

# Structure of Solid Matter Under Super-Earth Conditions

*Kavli Institute for Theoretical Physics, Santa Barbara, 2/23/2015*

*Physics of Exoplanets: From Earth-sized to Mini-Neptunes*

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 Lawrence Livermore  
National Laboratory

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# We have built a broad base of academic collaborators



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- **Additional Collaborators / Consultants**
  - Andrew Comley, Brian Maddox, Chris Wehrenberg, Hye-Sook Park, and Bruce Remington
- **Plus farget fabrication, Omega and NIF facility and diagnostic teams.**

\*Currently, Washington State University  
\*\*Currently, University of Edinburgh  
\*\*\*Currently, Harvard University  
\*\*\*\*Currently, DESY



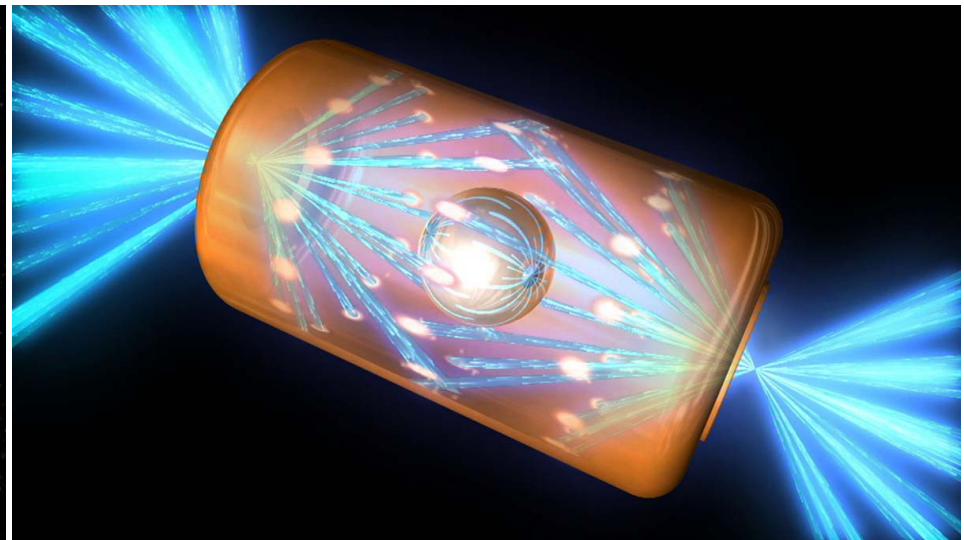
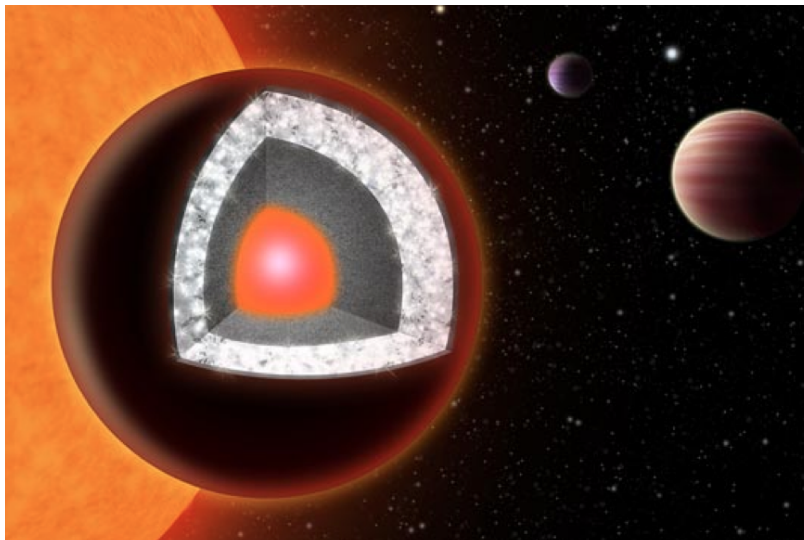
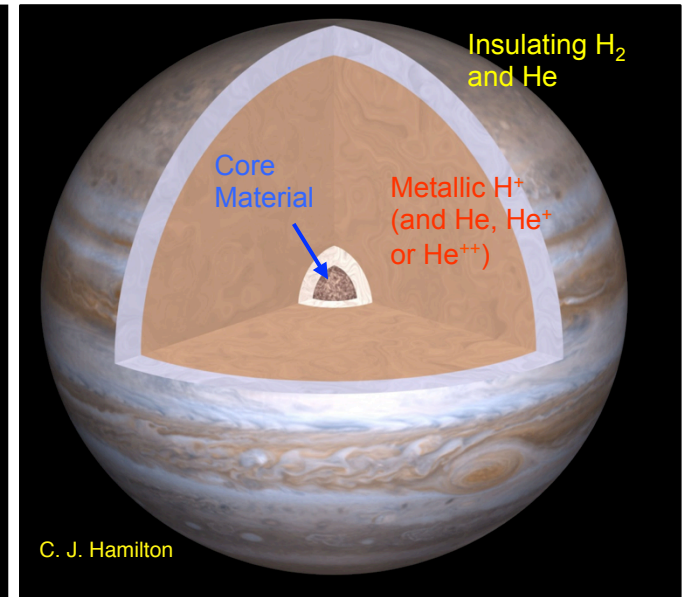
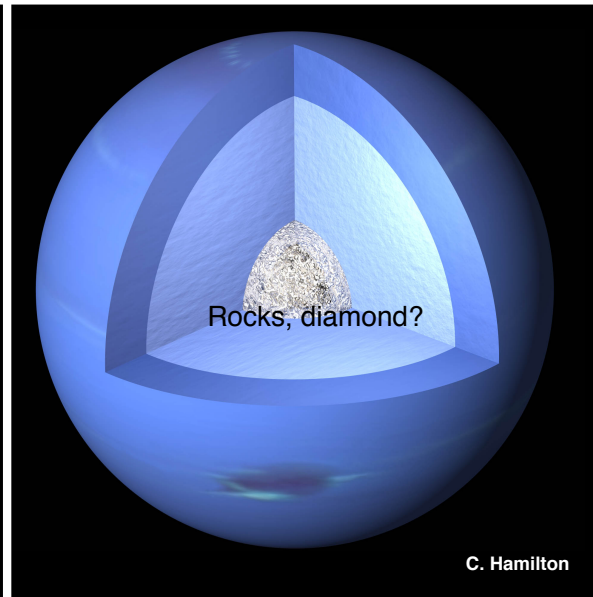
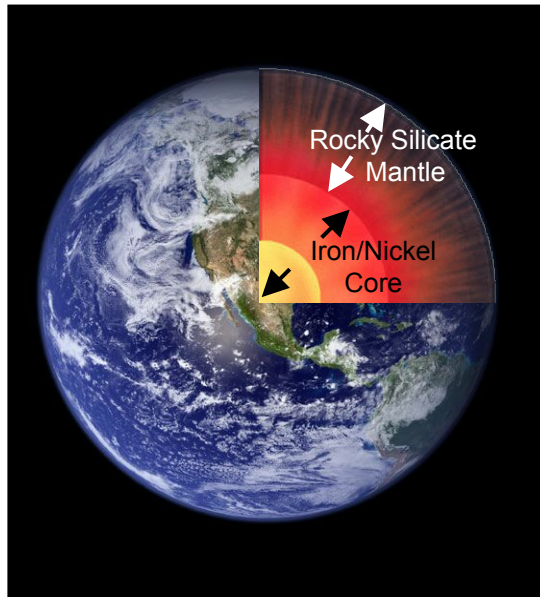
## Outline

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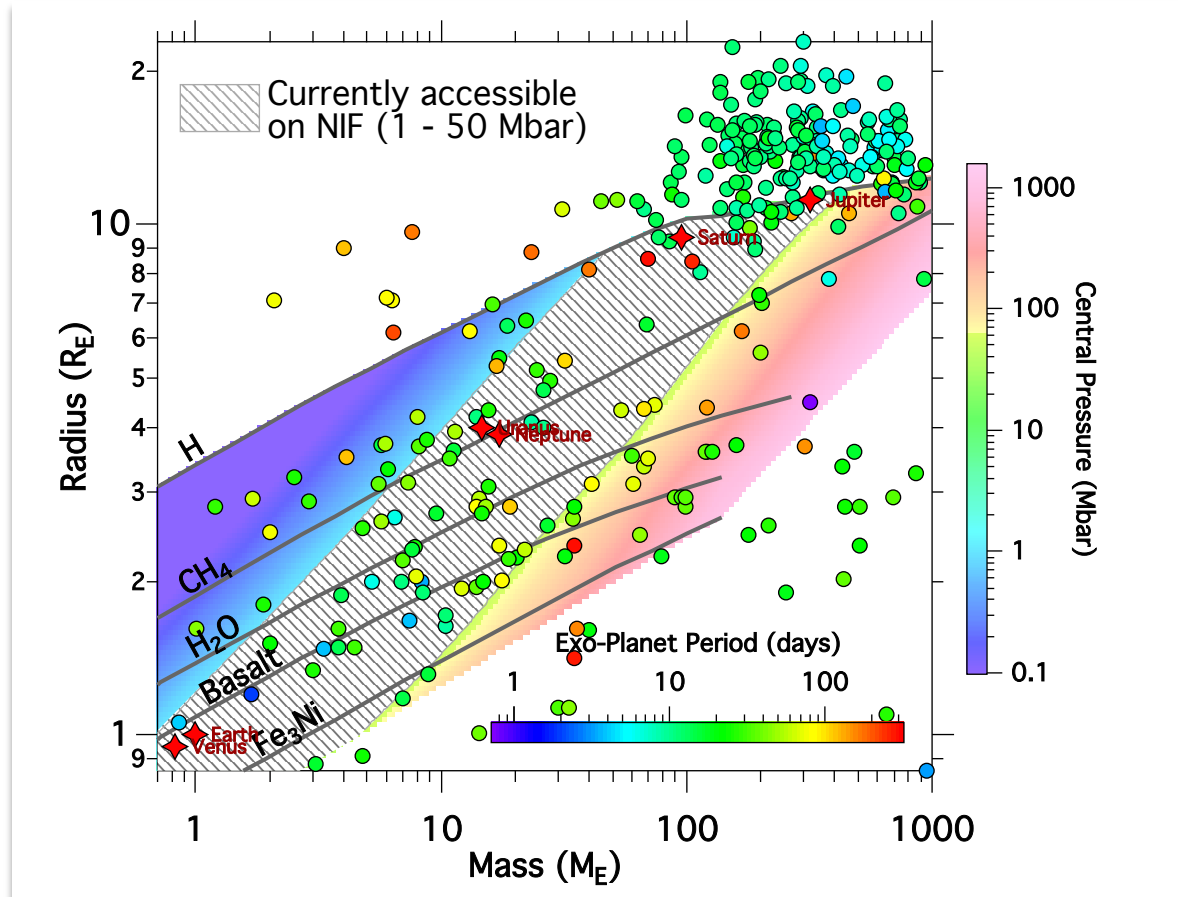
- **Introduction**
- **Ramp-Compression  
Stress-Density EOS**
- **X-Ray Diffraction at  
Omega and NIF**
- **Future Experiments**

# Matter at High Energy Density (HED) is found throughout our universe

1 Mbar = 100 GPa = 0.1 TPa



# High pressures have particular relevance to the interiors of planets

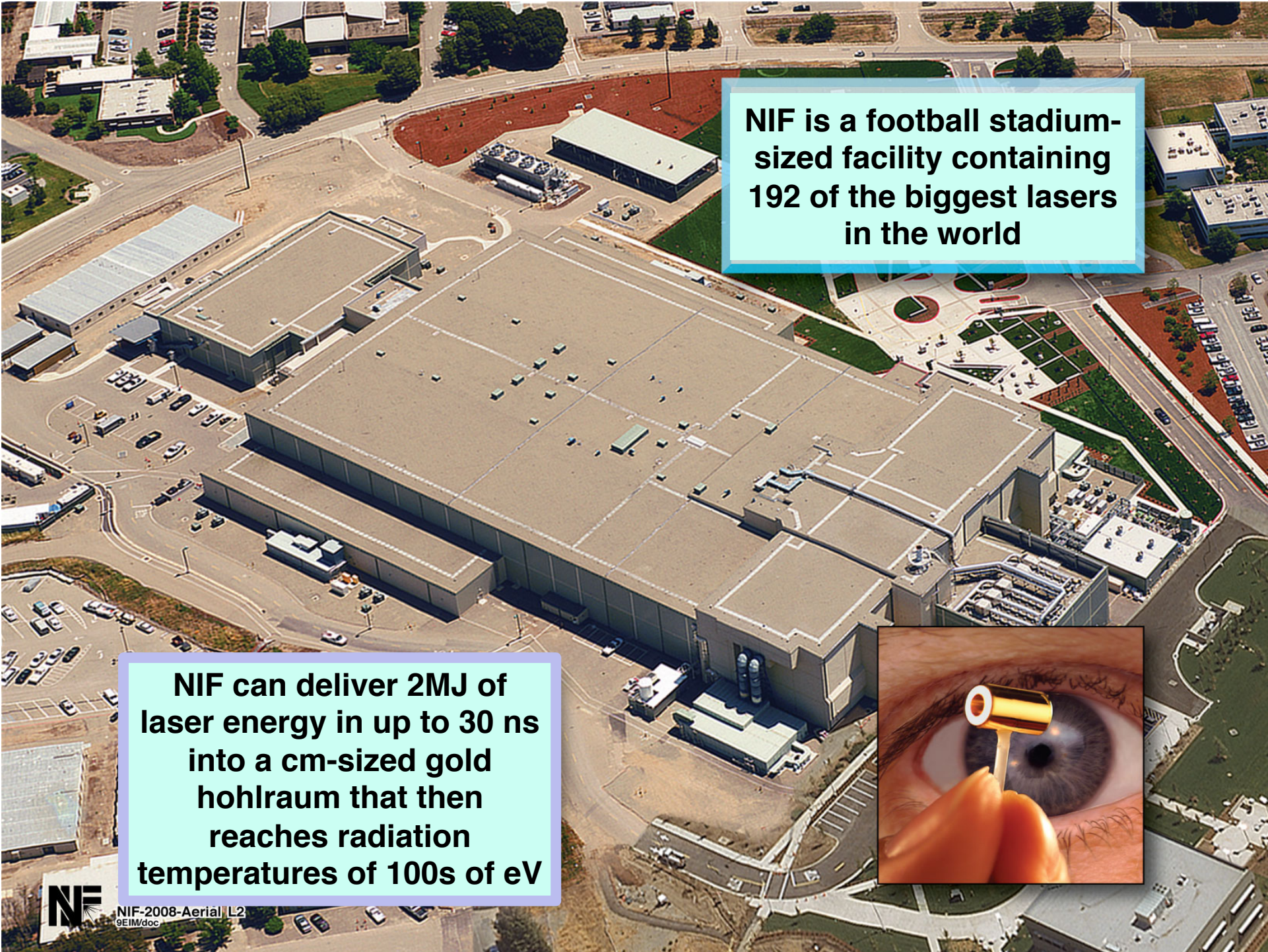


As of February 21, 2015:  
 1890 planets  
 1189 planetary systems  
 477 multiple planet systems  
 (<http://exoplanet.eu>)

1189 transiting exo-planets  
 have been confirmed ~405  
 with known mass and radius.

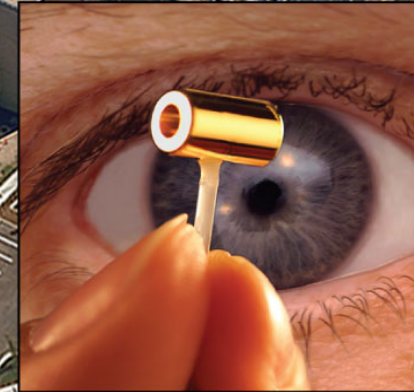
The mass-radius plot is our  
 best way to constrain the  
 interior make-up of the  
 planets.

**We can study materials at rocky-planet core pressures for 0.5–20 earth masses in the laboratory**

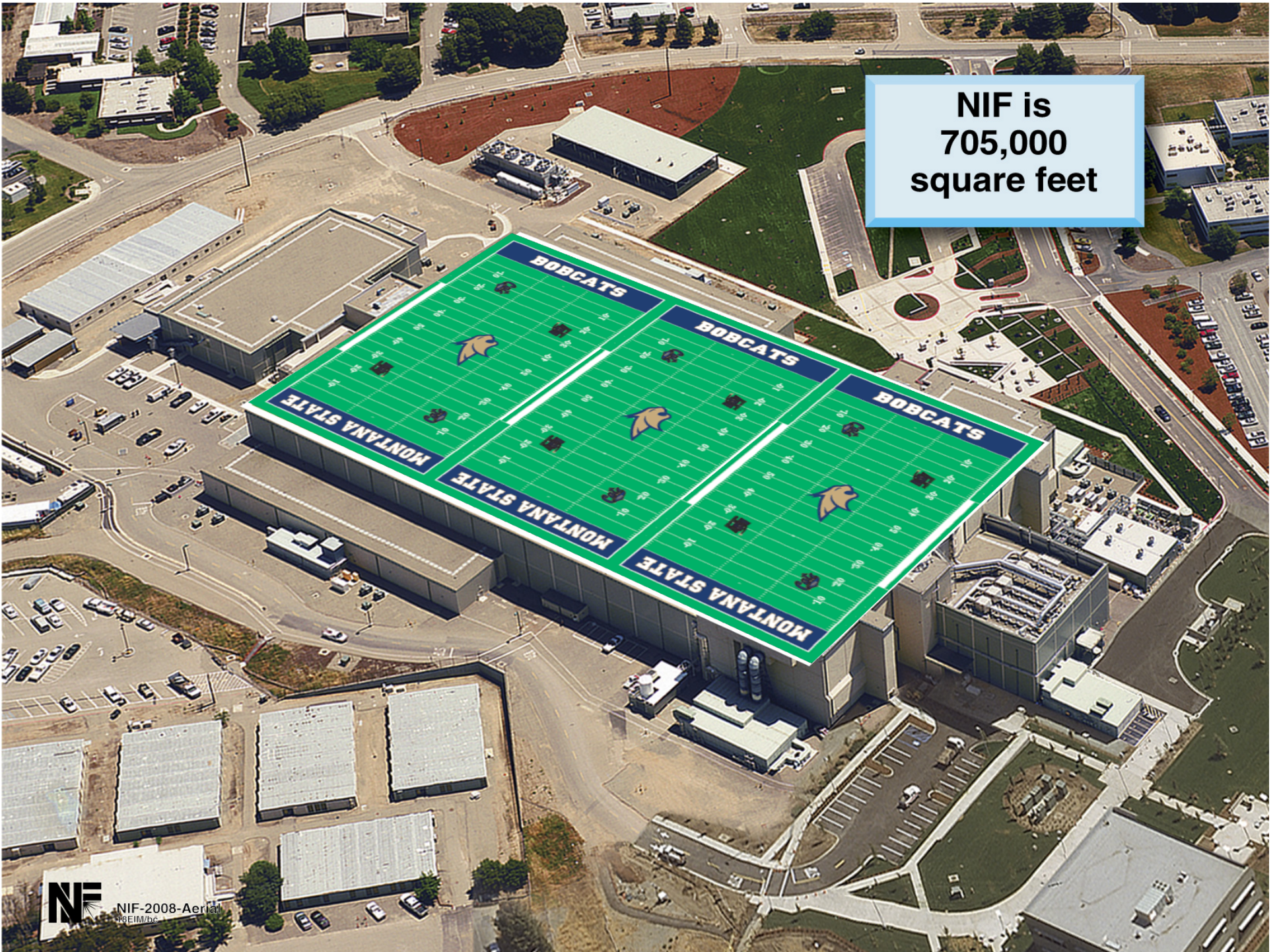


**NIF is a football stadium-sized facility containing 192 of the biggest lasers in the world**

**NIF can deliver 2MJ of laser energy in up to 30 ns into a cm-sized gold hohlraum that then reaches radiation temperatures of 100s of eV**



**NIF is  
705,000  
square feet**



NIF-2008-Aerial  
©EIM/bc

**Finished LB2  
Installation Qualification  
March 31, 2008**



NIF-0508-14729  
12EHW/cfs

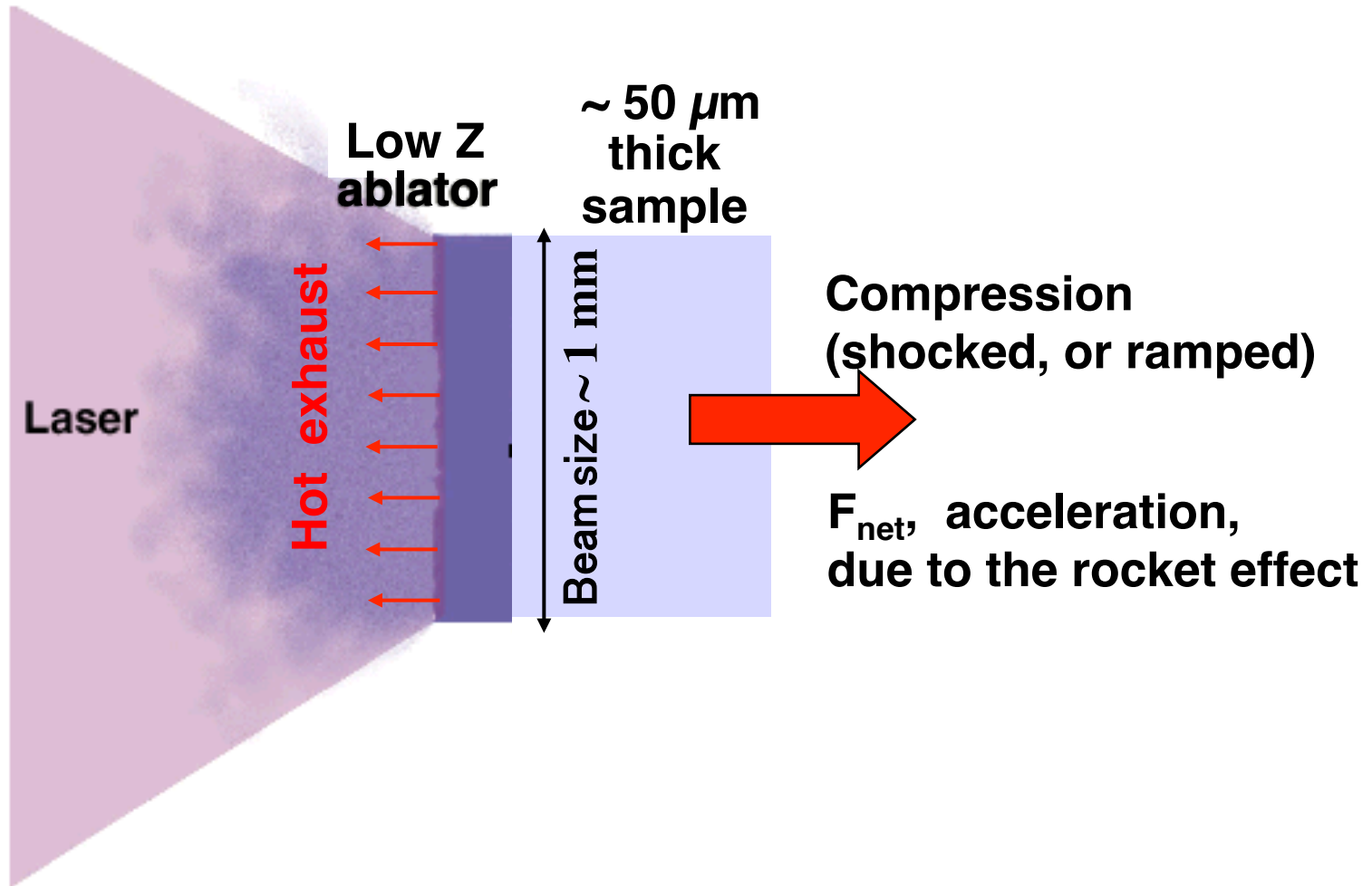


# Inside the Target Chamber



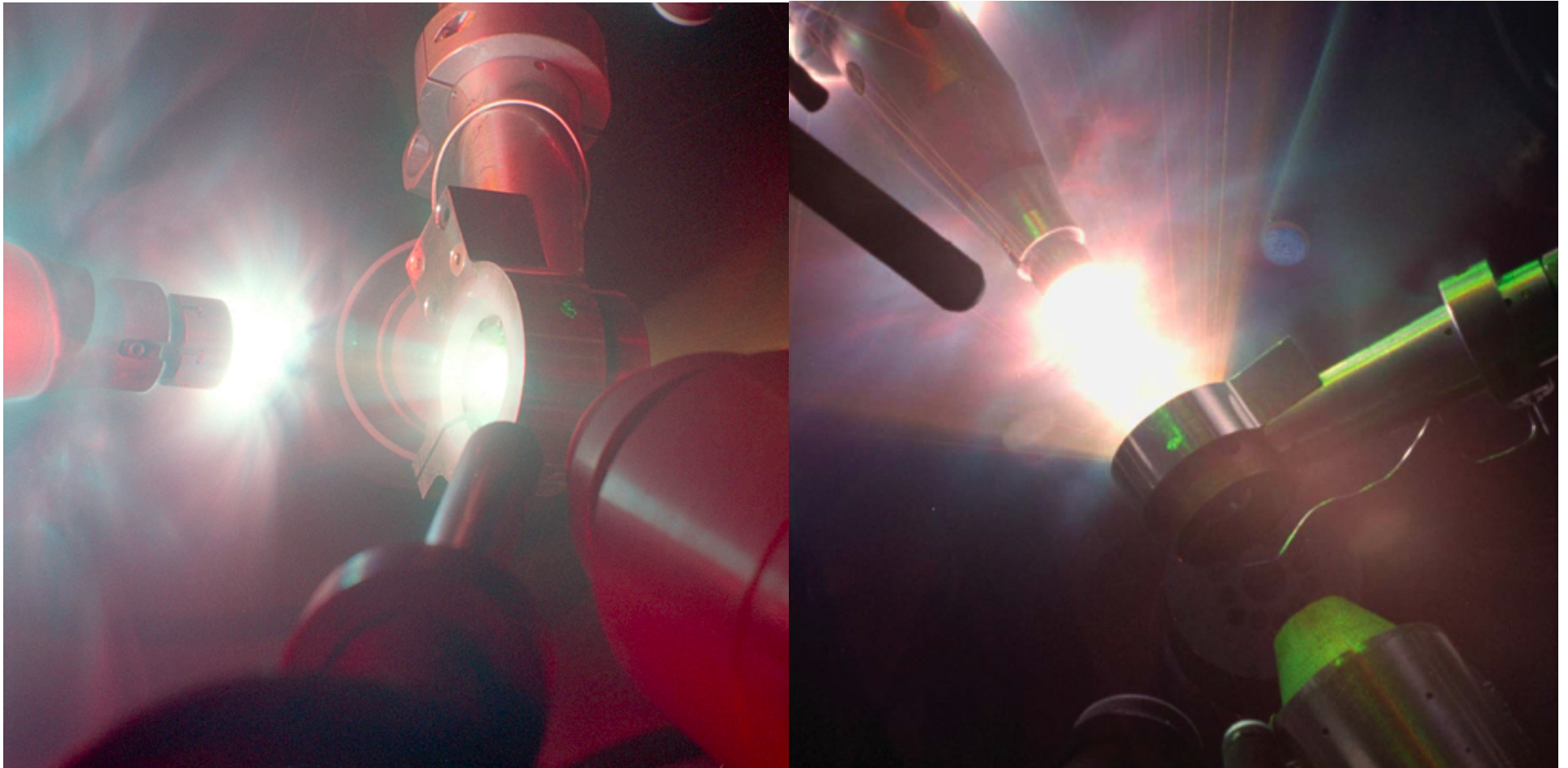


# Laser Ablation Drive



1 Mbar = 100 GPa = 0.1 TPa

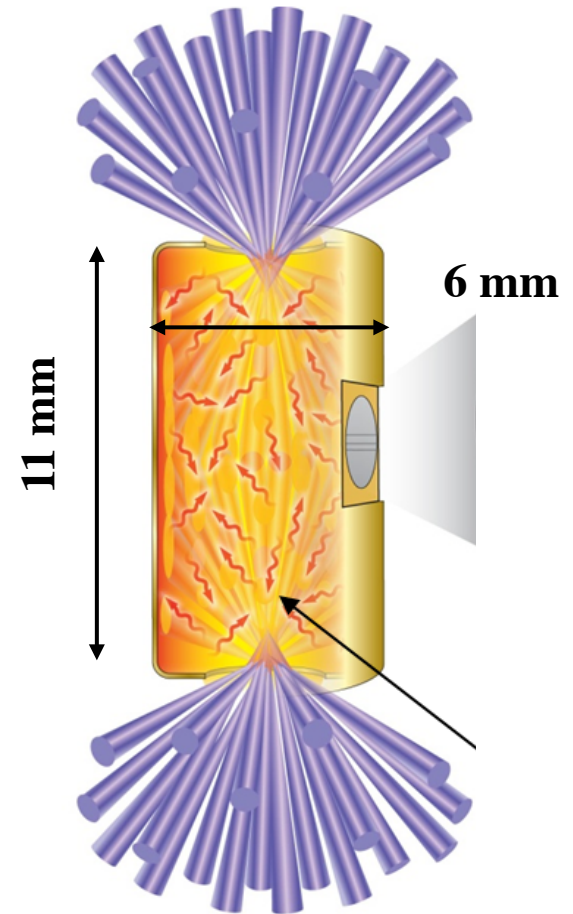
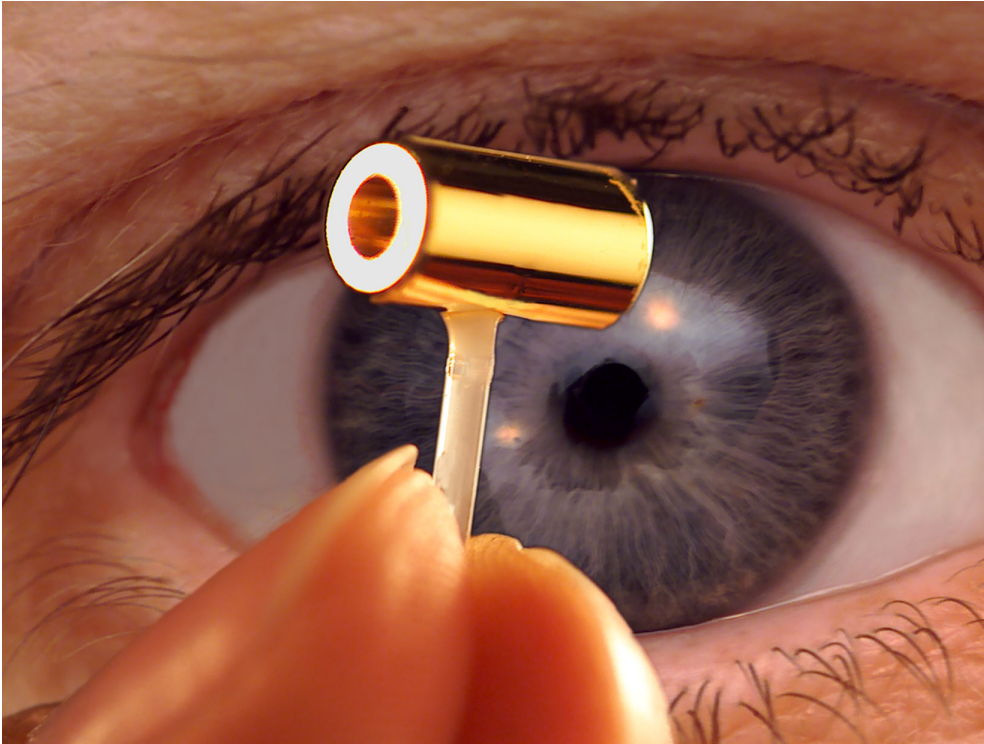
**High pressures result from the rocket effect generated by laser-induced ablation.**



**Time-integrated photos of shots at the Omega laser (60 beams, 30 kJ) at University of Rochester**

# A uniform photon field supplied by a gold radiation cavity or *Hohlraum* ensures good drive planarity

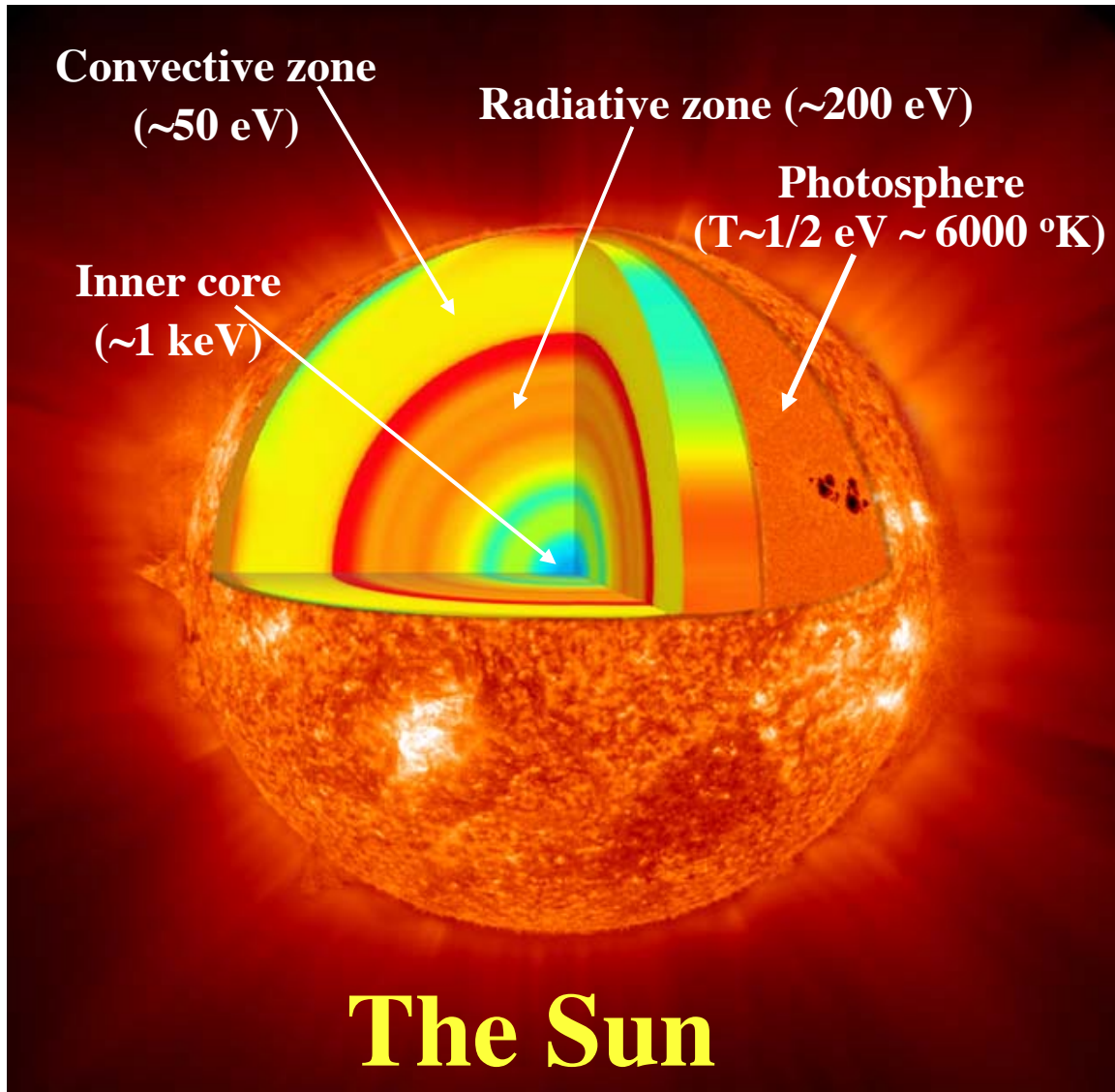
$$1 \text{ Mbar} = 100 \text{ GPa} = 0.1 \text{ TPa}$$



Typical  $T_{rad}$  of 200 eV will generate pressures of about 40 Mbar



## How hot is 200 eV?



- 200 eV = 2 million degrees
- 200 eV = 400 x temperature at the surface of sun
- 200 eV = the temperature about half way to the center of the sun, in the radiative zone



# Using the NIF we will explore Extreme Compression Science

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## **We want to measure:**

Stress-Density

Temperature

Melting

Solid-Solid Phase Transitions

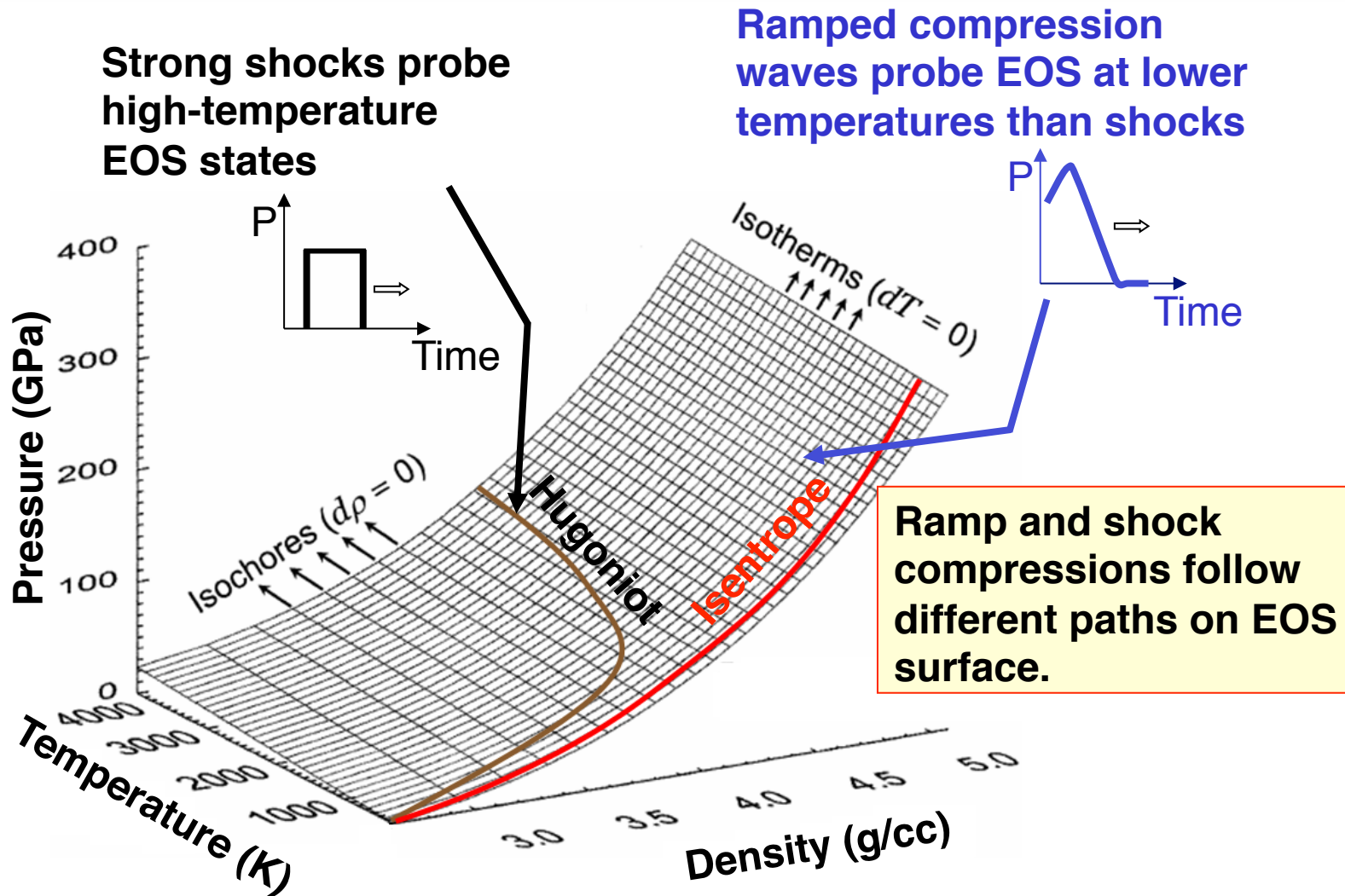
Structure

Texture

Strength

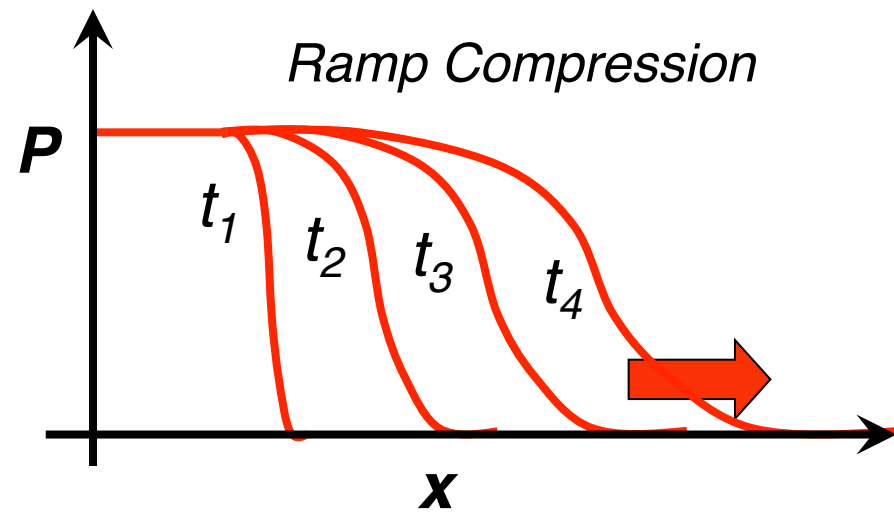
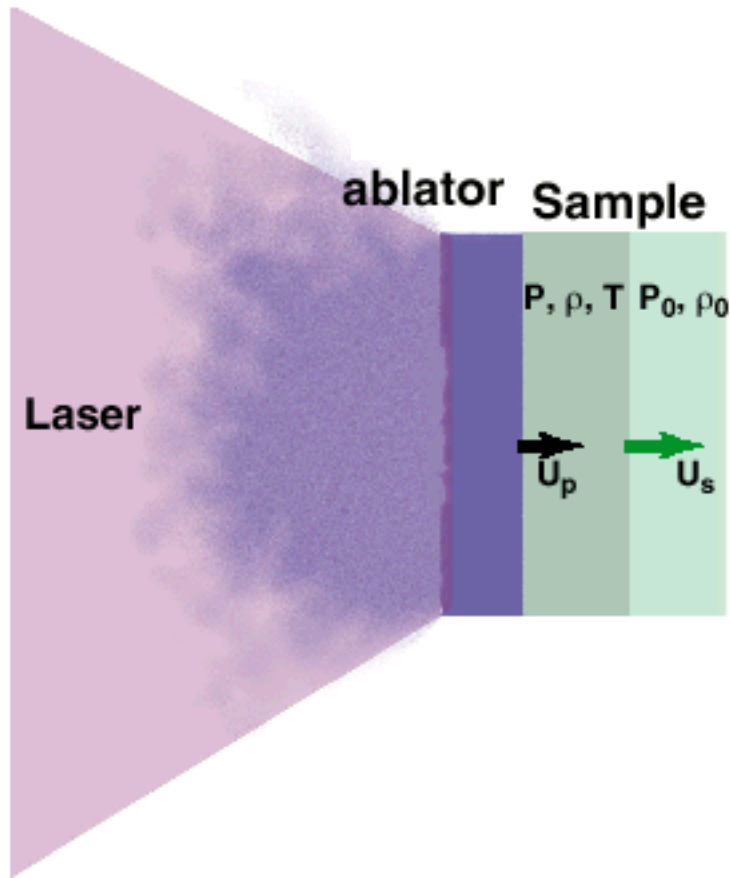


# Equilibrium thermodynamics is described by an equation-of-state (EOS) surface





# Ramp compression by variable drive intensity

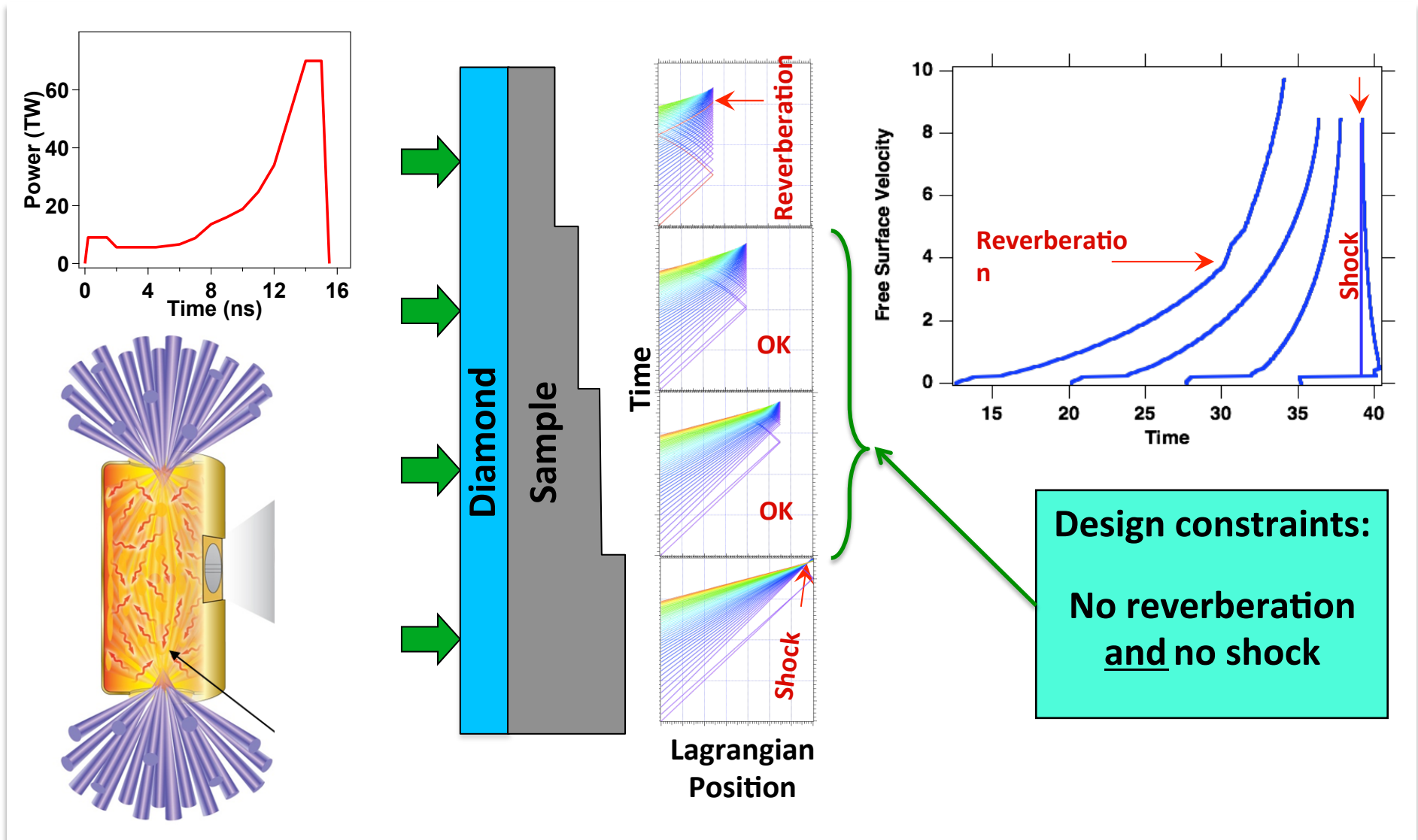


Ramp Compression -> Lower Temperature



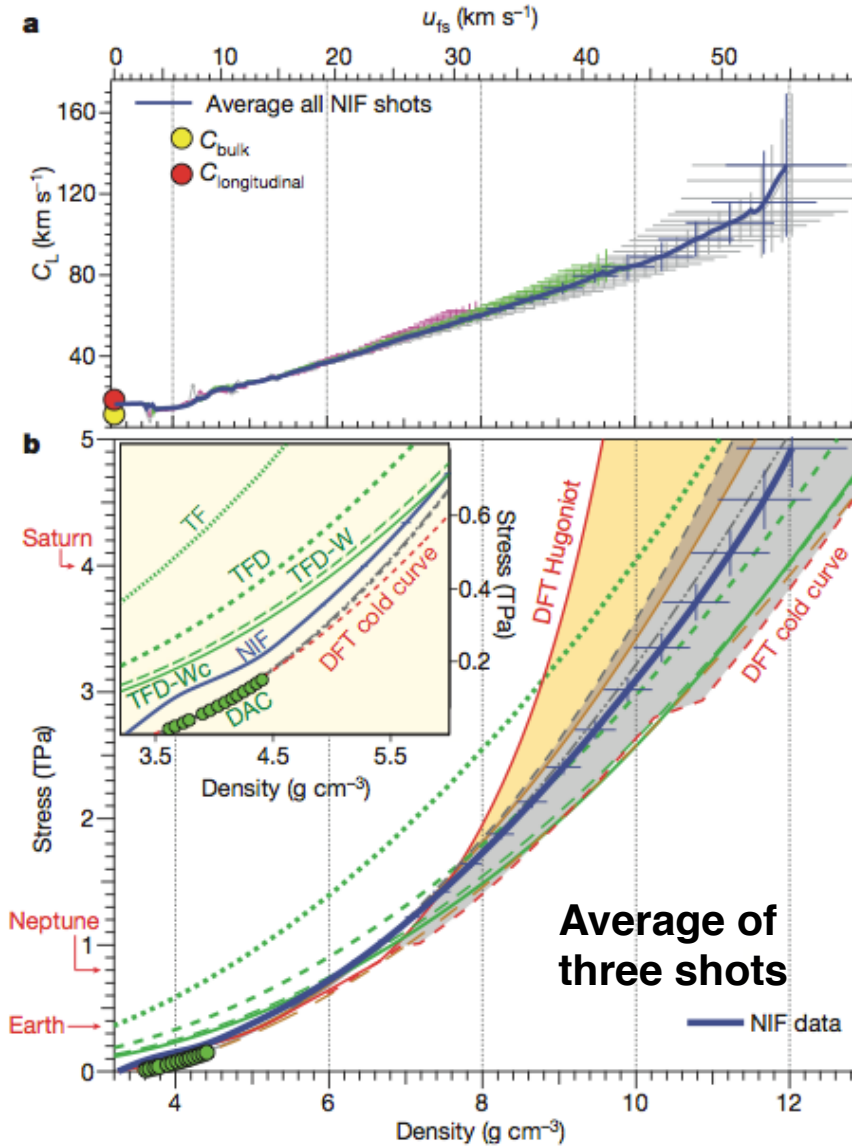
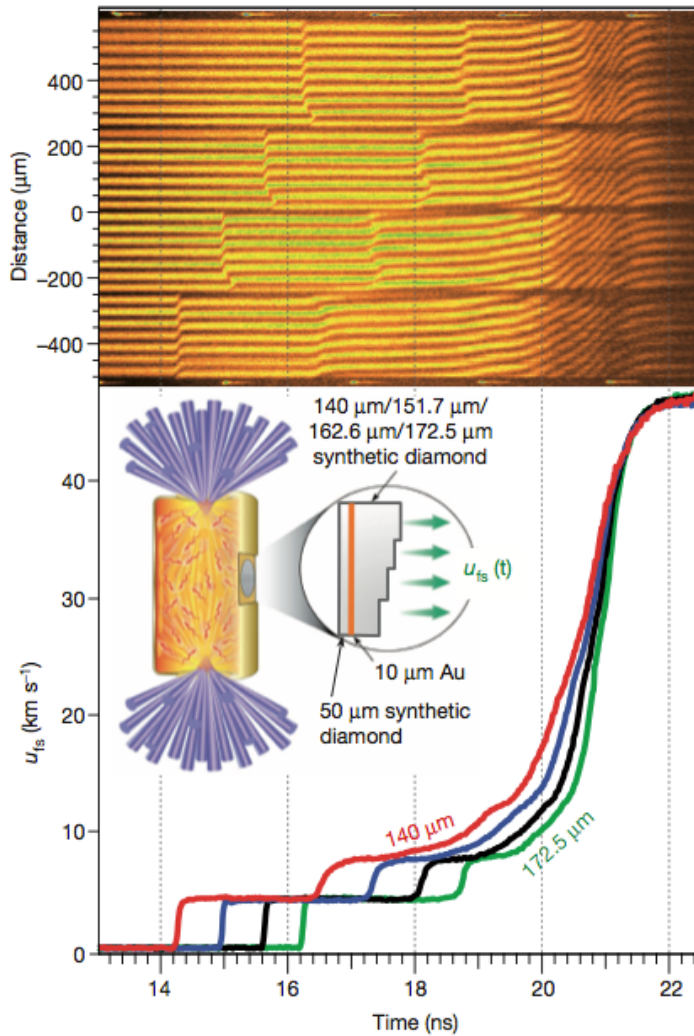


# Ramp loading, EOS (stress-density) determined from free-surface velocity measurements



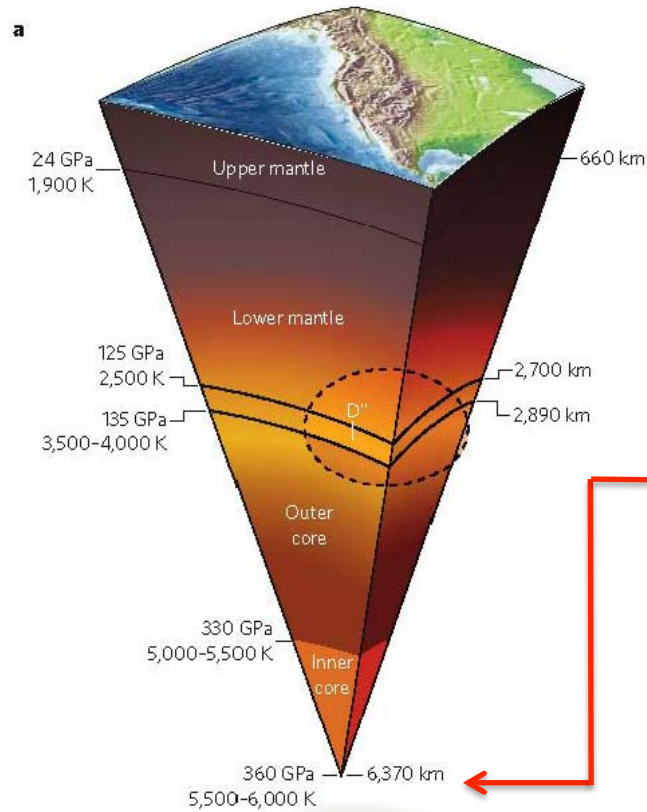
# Ramp-compression EOS of nano-crystalline diamond to 50 Mbar.

1 Mbar = 100 GPa = 0.1 TPa

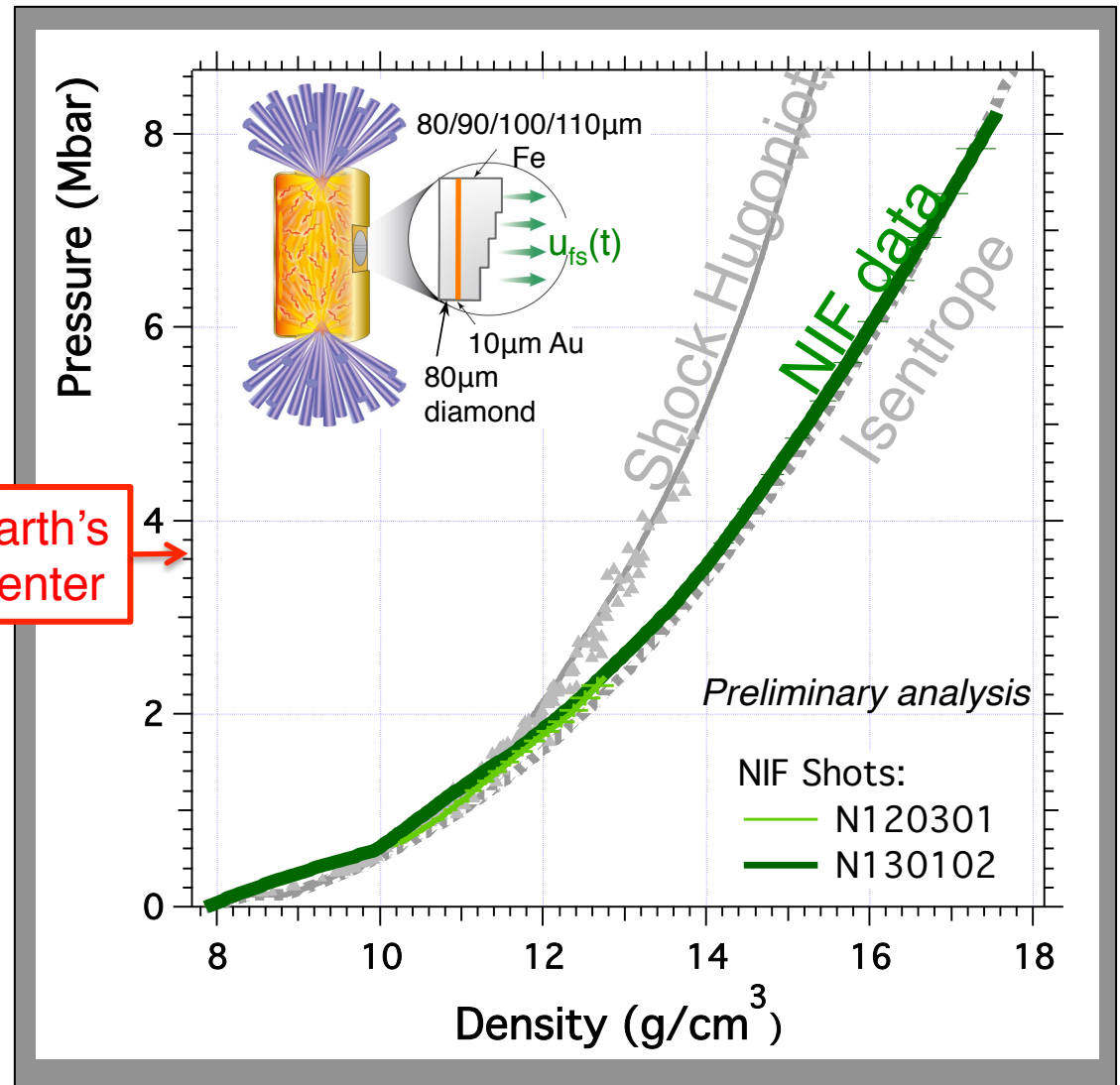


(Smith, et al., Nature, 2014)

# Recent shots on NIF have measured the equation of state of Fe at 8 Mbar, >2x pressure of Earth's core



Earth's Center



**But, we wanted to measure...**

Stress-Density

Temperature

Melting

**Solid-Solid Phase Transitions**

**Structure**

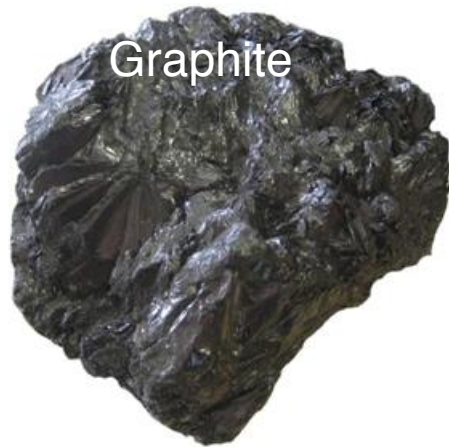
**Texture**

**Strength**

So we developed an X-ray diffraction  
platform for Omega and NIF

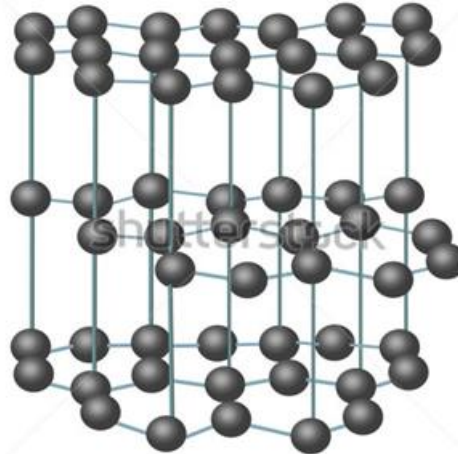


# Thermo-mechanical properties can vary significantly between structures



Graphite

## Atomic Structure

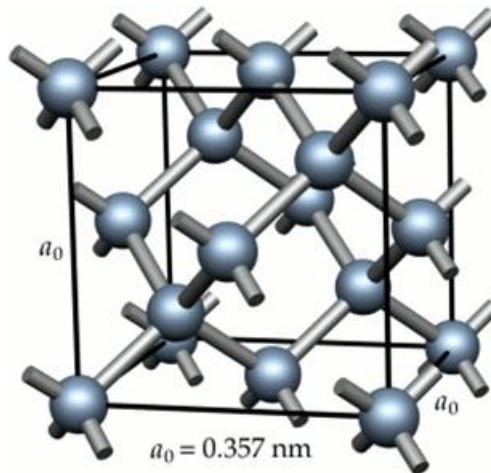


## Physical Properties

	Graphite	Diamond
Density (g/cm <sup>3</sup> )	2.2	3.51
Bulk Modulus (GPa)	34	440
Coefficient of Thermal Expansion (K <sup>-1</sup> )	7.8 x 10 <sup>-6</sup>	1.1 x 10 <sup>-6</sup>
Strength (GPa)	< 0.2	>110



Diamond



**Structure difference leads to:**  
**1.6x difference in density**  
**10x difference in compressibility**  
**500x difference in strength**

# Surprising phases have been discovered at high compression

1 Mbar = 100 GPa = 0.1 TPa

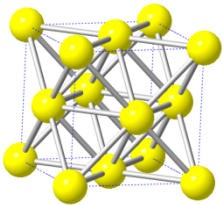


**Traditional view that *all* materials become simple at high pressure is incorrect!**

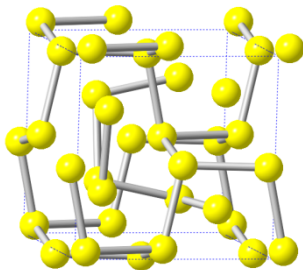
“... what the present results most assuredly demonstrate is the importance of pressure in revealing the limitations of previously hallowed models of solids”

–Neil Ashcroft (2009).

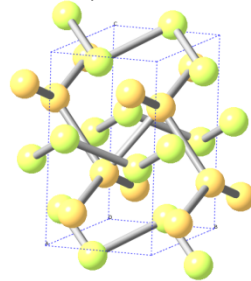
FCC, 65 GPa



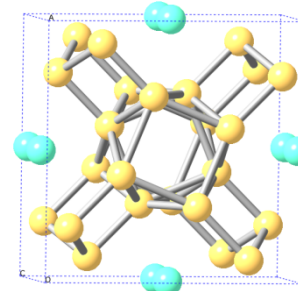
cl16, 108 GPa



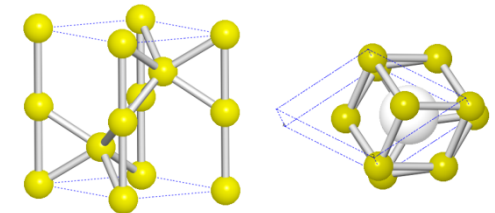
oP8, 119 GPa



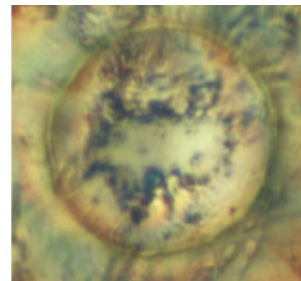
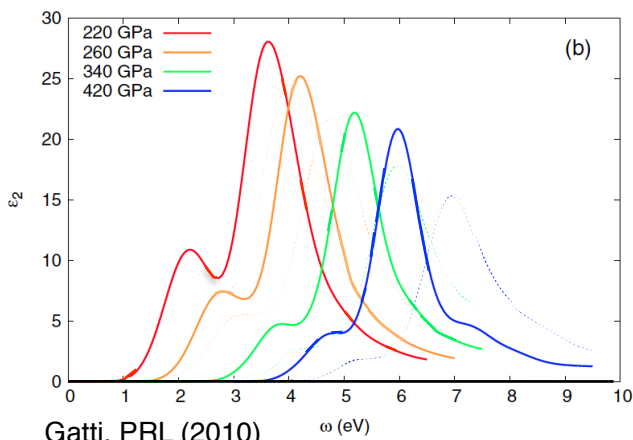
tl19, 147 GPa  
Incommensurate



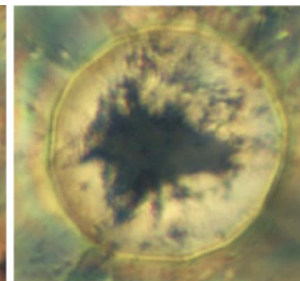
hP4, 190 GPa  
Insulating, Transparent  
Electride



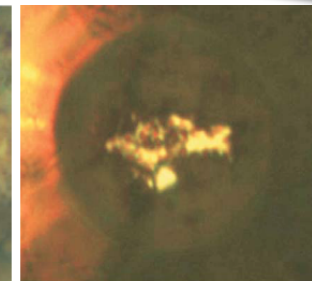
**Increasing Structural Complexity**



120 GPa



156 GPa



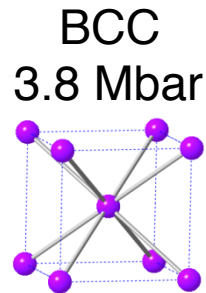
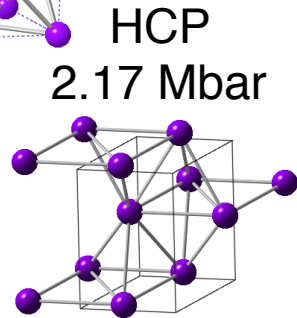
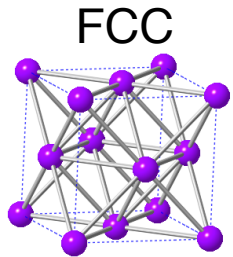
199 GPa Ma, Nature (2009)

# High pressure phases of aluminum are also predicted to be complex

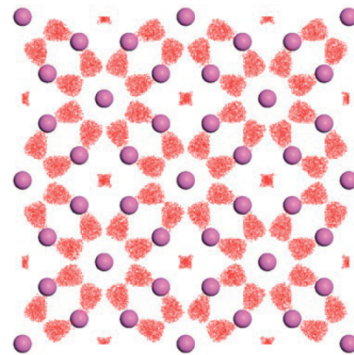
1 Mbar = 100 GPa = 0.1 TPa



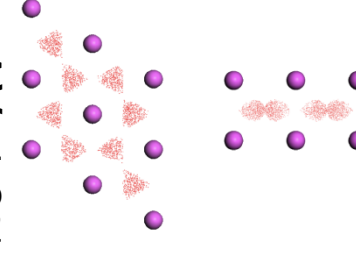
Pickard and Needs, Nature Materials (2010).



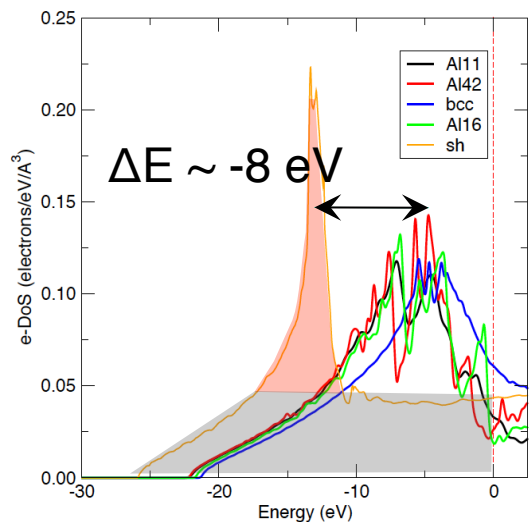
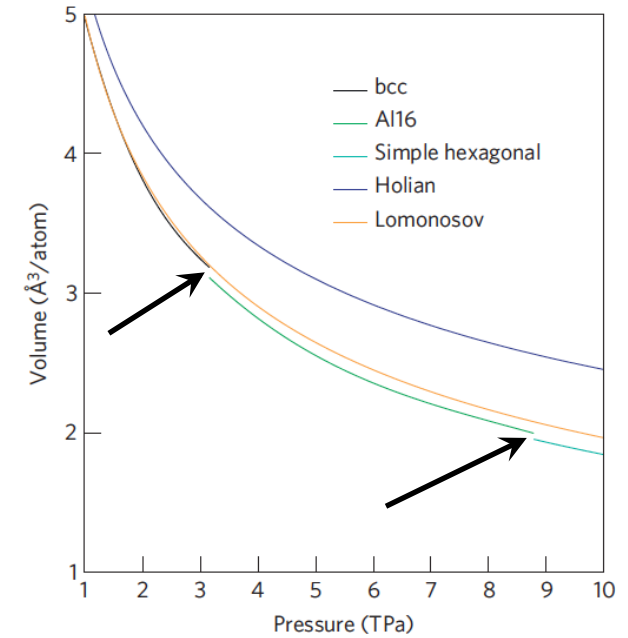
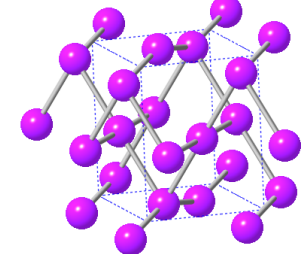
**Host-Guest structure of Ba-IVa (Incommensurate Electride)**  
32-88 Mbar



**Simple Hexagonal Electride**  
88 – 100 Mbar



**CMMA Electride**  
> 100 Mbar

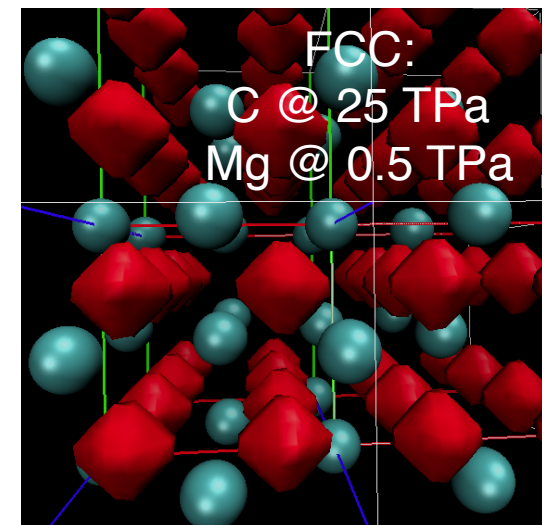
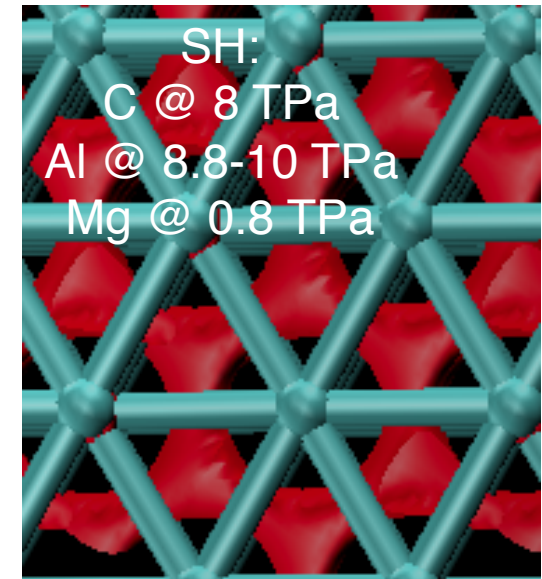
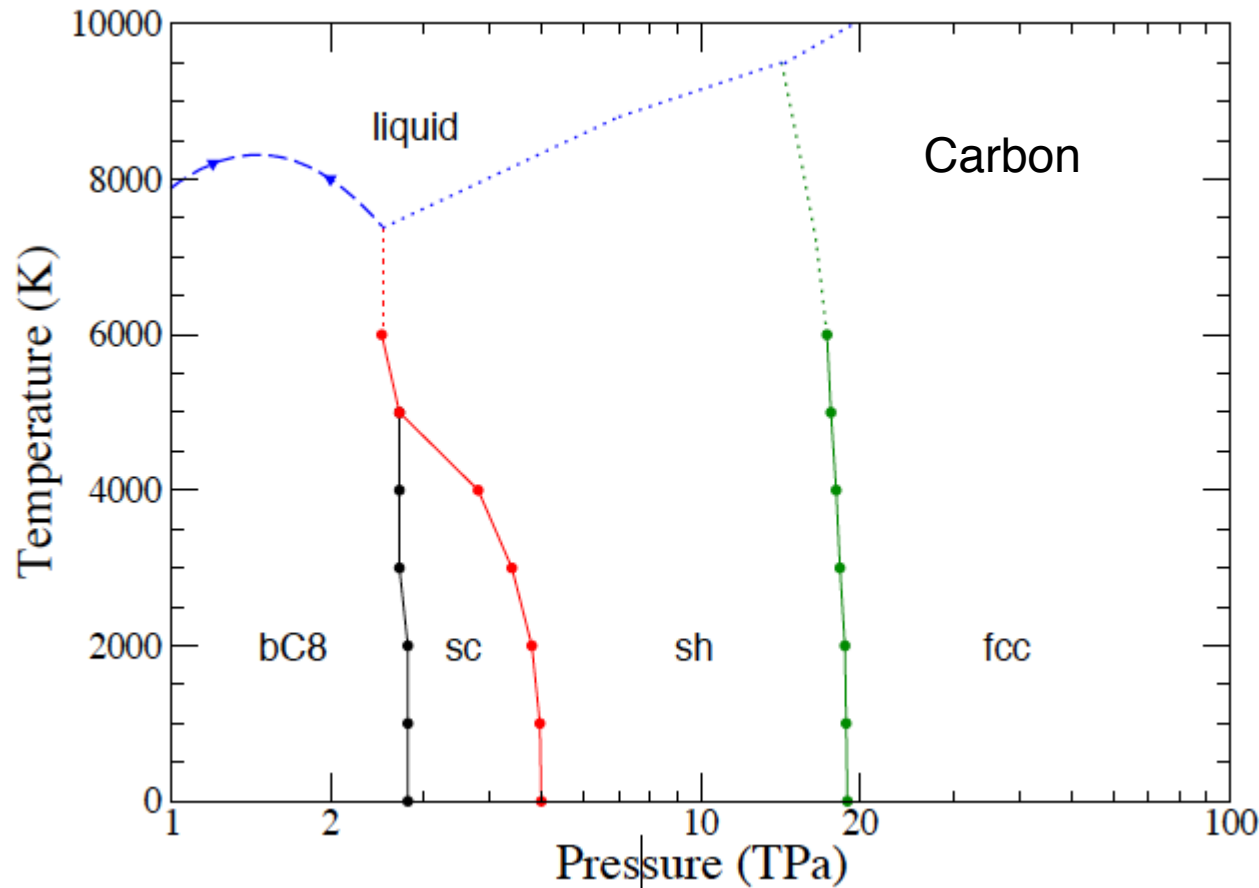


$\Delta V \sim 2.8\%$

$\Delta V \sim 1.8\%$

“All structures near 300 Mbar are far from close packed”

# At even higher pressures carbon is also predicted to adopt electride phases.



Canales, Pickard, Needs, Phys. Rev. Lett. 108, 045704 (2012)

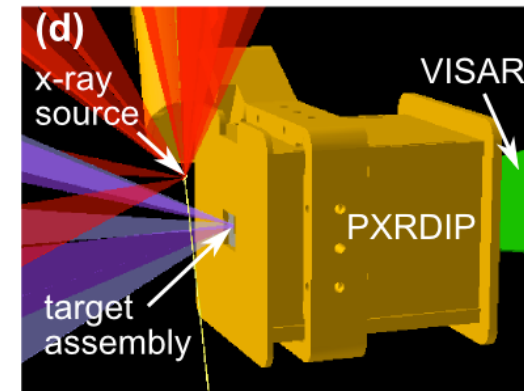




# In situ diffraction gives critical data:

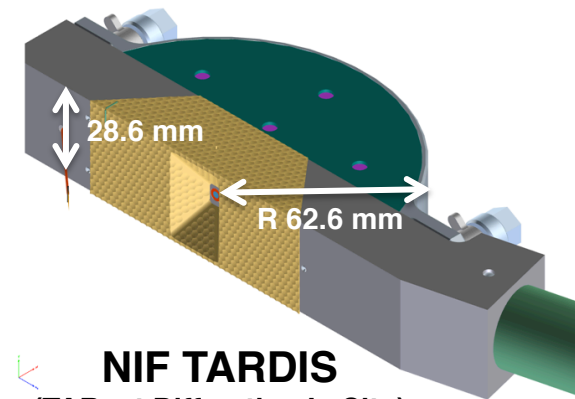
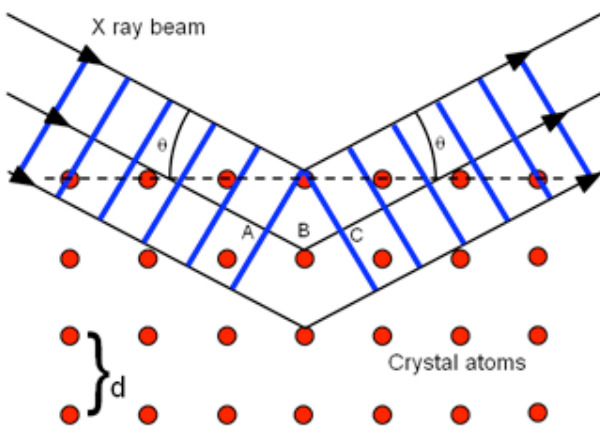
- Crystal structure / phase diagram
- EOS
- Phase-transition mechanisms
- Deformation texture / microstructure
- Potential to determine liquid structure

- Target and diagnostics are simple
- We have done 22 NIF TARDIS shots



Demonstrated at Omega, PXRDIIP

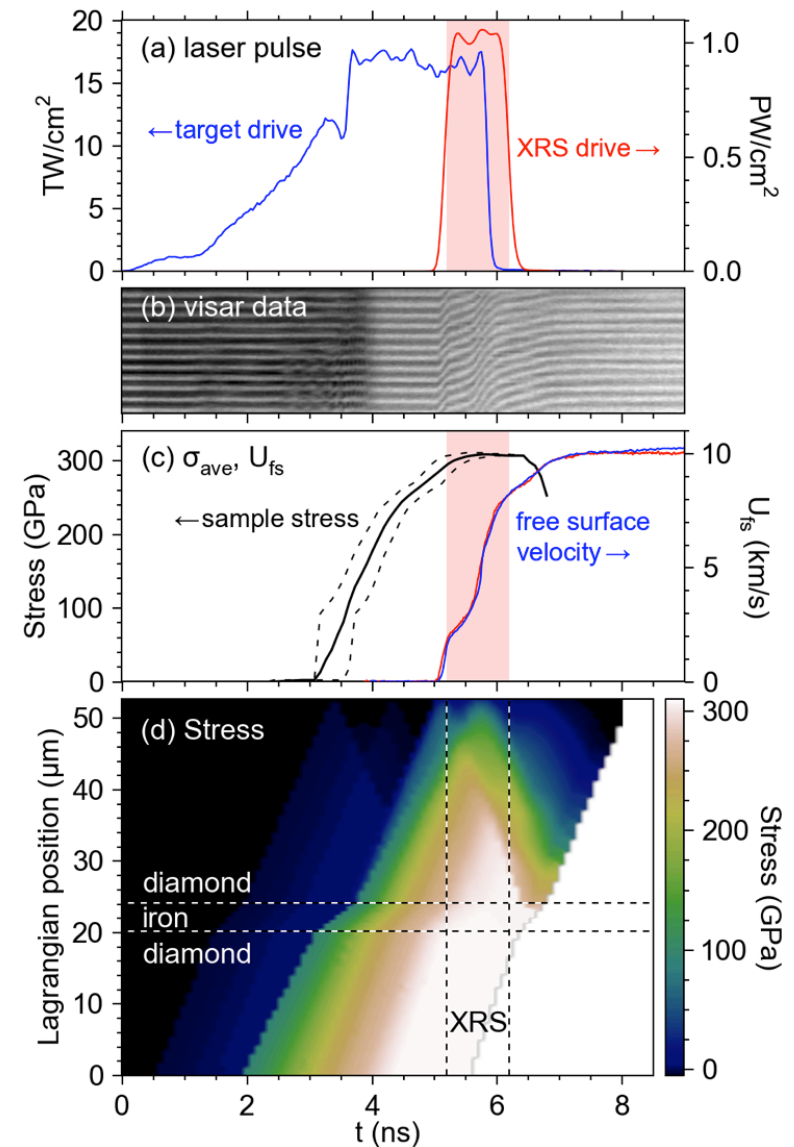
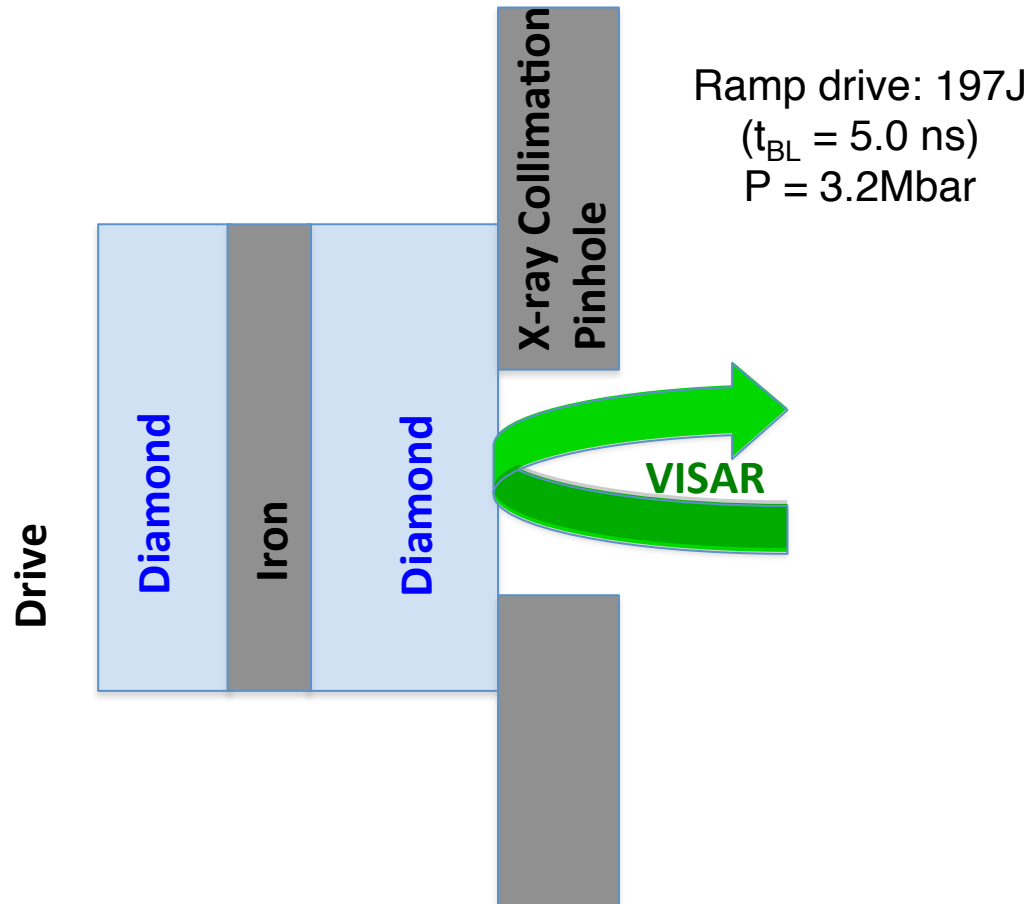
(Powder X-Ray Diffraction Image Plates)



NIF TARDIS (TARget Diffraction In Situ)

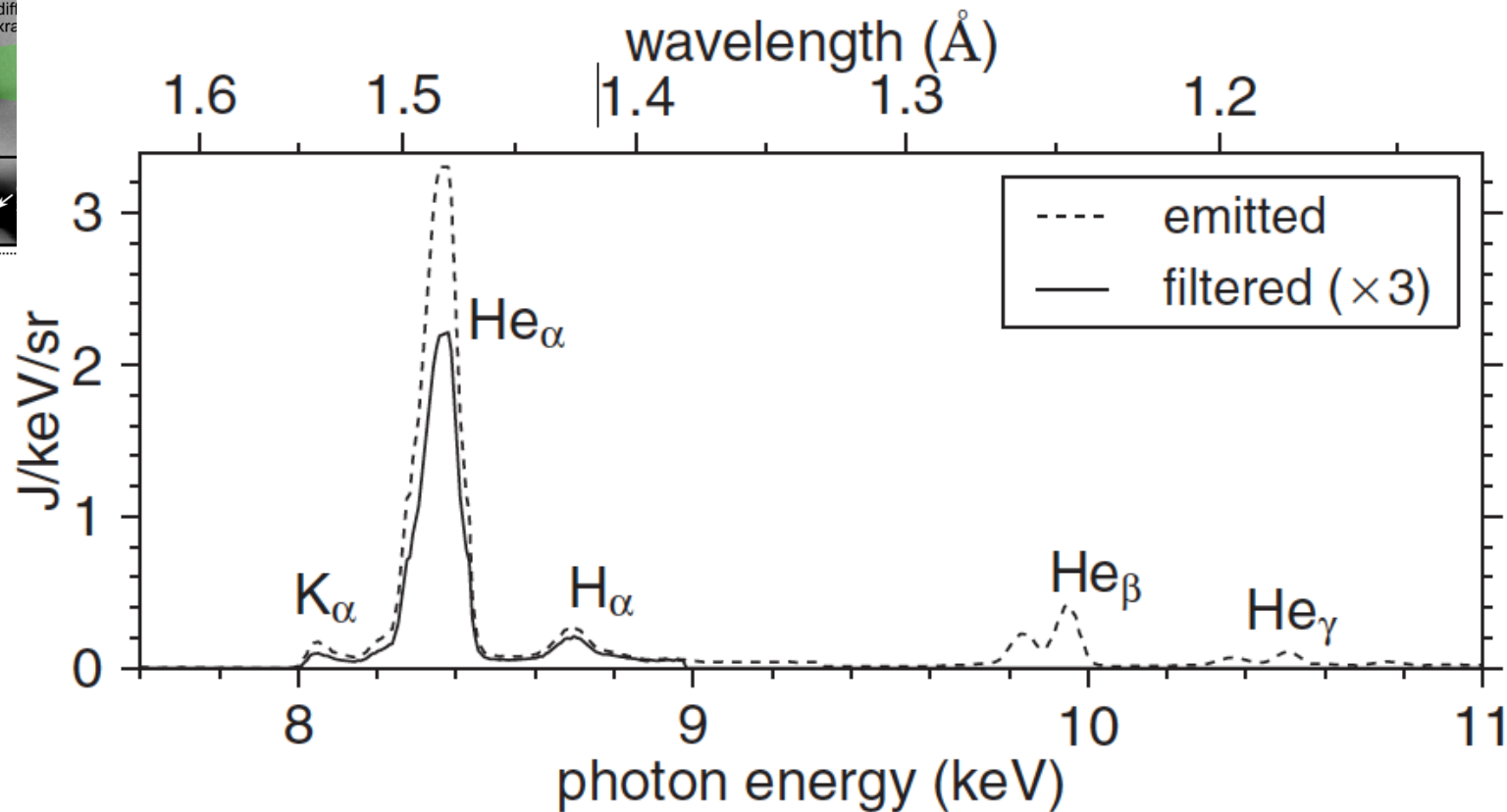
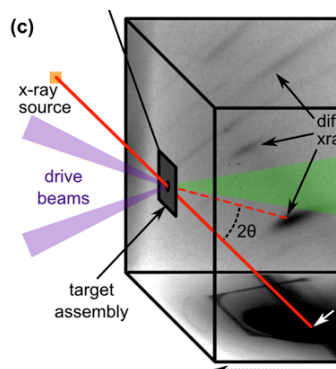


# We use diamond-sandwich targets to obtain uniform stress density conditions after ramp compression



We determine stress by backward propagation of the diamond free-surface velocity, assuming that we know the EOS of diamond.

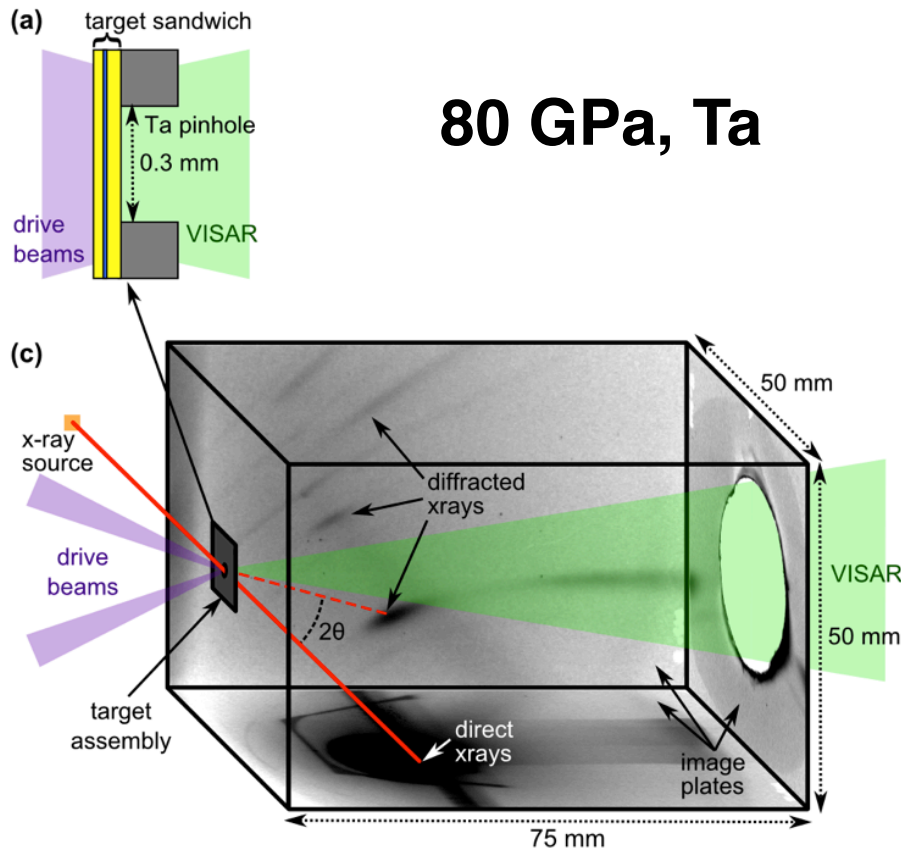
# Quasi-monochromatic beam by thermal emission of Cu He- $\alpha$ line.



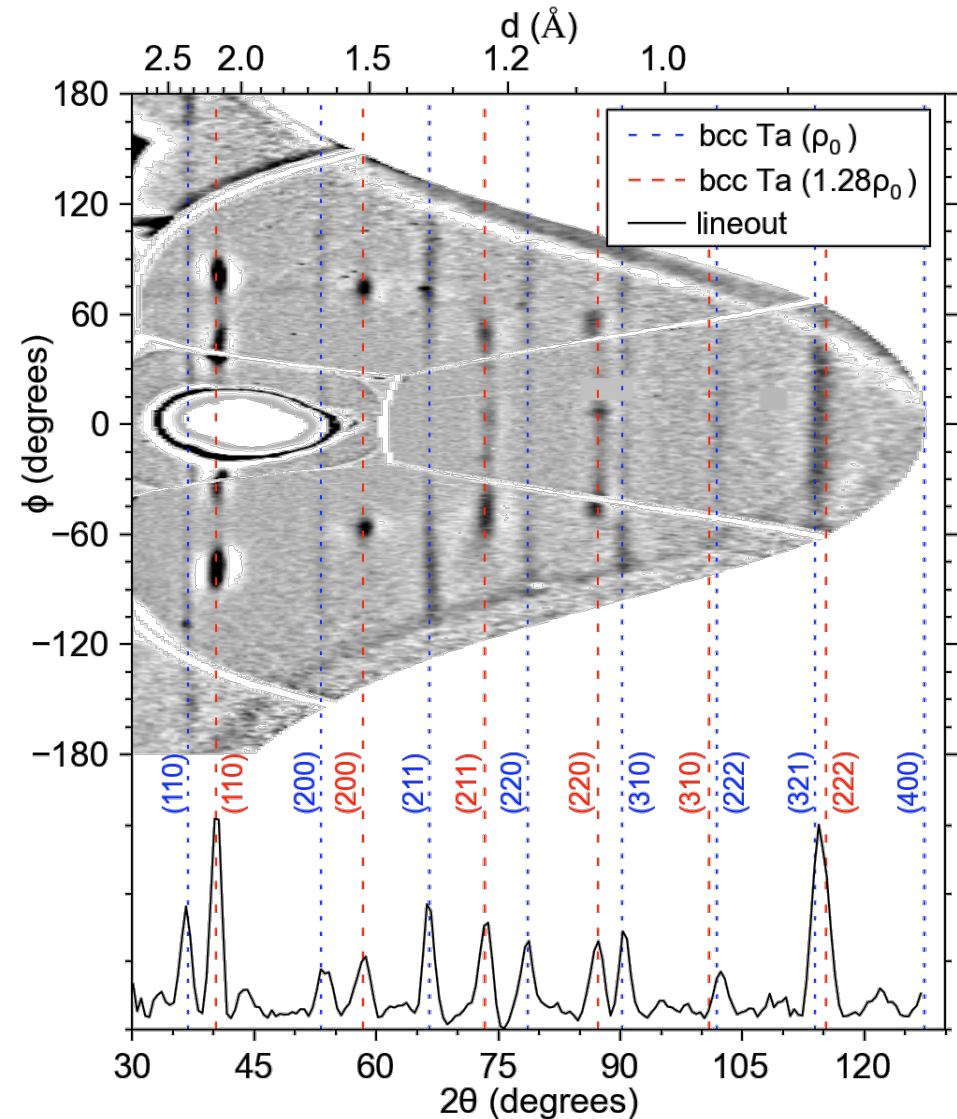
**$10^{11}$  -  $10^{12}$  photons incident on sample**  
**3.5% bandwidth**



# In situ diffraction provides crystal structure. Demonstrated at Omega



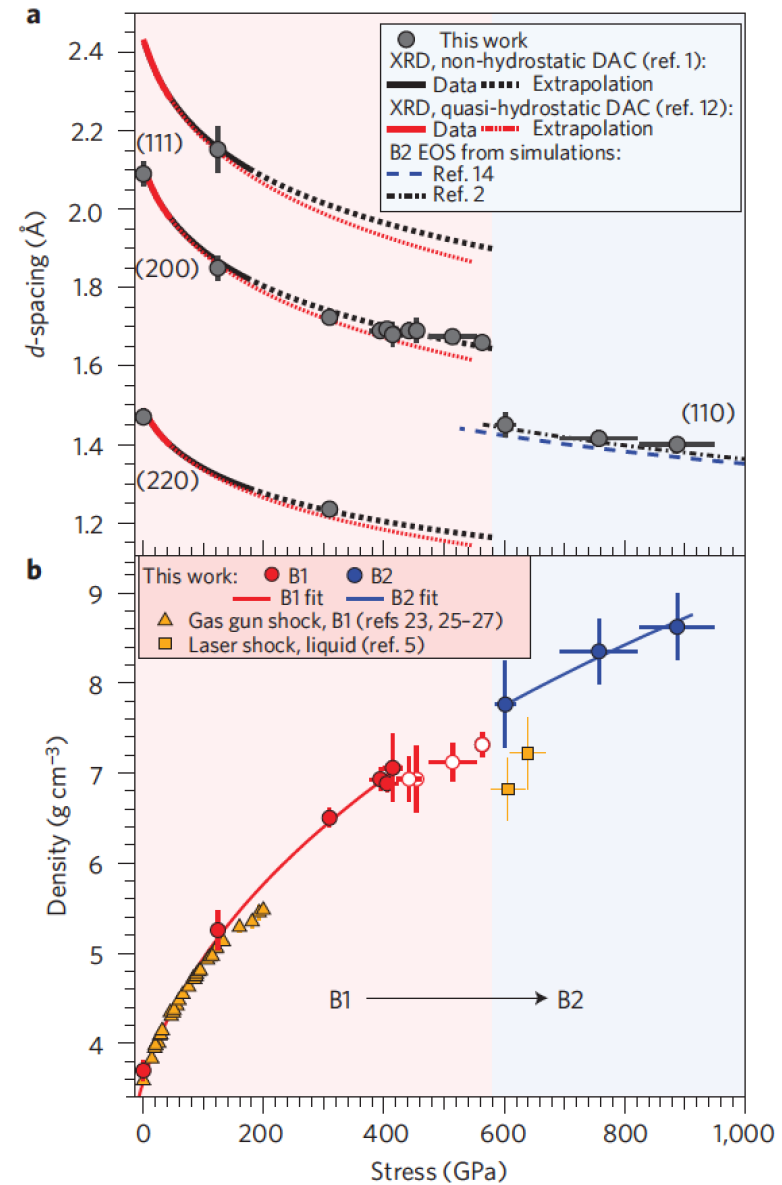
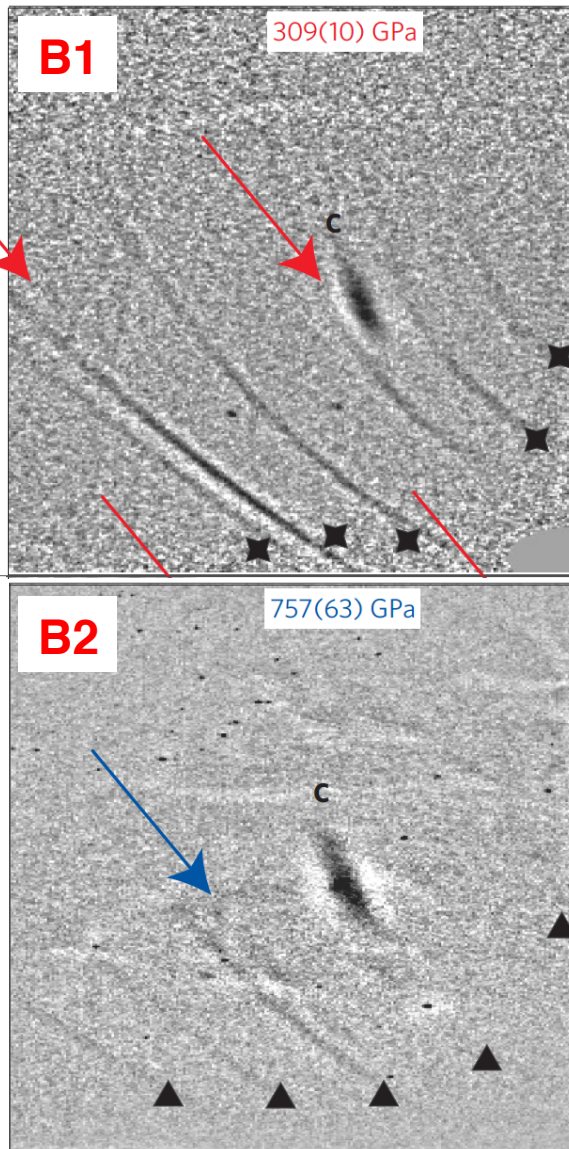
Rygg, et al., RSI, **83**, 113904 (2012)



De-warped image plate data



# We observed the B1-B2 phase transition in MgO

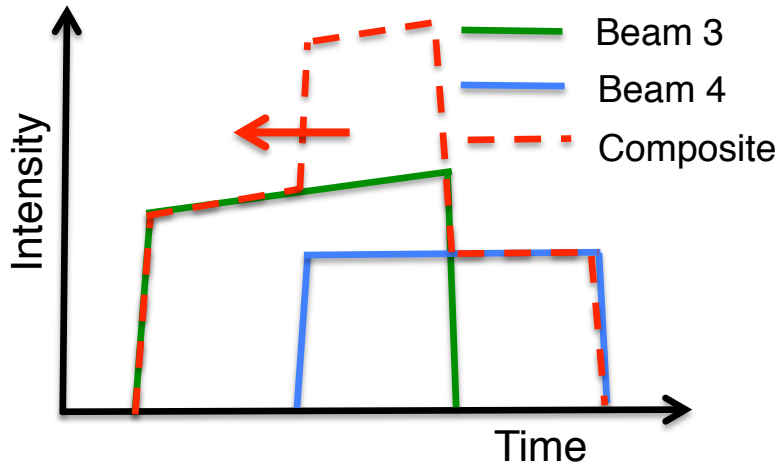


# We have observed Shock-Melt – Refreeze for first time ever in Sn at Omega

1 Mbar = 100 GPa = 0.1 TPa

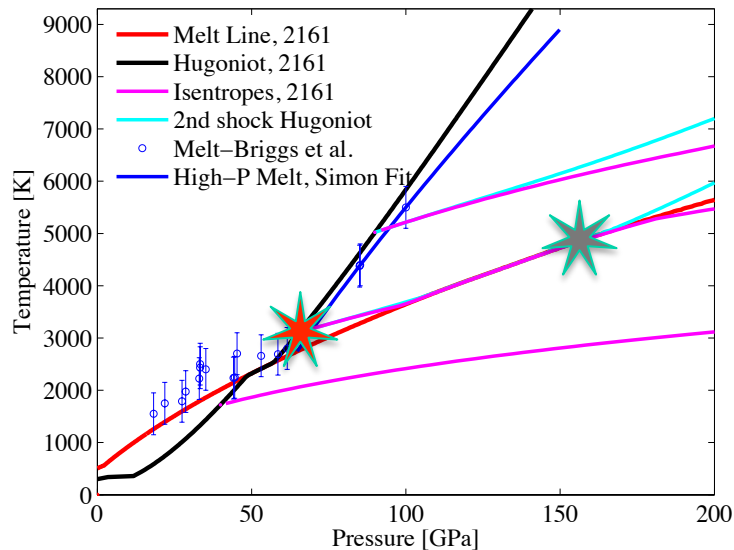


[May 28, 2014]

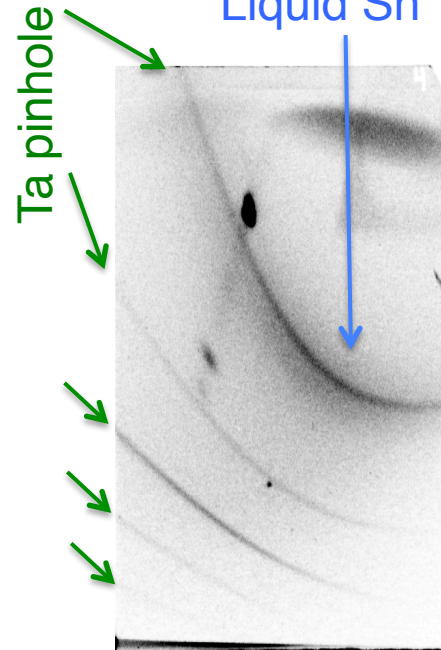


Shot 18450  
Long Delay  
=> All Liquid

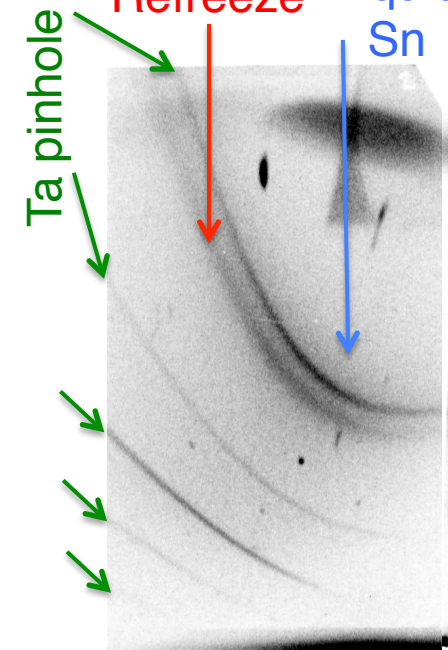
Shot 18452  
Reduced Delay  
=> Liquid + Refreeze



Diffuse  
Liquid Sn



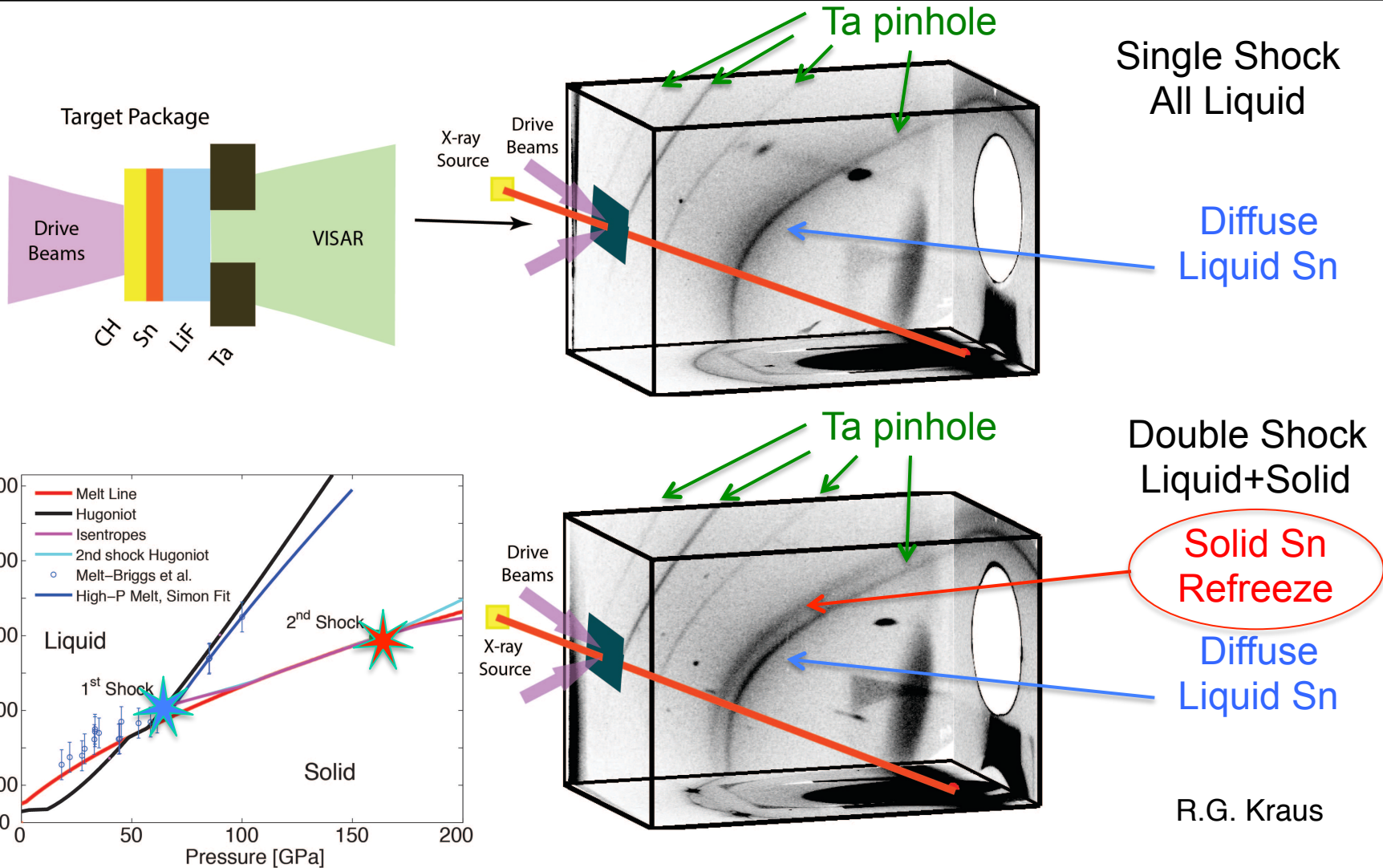
Solid Sn  
Refreeze Liquid Sn



Rick Kraus, Federica Coppari

# Shock-Melt, Refreeze was observed for first time ever in Sn at Omega

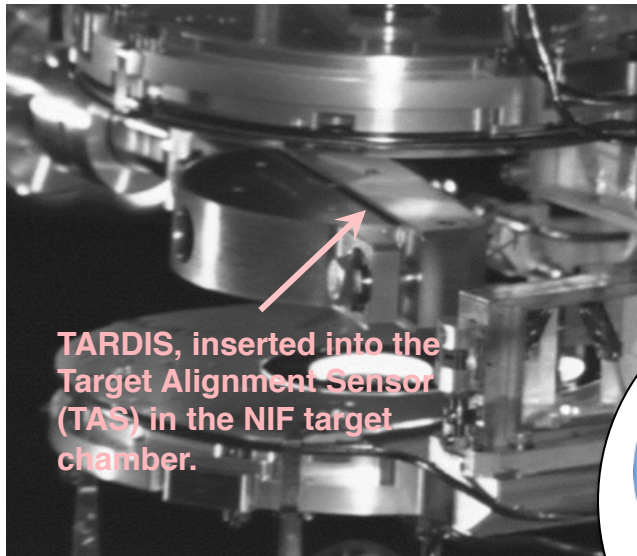
1 Mbar = 100 GPa = 0.1 TPa



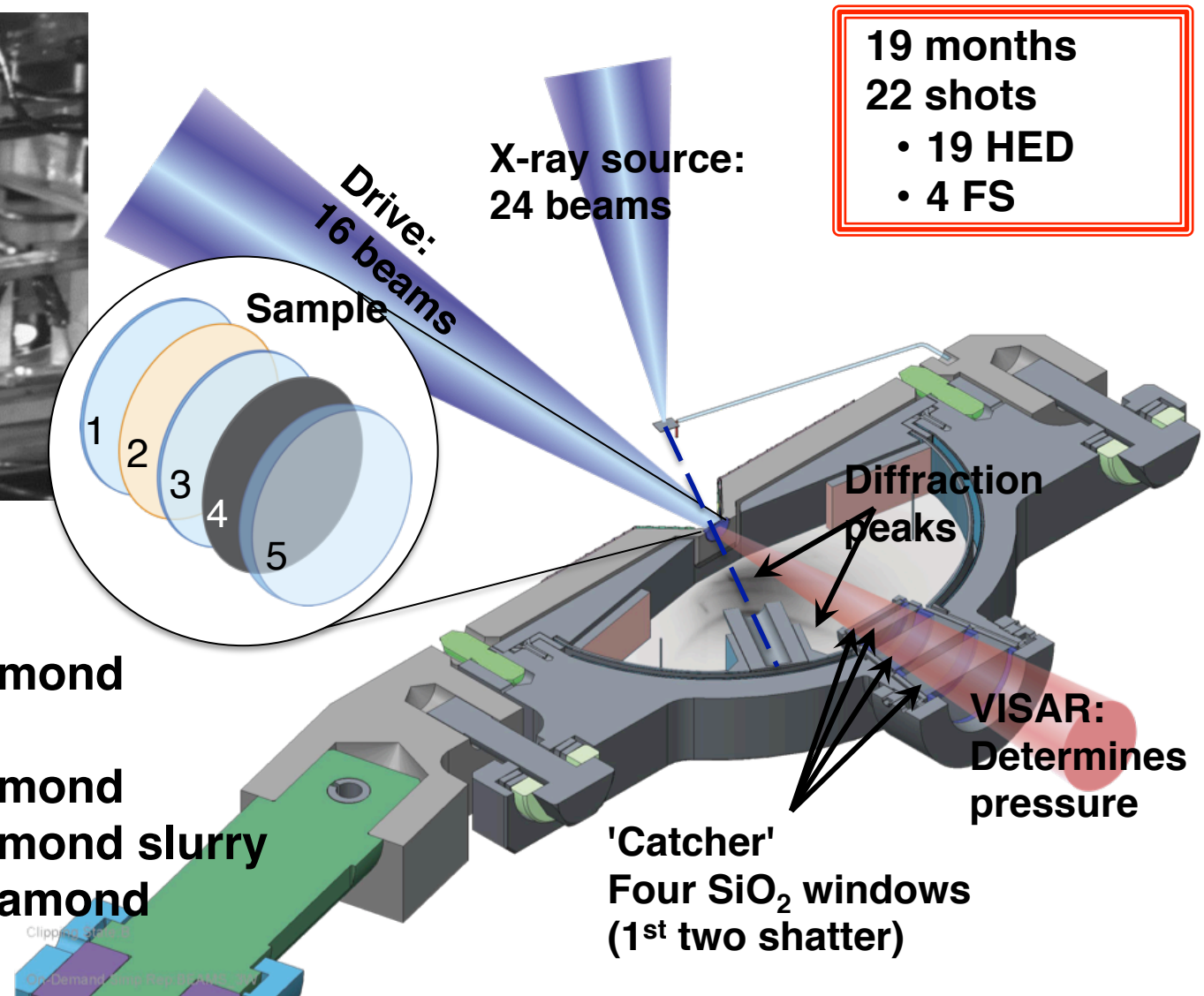
**NIF Discovery Science campaign to measure Fe melt line from 5-20 Mbar (~4-20 M<sub>E</sub>). Led by R. Hemley and R. Kraus, beginning in Oct.**



# TARDIS: TARget Diffraction In-Situ diagnostic for X-ray diffraction experiments on NIF



TARDIS, inserted into the Target Alignment Sensor (TAS) in the NIF target chamber.



**19 months**  
**22 shots**

- 19 HED
- 4 FS

## Sample:

- 1: 40 μm diamond
- 2: 2 μm gold
- 3: 40 μm diamond
- 4: 40 μm diamond slurry
- 5: 150 μm diamond

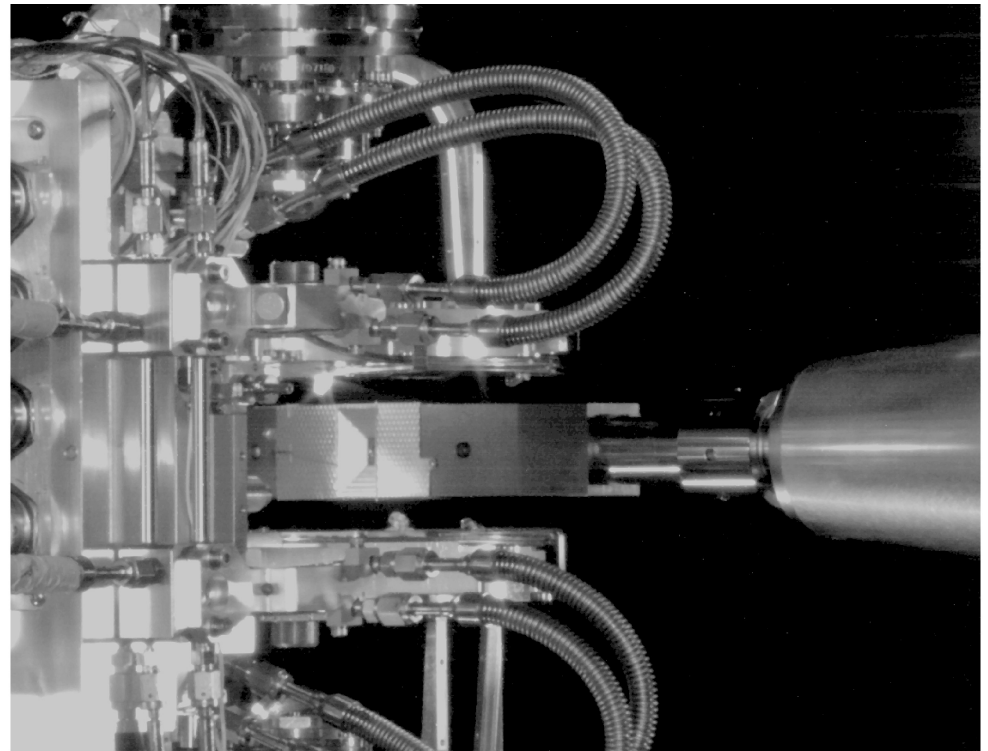
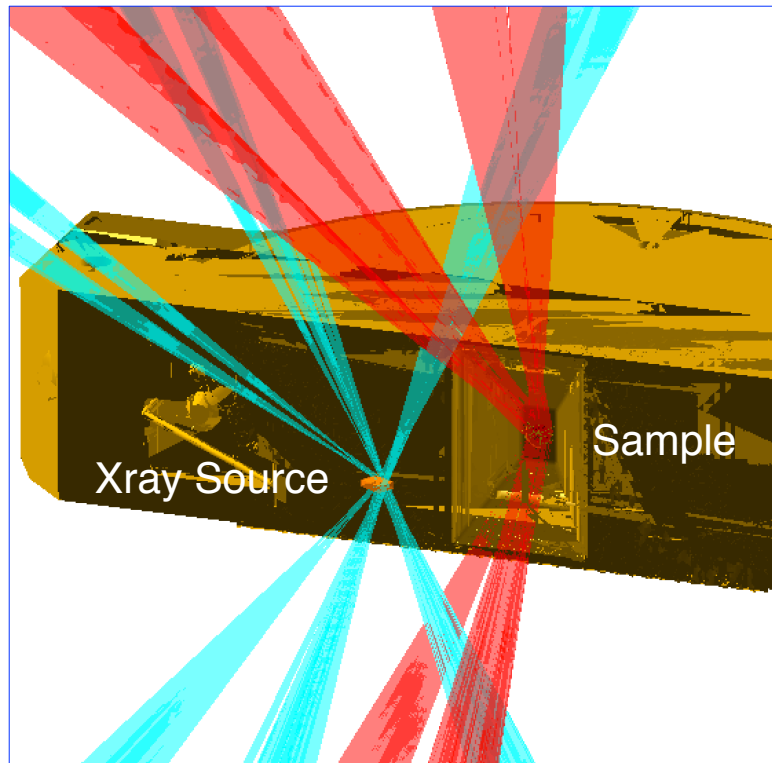


# This year we began angle-dispersive x-ray diffraction on the NIF

1 Mbar = 100 GPa = 0.1 TPa



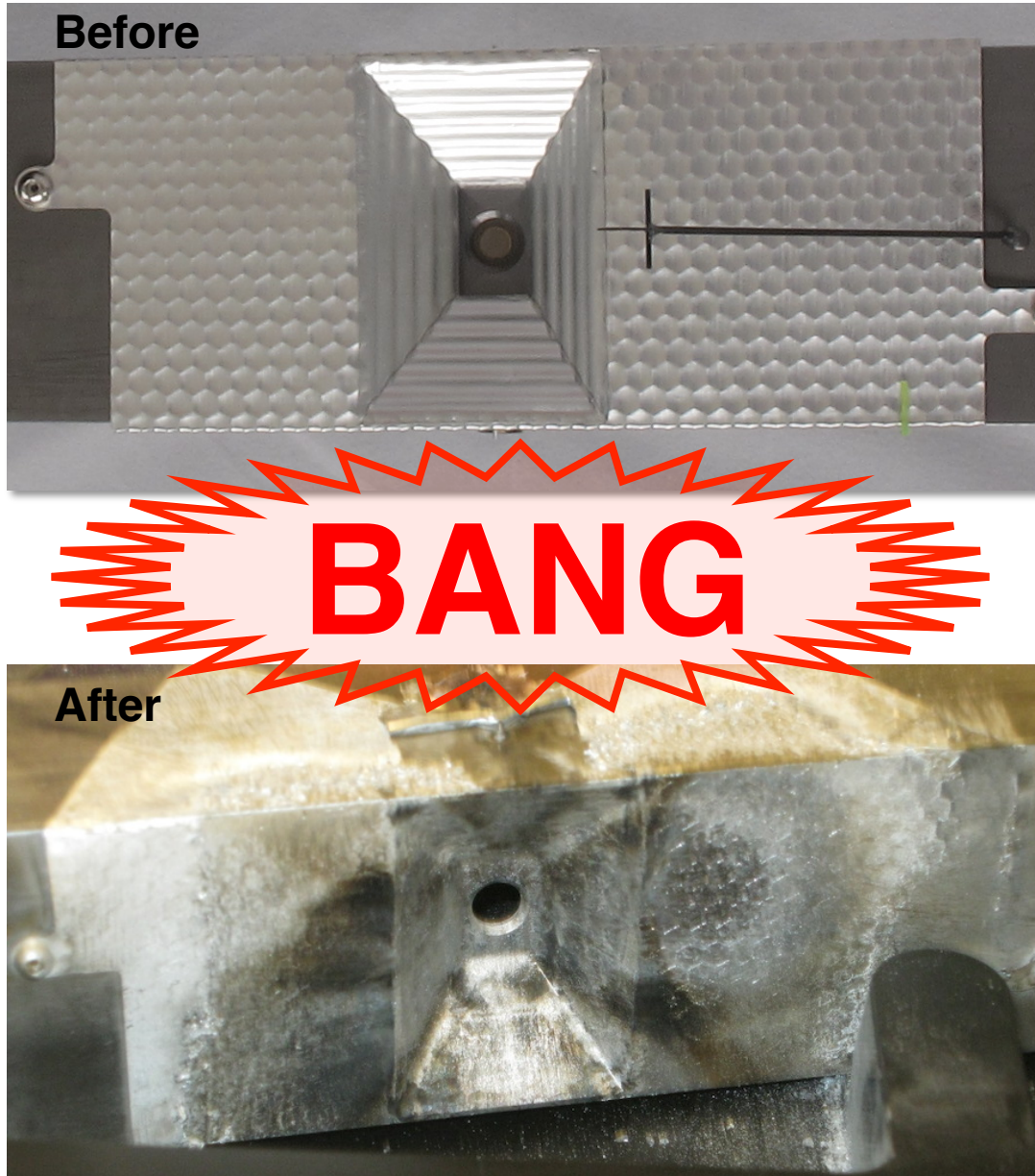
**TARDIS = TARget Diffraction In Situ**



The TARDIS is a modified version of the PXRDIP used on Omega.

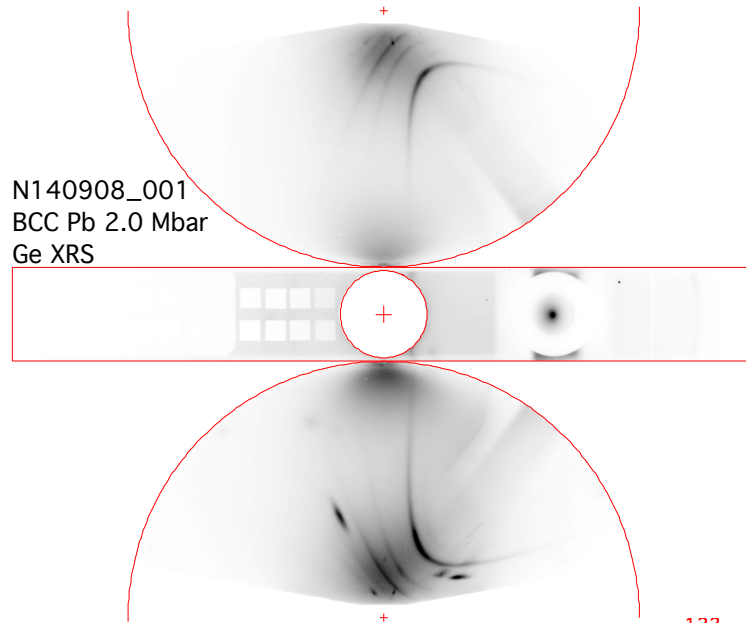
Target sustains significant damage, but the support does not

1 Mbar = 100 GPa = 0.1 TPa

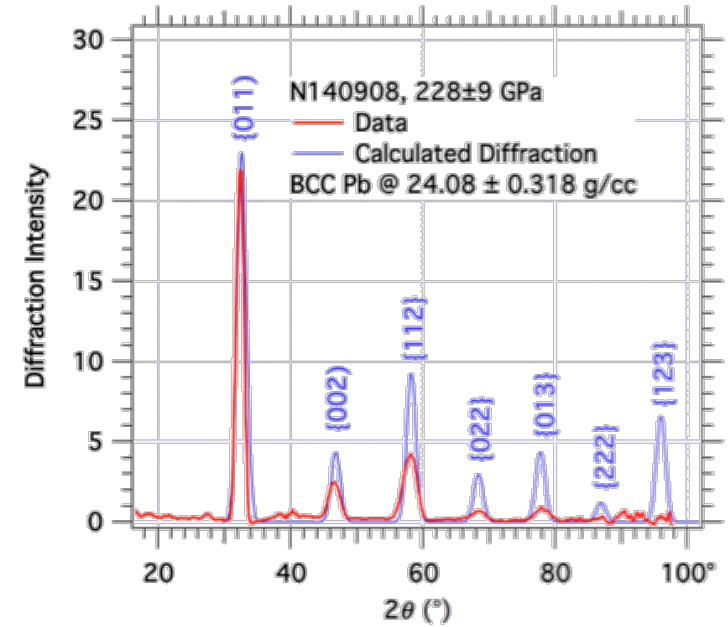
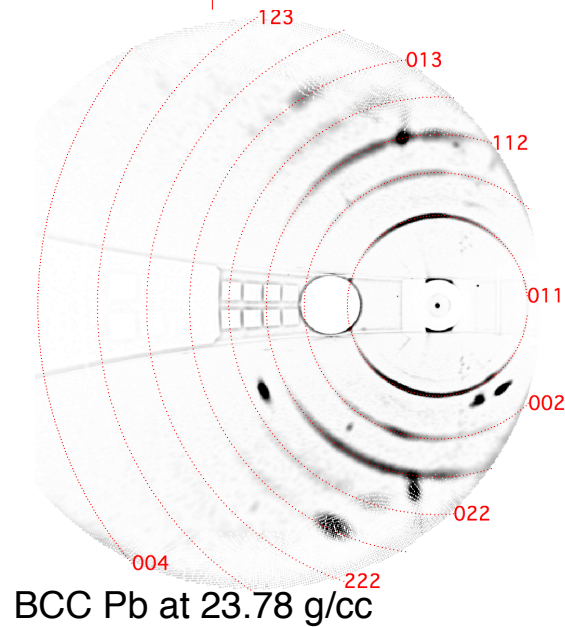
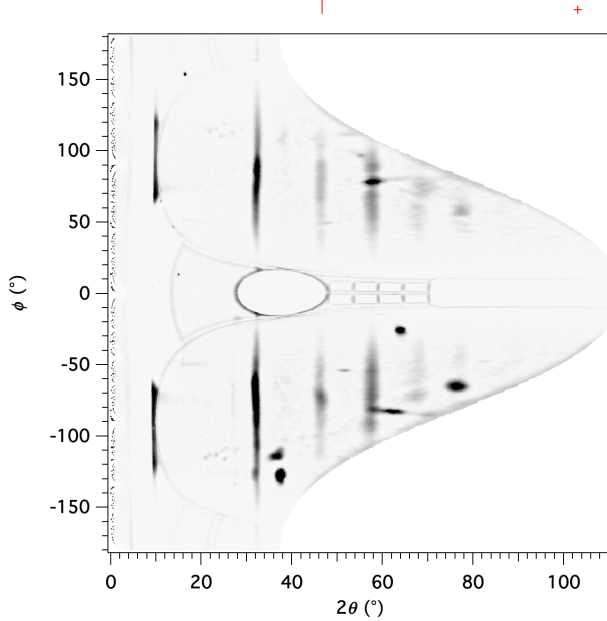
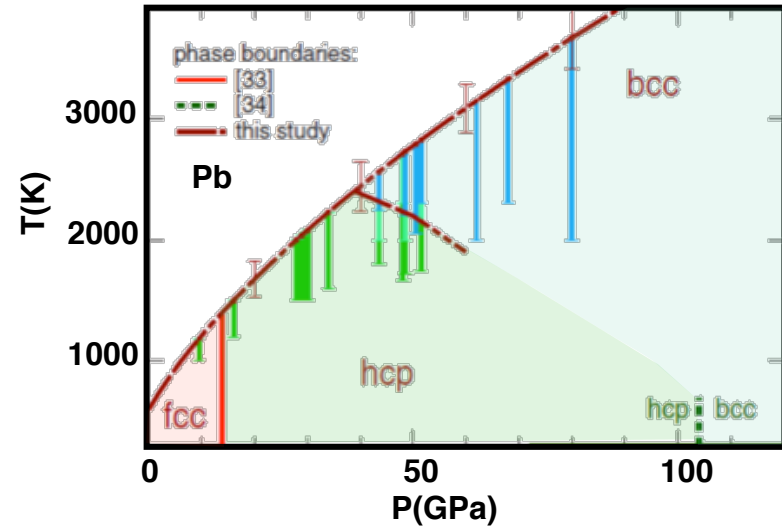




# At least 5 BCC diffraction lines for Pb at 2.0 Mbar

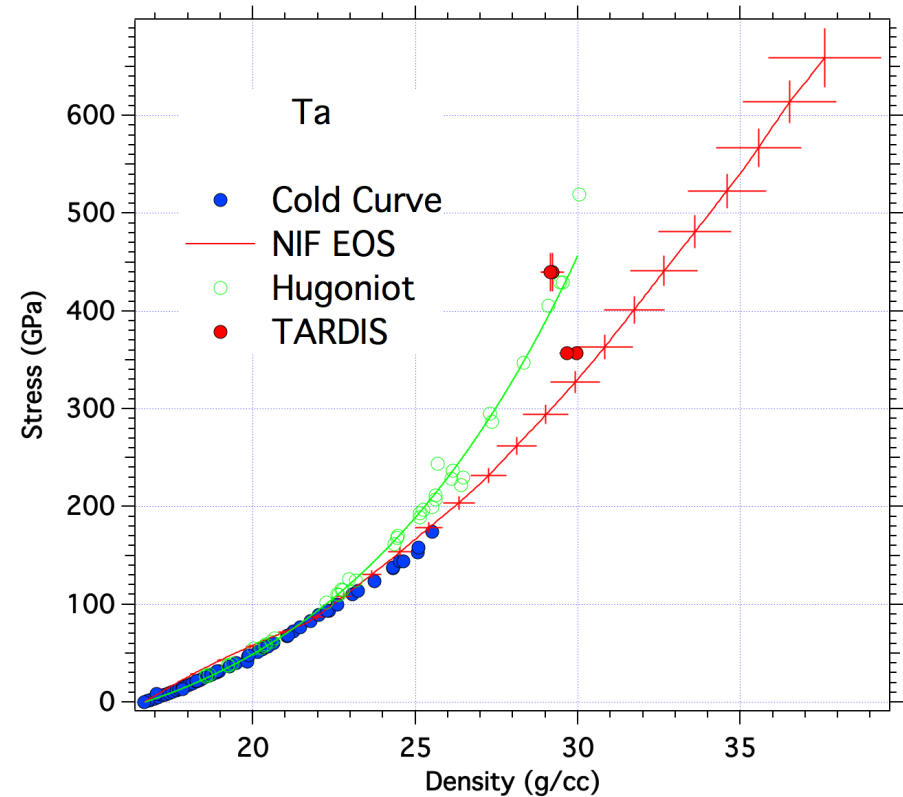
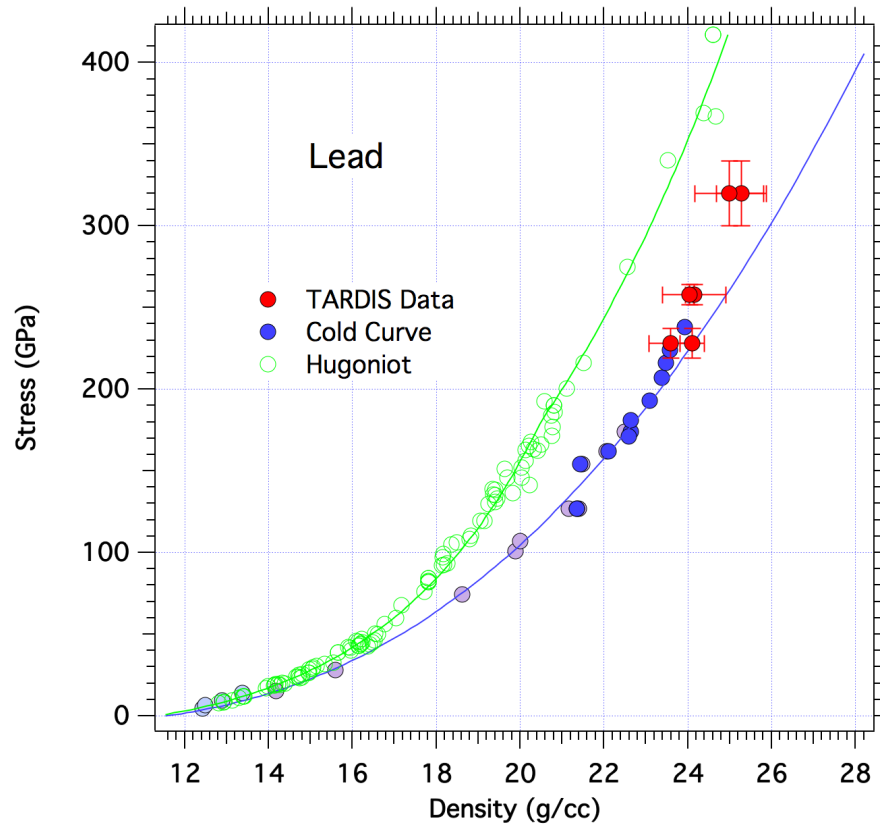


Pb Phase diagram [Dewaele, PRB (2007)]





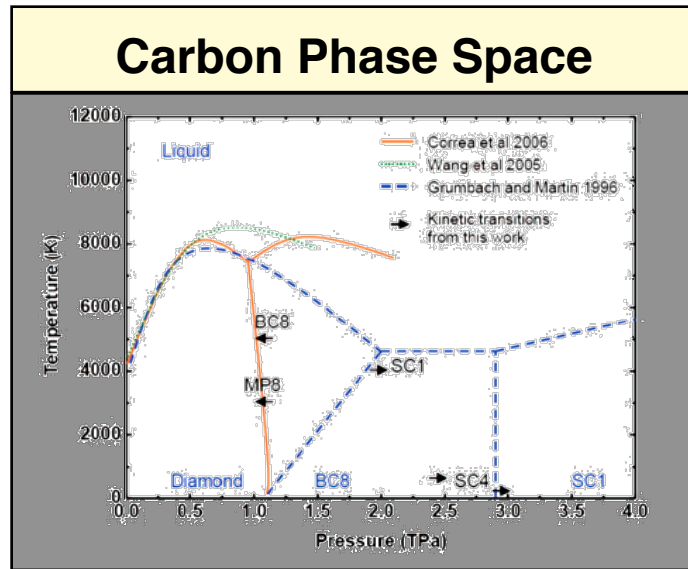
# Preliminary Stress-Density Results



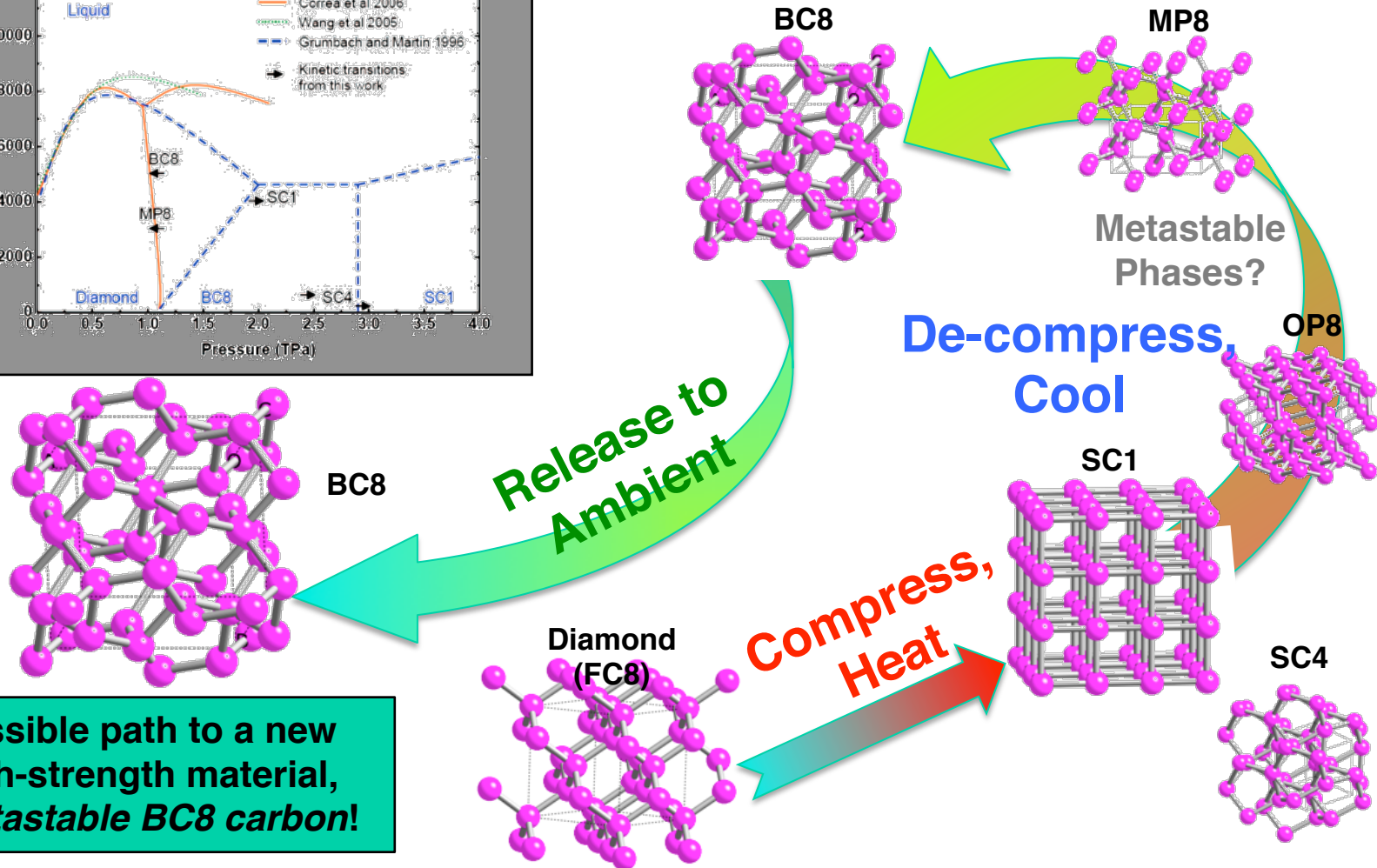
!!! Stress, Density, and Phase  
are very preliminary !!!

# Current Fundamental Science on NIF campaign to try to locate BC8 phase of carbon

1 Mbar = 100 GPa = 0.1 TPa

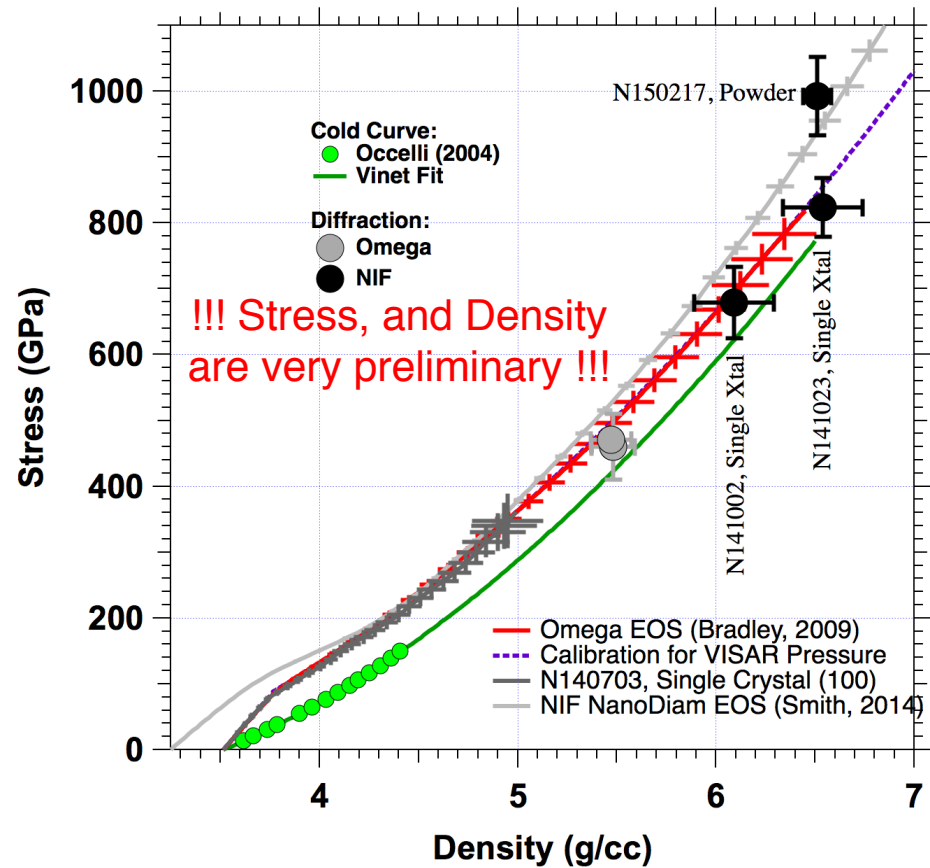
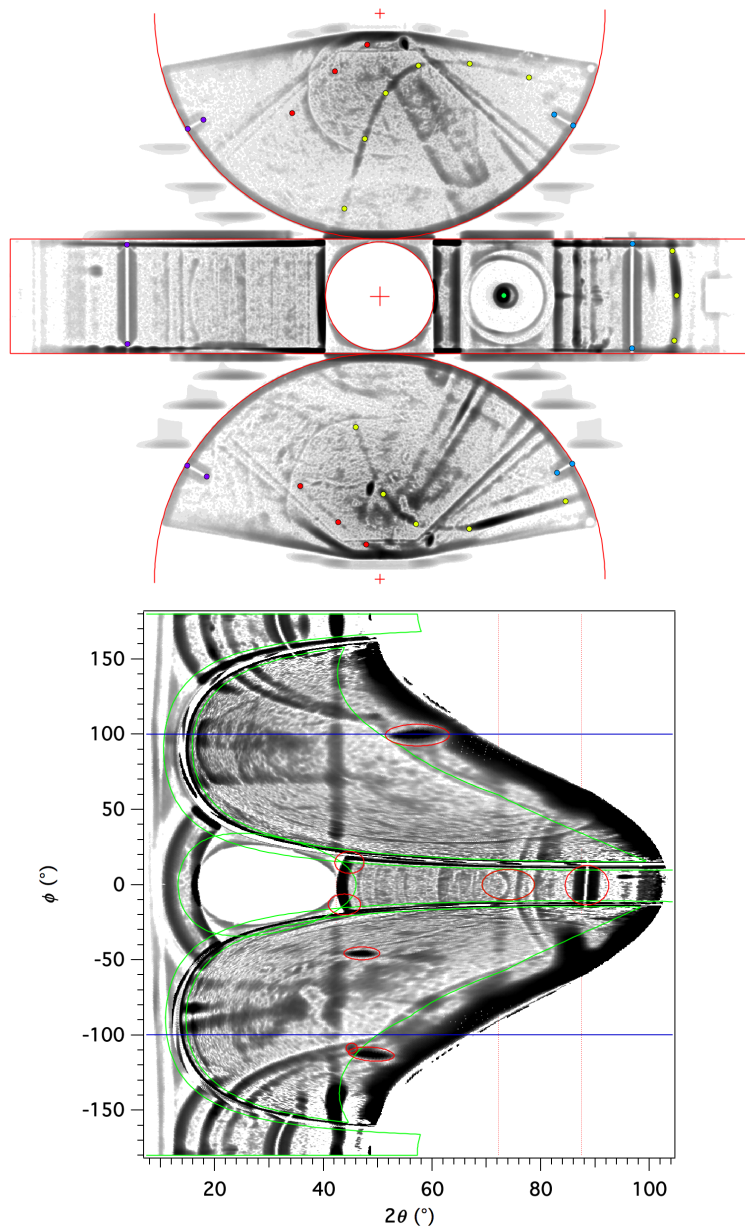


Sun, Klug, and Martonak, JCP 2009



Possible path to a new high-strength material, *Metastable BC8 carbon!*

# We had only seen highly-structured diffraction from diamond. On Monday we saw power diffraction.



Diffraction of carbon structures at 1 TPa

# Outstanding Issues with Dynamic-Diffraction Experiments

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## **Validate the accuracy of our stress determination**

- Effect of strength in diamond is uncertain
- Use different sandwich materials, e.g.: Diamond, LiF, MgO

## **Experimentally constrain the temperatures we reach**

- Heating by: thermal conduction, plastic work, shock formation, etc.
- Debye-Waller factor in diffraction
- Debye-Waller factor in EXAFS
- Thermal-expansion in diffraction

## **Explore systematics of rate-dependent phase transitions**

- Simple structures may form more rapidly than complex structures
- Explore phase diagrams on multiple platforms

## **Improve signal to noise ratios**

- Lower ablation plasma and other background
- Use higher energy x-rays

## **Develop cheaper targets**