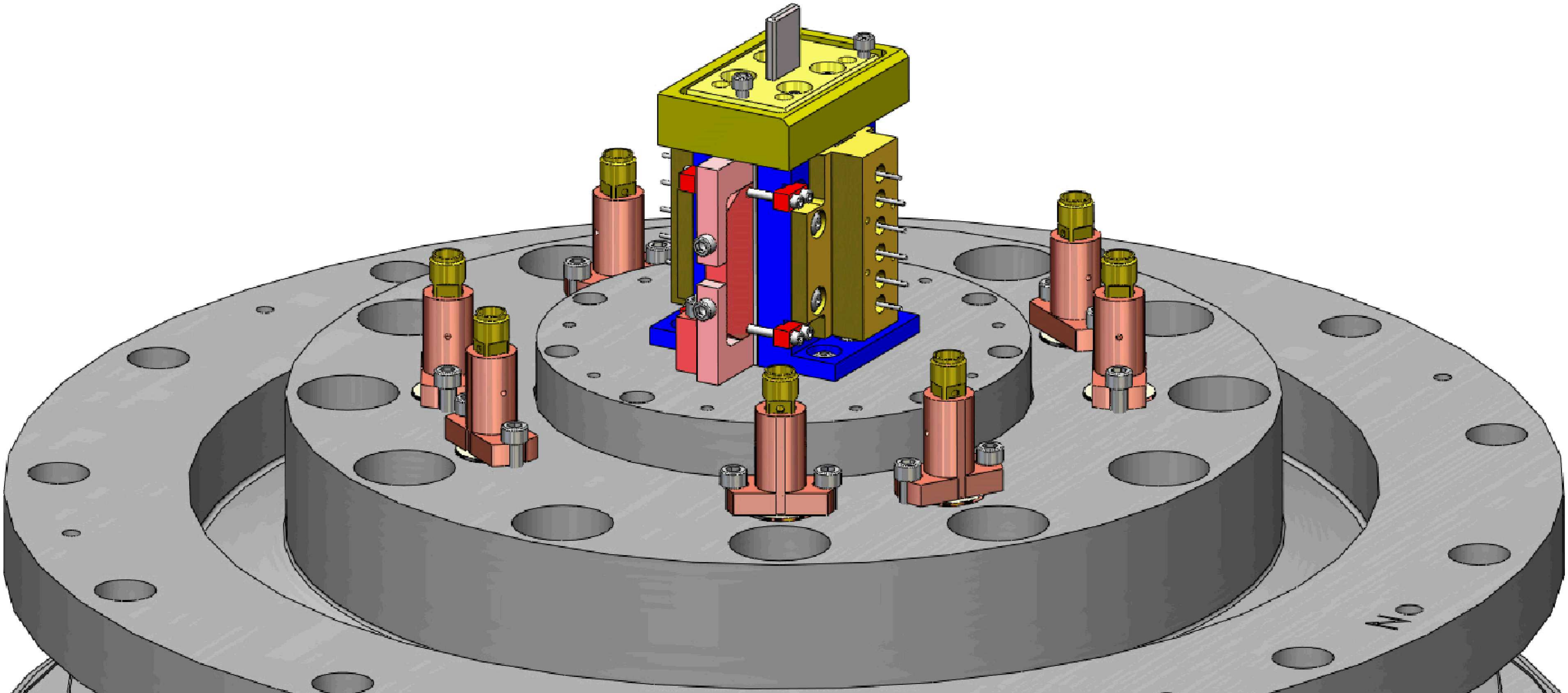
$J \times B$ magnetic force transferred to electrode material



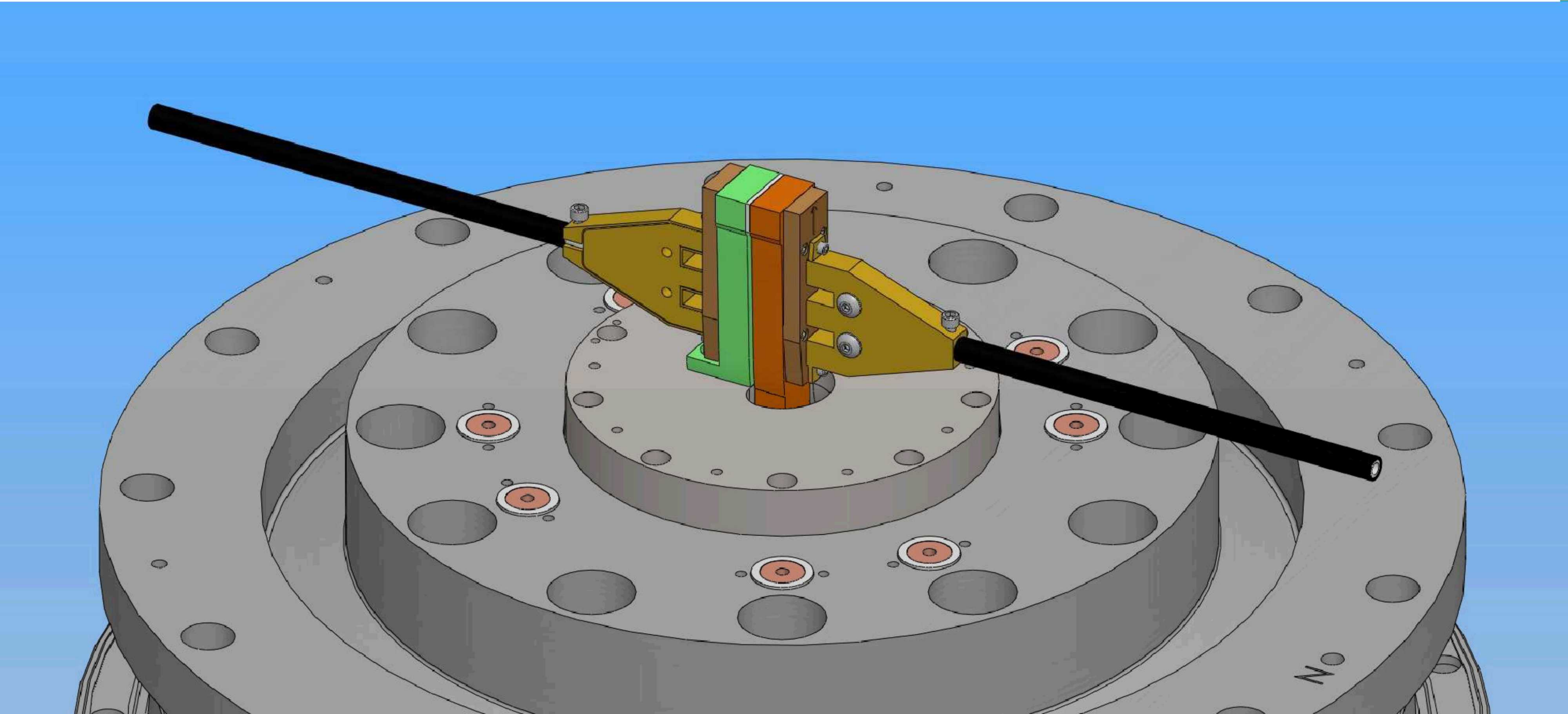


Hypervelocity flyer plate platform on the Sandia Z Machine

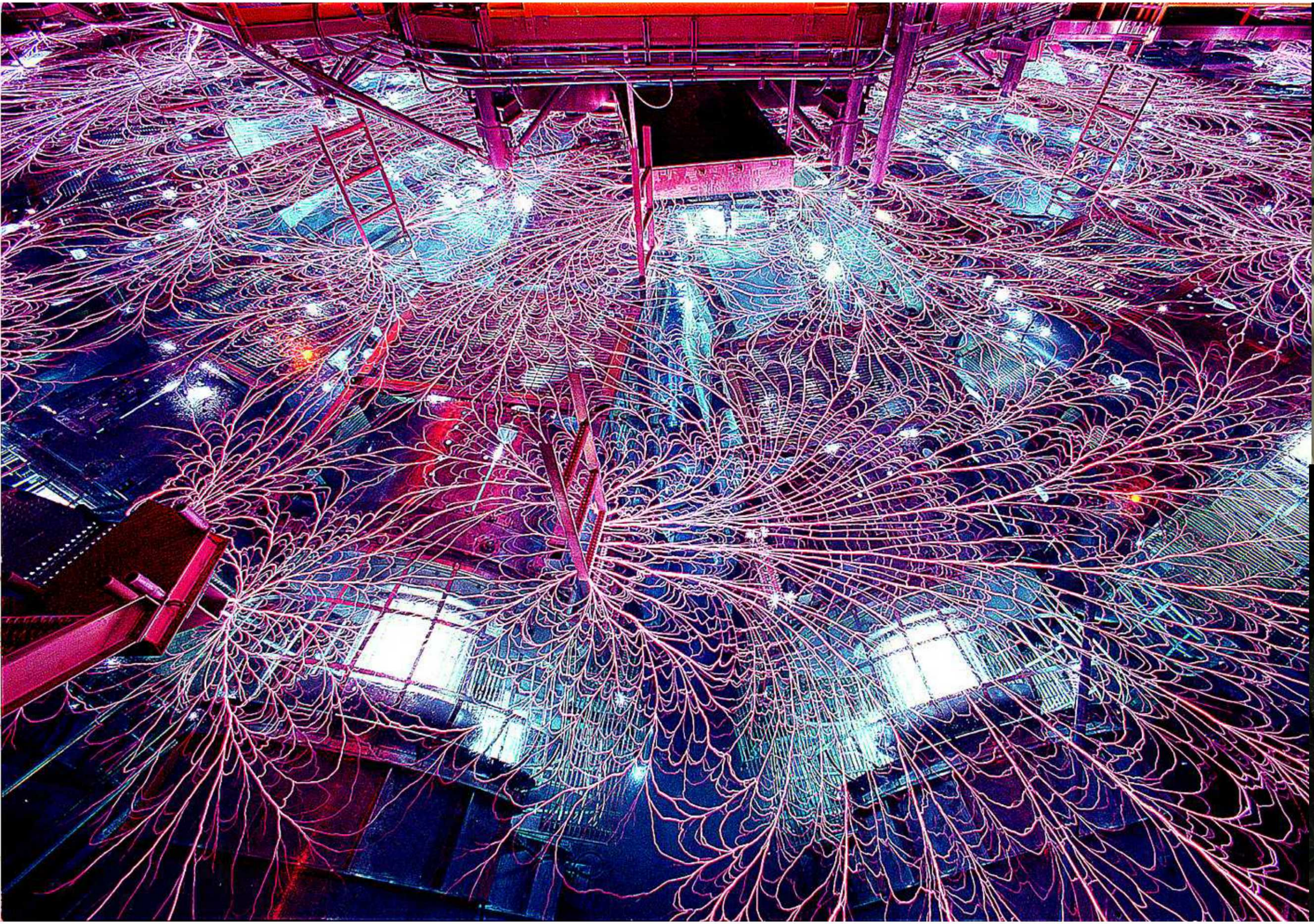
Typical coaxial load on Z

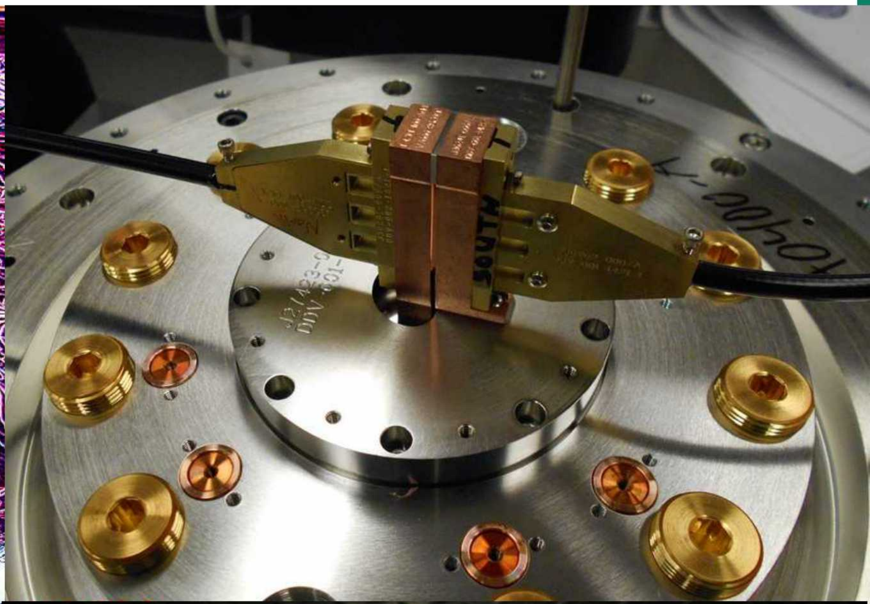


Typical stripline load on Z

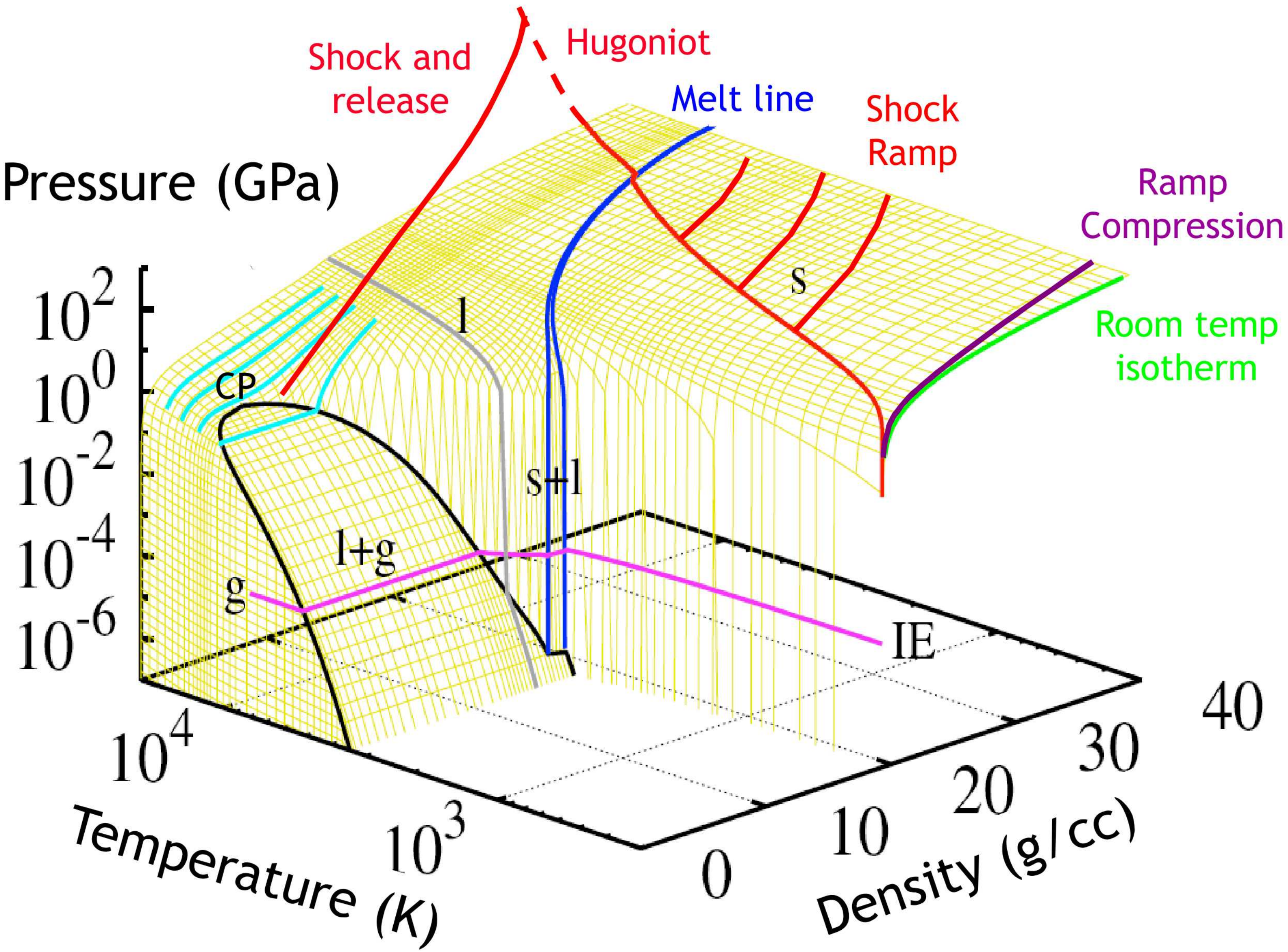


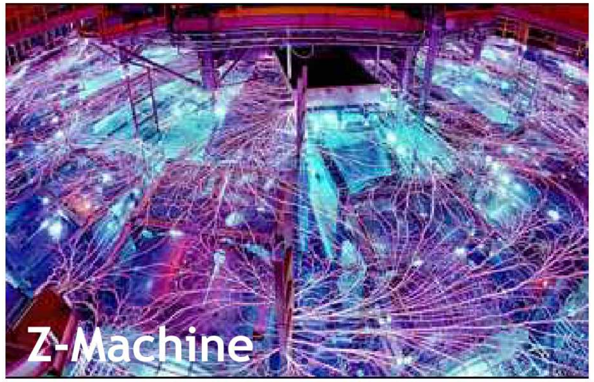
Pulsed Power

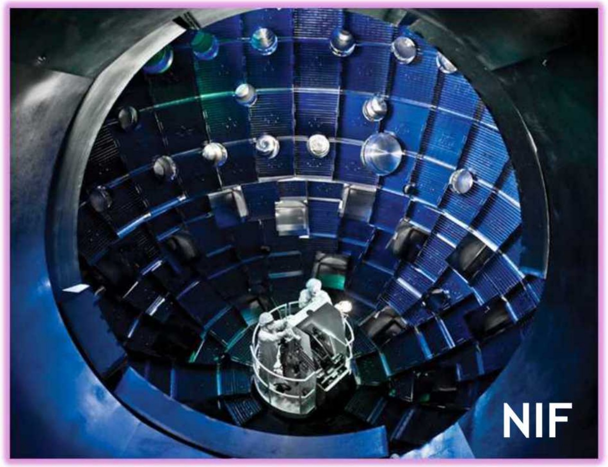




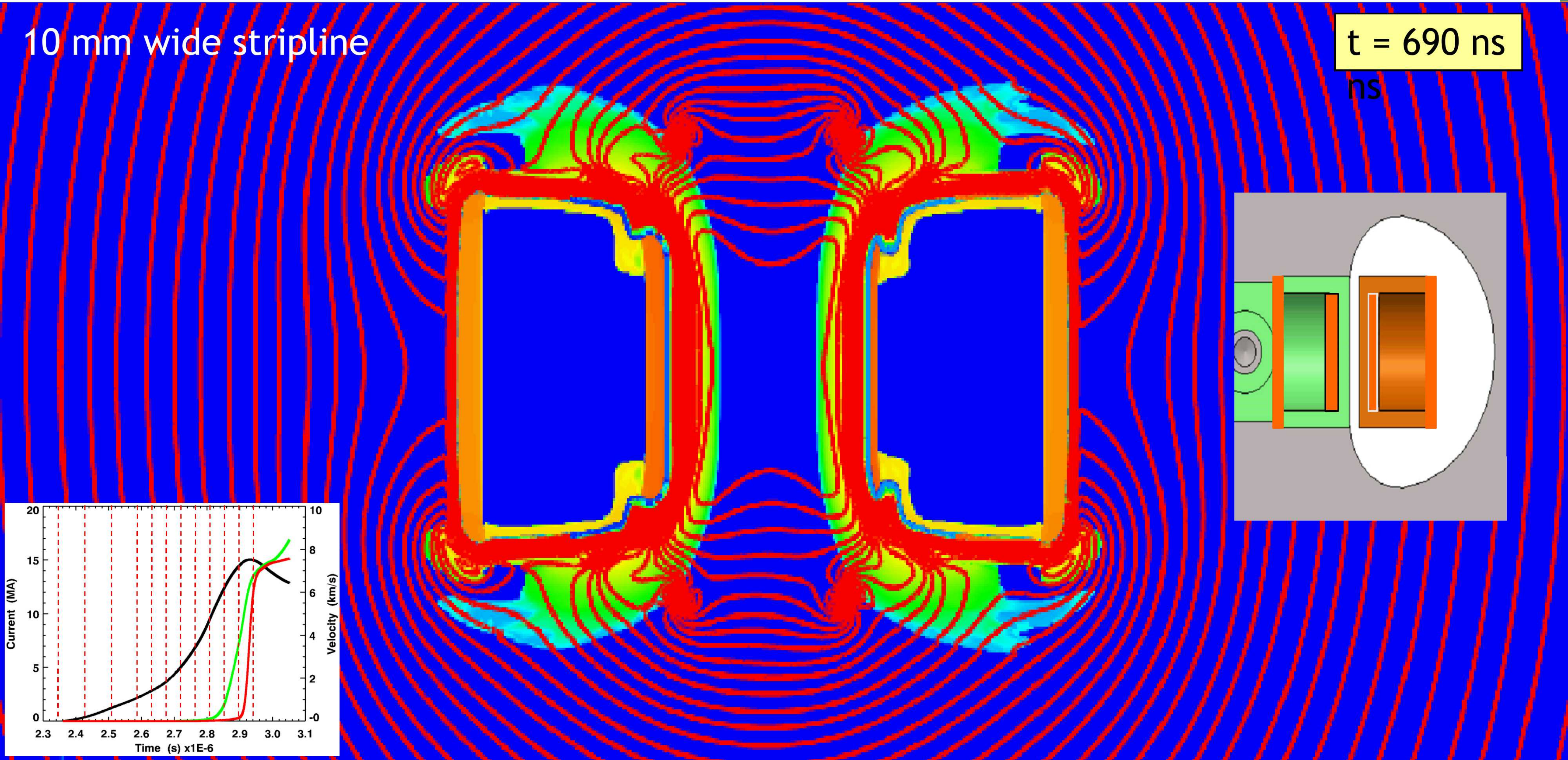
Advanced experimental platforms







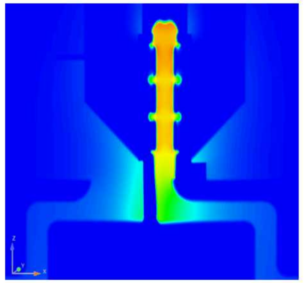
Fully self-consistent, 2D MHD simulations required



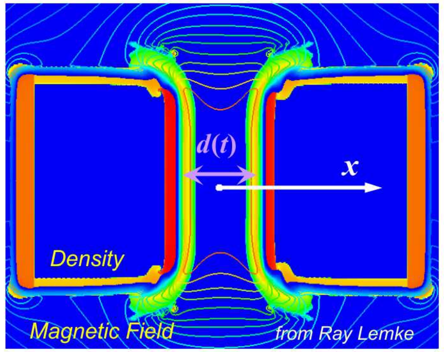
Integration of theory, computation, and experiment required

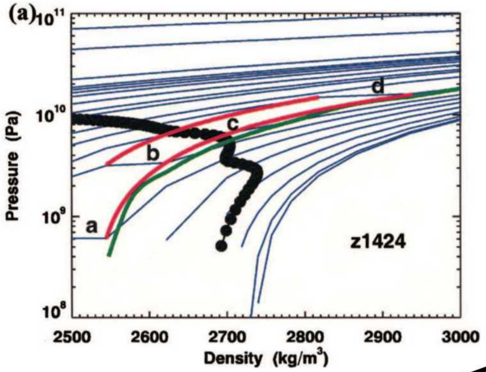
ALEGRA ...
The Shock and Multiphysics Family of Codes

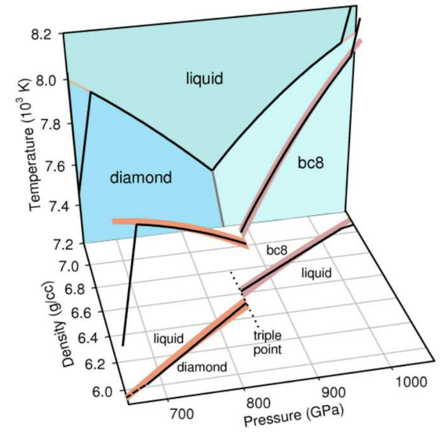
DAKOTA

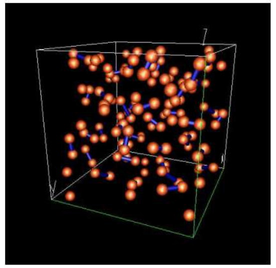


$$\sigma_{\mathbf{k}}(\omega)=\frac{2\pi e^2\hbar^2}{3m^2\omega\Omega}\sum_{\alpha=1}^{3}\sum_{j=1}^{N}\sum_{i=1}^{N}(F(\varepsilon_{i,\mathbf{k}})-F(\varepsilon_{j,\mathbf{k}}))\left|\left\langle\Psi_{j,\mathbf{k}}\left|\nabla_{\alpha}\right|\Psi_{i,\mathbf{k}}\right\rangle\right|^2\delta(\varepsilon_{j,\mathbf{k}}-\varepsilon_{i,\mathbf{k}}-\hbar\omega)$$

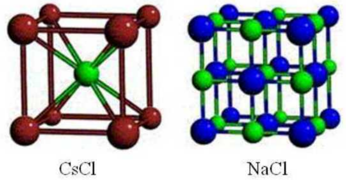


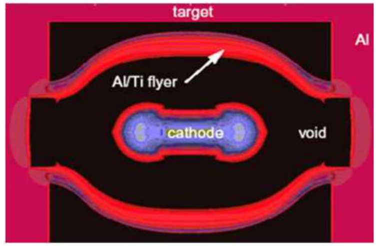


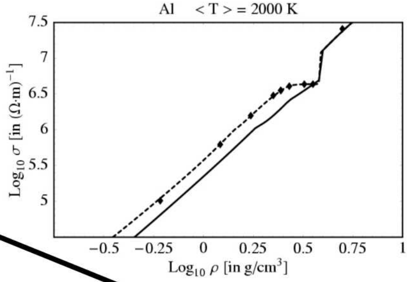


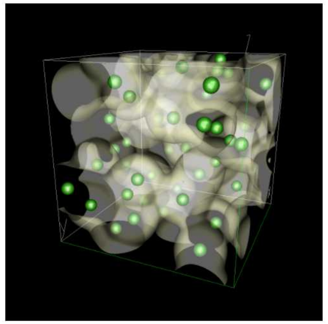


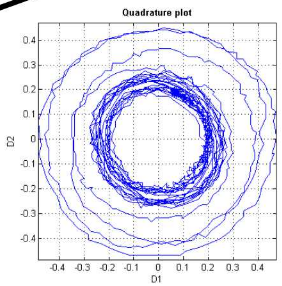
Vienna Ab-initio Simulation Package

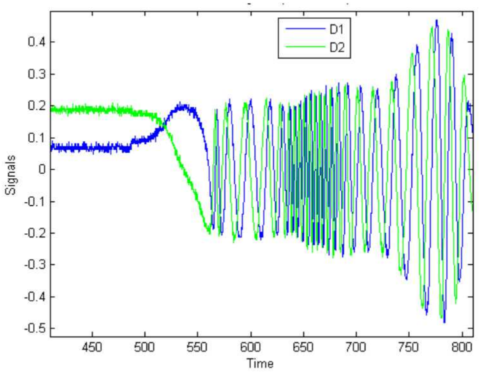


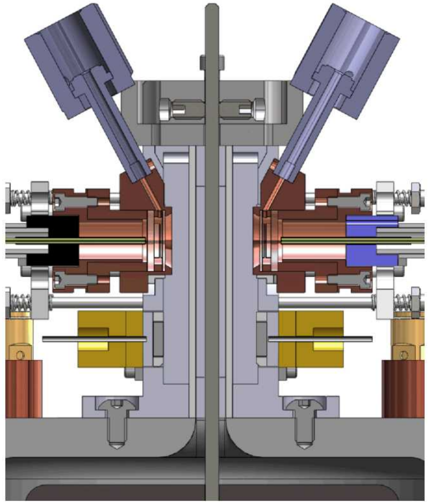


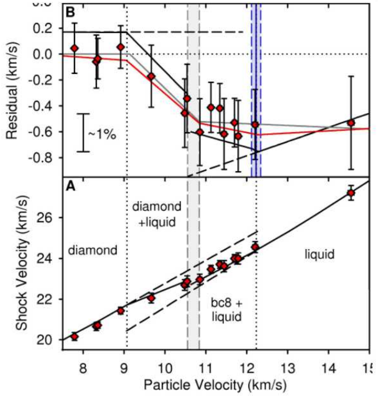


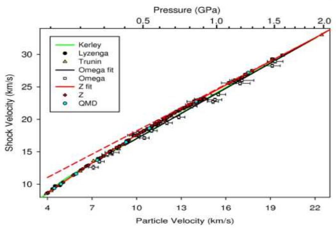






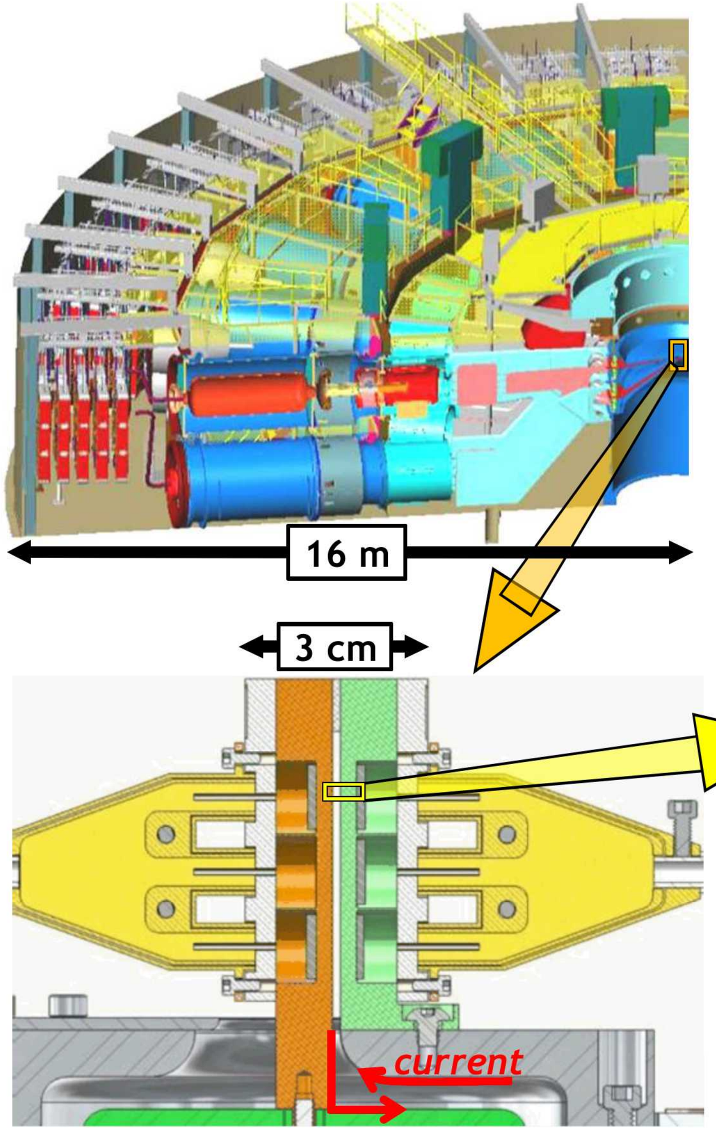






Stripline short-circuit loads on the Z machine can produce planar shockless compression of solids to 400+ GPa

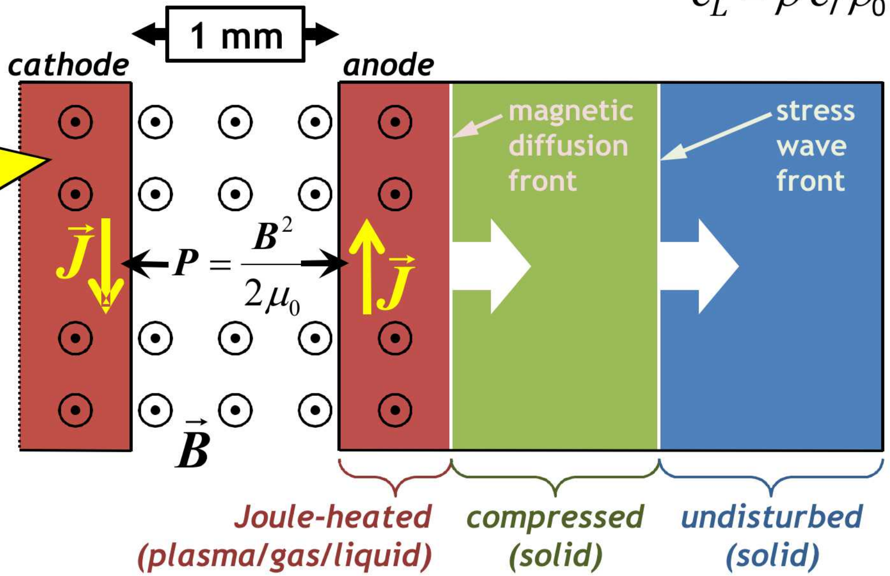
- current pulse of 7-26 MA delivered to load
- controllable pulse shape, rise time 100-1500 ns
- stripline = parallel flat-plate electrodes shorted at one end, identical loading of sample pairs
- magnetic ($\boldsymbol{J}\times\boldsymbol{B}$) force induces ramped stress wave in electrode material
- stress wave propagates into ambient material, de-coupled from magnetic diffusion front

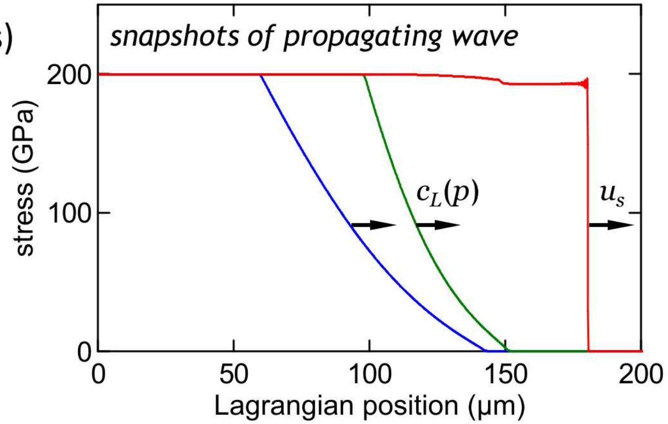


- sound speed c increases with pressure (normal materials)
- ramp steepens into a shock

$$c^2 = (\partial P/\partial \rho)_s$$

$$c_L = \rho\, c/\rho_0$$





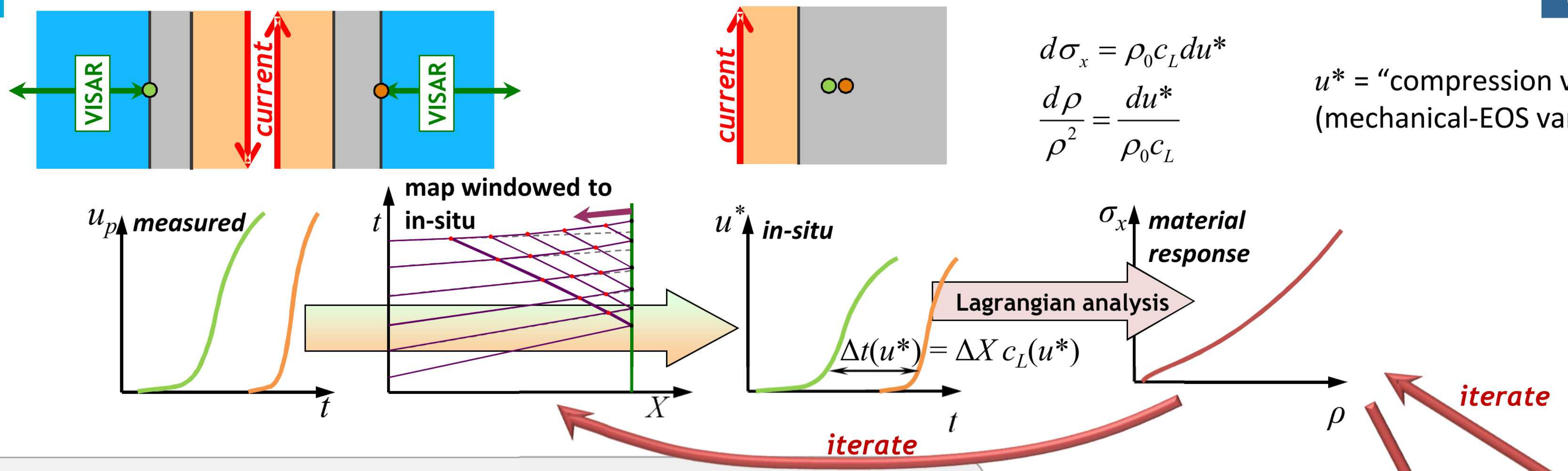
principal Hugoniot

principal isentrope (dS = 0)

RTP

Lagrangian analysis can extract compressibility

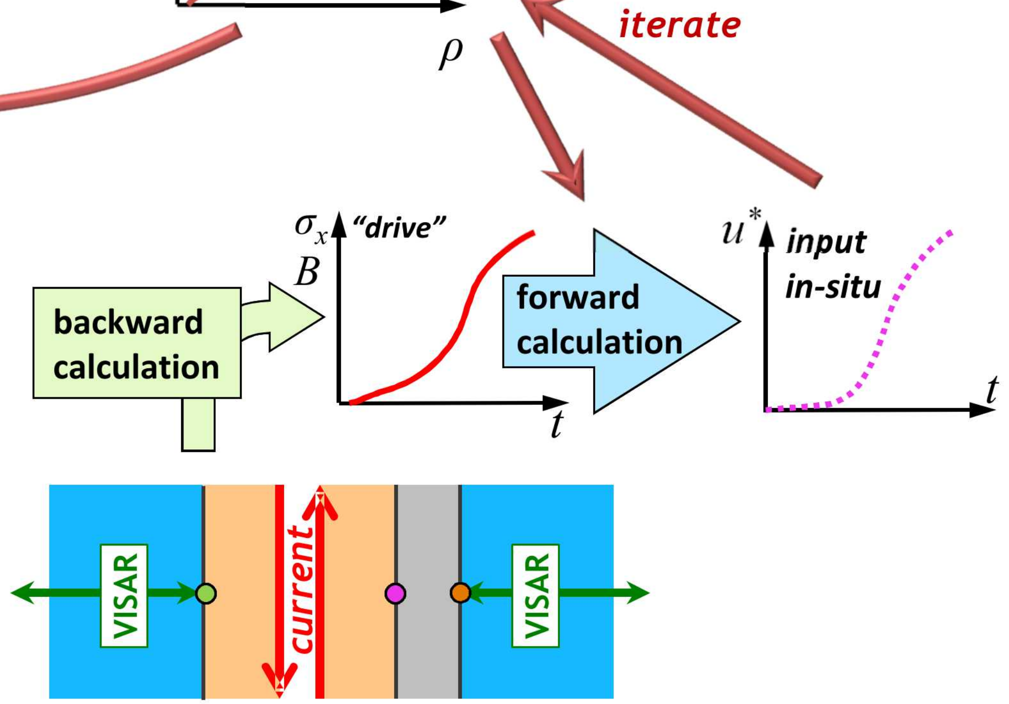
Ramp



$$d\sigma_x = \rho_0 c_L du^*$$

$$\frac{d\rho}{\rho^2} = \frac{du^*}{\rho_0 c_L}$$

u^* = “compression velocity” (mechanical-EOS variable)



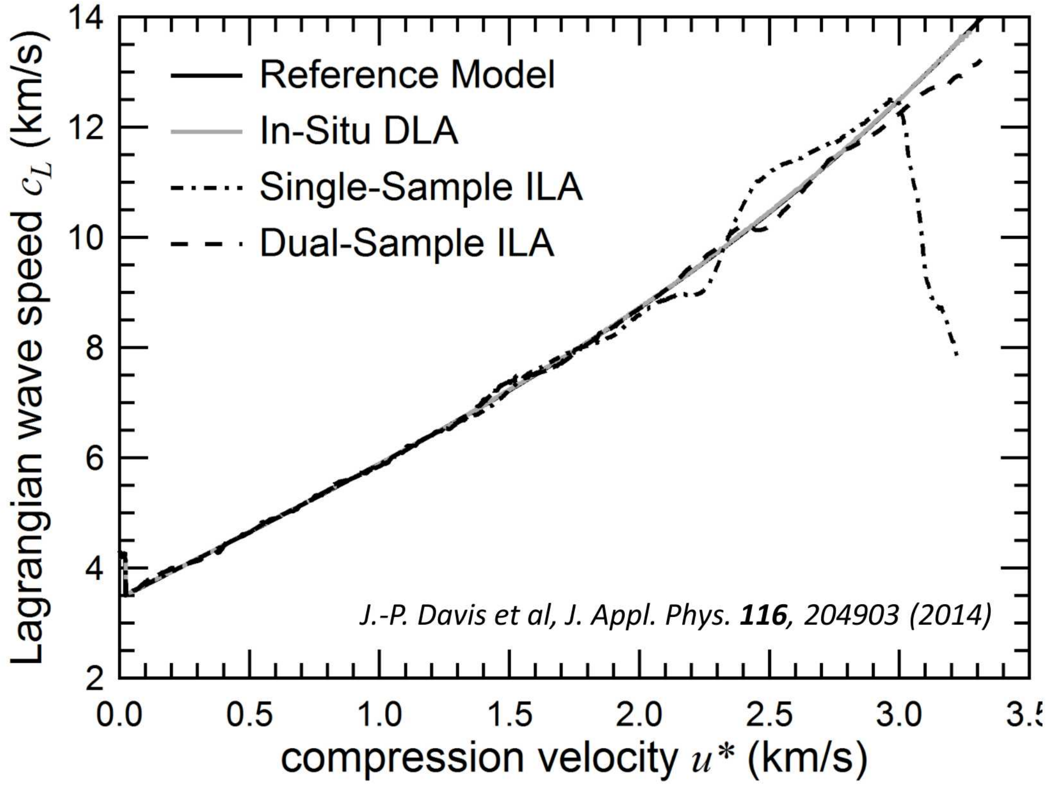
Single-sample approach

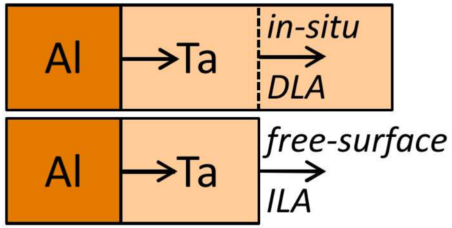
- in-situ measurements → Direct Lagrangian Analysis (DLA)
- real measurements are free-surface or window-interface
  - <u>map measured $u(t)$ into in-situ $u^*(t)$</u>, then apply DLA
  - **shockless compression:** map by iterative characteristics technique[1]
    - referred to as **Iterative Lagrangian Analysis (ILA)**
  - <u>single-sample</u>: use “zero-thickness” sample velocity from drive
    - *deduce B-field from drive velocity using 1-D MHD simulation*
    - *outer-loop iteration of simulating electrode/sample velocity*
    - ***advantage** = greatly reduce effect of thickness uncertainty*
    - ***advantage** = amenable to forward-only analysis (optimize models)*
    - ***disadvantage** = requires accurate electrode models, code physics*

[1] *S. D. Rothman & J. Maw, J. Physique IV **134**, p745 (2006)*

LiF windows alleviate ILA errors due to elastic sound speed in local regions of decompression for high-strength materials

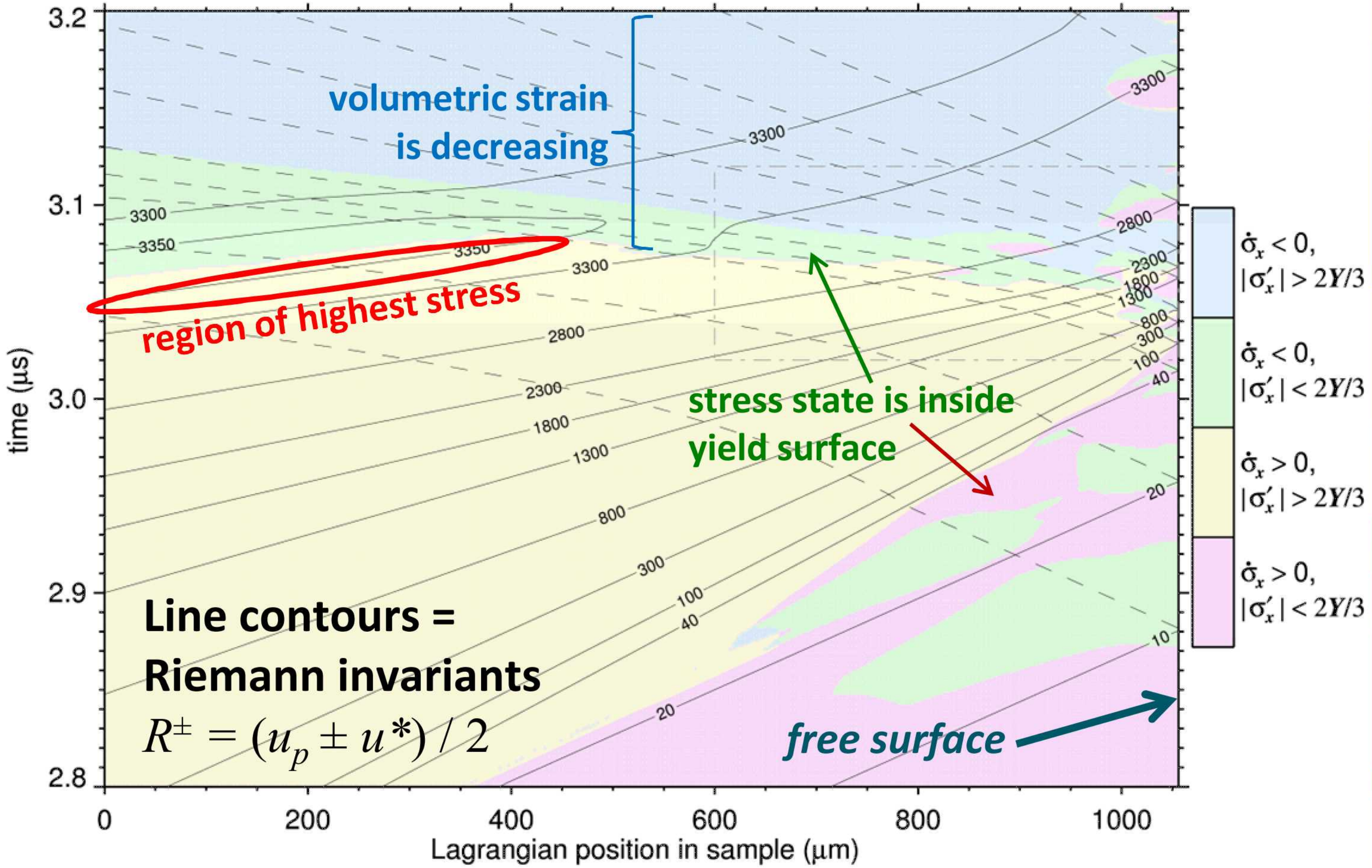
Ramp





Simulations of free-surface Ta experiments

Pulse-shape design can help, but not enough

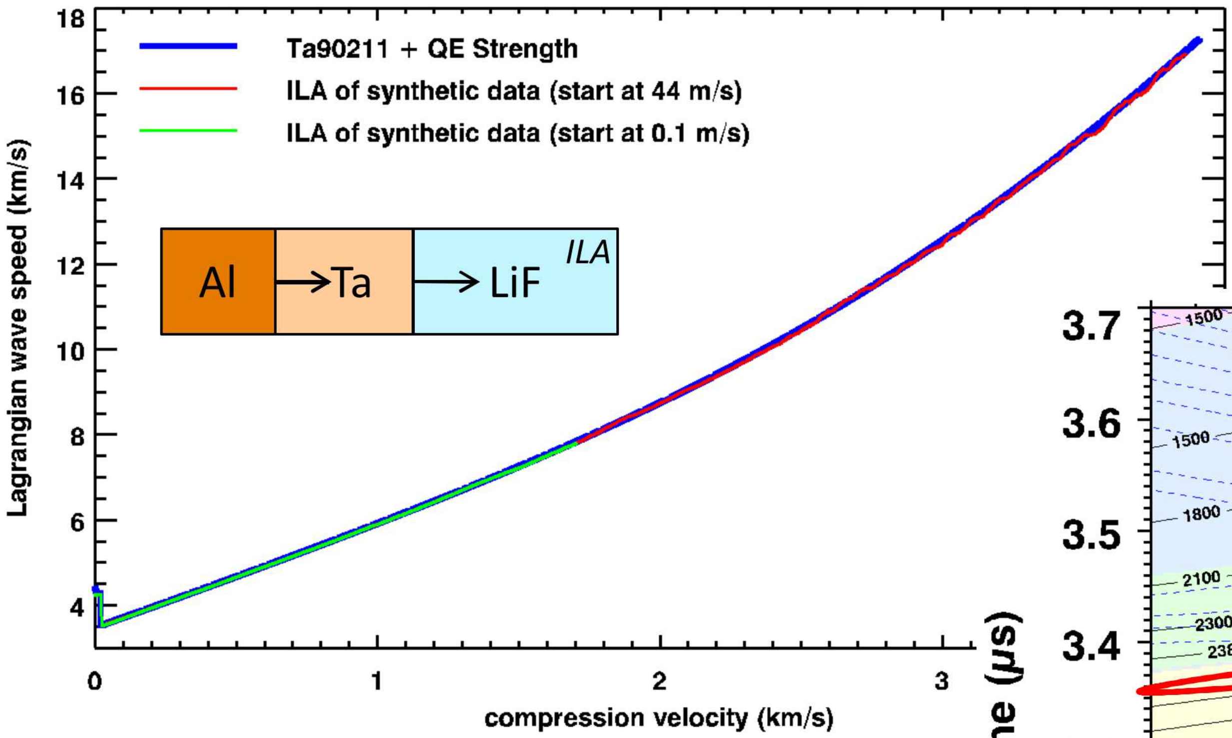


- **Reference model** = Sesame 90210[1] + Steinberg-Guinan fit to ramp-release strength data[2]
- Strength interaction with free surface (ILA)
  - → Localized deviations in apparent $c_L(u^*)$
  - → Partial cancellation in dual-sample case

[1] *C. Greeff et al, AIP Conf. Proc.* ***1195**, 681 (2009)*
[2] *J. L. Brown et al, J. Appl. Phys.* ***115**, 043530 (2014)*

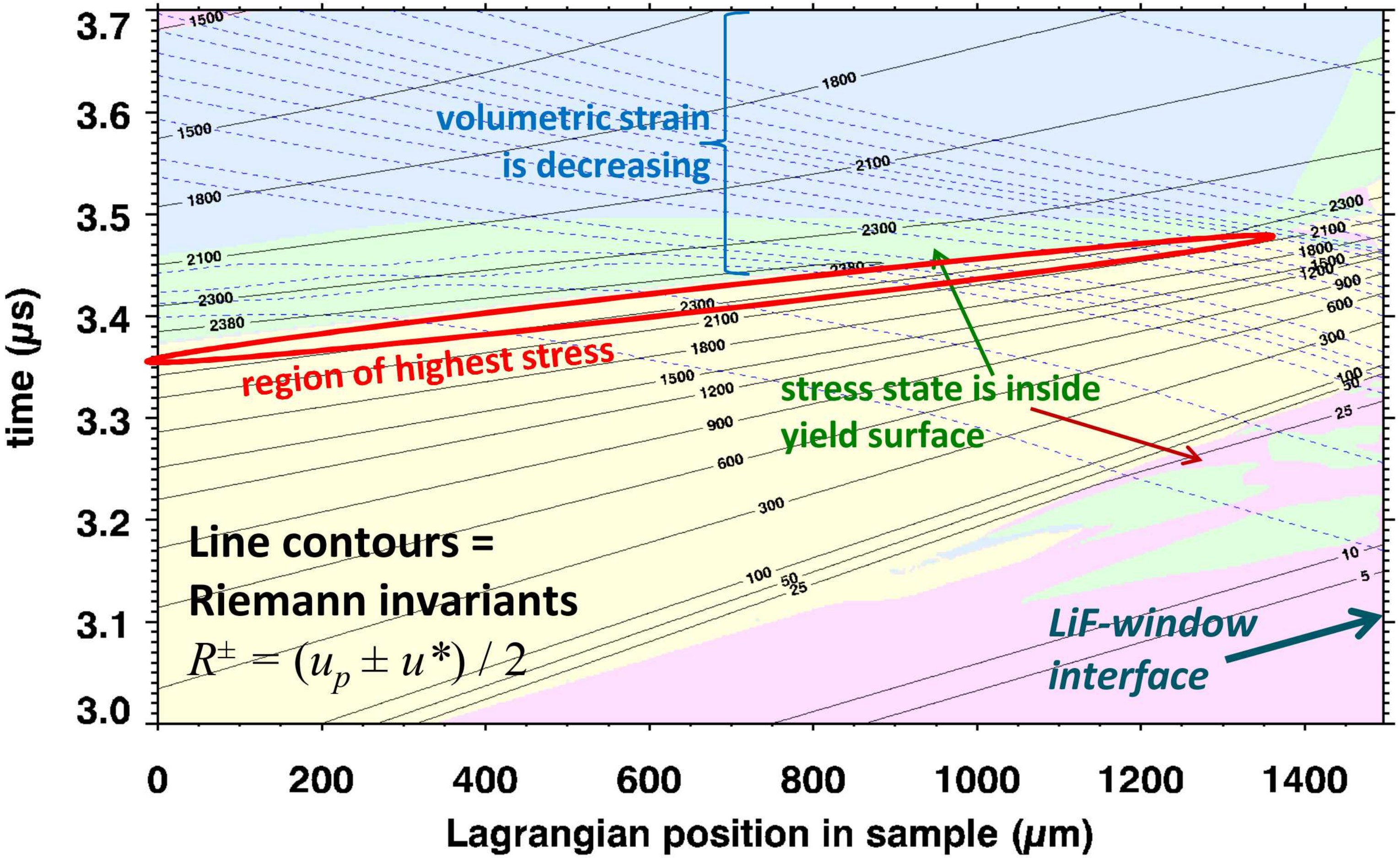
LiF windows alleviate ILA errors due to elastic sound speed in local regions of decompression for high-strength materials

Ramp



Simulations of LiF-windowed Ta experiments

LiF window significantly reduces extent of decompression regions



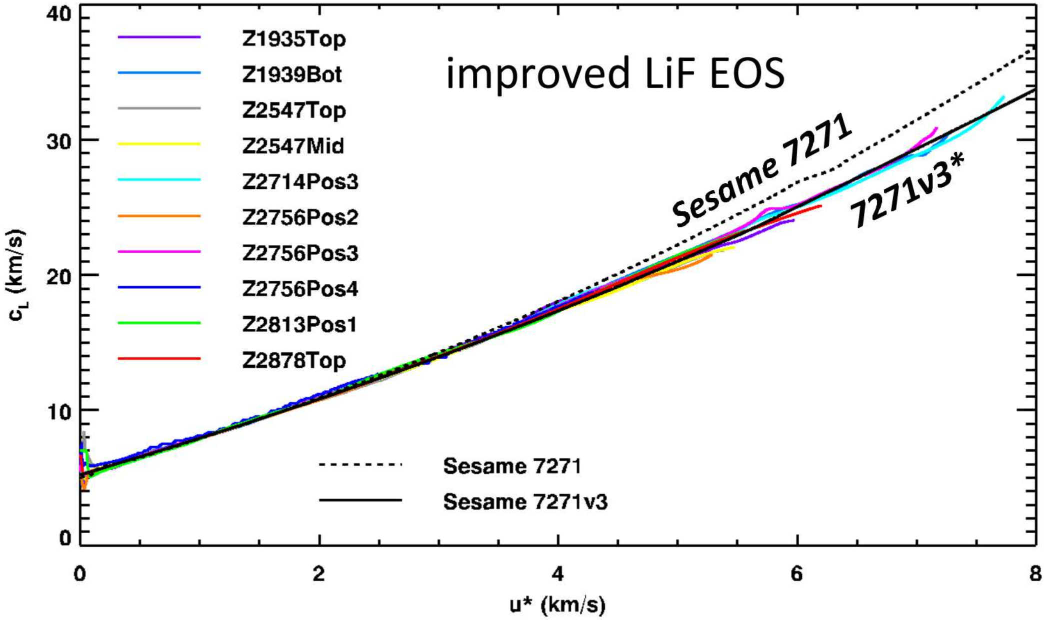
- **Reference model** = Sesame 90210[1] + Steinberg-Guinan fit to ramp-release strength data[2]

[1] *C. Greeff et al, AIP Conf. Proc.* ***1195****, 681 (2009)*

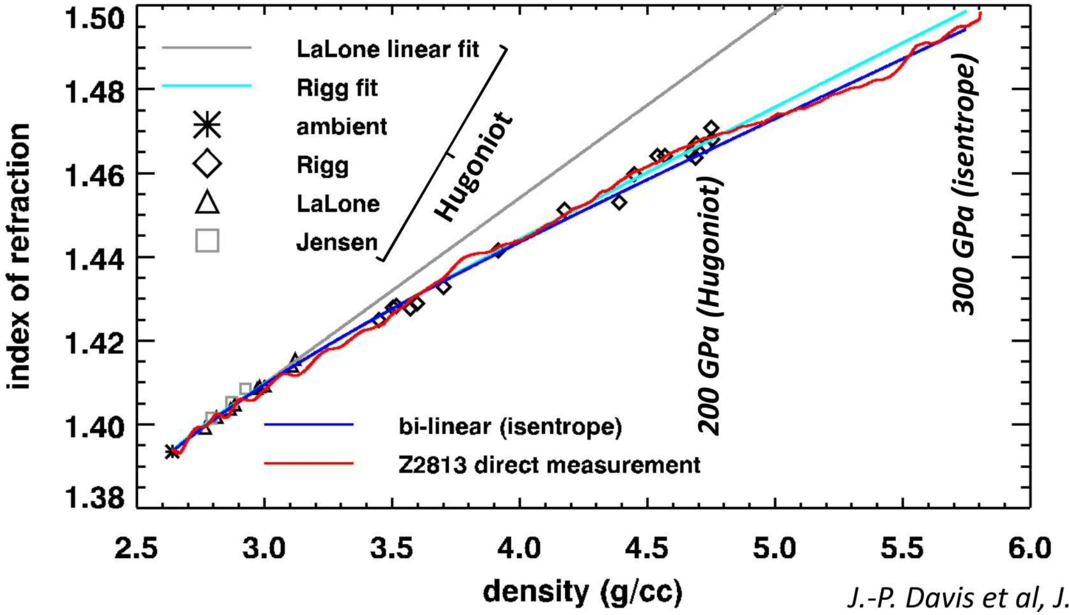
[2] *J. L. Brown et al, J. Appl. Phys.* ***115****, 043530 (2014)*

Results thus far suggest current models for the mechanical and optical response of LiF are adequately accurate

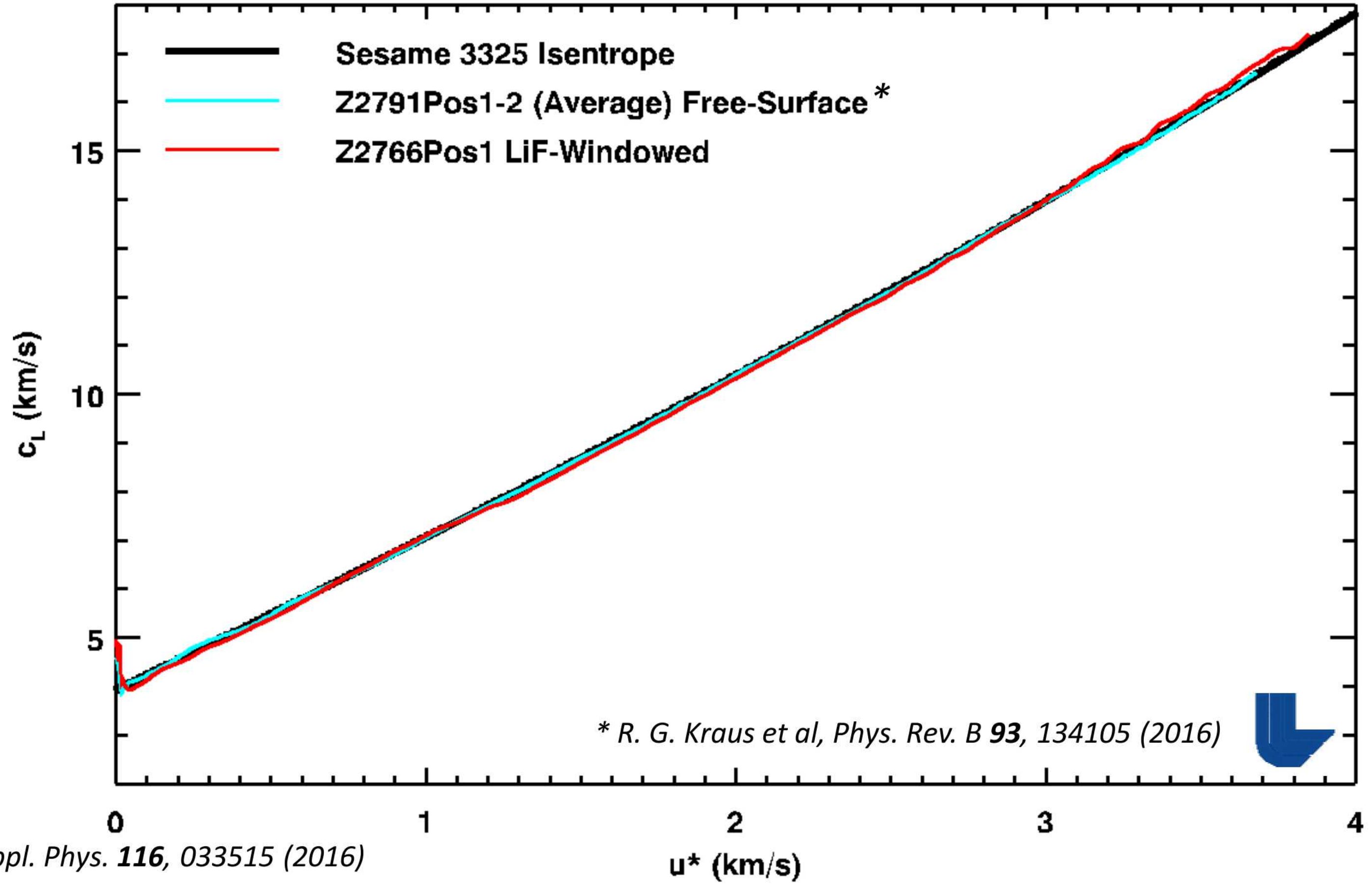
Ramp



- refractive index non-linear in density
- 1-D hydrocode computes $u_{apparent}$ from given u_{true}
- update u_{true} from measured $u_{apparent}$
- iterate until simulation matches measured $u_{apparent}$



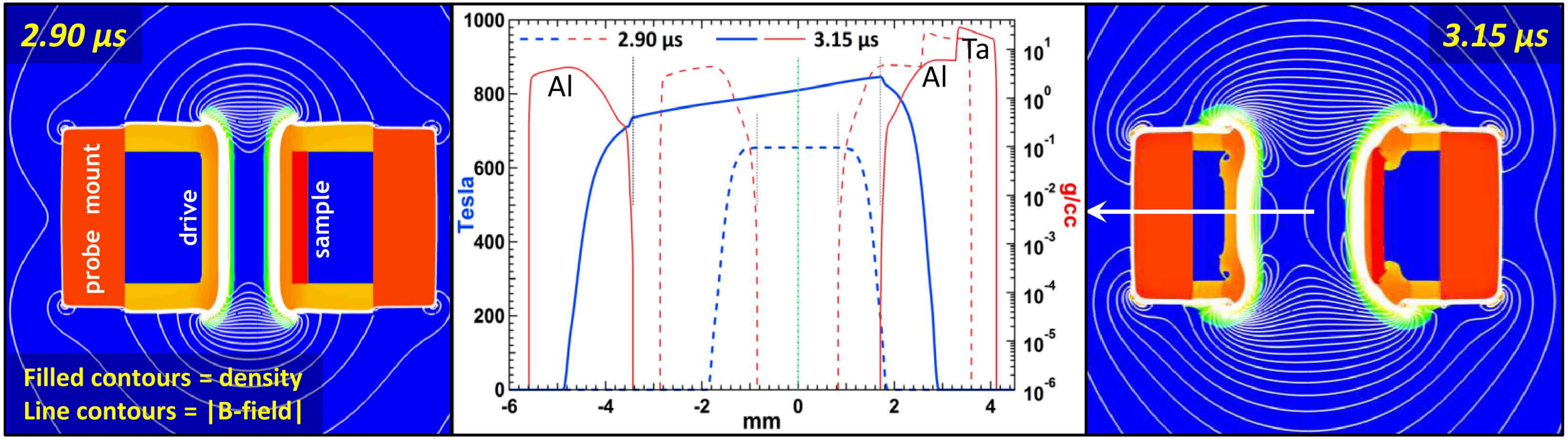
J.-P. Davis et al, J. Appl. Phys. **116**, 033515 (2016)

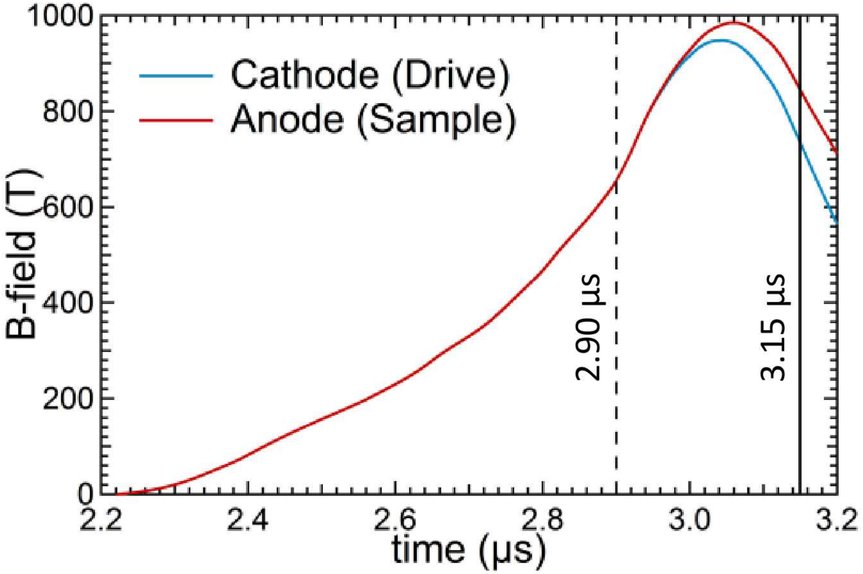


* R. G. Kraus et al, Phys. Rev. B **93**, 134105 (2016)

2-D MHD can correct for asymmetry in magnetic drive

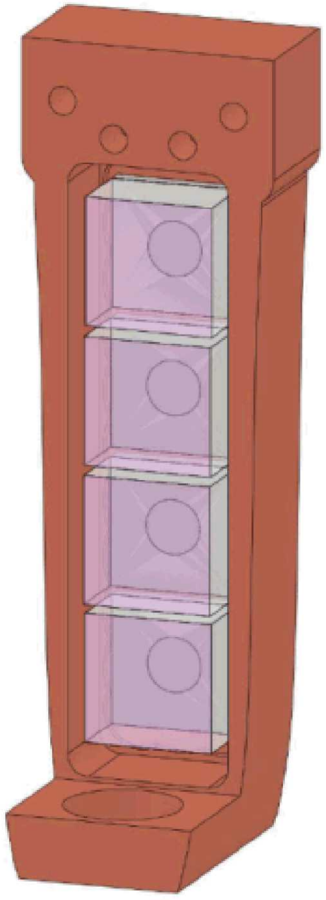
Snapshots with line-outs from Alegra simulation of Z2434 mid-height position



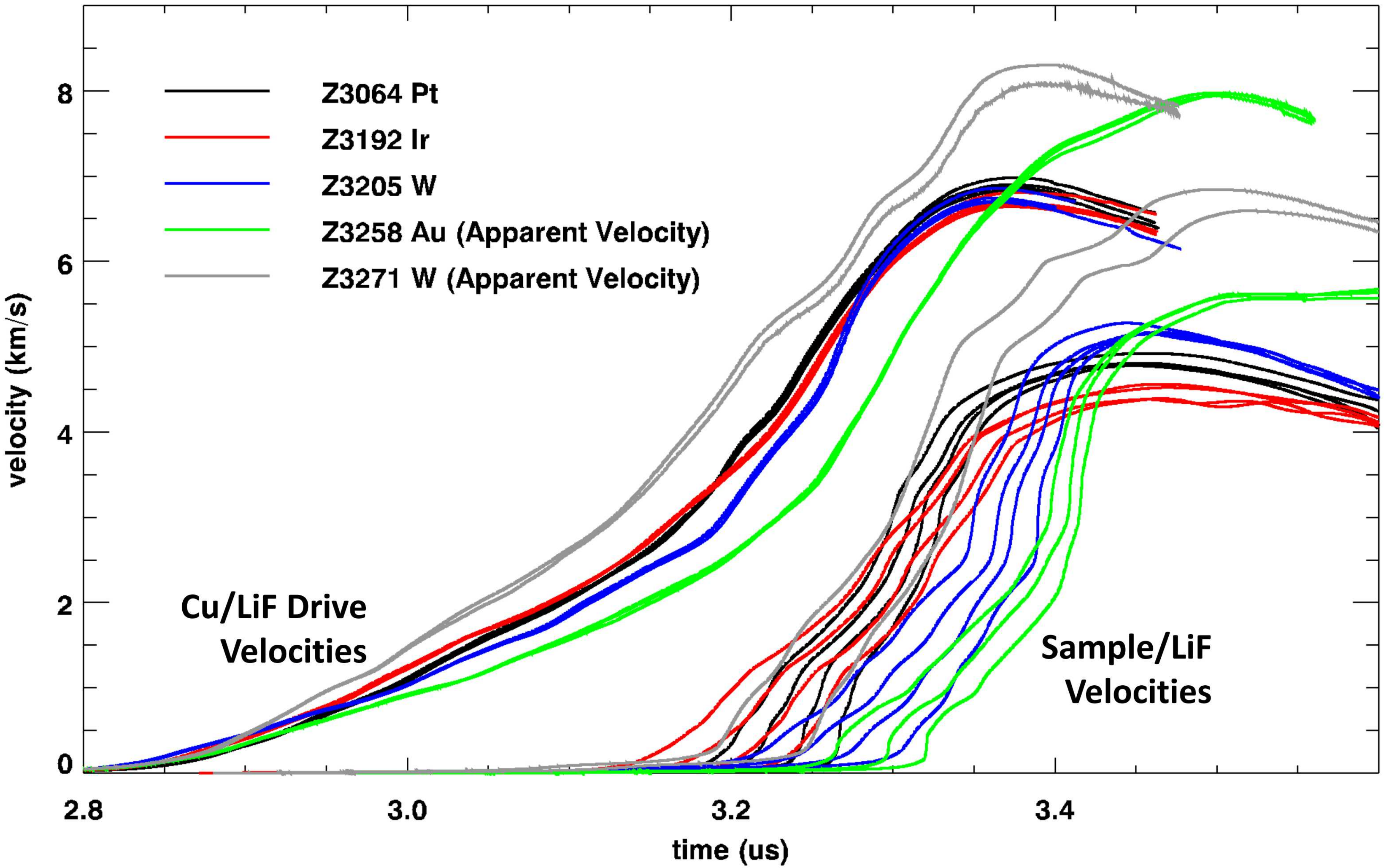


- Asymmetric wave reverberations in electrodes
  - Left (drive): reflection from free surface
  - Right (sample): reflection from high-impedance material
- Resulting 2-D effects cause asymmetric B-field topology
- Can occur prior to time of peak current
- Use 2-D B-field Sample/Drive ratio to correct 1-D B-field
  - Only if experiment is really 2-D!

→ ***rectangular samples and panel features***

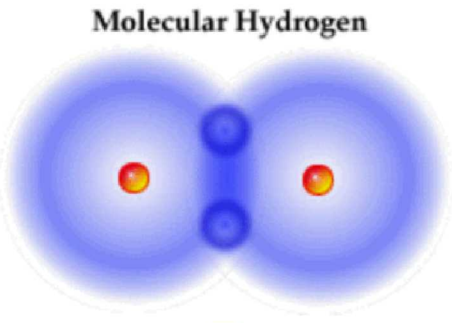


Velocimetry data accumulated in past two years on several metal standards has yet to be fully analyzed

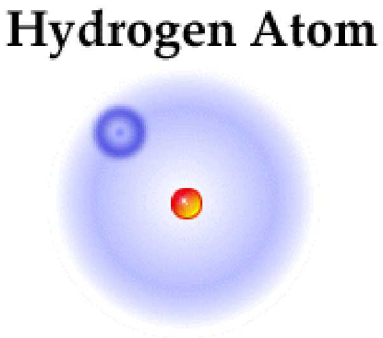


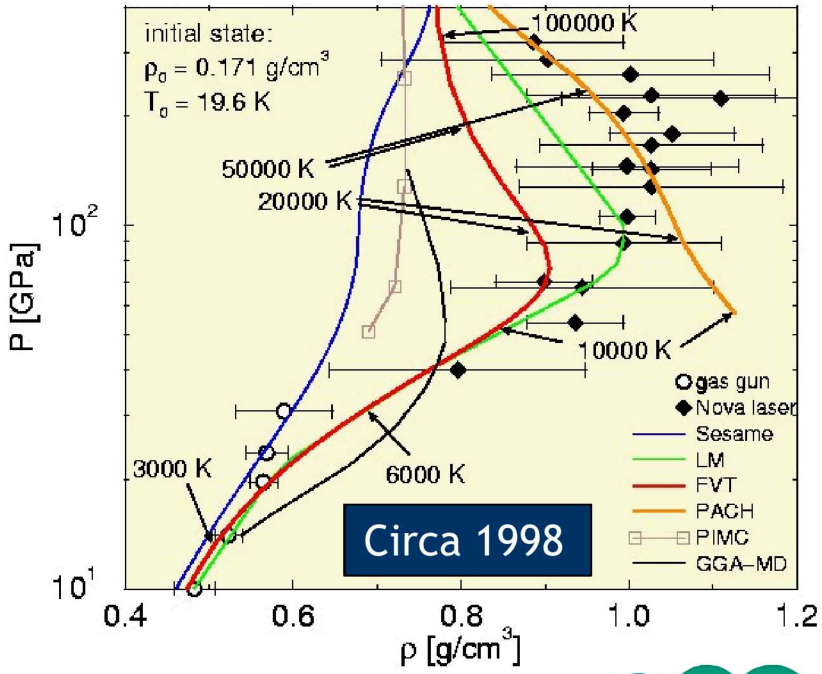
QMD calculations of the hydrogen/deuterium Hugoniot

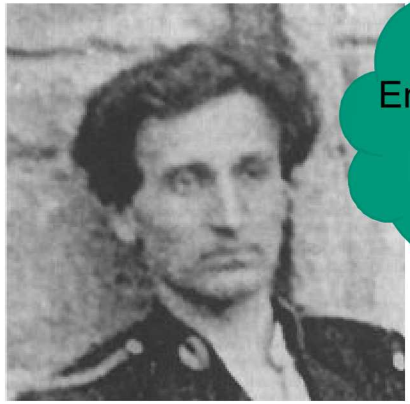
Shock



High Temperature
High Pressure

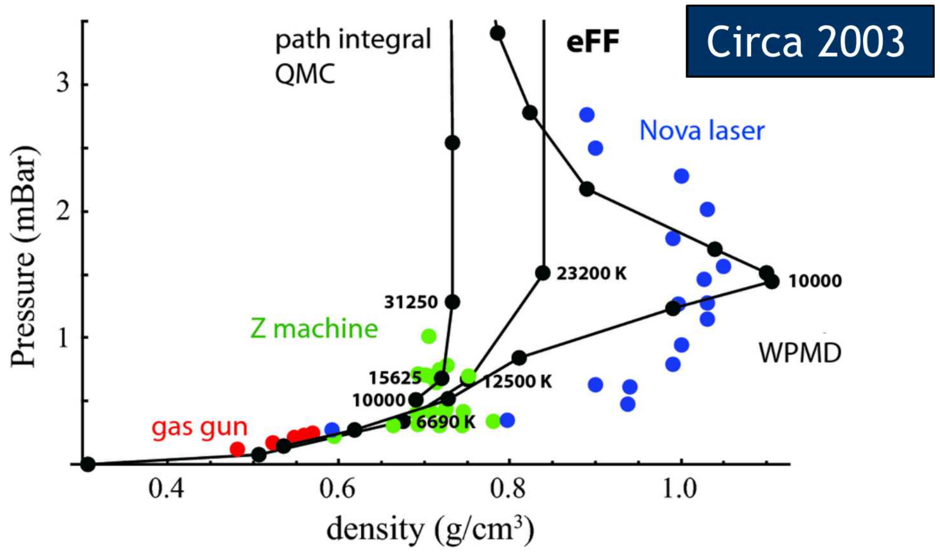


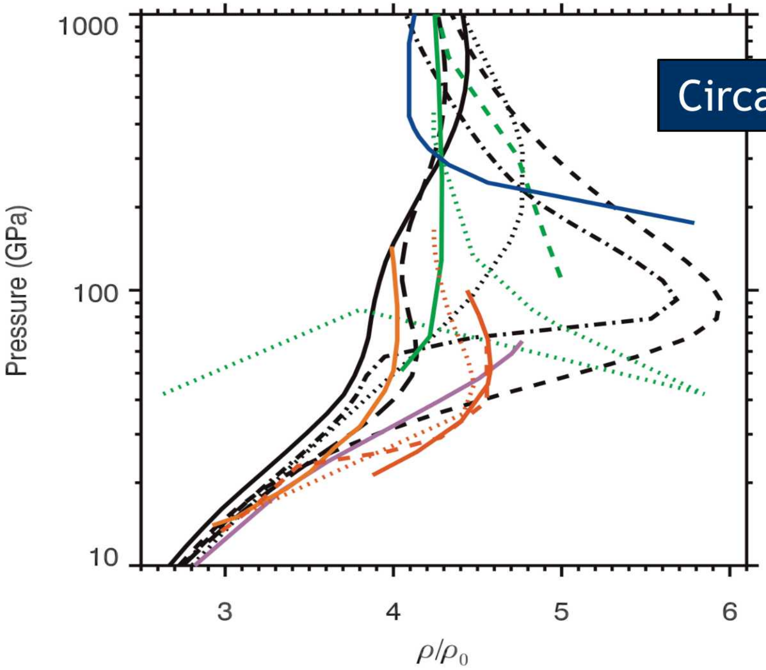




Pierre Henri Hugoniot

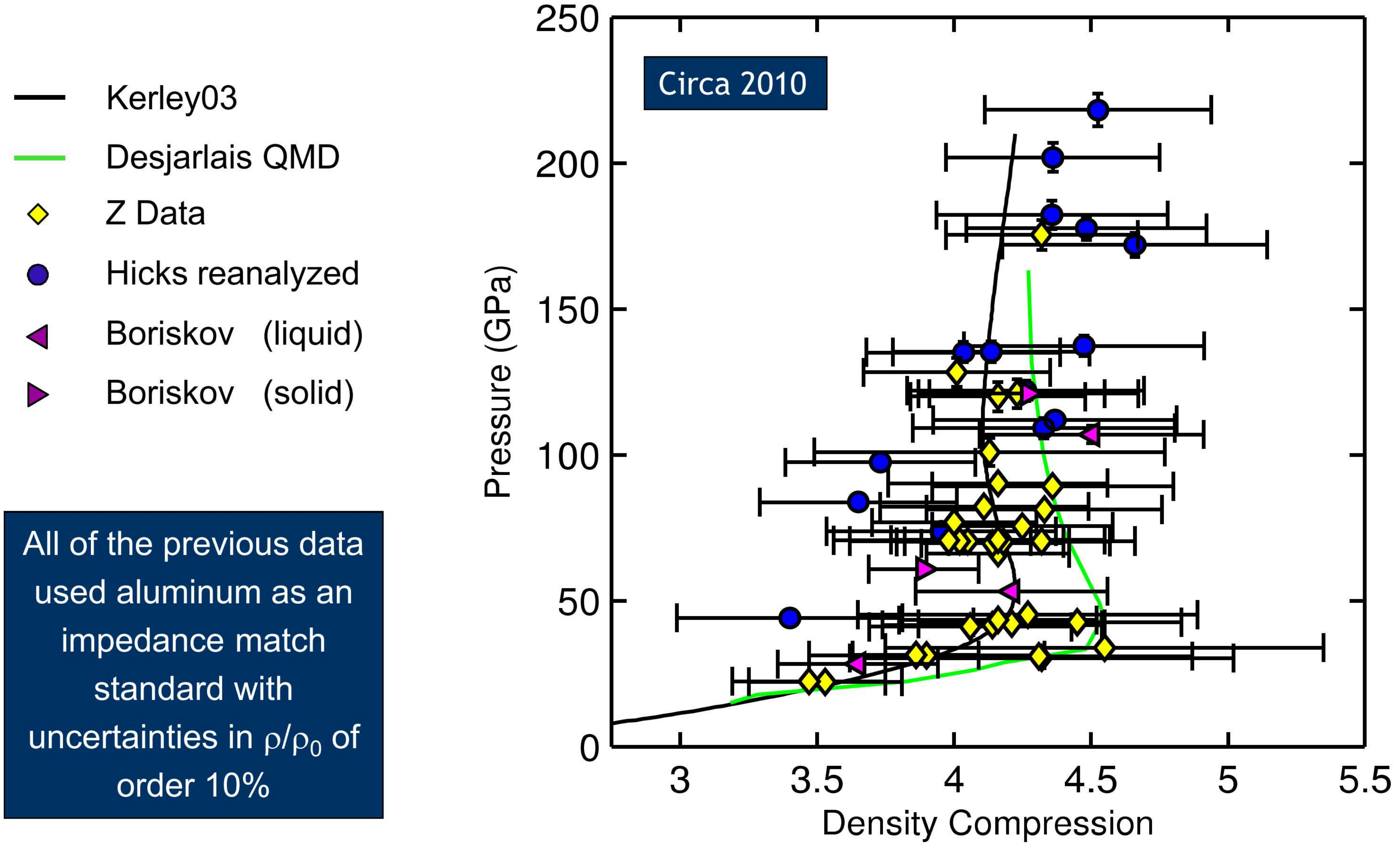
En fait, il n'est pas si simple





Chemical picture
Activity expansion (ACTEX)
Tight Binding
Path Integral Monte Carlo
Ensemble Monte Carlo
Density Functional Theory

Let's not just pick on the theorists…



All of the previous data used aluminum as an impedance match standard with uncertainties in ρ/ρ_0 of order 10%

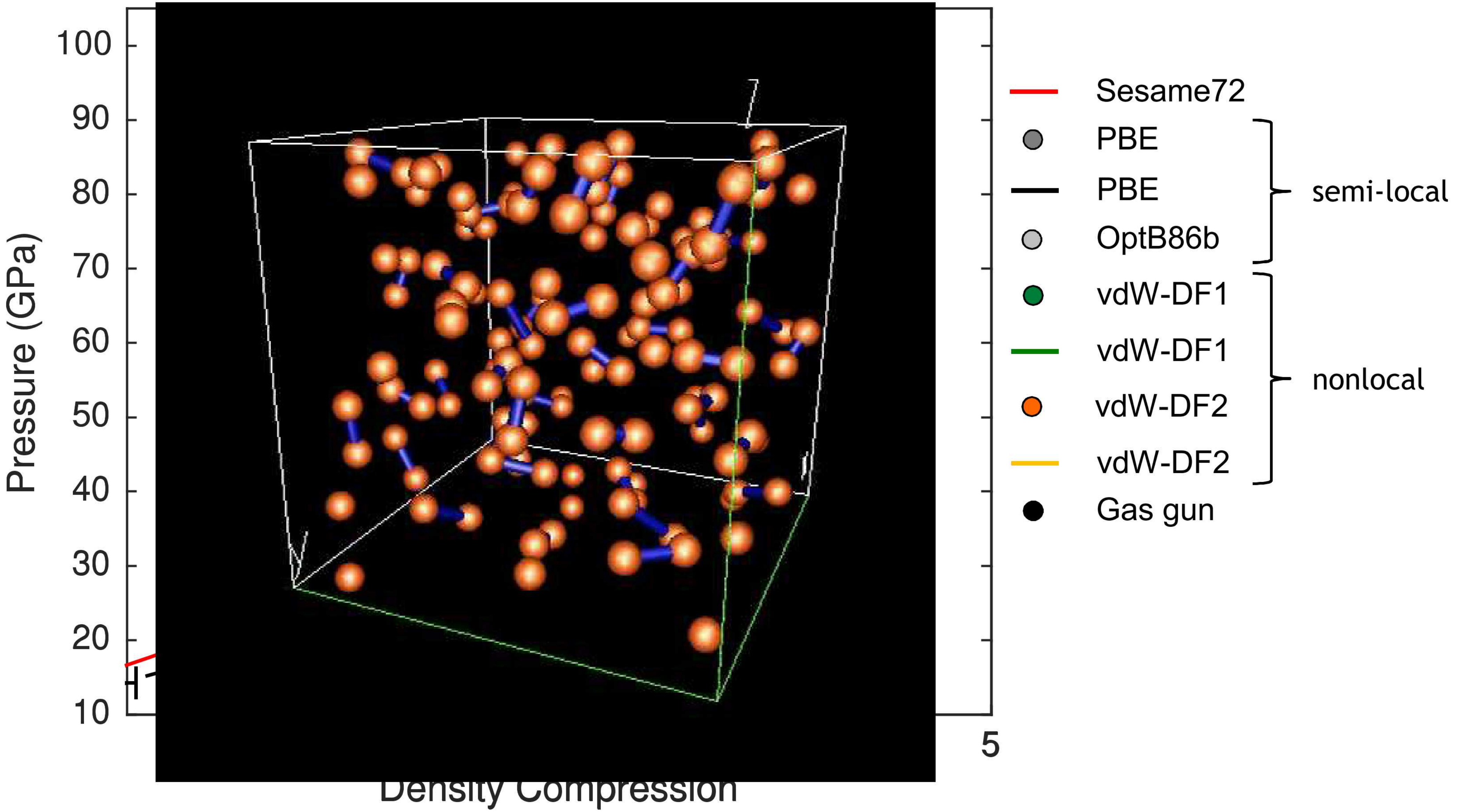
Boriskov et al., PRB 71, 092104 (2005)

Knudson et al., PRB 69, 144209 (2004)

Hicks et al., PRB 79, 014112 (2009)

Current state-of-the-art: deuterium Hugoniot

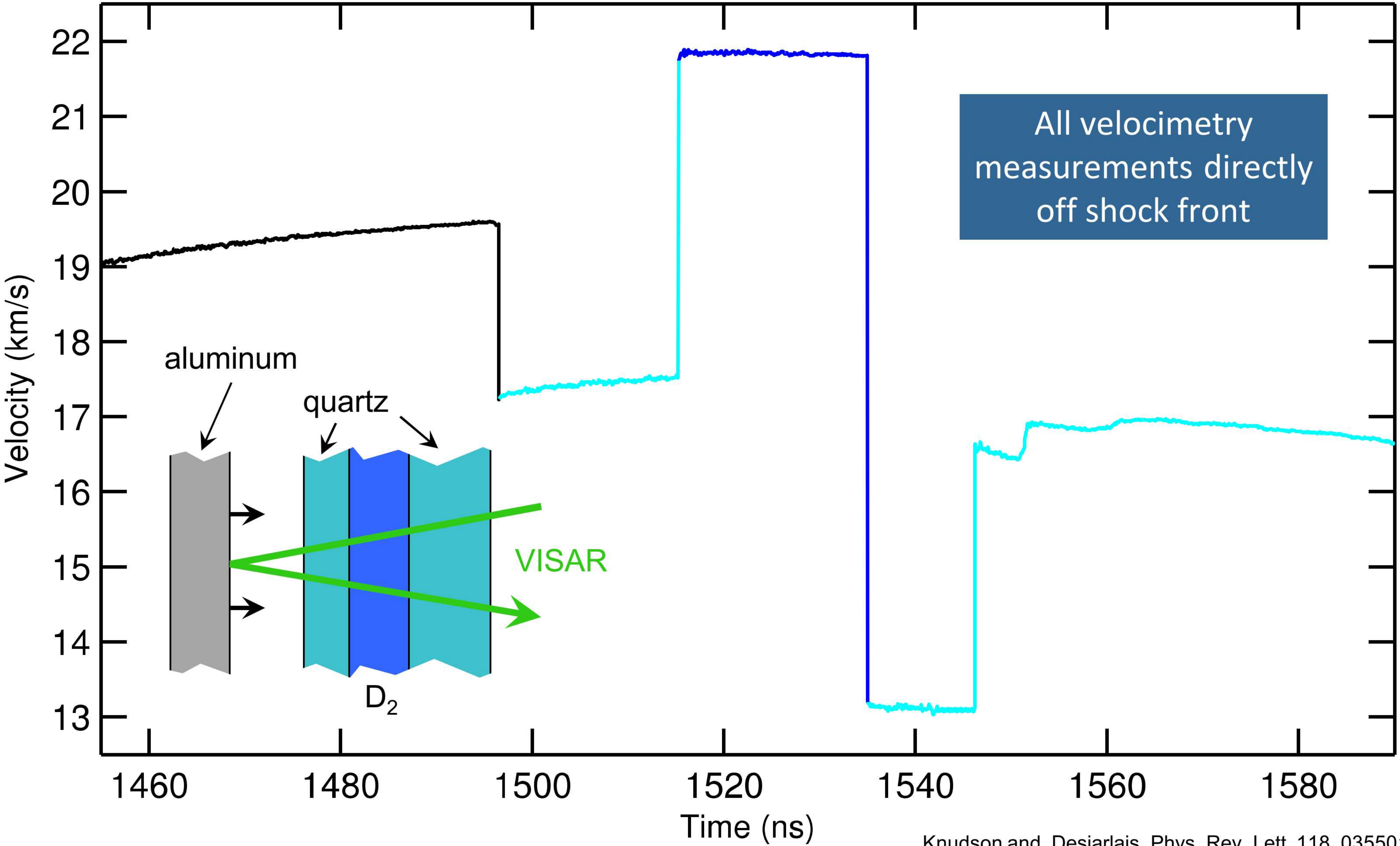
Shock



Knudson and Desjarlais, Phys. Rev. Lett. 118, 035501 (2017)

High-precision Hugoniot experiments on deuterium

Shock



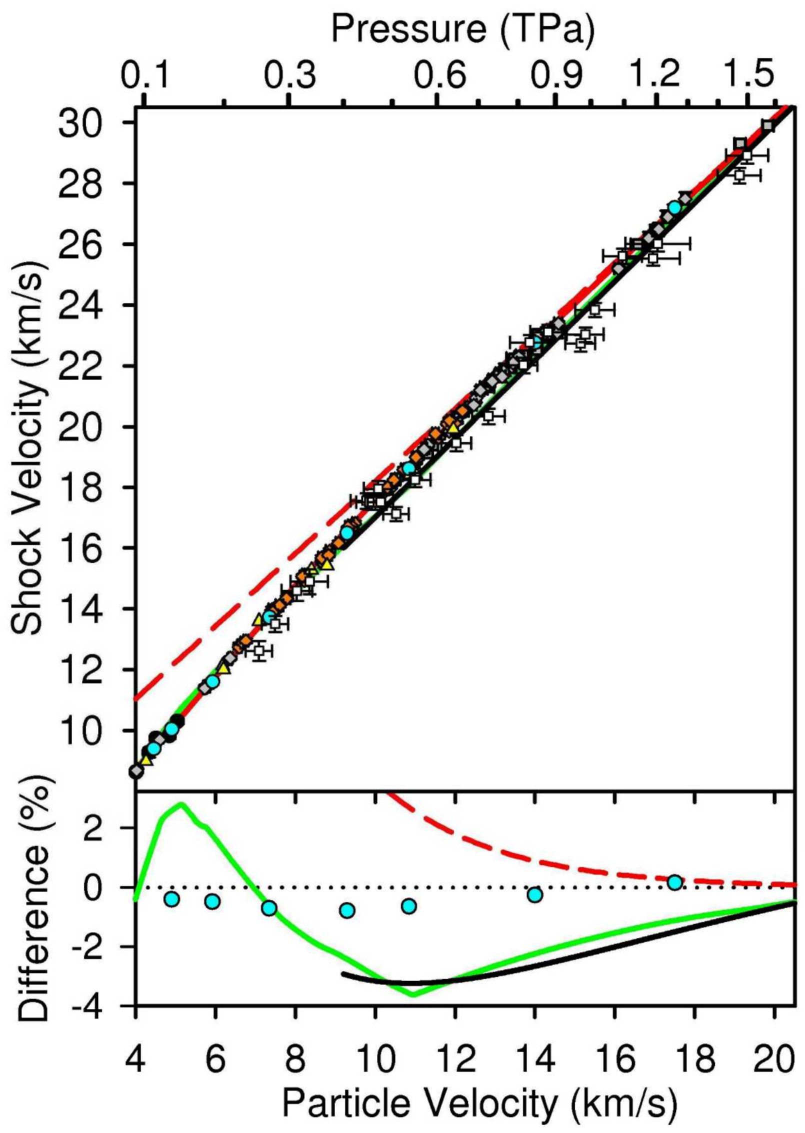
All velocimetry measurements directly off shock front

Knudson and Desjarlais, Phys. Rev. Lett. 118, 035501 (2017)

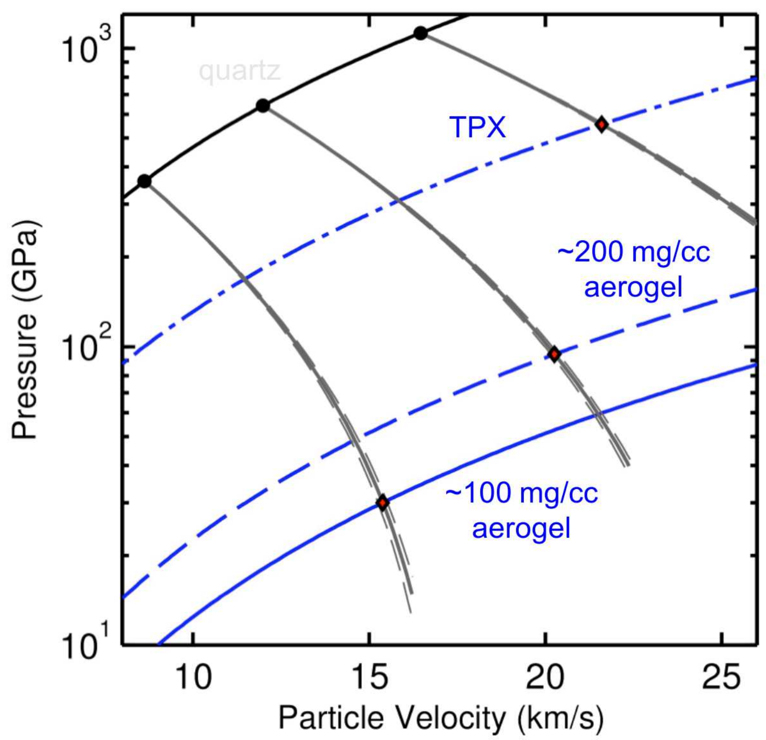
High-precision quartz standard developed on Z

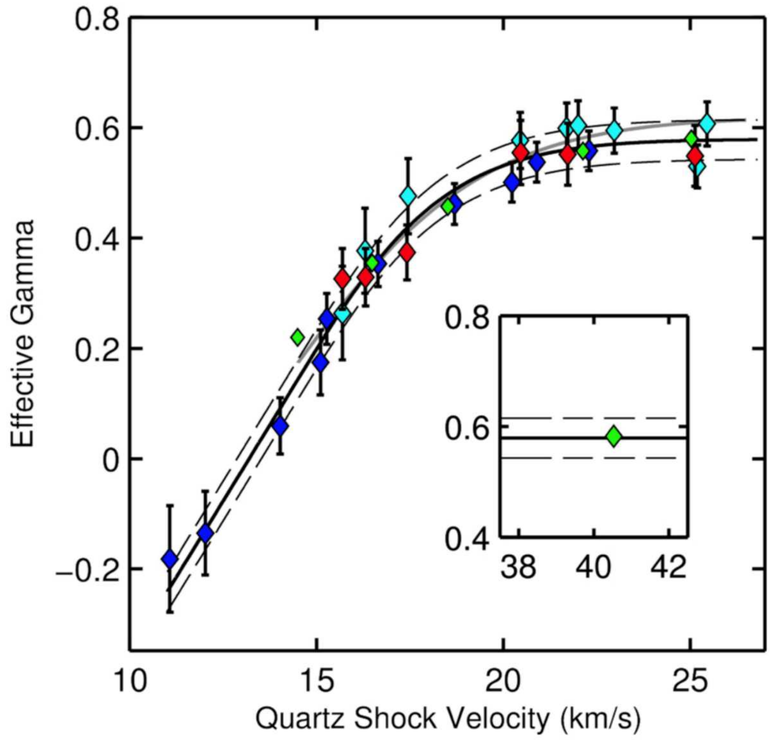
Shock

- Nearly 300 Hugoniot points for quartz have been obtained between 1 and 15 Mbar
- A release model was developed using release measurements obtained from TPX, and both ~200 mg/cc and ~100 mg/cc aerogel and based on insight gained from QMD calculations



Knudson and Desjarlais, PRL 103, 225501 (2009)

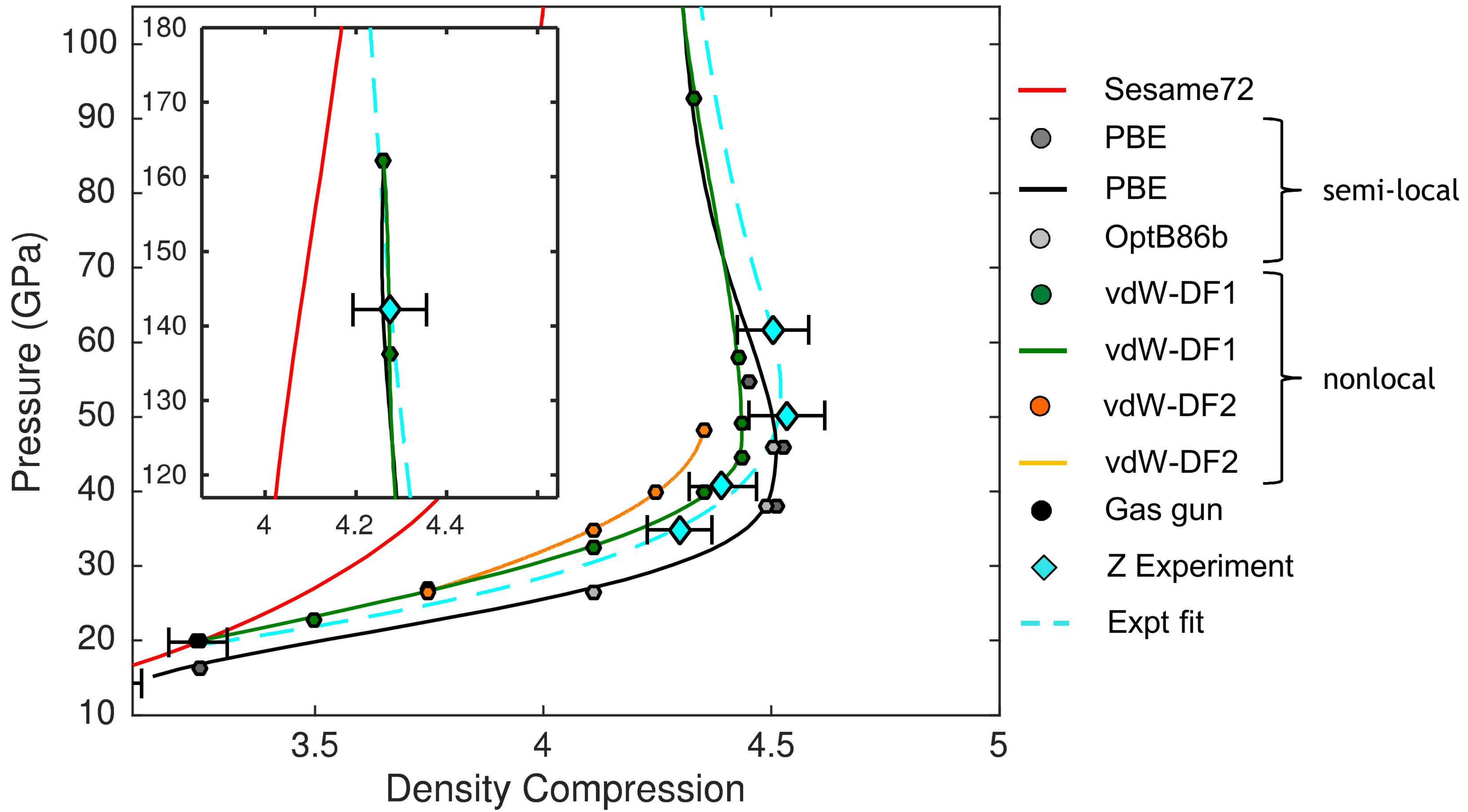




Knudson and Desjarlais, PRB 88, 184107 (2013)

High-precision Hugoniot data for deuterium

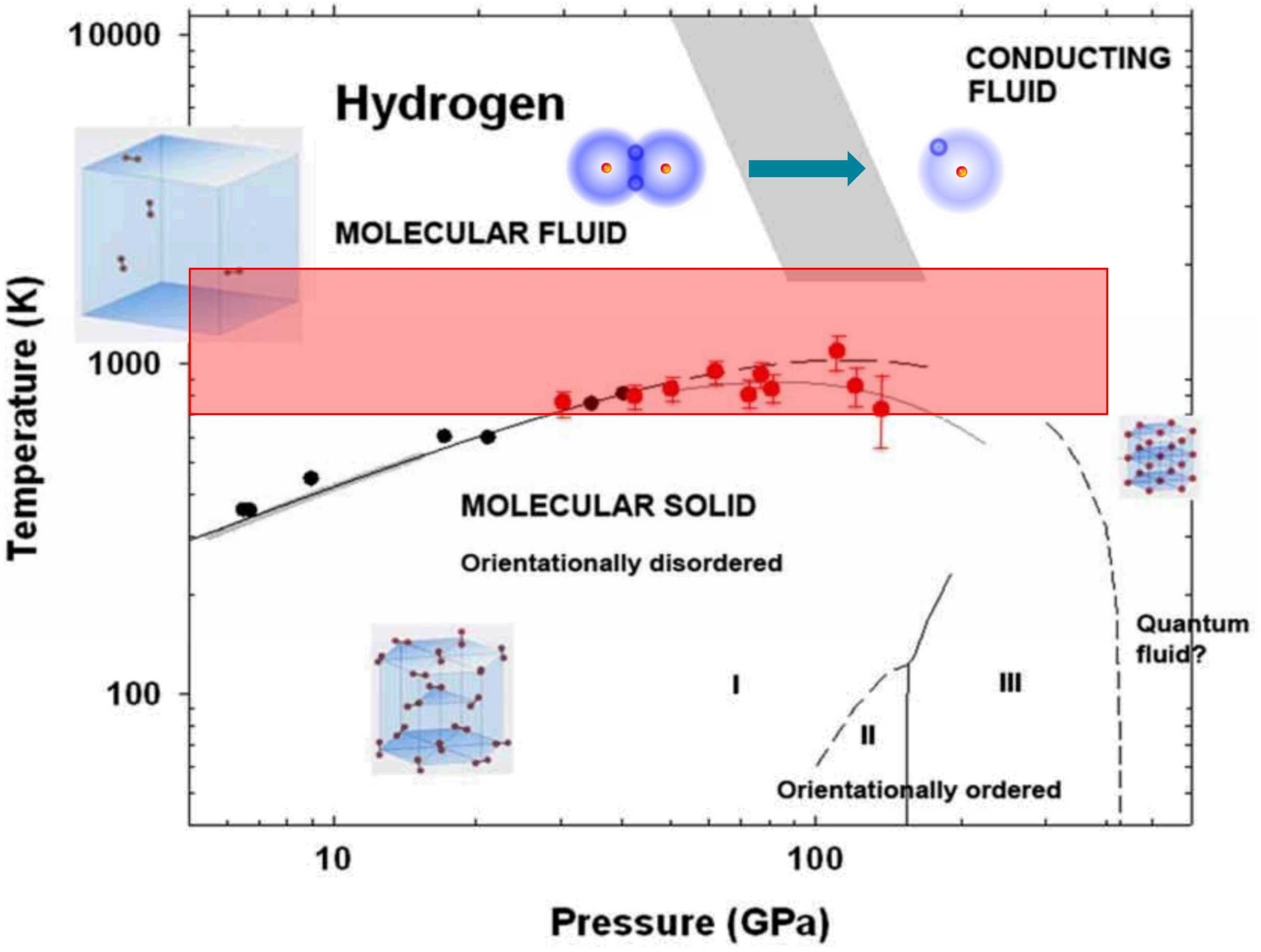
Shock

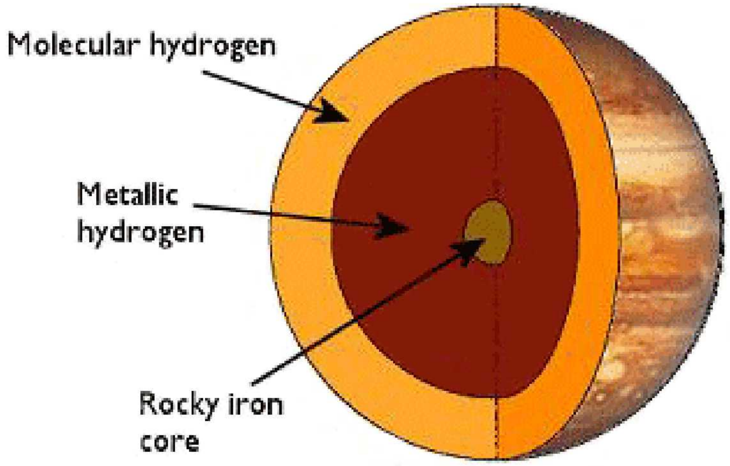


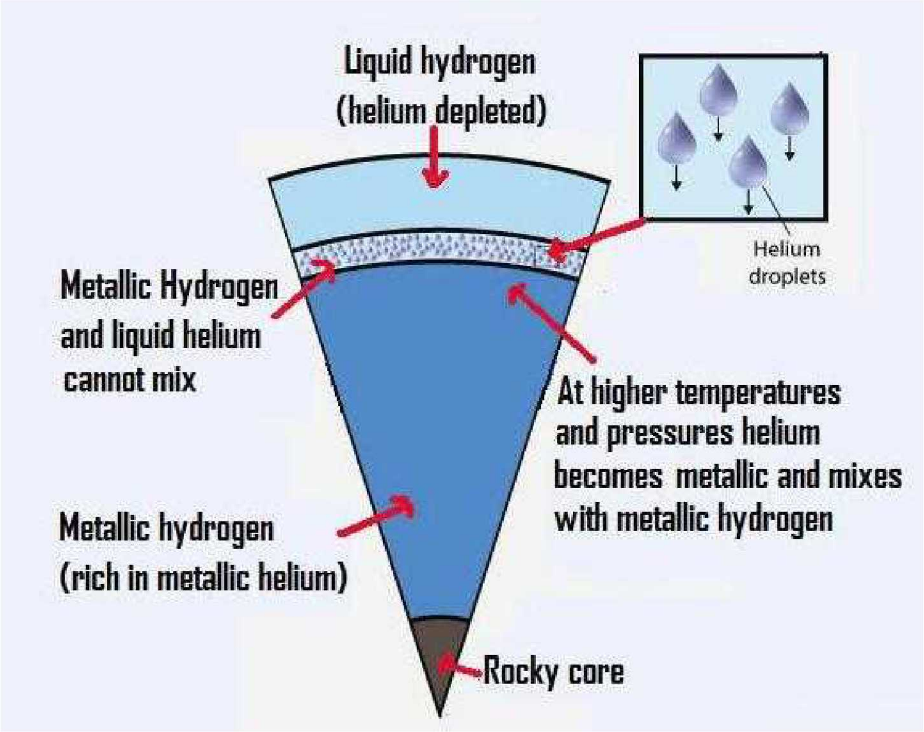
Knudson and Desjarlais, Phys. Rev. Lett. 118, 035501 (2017)

Metallization at high-density / low-temperature

Shock-ramp

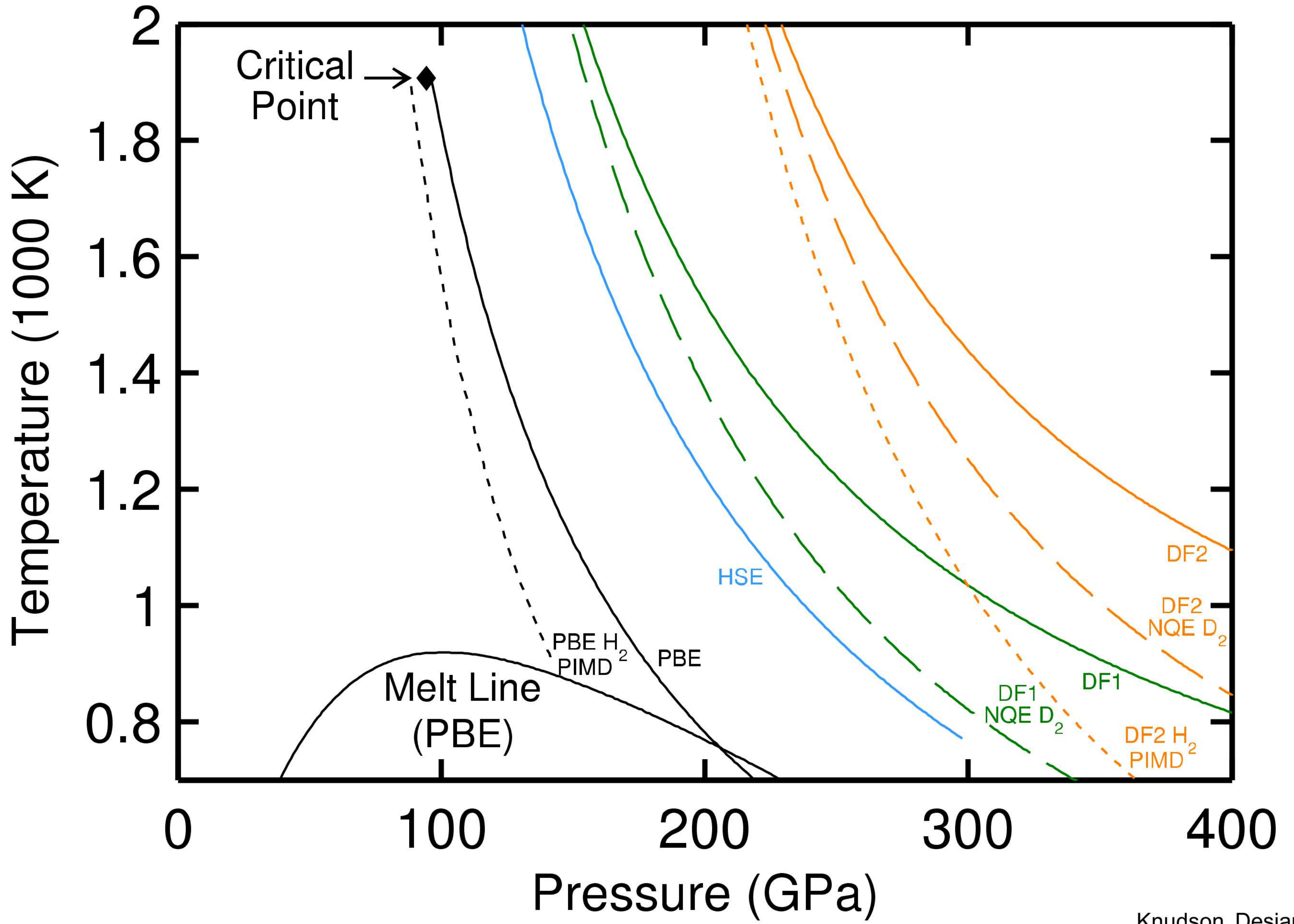






Metallization of hydrogen / deuterium

Shock-ramp

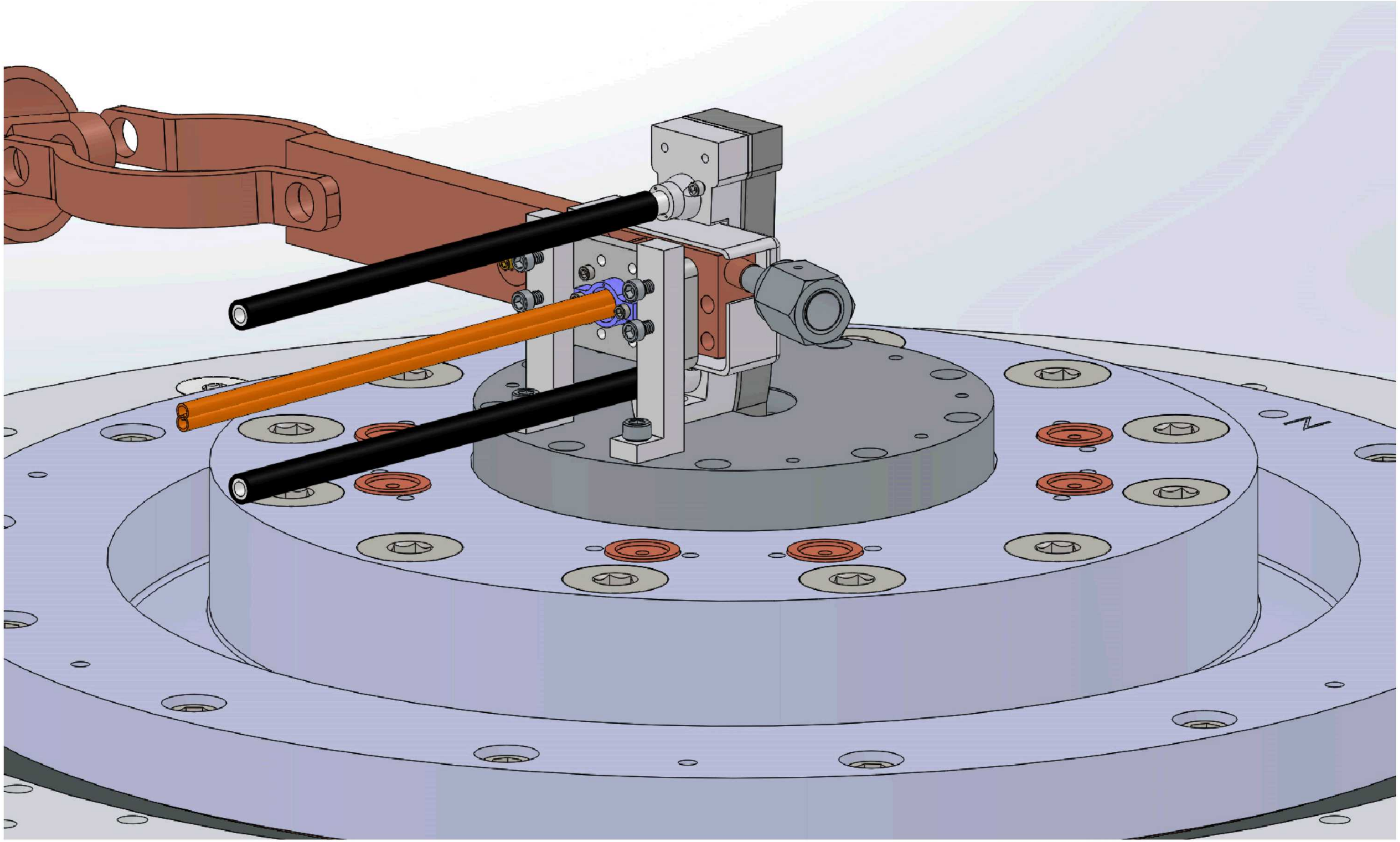


- **All functionals considered predict a first-order, liquid-liquid phase transition ending in a critical point at ~2k K**
- **This transition is concurrent with an insulator to metal transition (IMT)**
- **Low-density phase is mostly molecular, the high-density phase is mostly atomic**
- **Pressure and density of the transition is extremely sensitive to the particular exchange-correlation functional**

Knudson, Desjarlais, Becker, Redmer, et al. Science 348, 1455 (2015)

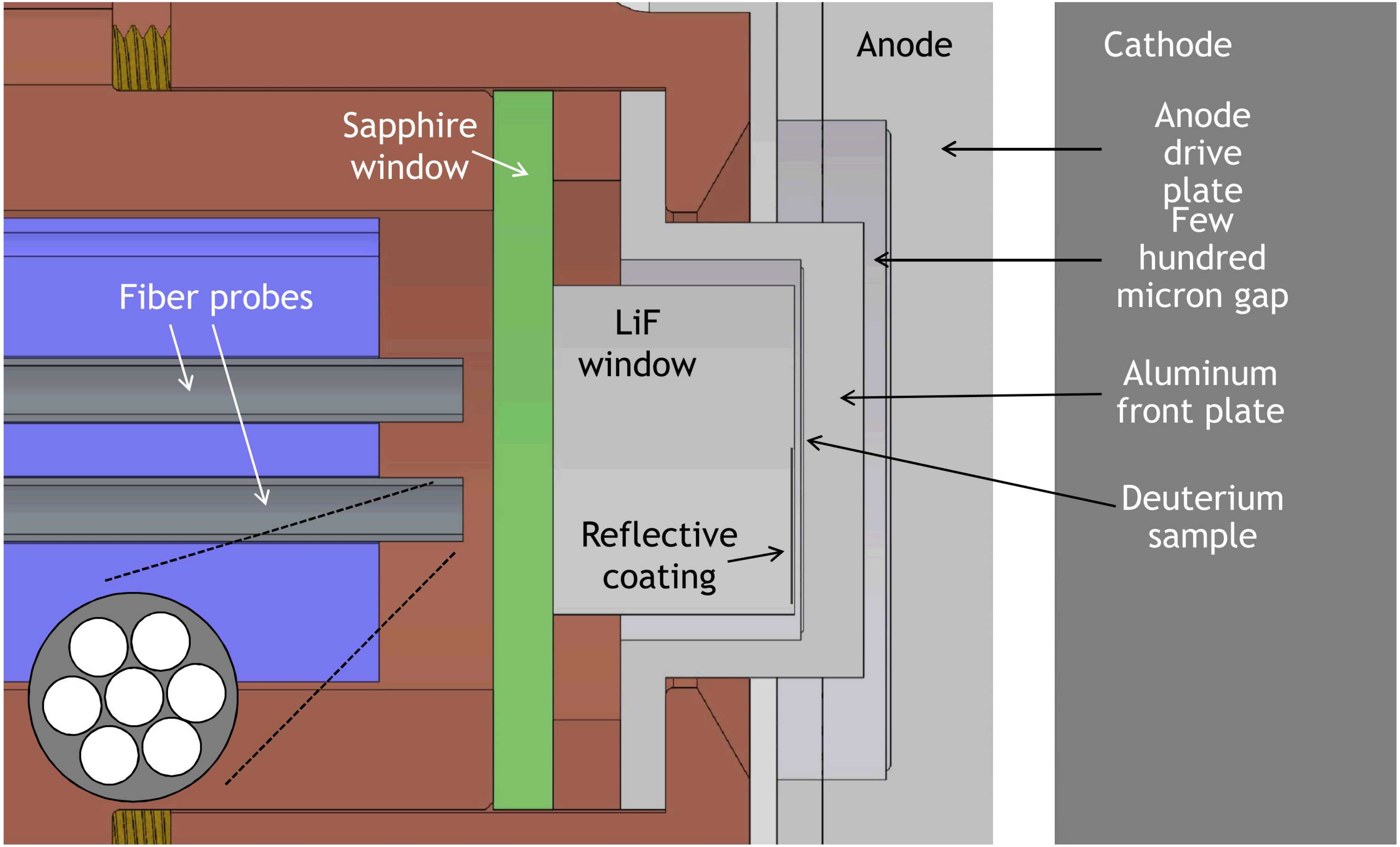
Experimental configuration

Shock-
ramp



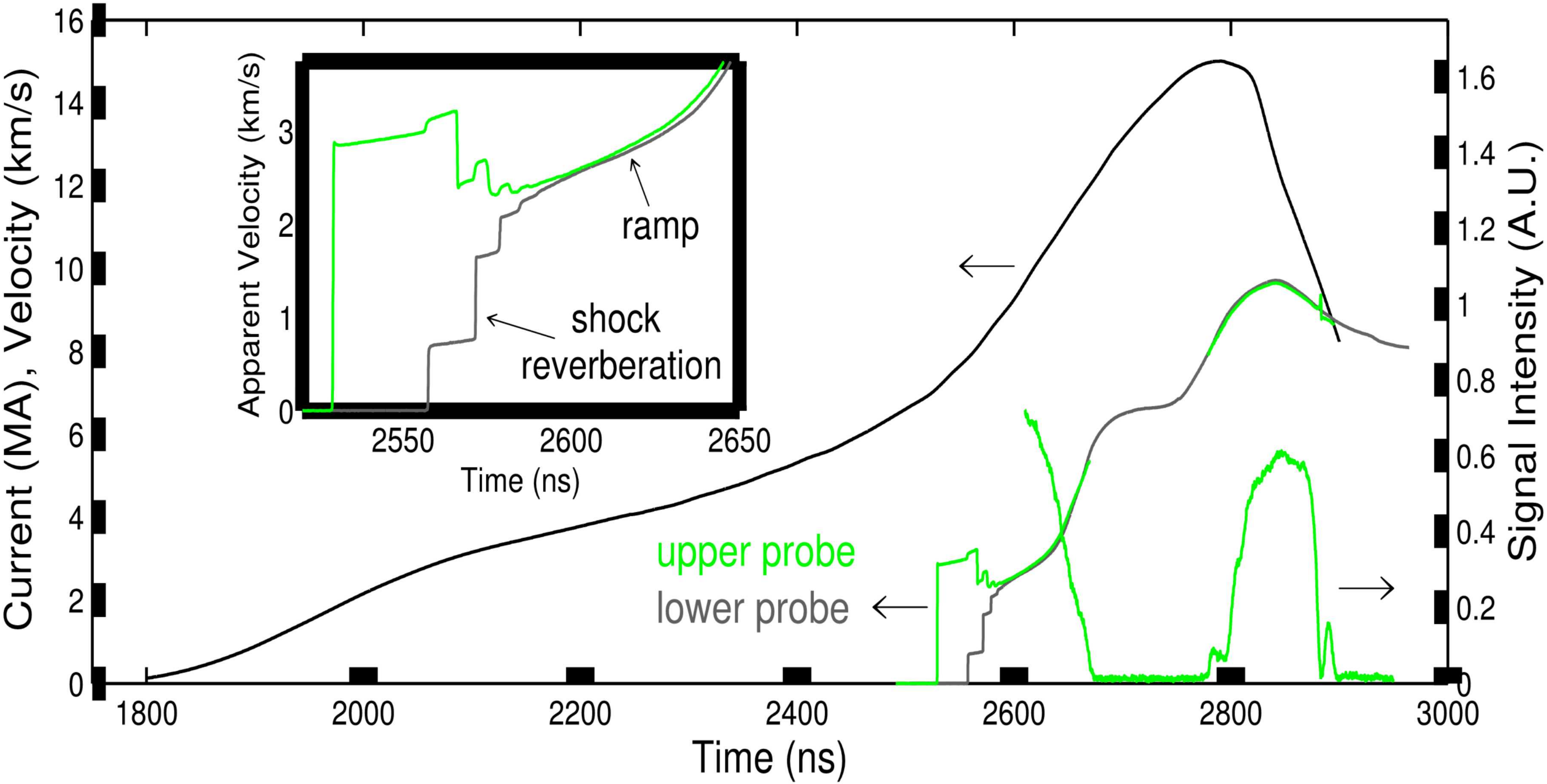
Knudson, Desjarlais, Becker, Redmer, et al. Science 348, 1455 (2015)

Experimental configuration



Knudson, Desjarlais, Becker, Redmer, et al. Science 348, 1455 (2015)

Representative data



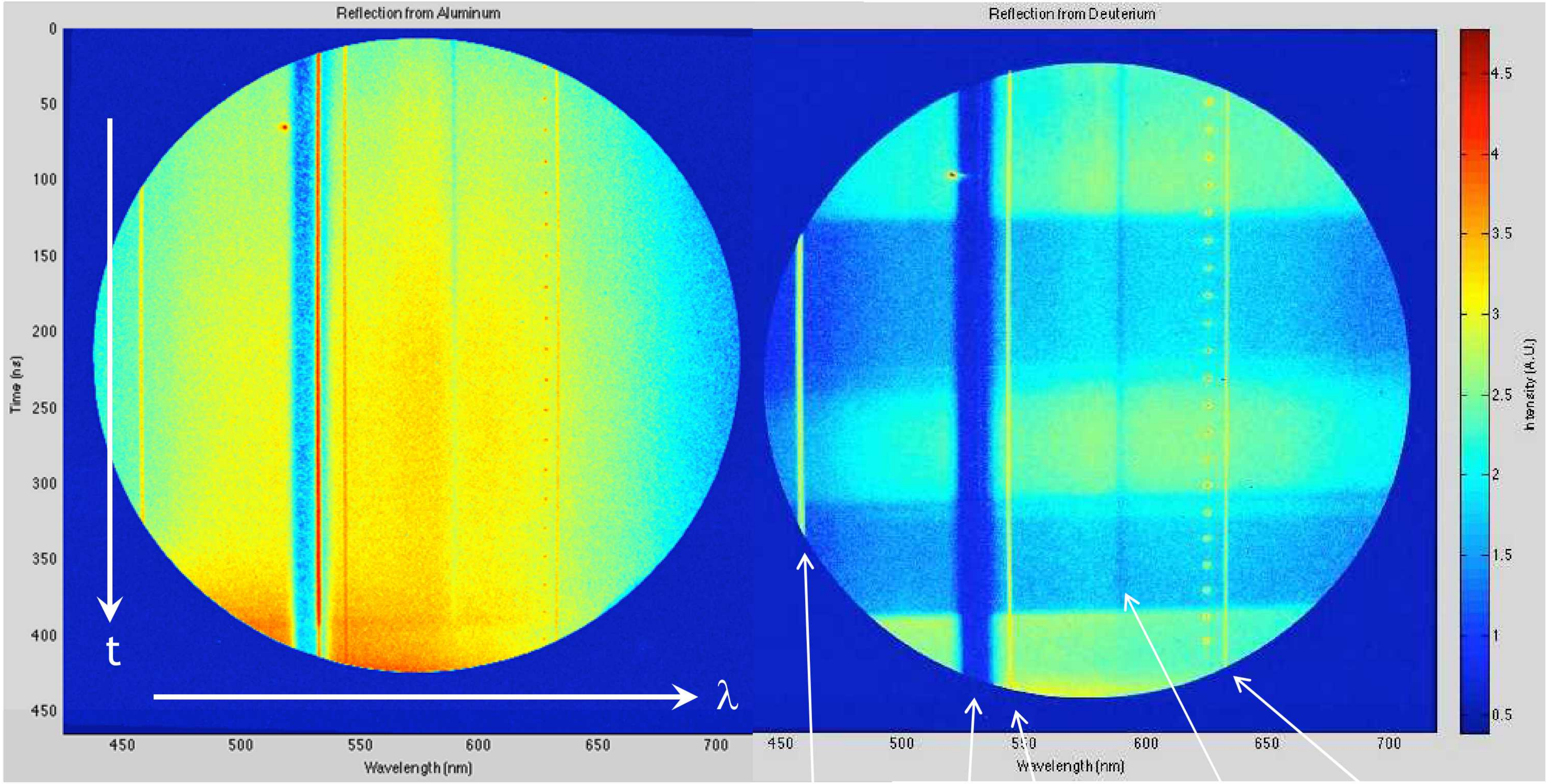
Knudson, Desjarlais, Becker, Redmer, et al. Science 348, 1455 (2015)

Comparison of reflectivity from aluminum and deuterium

Shock-ramp

Reflection from aluminum coating

Reflection from deuterium



Wavelength range ~450-700 nm

457.9 nm

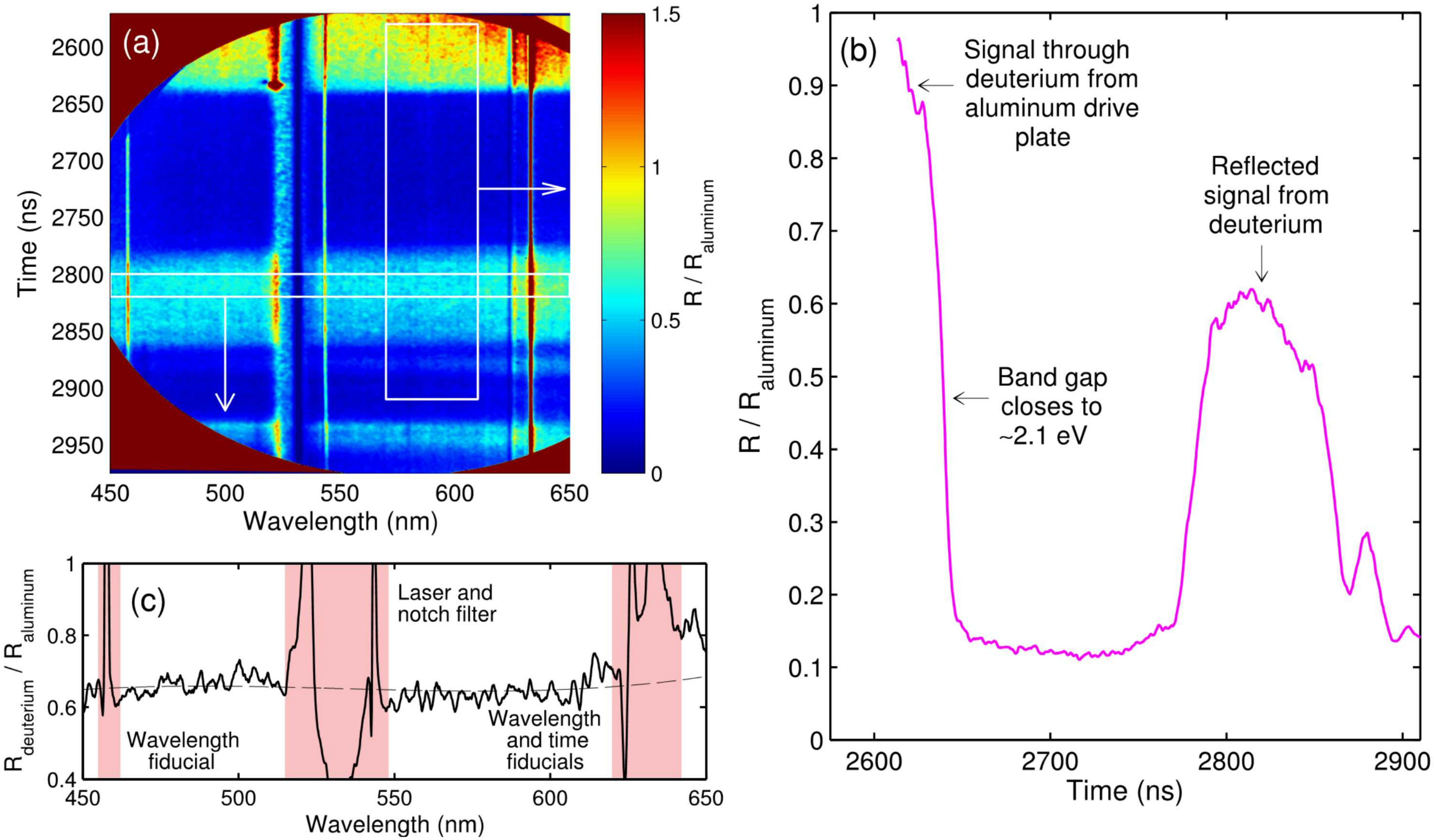
532 / 543.5 nm

589.3 nm

633 nm

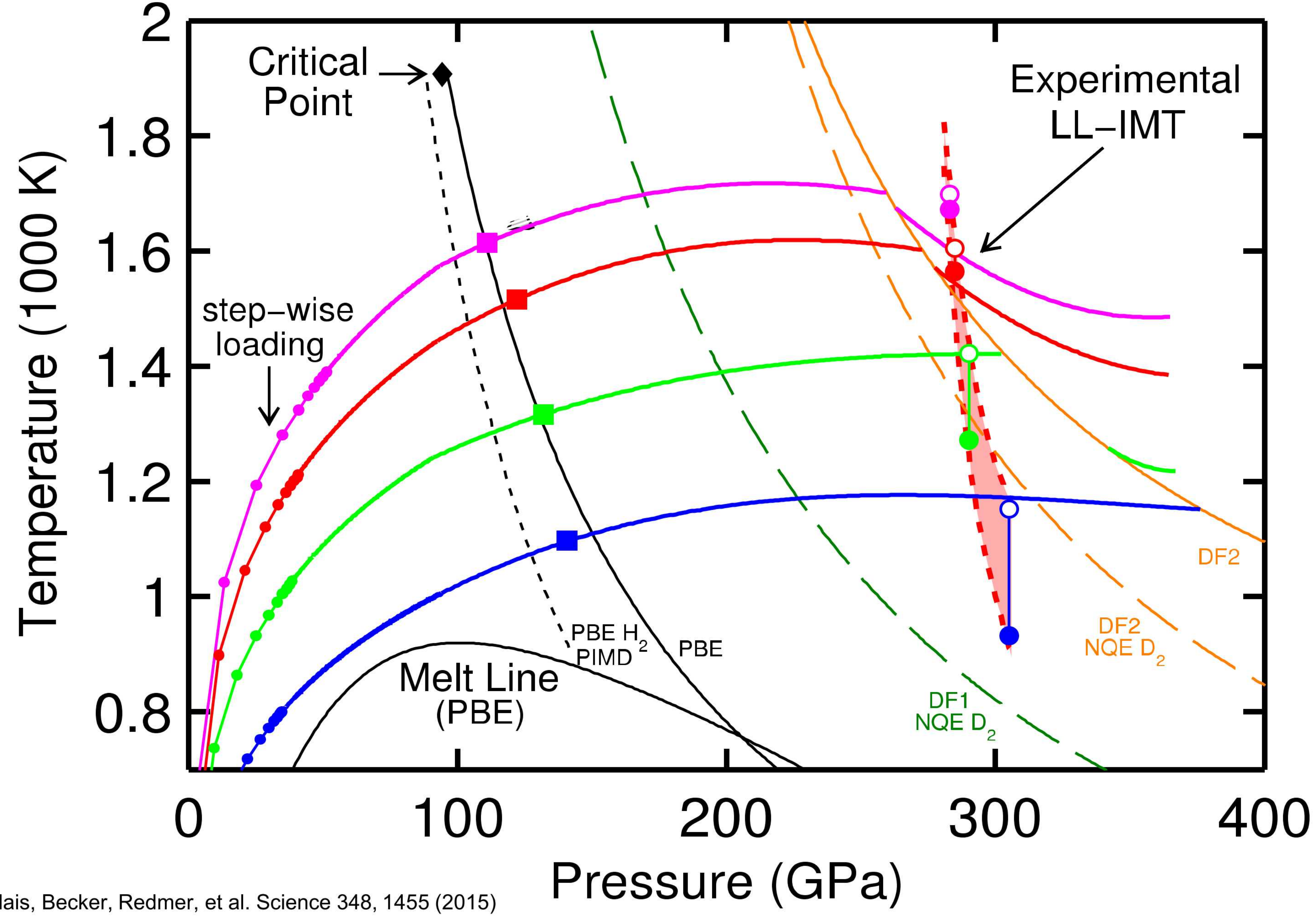
Knudson, Desjarlais, Becker, Redmer, et al. Science 348, 1455 (2015)

Wavelength dependence of reflectivity indicative of a metal



Knudson, Desjarlais, Becker, Redmer, et al. Science 348, 1455 (2015)

Liquid-liquid, insulator-to-metal transition (LL-IMT)

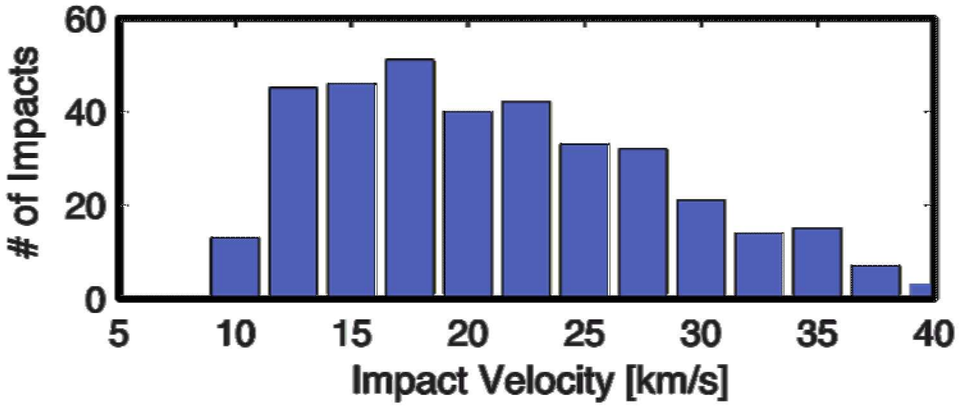


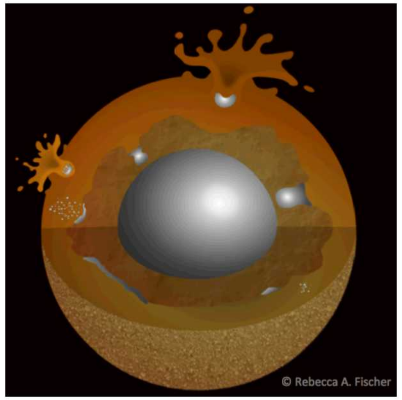
Knudson, Desjarlais, Becker, Redmer, et al. Science 348, 1455 (2015)

Vaporization key mechanism during planet formation and evolution

Shock-release

Simulations of planetary dynamics suggest high impact velocities





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.

Large uncertainty in onset of vaporization

Does an iron meteor:

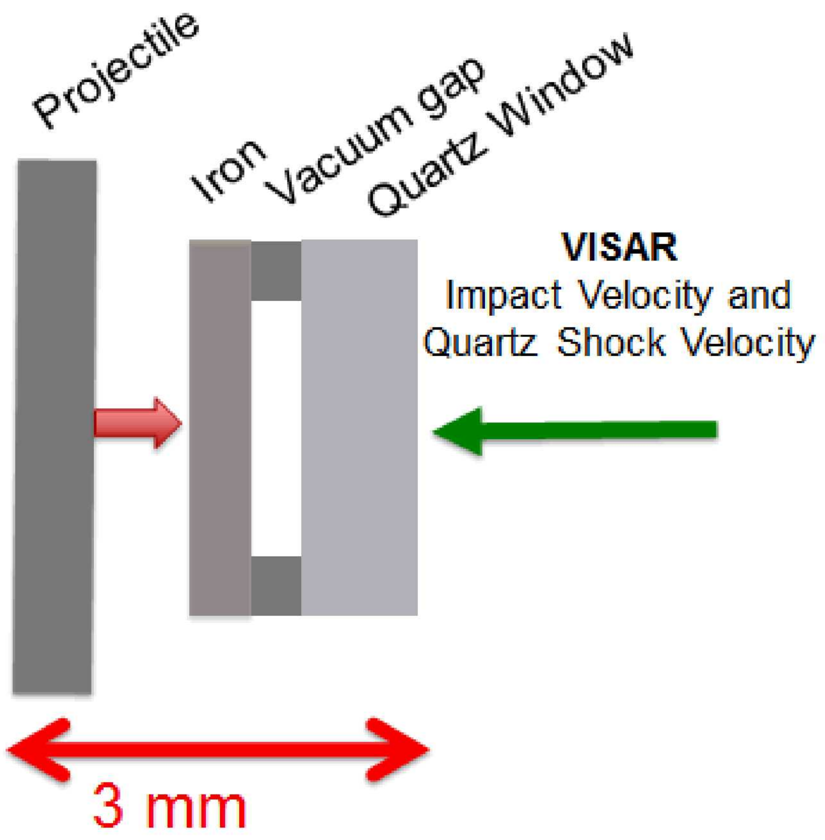
- plow into a planet as a bullet?
- splatter as a drop of rain?
- vaporize into a cloud of iron to return as iron rain?

The outcome depends on the HED properties of iron – particularly vaporization

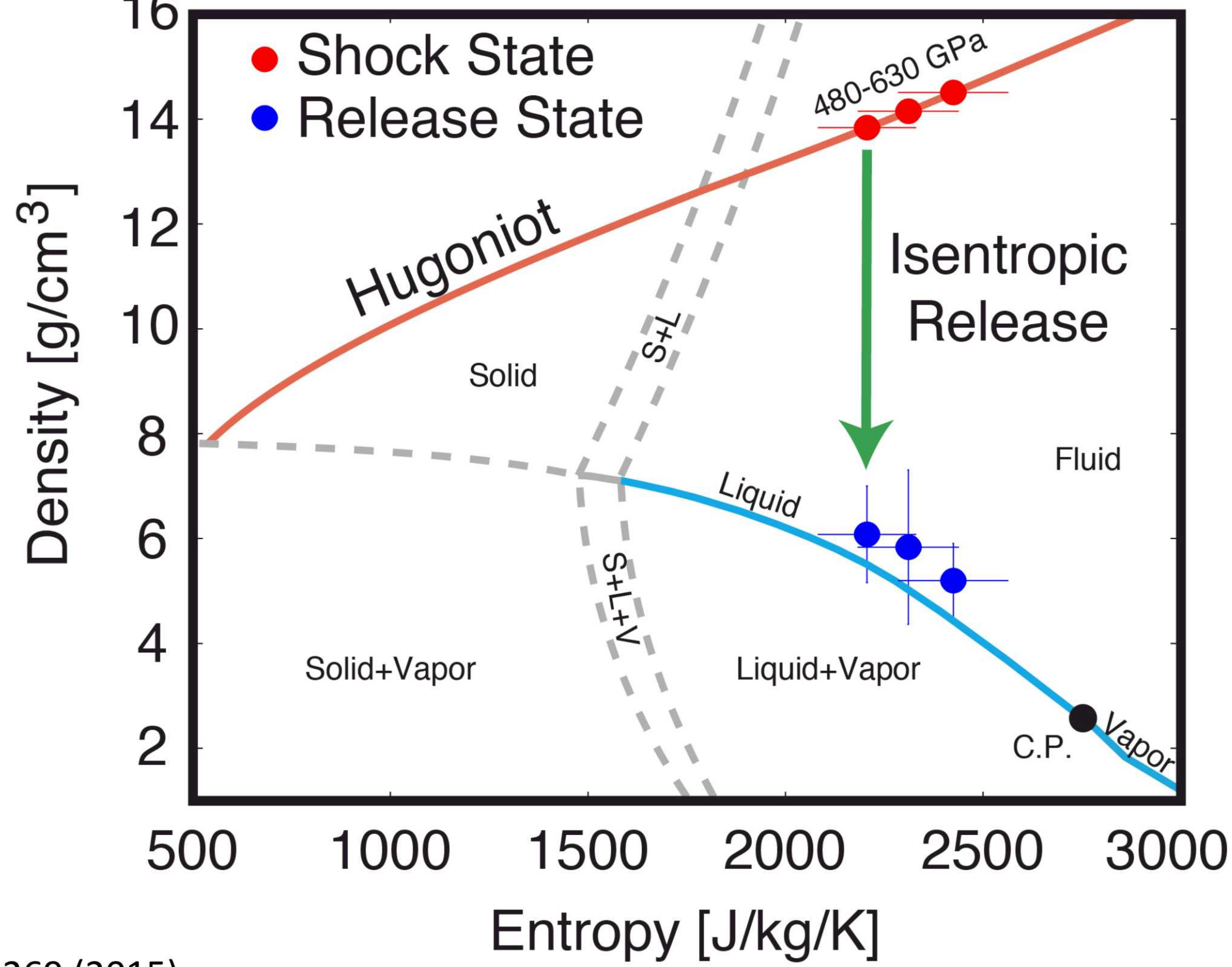
N-body simulations from Raymond et al. 2009

Vaporization by planet forming impacts can be studied on Z

- Flyer plates on Z can exceed 40 km/s
- Liquid-vapor dome located via shock-release experiments

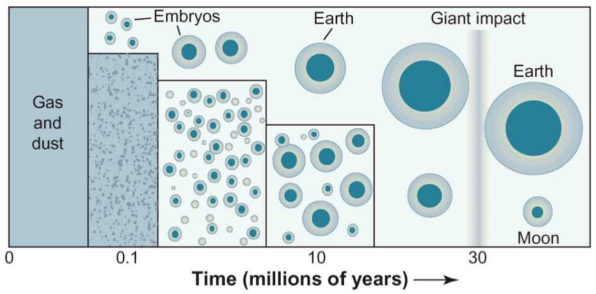


Iron Shock and Release Data

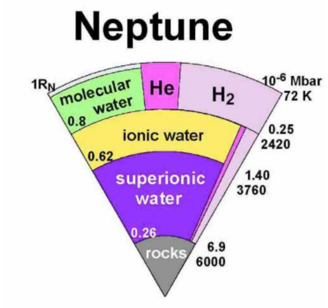


R.G. Kraus et al., *Nature Geoscience* 8, 269 (2015)

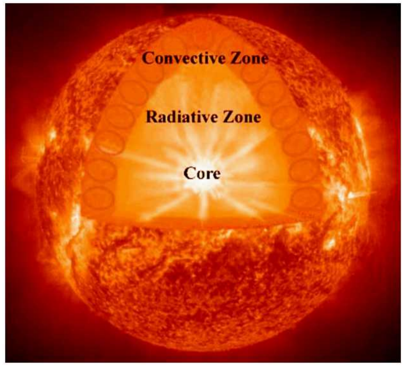
Z Fundamental Science Program is a growing community



Earth and super earths
Properties of minerals and metals



Jovian Planets
Water and hydrogen



Stellar physics
Fe opacity and H spectra

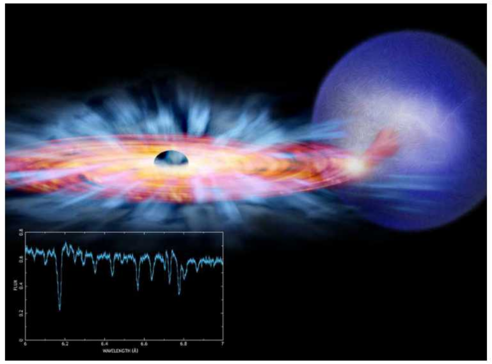


Photo-ionized plasmas
Range of ionization param. ξ

12+ students are currently involved

Resources over 10 years

- 115 dedicated ZFSP shots (5-7% of all Z shots)
- Ride-along experiments on Z program shots, guns, DICE, and THOR

Science with far-reaching impact

- Nature, Nature Geoscience, SCIENCE
- 7 Phys. Rev. Lett, 3+ Physics of Plasmas, 5+ Physical Review (A,B,E)
- More than 40 total peer reviewed publications and 10 conference proceedings
- 70+ invited presentations

Popular outreach

- National Public Radio, “All things considered”, 2014
- Discover Magazine
  - Reportage 9/16/2012
  - *Iron rain #62 in top 100 Science stories in 2015*
- Albuquerque Journal Front Page 9/2017
- Twice local TV coverage on planetary science

ZFS Program has transitioned to a yearly Call for Proposals

ZFSP is a core part of our research strategy

- 100+ dedicated shots since the start in 2011
- About 10% of the shots on Z, so 15 per year
- 4 -7 independent projects

Proposal format

- 12 page research narrative
- Shot plan, target- and diagnostics needs, etc
- PI CV/resume

Review

- Facility review for safety and readiness (target, diagnostics)
- Review of scientific relevance and impact by an independent review panel

ZFSP 2020 workshop TBD, Albuquerque

- Sunday evening – Wednesday afternoon
- Typically been held at Hotel Andaluz, downtown ABQ

Two-year award period

Sandia National Laboratories
Pulsed Power Sciences

Call for Proposals Package for the Z Facility Fundamental Science Program for the Period July 1, 2020 to June 30, 2022

Issue Date: June 17, 2019

Due Date: September 16, 2019

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QMD Calculations

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Planetary Modeling

Nadine Nettelmann
Andreas Becker
Ronald Redmer

Pulse Shaping

Ray Lemke
Jean-Paul Davis
Chris Seagle
Mark Savage
Ken Struve
Keith LeChien
Brian Stoltzfus
Dave Hinshelwood

Sandia National Laboratories

Entire Z crew

University of Rostock