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X-Ray Diffraction on NIF#

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X-Ray Diffraction on NIF

NIF Users Group Meeting

LLNL, 2/15/2012

Jon Eggert (LLNL)

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Team

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- **University of Oxford**
  - J. Wark, A. Higginbotham, M. Suggit, G. Mogni
- **National Research Council of Canada**
  - D. Klug, Y. Yao
- **Washington State University**
  - C.S. Yoo
- **AWE Aldermaston**
  - N. Park
- **Osaka University**
  - K. Shigemori, K. Shimizu
- **University of Rochester**
  - Tom Boehly

- **Additional Collaborators / Consultants**
  - A. Lazicki, F. Coppari, D. Hicks, Y. Ping, D. Swift
  - Andrew Comley, Brian Maddox, Hye-Sook Park, and Bruce Remington
  - M. McMahon, T. Duffy

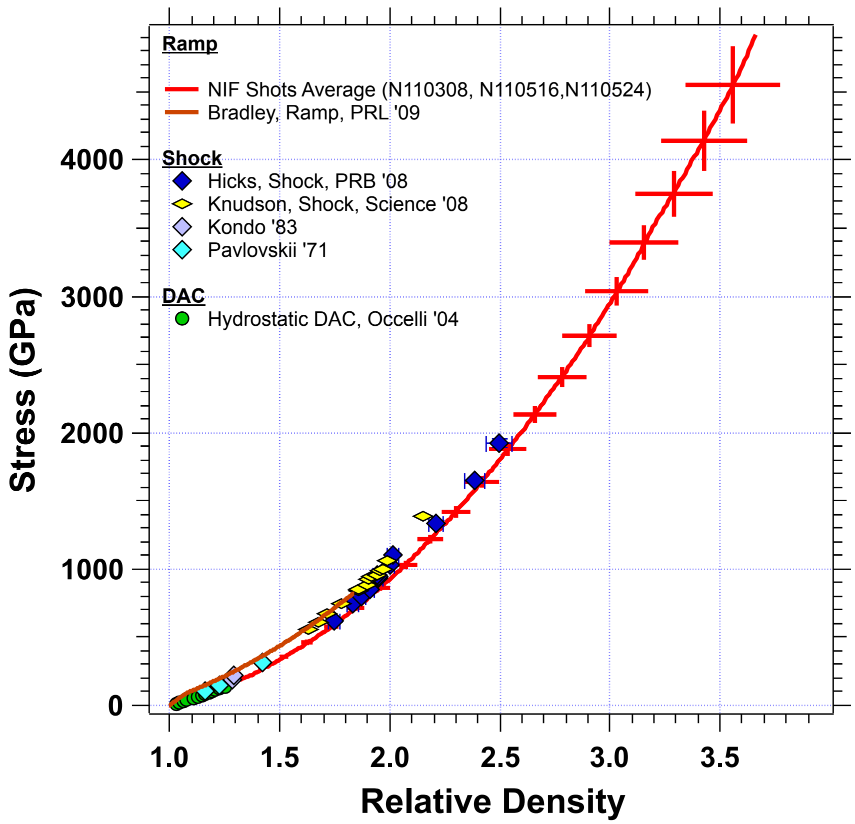
The National Ignition Facility (NIF) is currently a 192 beam, 1.6 MJ laser

We have an unprecedented opportunity to perform extraordinary basic HED science.
In particular, highly-compressed material science.

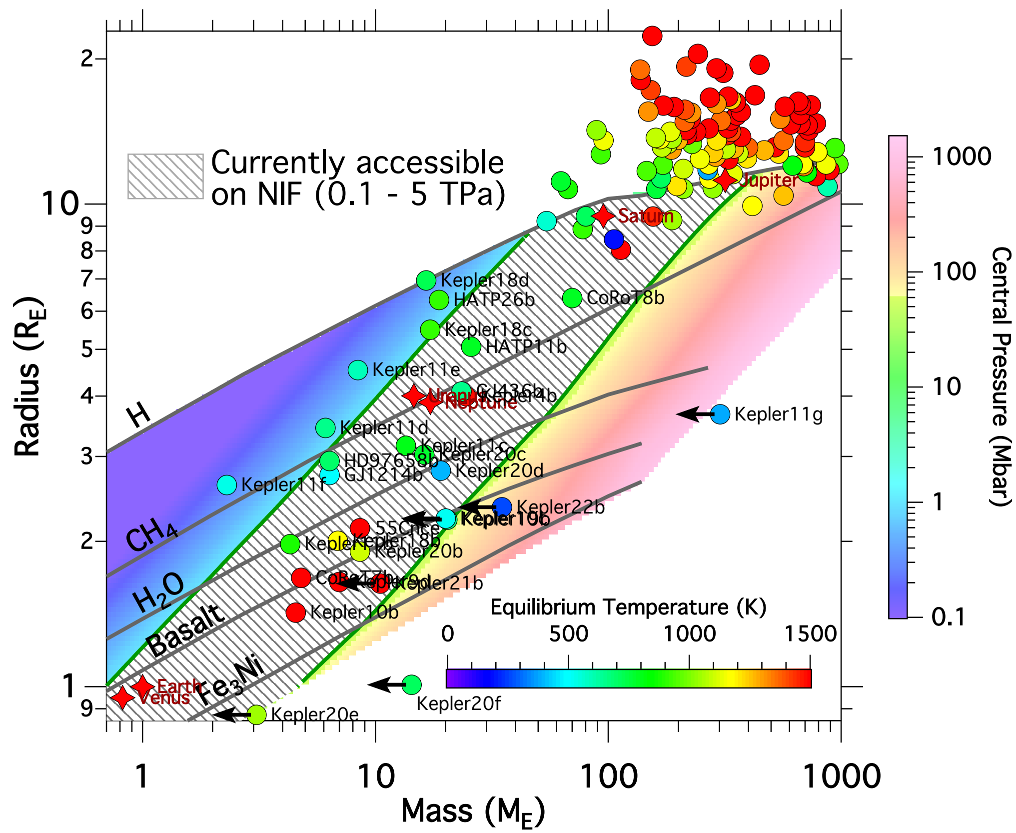
Target chamber with steel frameworks for catwalks being installed.

NIF Ramp-Compression Experiments have already made the relevant exo-planet pressure range from 1 to 50 Mbar accessible.

We measured stress-density up to 5 TPa on NIF.



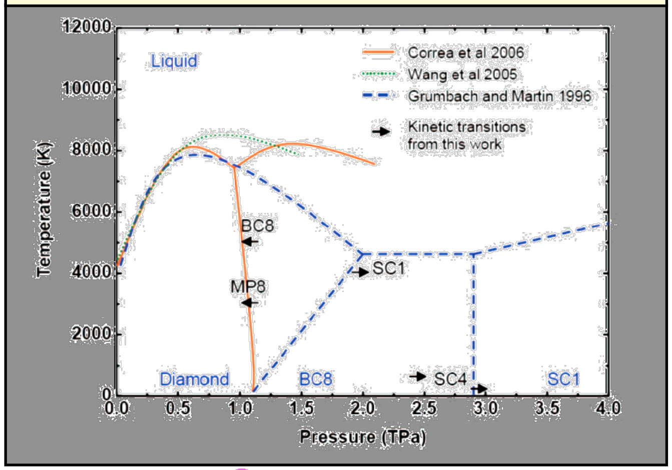
187 transiting exoplanets as of December 29, 2011, http://exoplanet.eu/

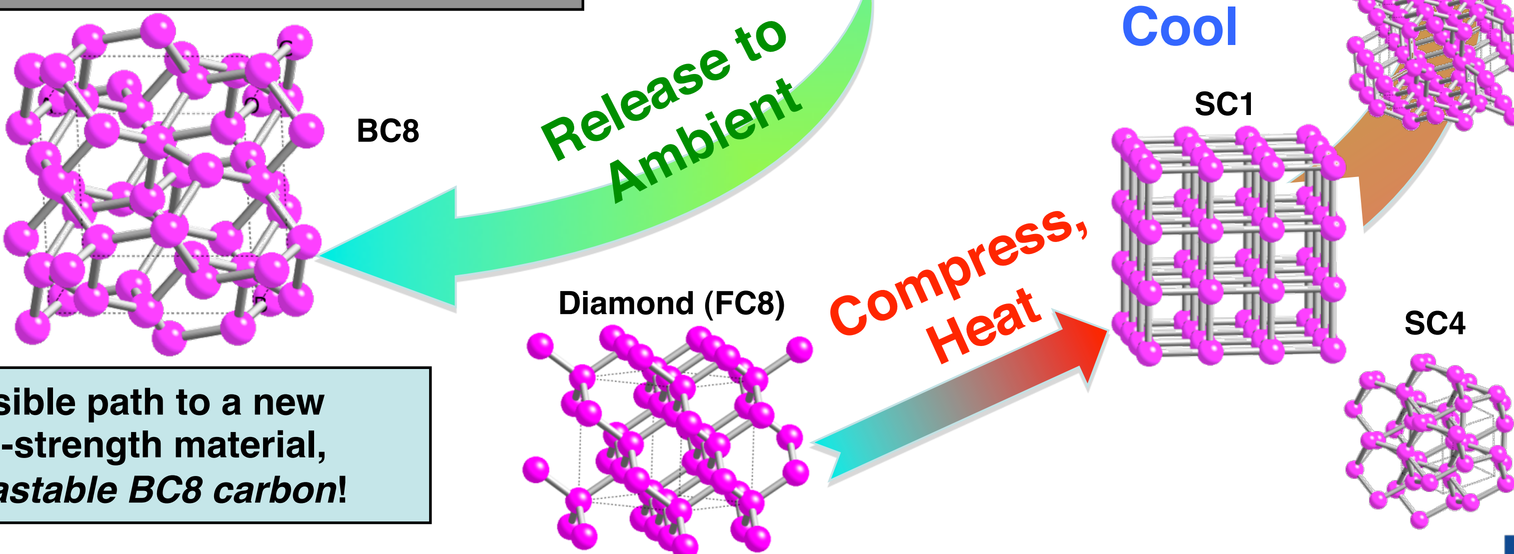


Our NIF experiments have demonstrated that we can access the relevant pressure composition region for exo-planet interiors.

We Proposed to Study Carbon Phases by X-Ray Diffraction on NIF

Carbon Phase Space

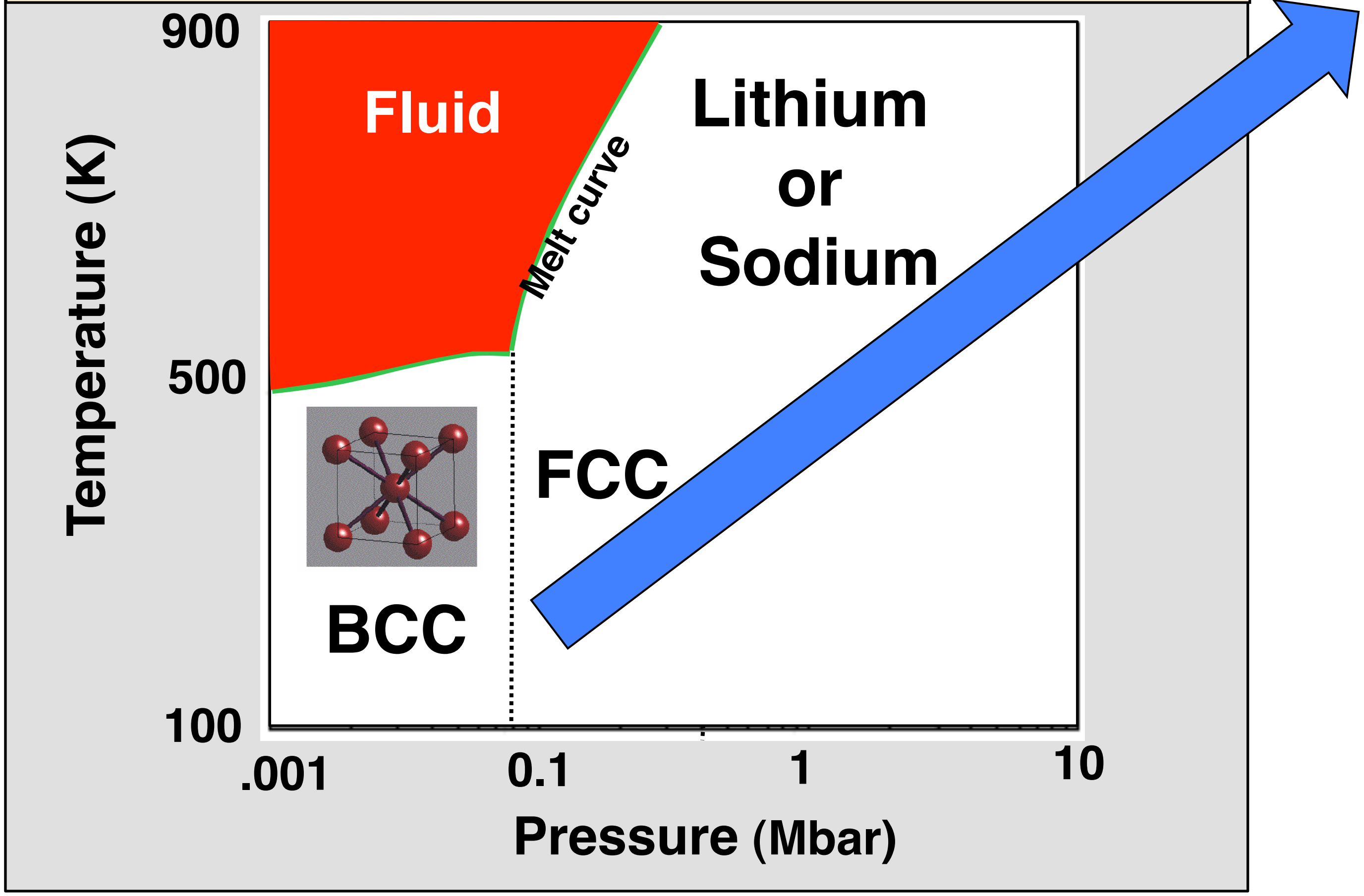




Possible path to a new high-strength material, *Metastable BC8 carbon*!

Just a few years ago, ultra-high pressure phase diagrams for materials were very "simple"

Melt curves followed a Lindeman law, structures were simple, and conductivities increased at high pressure



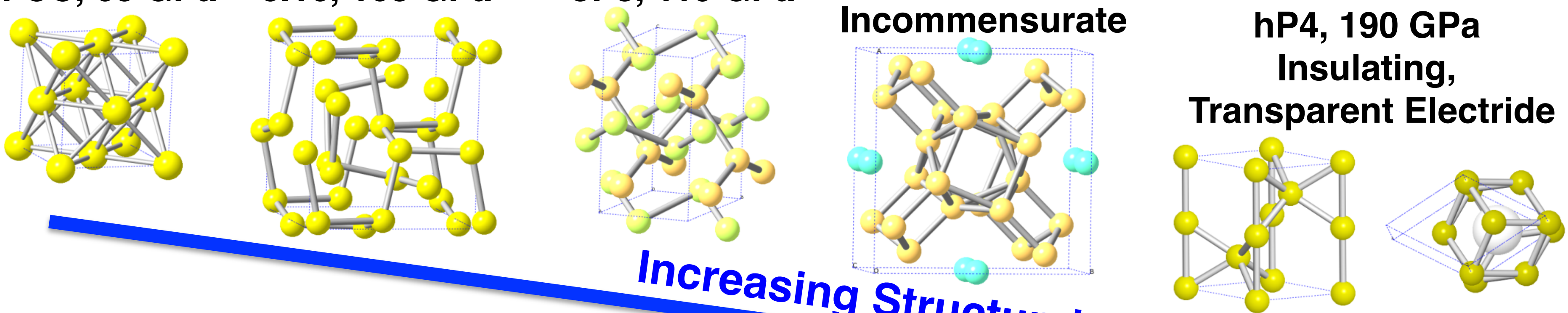
Physics Gets Simple!

New experiments and theories point out surprising and decidedly complex behavior at the highest pressures considered.

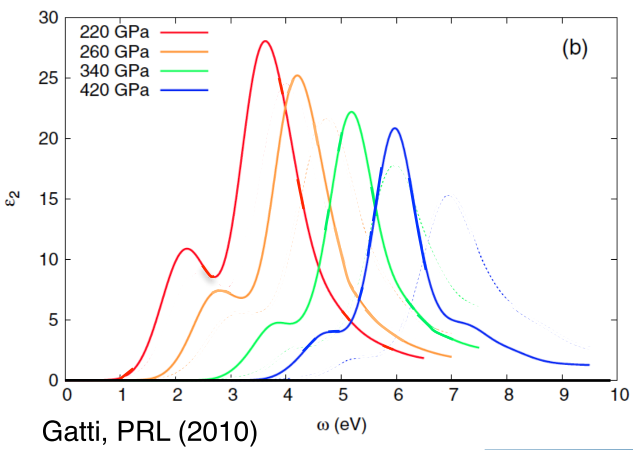
Traditional view: All materials become simple at high pressure appears to be incorrect!

> **“. . . 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 | cI16, 108 GPa | oP8, 119 GPa | tI19, 147 GPa Incommensurate | hP4, 190 GPa Insulating, Transparent Electride

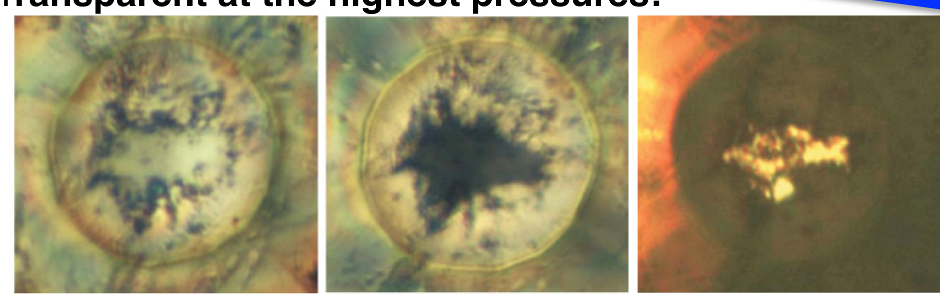


Increasing Structural Complexity



Gatti, PRL (2010)

Transparent at the highest pressures!



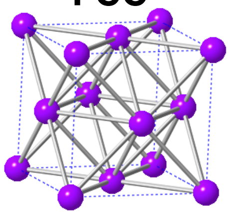
120 GPa | 156 GPa | 199 GPa

Ma, Nature (2009)

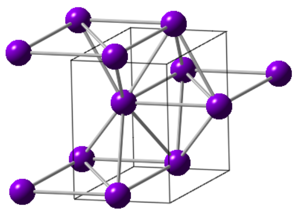
High pressures phases of aluminum are also predicted to be complex

Pickard and Needs, Nature Materials (2010).

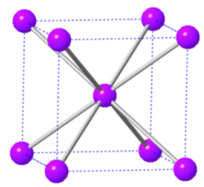
FCC



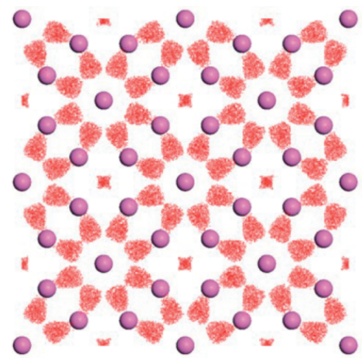
HCP
2.17 Mbar

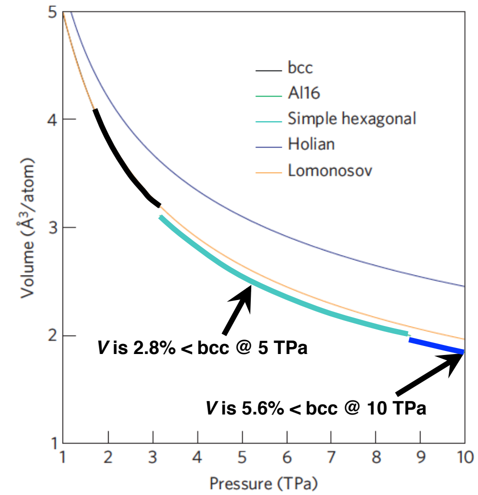


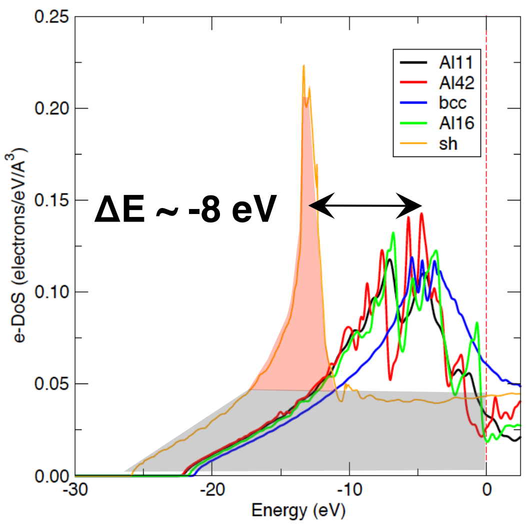
BCC
3.8 Mbar



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



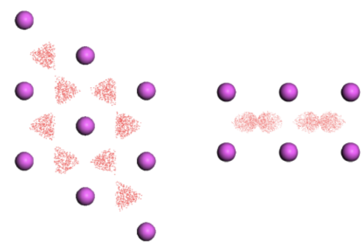




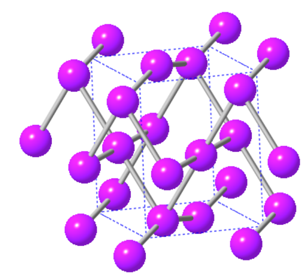
ΔV~2.8%

Simple Hexagonal Electride
88 – 100 Mbar

ΔV~1.8%



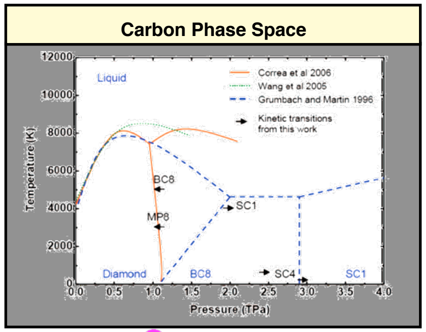
CMMA Electride
> 100 Mbar

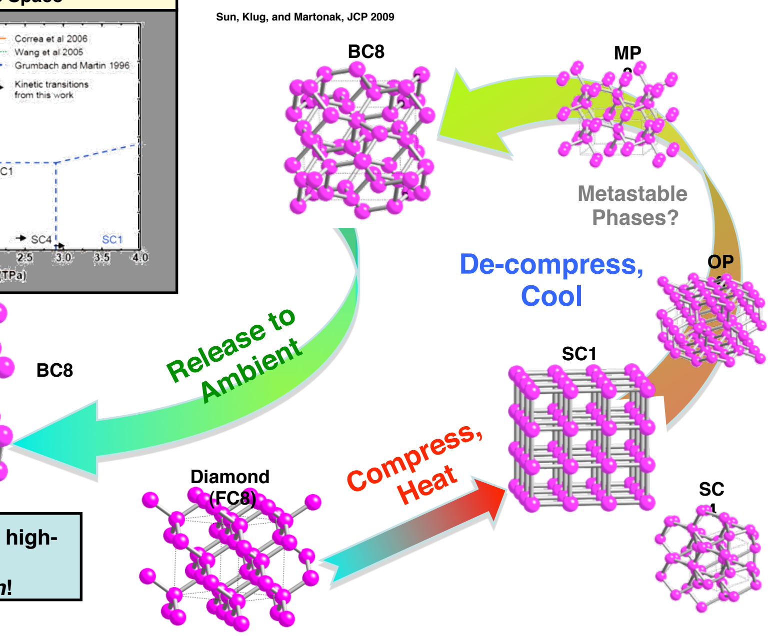


No predictions yet for melt line of aluminum

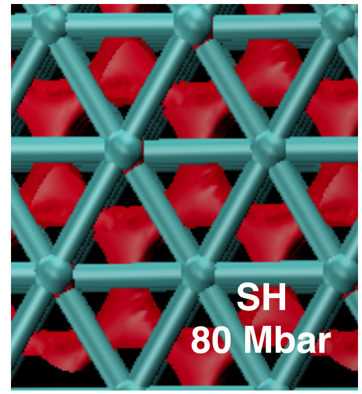
"all structures near 300 Mbar are far from close packed"

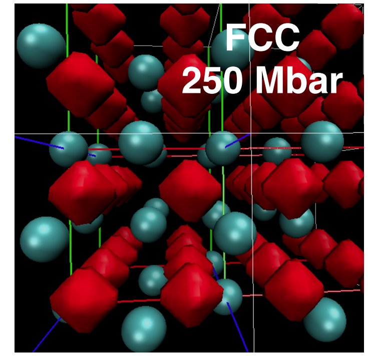
Recent metadynamics survey of carbon proposed a dynamic pathway among multiple phases

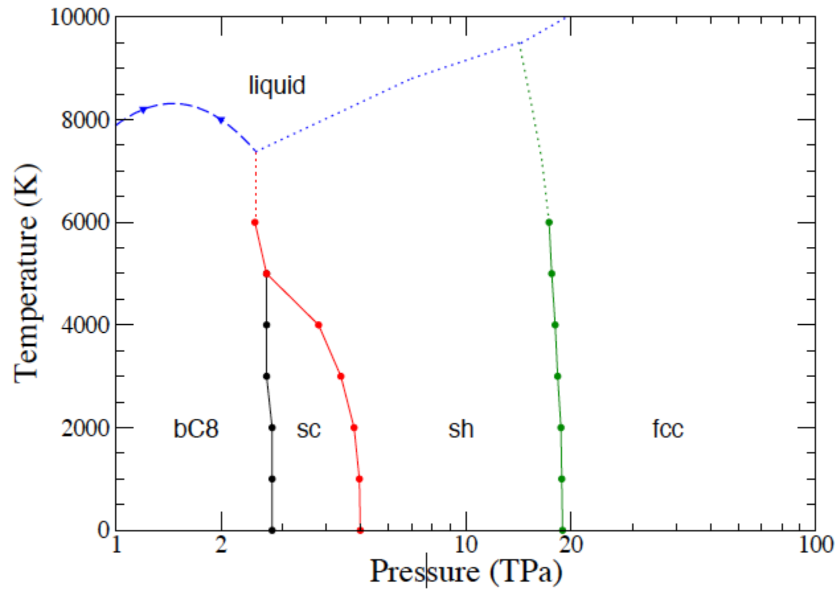




Possible path to a new high-strength material, *Metastable BC8 carbon*!







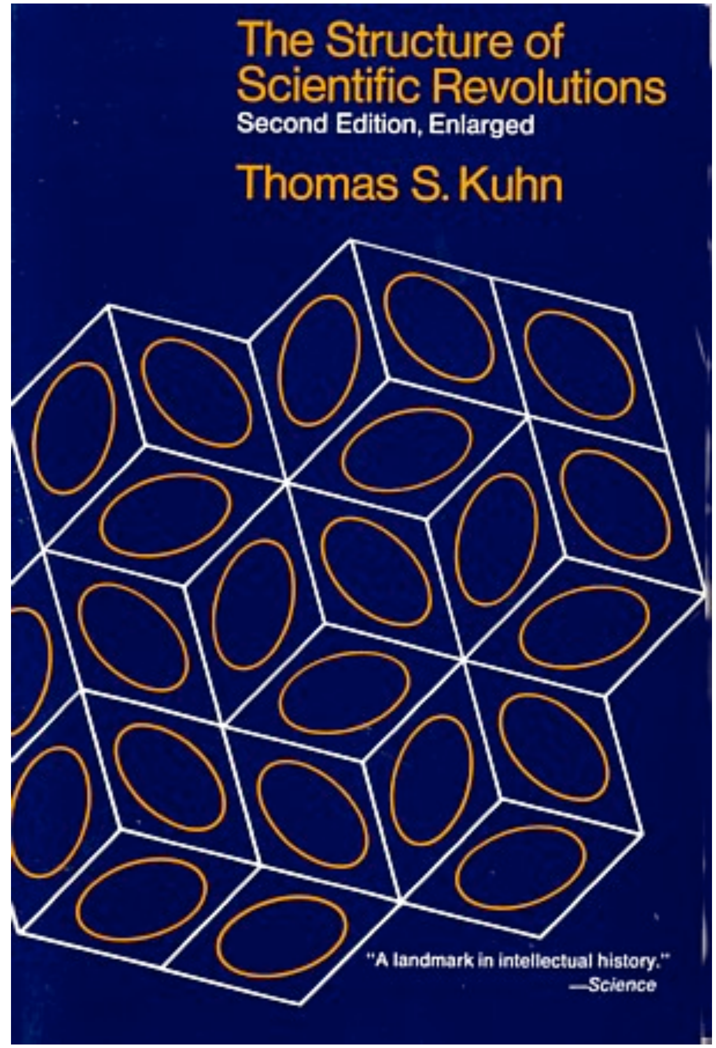
Canales, Pickard, Needs, Phys. Rev. Lett. 108, 045704 (2012)

A new paradigm. Really?

Are we really about to witness a true paradigm shift in extreme compressed-matter physics?

"Only as experiment and tentative theory are together articulated to a match does the discovery emerge and the theory become a paradigm"
–p 61

"Further development ordinarily calls for the construction of elaborate equipment, the development of an esoteric vocabulary and skills, and a refinement of concepts. . .."
–p 64



Facilitating new Paradigms in Extreme Compression and High Energy Density Science

We need to develop diagnostics and techniques to explore this new regime of highly compressed-matter science.

X-Ray Diffraction:

Understand the phase diagram / EOS / strength / texture of materials to 10's of Mbar

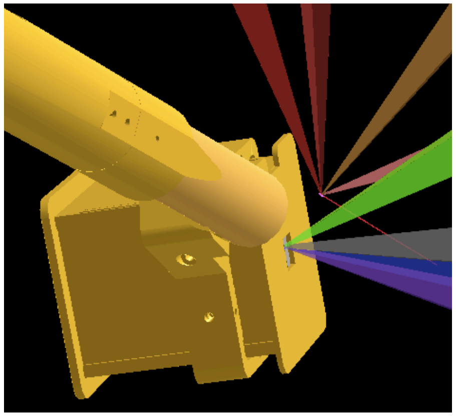
Strategy and physics goals:

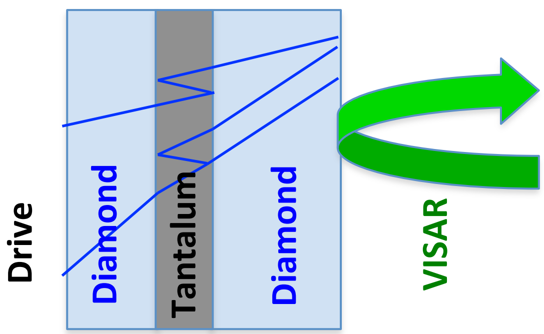
- Powder diffraction
- Begin with diamond
- Continue with metals etc.
- Explore phase diagrams
- Develop liquid diffraction

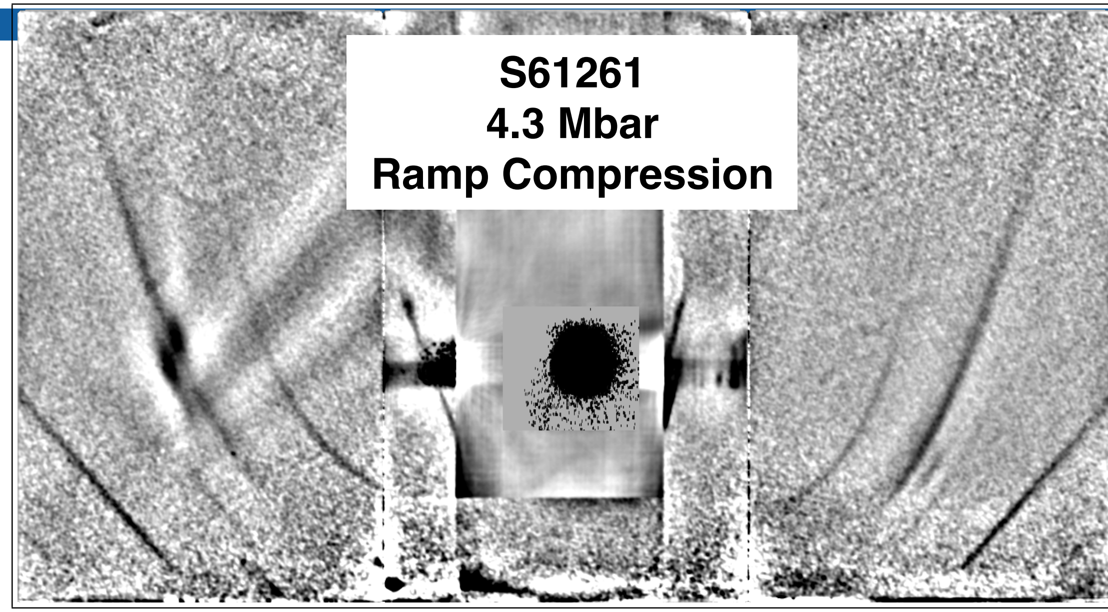
Reduce background / improve resolution

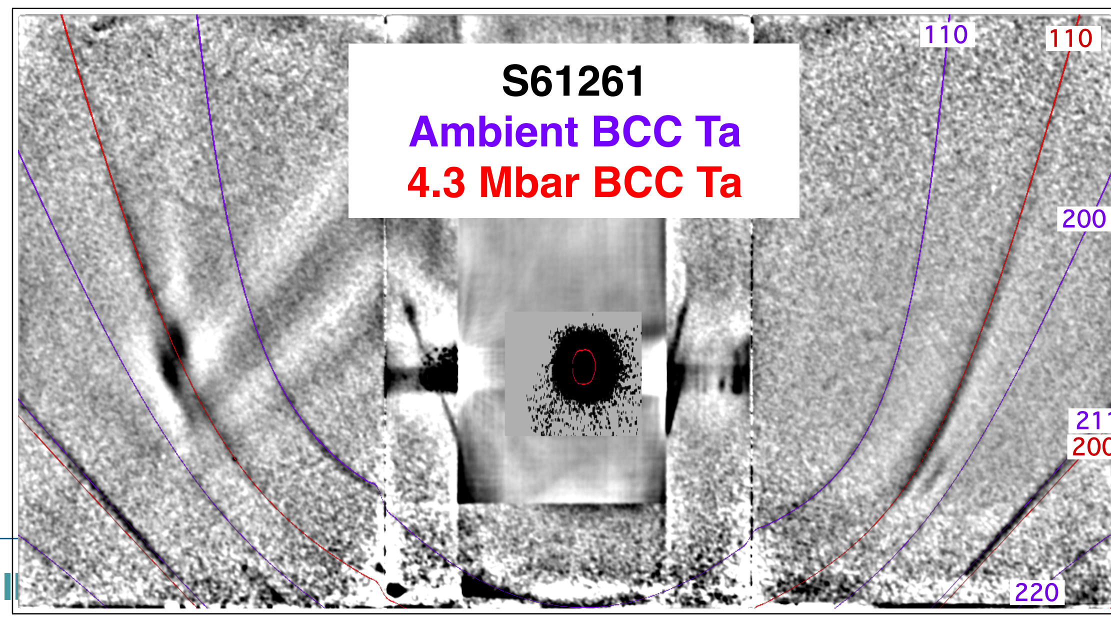
Powder x-ray diffraction of rolled foils on the Omega laser

We performed high-pressure x-ray diffraction on tantalum at the Omega laser







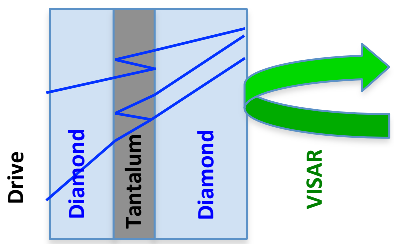


Diffraction data quality is roughly where DAC diffraction was in the '80s. We need to make similar strides.

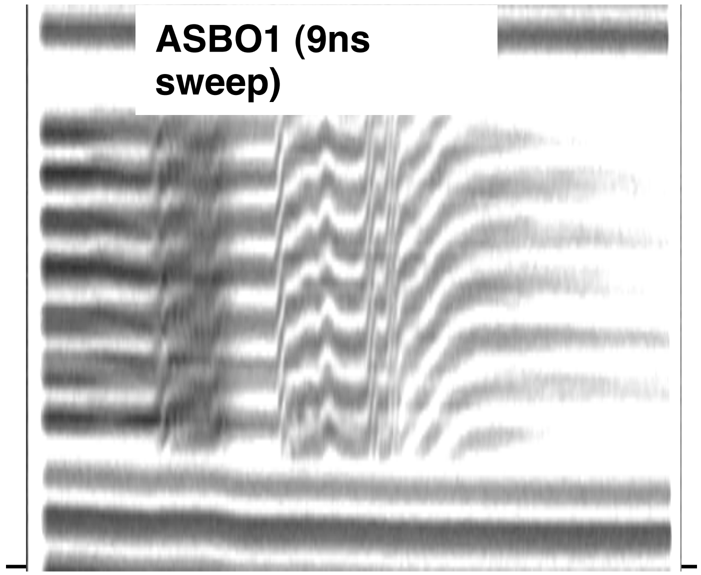
We determine stress by backward integration of diamond free-surface velocity

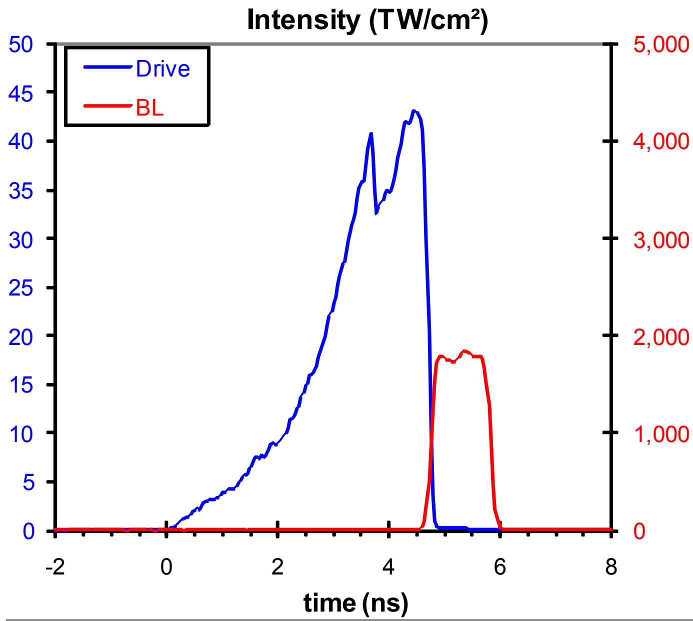
Shot 61261,
OMEGA 2011-0223

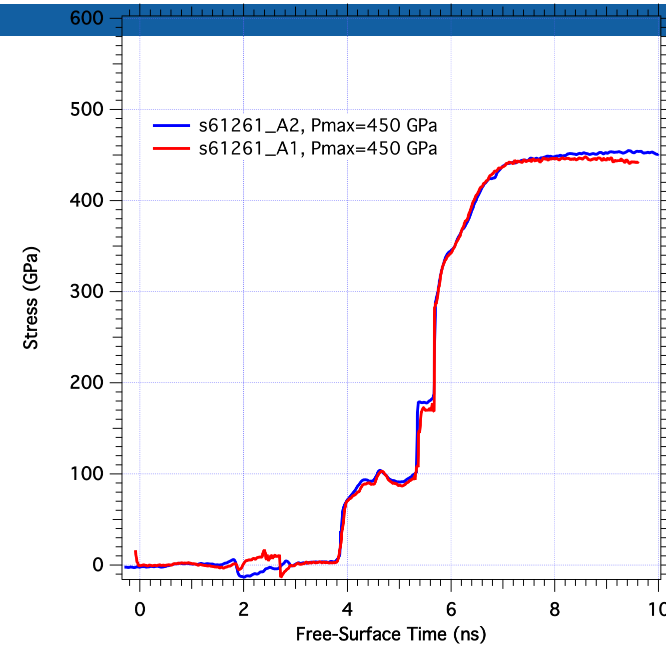
Target: C[17]Ta[3]C [40], BL: Fe

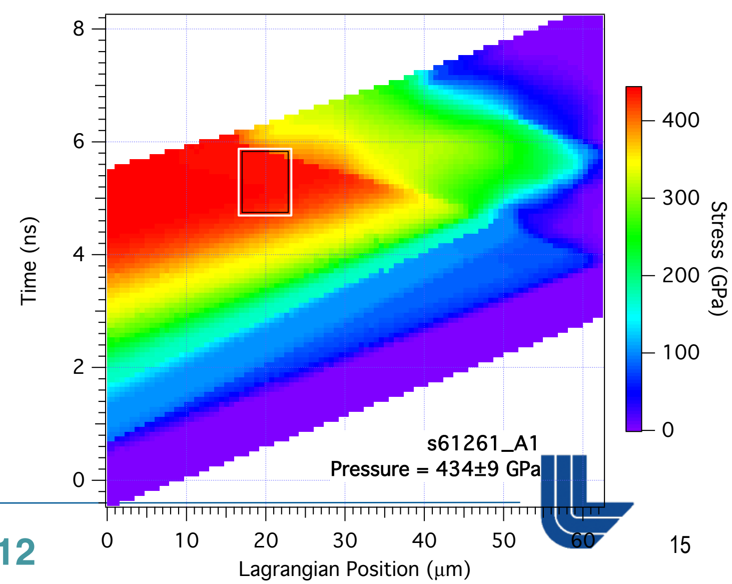


Ramp drive: 246 J
(t_{BL} = 4.6 ns)
P = 4.34±0.09 Mbar

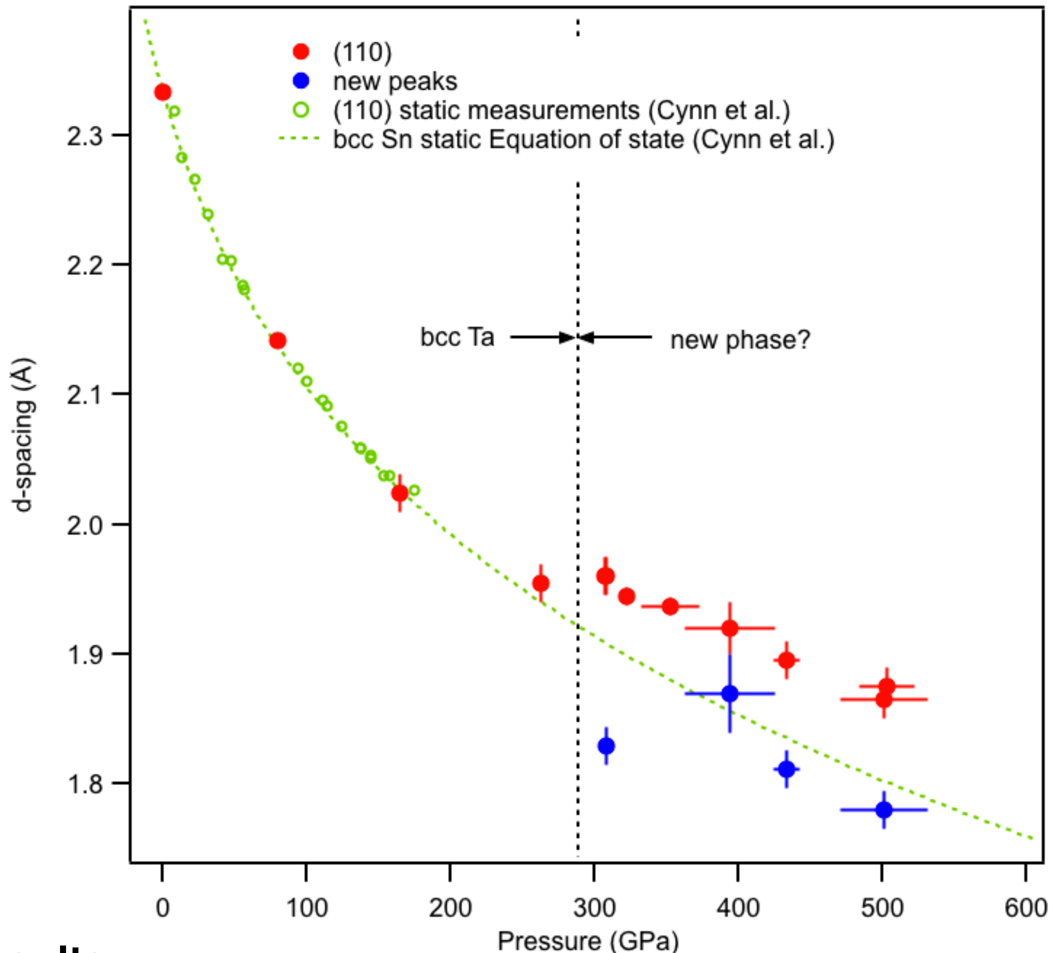




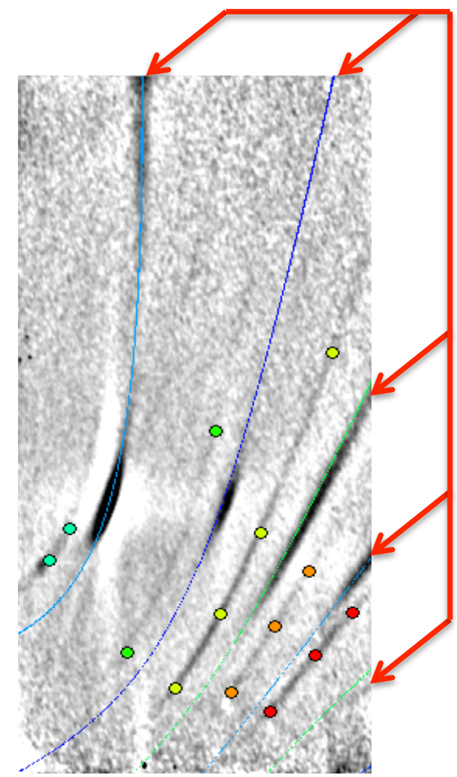




Tantalum diffraction on the Omega laser



bcc Ta at 100 GPa



Results:

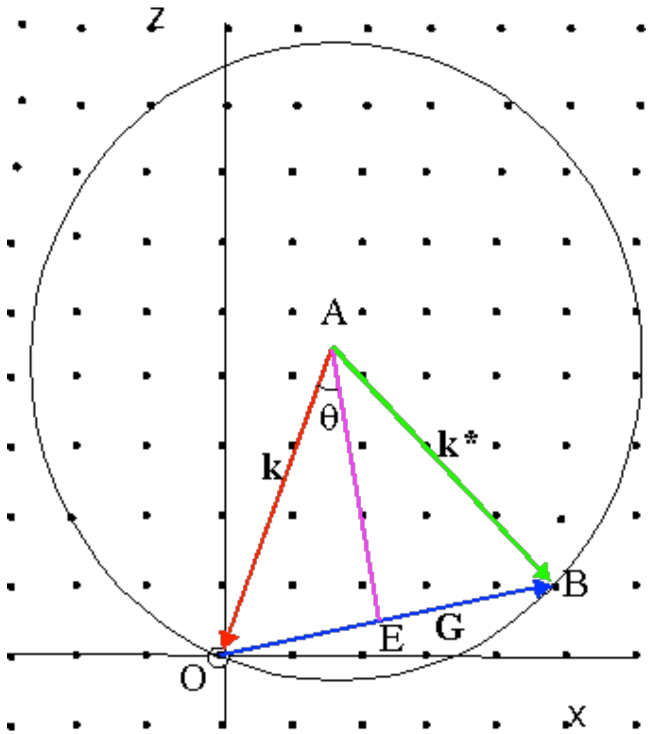
- **High-quality data at moderate pressure**
- **Extension of the bcc equation of state**
- **Indication of possible phase transition above 300 GPa**

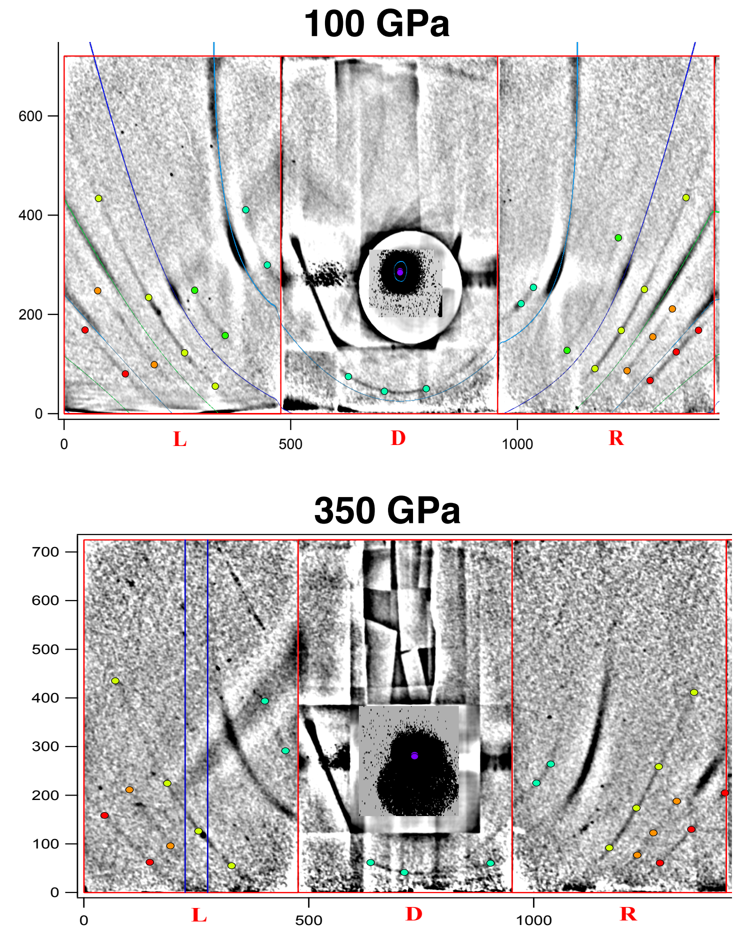
Further work:
Solve technical difficulties associated with diffraction above 600 GPa

Lessons learned on the Omega laser:

- Samples are cool enough to do crystalline diffraction up to near 1 Tpa, far above Hugoniot melt pressure
- Small number of reflections available is a major limitation in structure determination
- X-ray background is a primary concern
- Above ~300 GPa texturing is ubiquitous (for both single- and poly-crystalline materials)

Texture and the Ewald Sphere Construction





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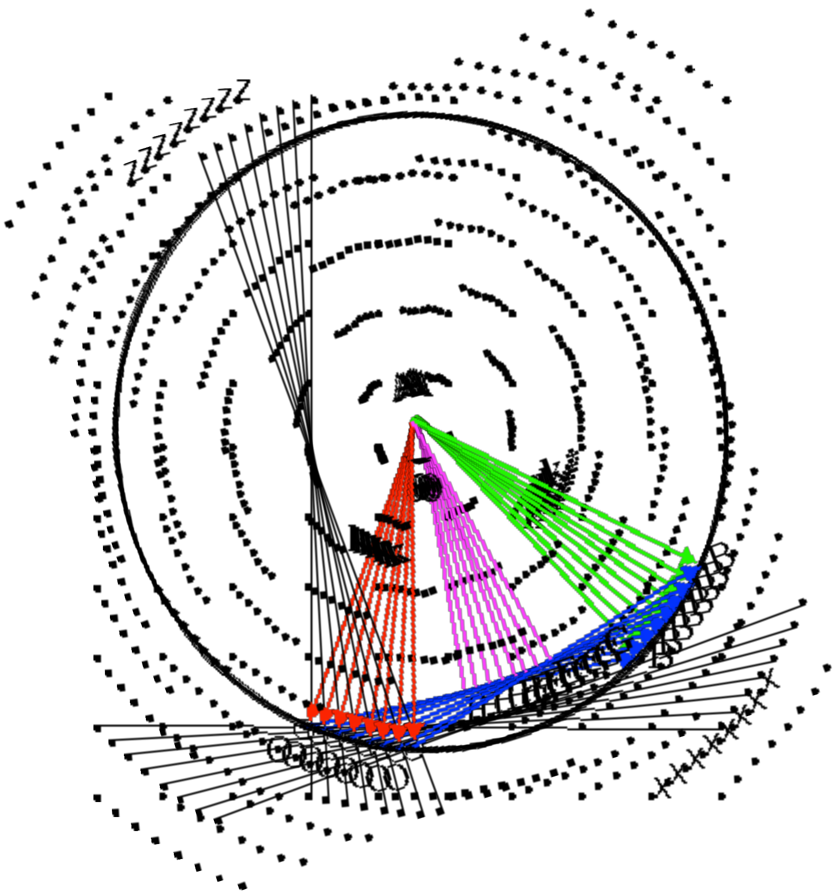
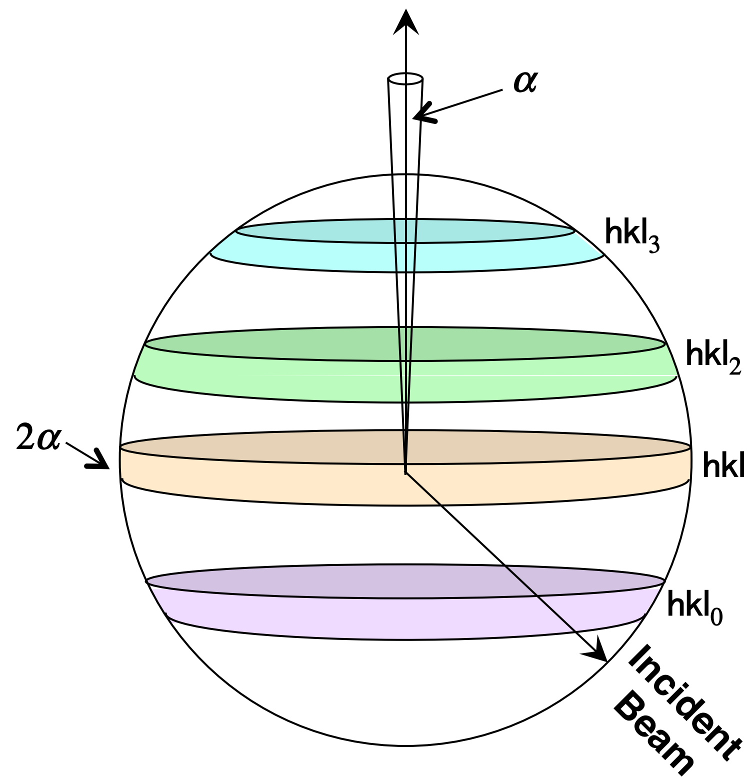
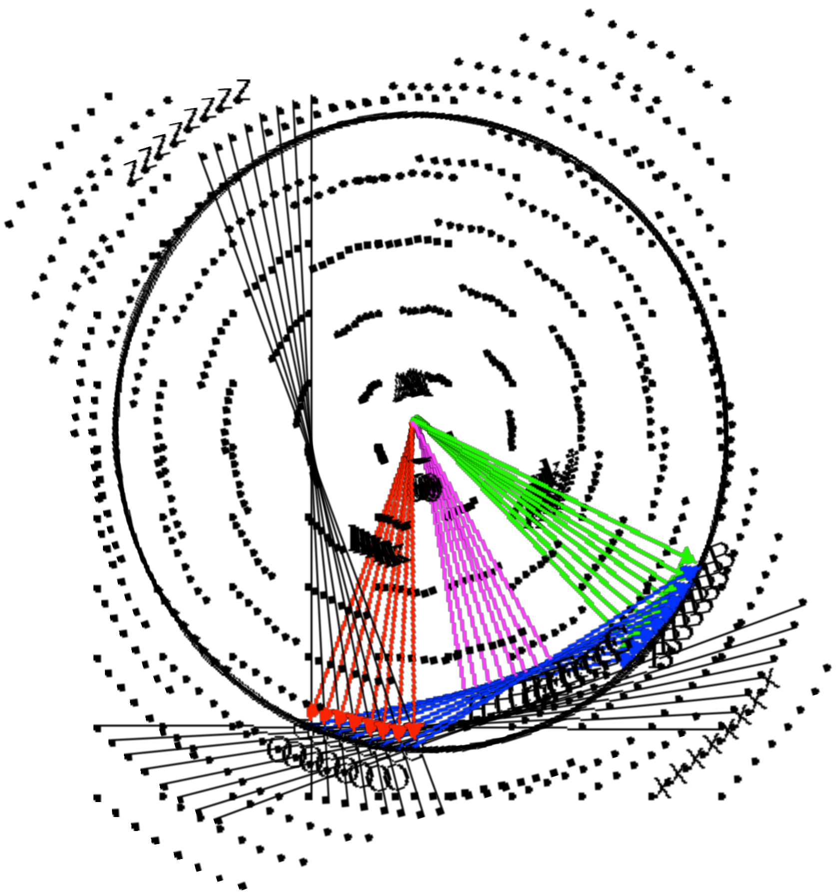
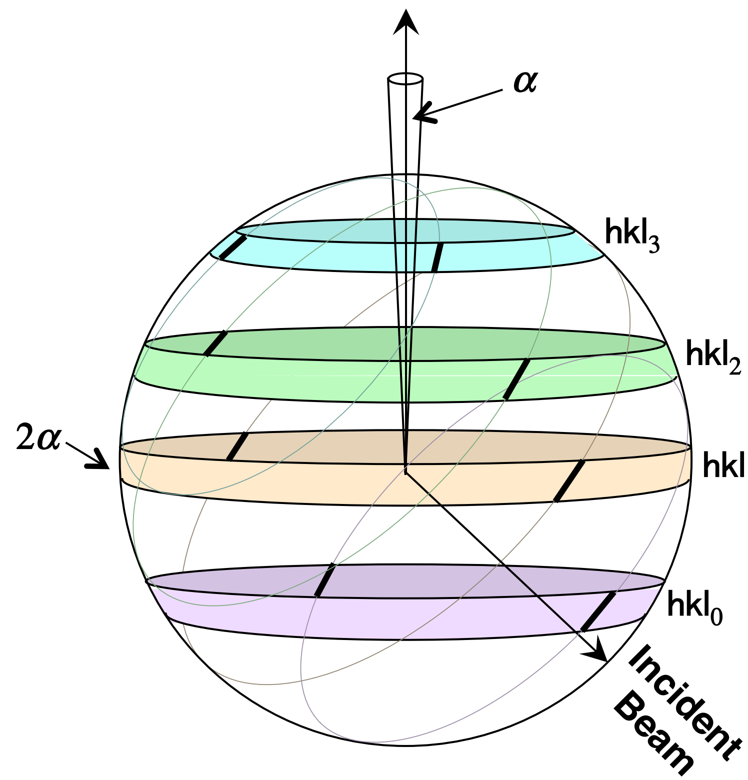




Texture and the Ewald Sphere Construction

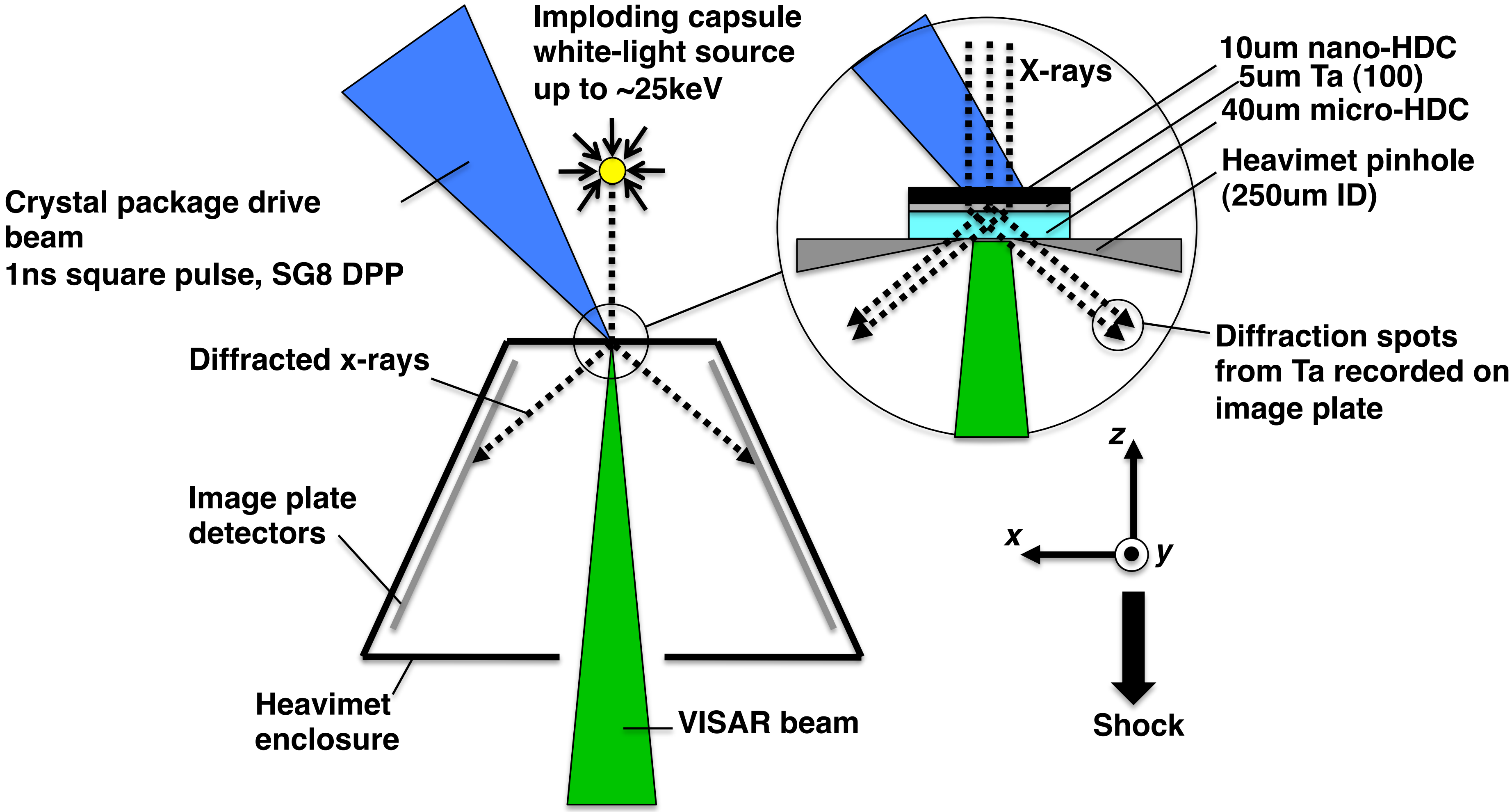




White light x-ray diffraction of single crystals on the Omega laser

Experiments performed by Andrew Comley, Brian Maddox, Jim Hawreliak, Hye-Sook Park, and Bruce Remington

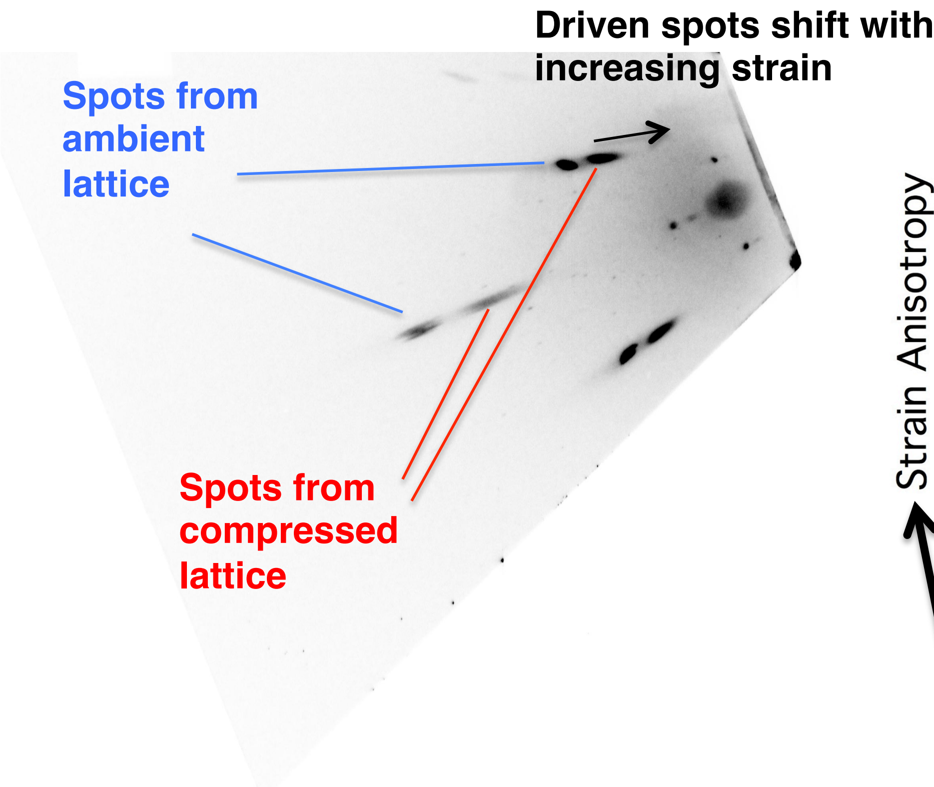
We probe shocked Ta (100) crystals in-situ using white-light Laue x-ray diffraction at the OMEGA laser facility



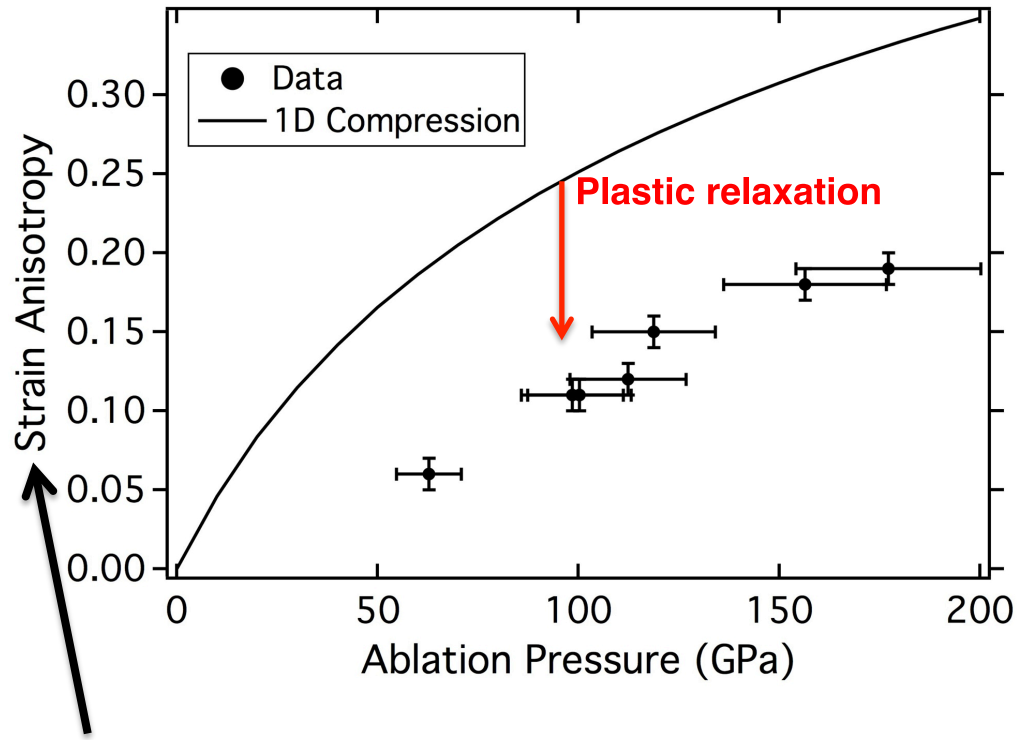
Thanks to Andrew Comley, Brian Maddox, Hye-Sook Park, and Bruce Remington

Fitting the diffraction pattern yields the strain anisotropy (difference in strains in shocked and transverse directions) of the compressed unit cell

Example of Laue x-ray diffraction data



Strain vs. Pressure



- **Von Mises Stress (Strength) = 2C’ x strain anisotropy**
- **C’ = (C_{11} – C_{12}) / 2 where C_{11} and C_{12} are elastic constants**

Thanks to Andrew Comley, Brian Maddox, Hye-Sook Park, and Bruce Remington

Guiding principles for fielding x-ray diffraction on NIF:

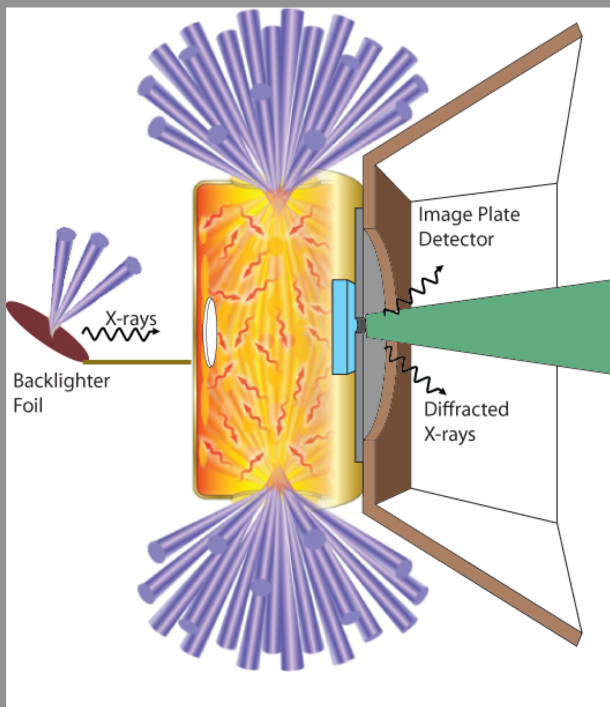
- Design and field a diagnostic useful to a wide range of experiments
  - Powder diffraction
  - White-light single crystal Laue
  - EXAFS
- Employ successful designs from Omega
- Enable both direct and indirect drive configurations
- Explore advanced concept possibilities
- Concentrate on reducing background, increasing resolution, and increasing the number of reflections observed

Pathway to the NIF

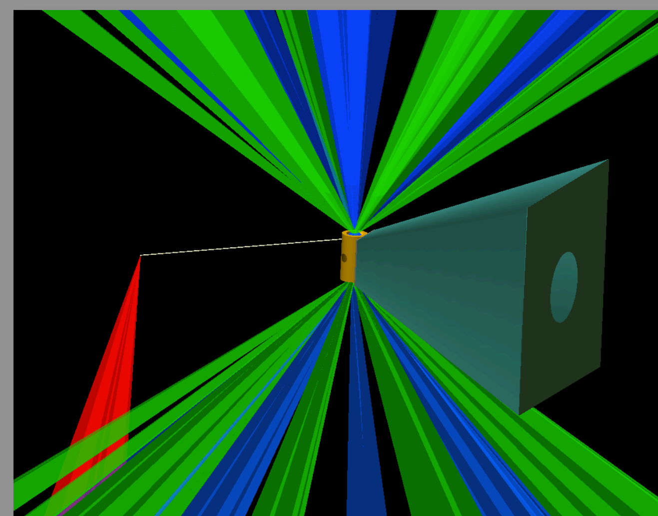
- <u>Diagnostic development</u>
  - Responsible Scientist: Ray Smith
  - Responsible Individual: John Dzenitis
  - Qualify diagnostic for
    - Debris
    - Survivability
  - Determine
    - Optimum shielding for hohlraum drive
    - Optimum backlighter energy
  - CDR planned in 2 months
- <u>Shot Plan</u>
  1. Diagnostic Damage assessment (½ Energy – 500 GPa)
  2. Noise Level measurement of Image plates
  3. Low (1 - 1.2 TPa)
  4. Middle (1.7 – 2.0 TPa)
  5. High (2.5 – 3.0 Tpa)

We will combine the XRD capability from Omega and the successful drive already used on the NIF

Target Geometry



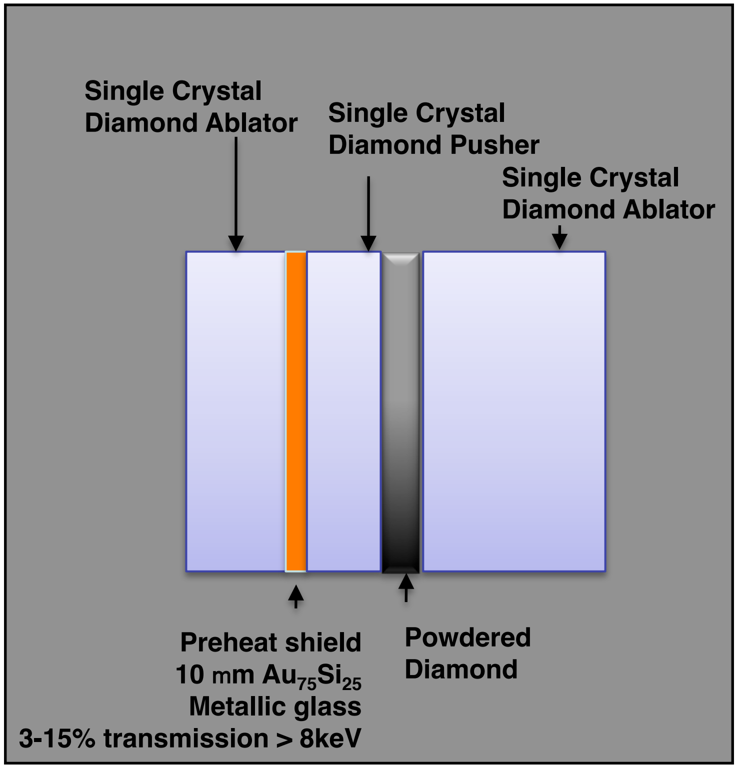
VISRAD Model



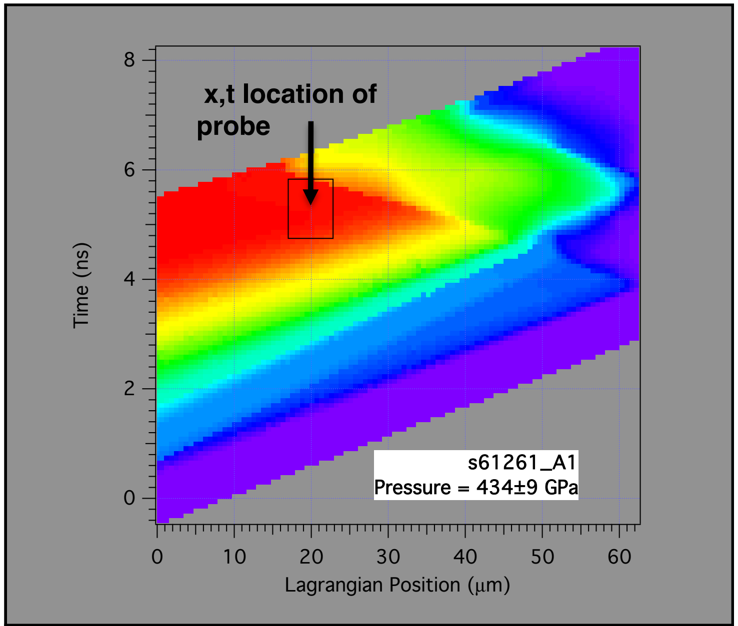
Using 176 beams to drive the holhraum leaves 4 quads for the backlighter

The NIF targets will draw on Omega design and experience

Diffraction Target



Pressure Profile

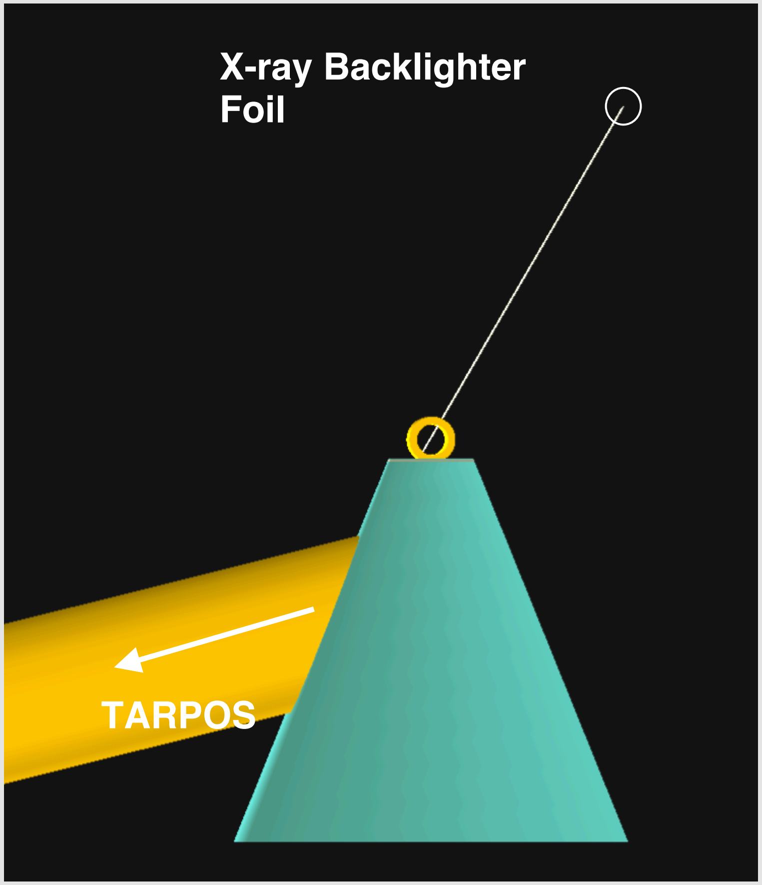


Using the free surface velocity to back integrate the pressure profile through the diamond

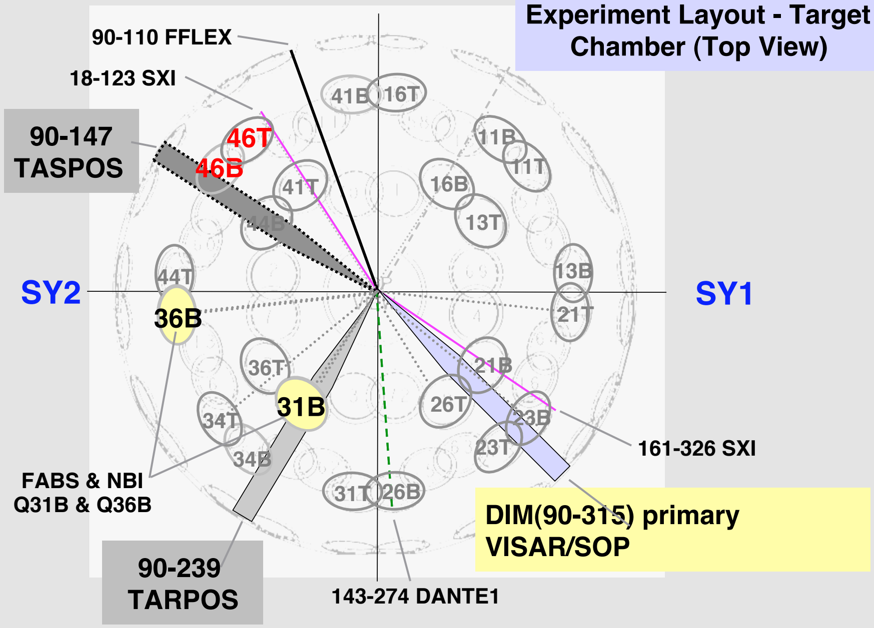
Using target components which will not contribute to the diffraction signal we ensure we probe a limited temporal and spatial region at the peak pressure

Diagnostic configuration

Primary XRD diagnostic on TARPOS

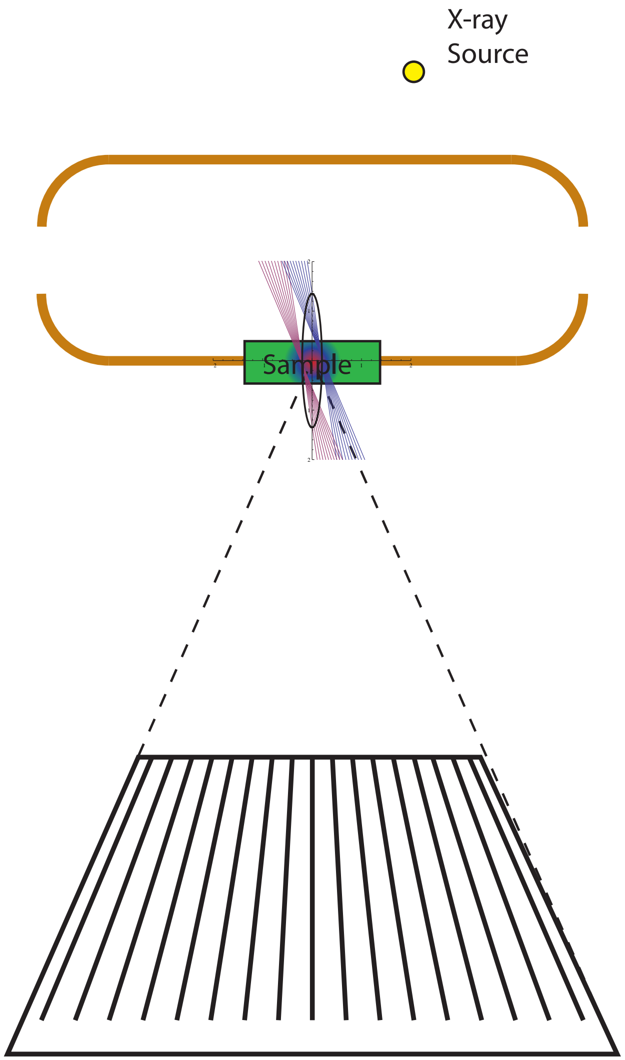


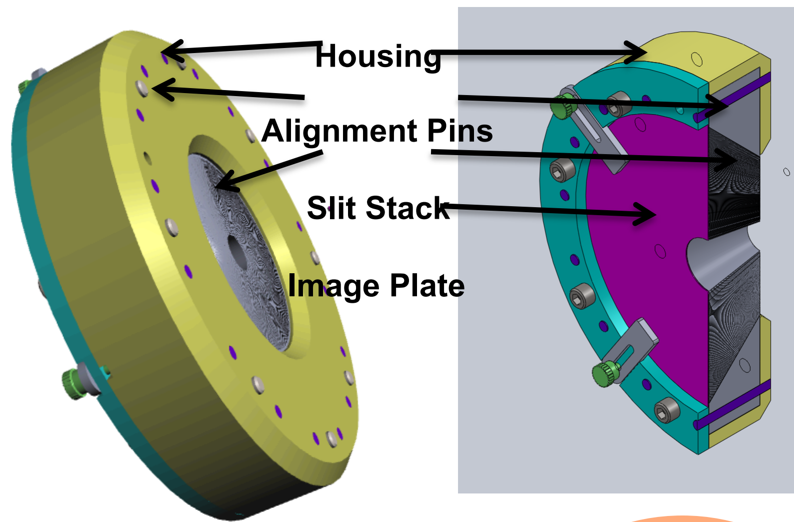
Experiment Layout - Target Chamber (Top View)

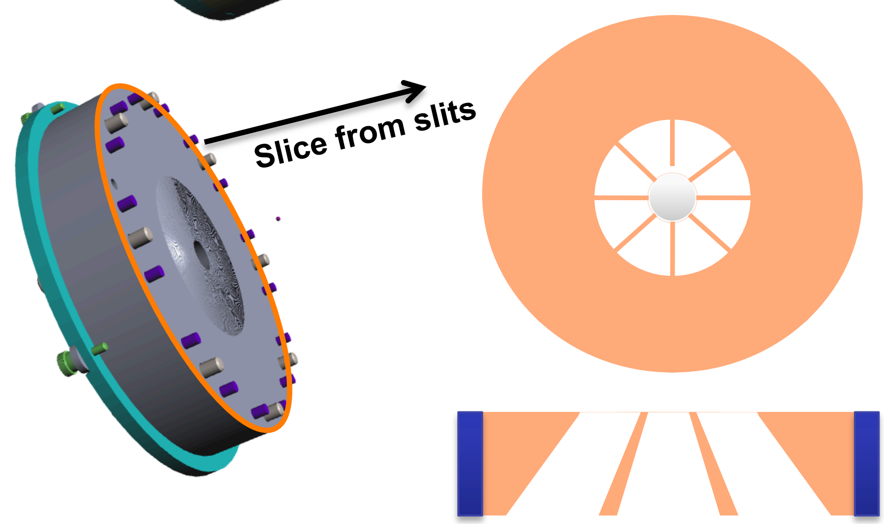


Diagnostic	Port	Priority
VISAR/SOP	90-315	1
DANTE-1	143-274,64-350	1
SXI-1,2	161-126, 18-123	3
FABS/NBI	Q31B, Q36B	3
FFLEX	90-110	3

Advanced Designs: Soller Slits.





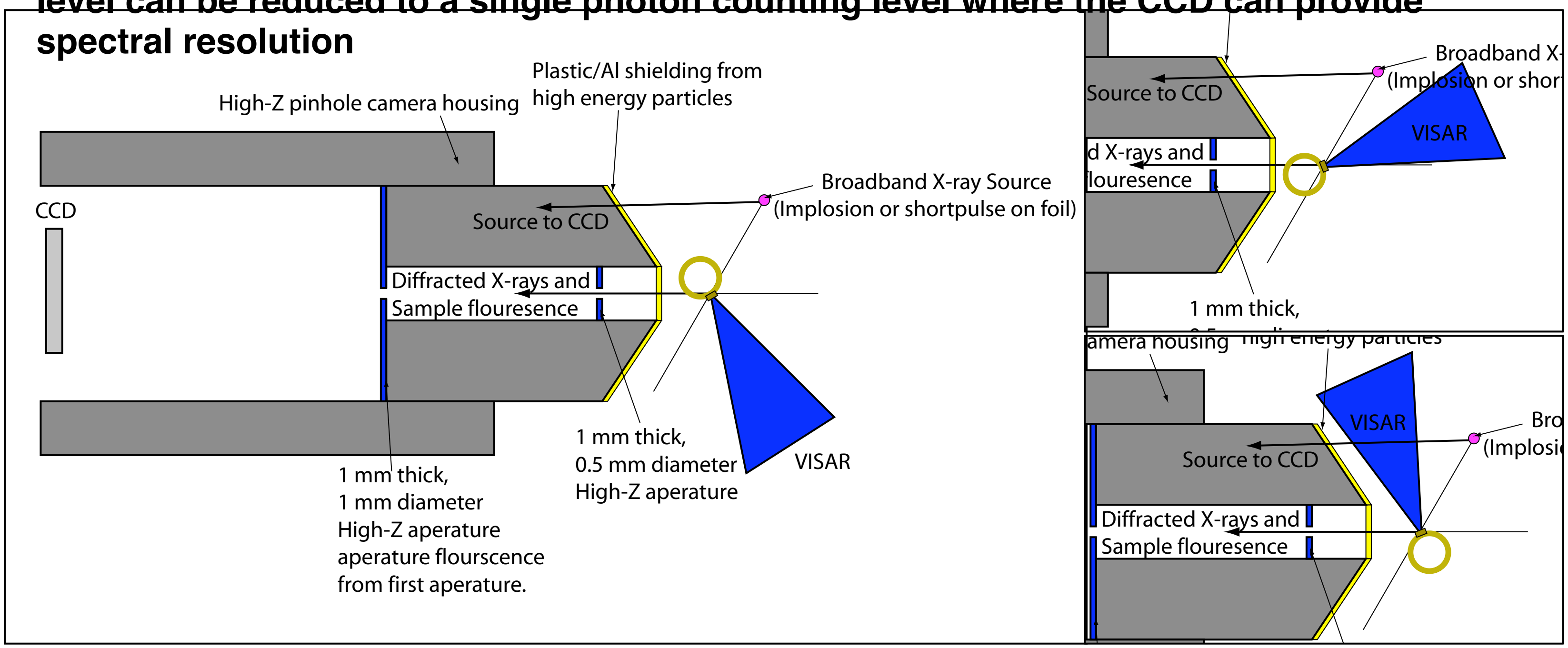


Stack layers with slightly larger patterns to assemble 2D array of slits

Advanced Designs: Energy / Angle Dispersive Diffraction

Using a broadband x-ray source and a fixed location energy dispersive detector we can resolve different lattice planes at different energies ($\lambda = 2d \sin\theta$ where θ is fixed and λ varies as d)

The example geometry shown below is similar to a pinhole camera which images the sample material onto a CCD. By filtering and use of small pinhole apertures the single level can be reduced to a single photon counting level where the CCD can provide spectral resolution



This design would allow coincident EXAFS measurements


Thanks