Working Under Intense Pressure at Omega (X-Ray Diffraction from Laser-Compressed Crystals: Experiments and Simulations)

Justin Wark
Department of Physics
Clarendon Laboratory
University of Oxford

Omega Users' Meeting
April 27th 2011, LLE, Rochester

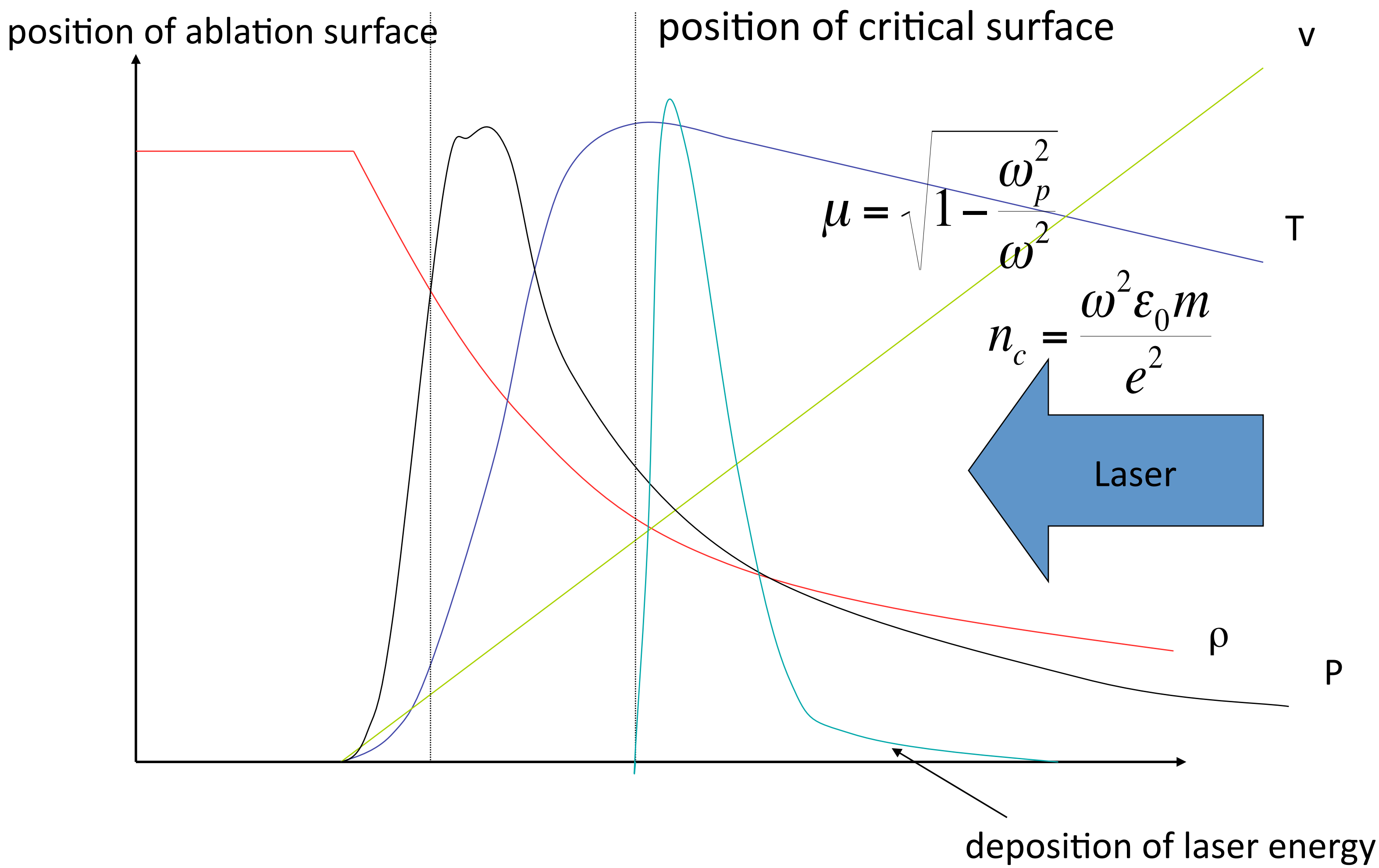
J.S. Wark,[1] E. Bringa,[2] G. Collins,[3] A. Comley,[4] J. Eggert,[3] J. Foster,[4] J. Hawreliak,[3] A. Higginbotham,[1] B. Maddox,[3] G. Mogni,[1] H.-S. Park,[3] N. Park,[4] B. Remington,[3] P. Rosen,[4] S. Rothman,[4] R. Rygg,[3] M. Suggit[1]

[1]Department of Physics, Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX1 3PU, United Kingdom
[2]Universidad du Cuyo, Mendoza, Argentina
[3]Lawrence Livermore National Laboratory, Livermore, CA 94550
[4]AWE, Aldermaston, Reading UK

Outline

- **Motivations:**
  - **Shock Physics - Plastic Flow and Phase Transitions.**
  - **(Quasi-) Isentropic Compression Experiments (ICE) – New Avenues in High-Pressure Solid-State Physics.**
- **Experiments.**
- **Modelling.**
- **Initial Successes.**
- **Future work….**

Plasma Parameters (1)



Laser Ablation Pressure

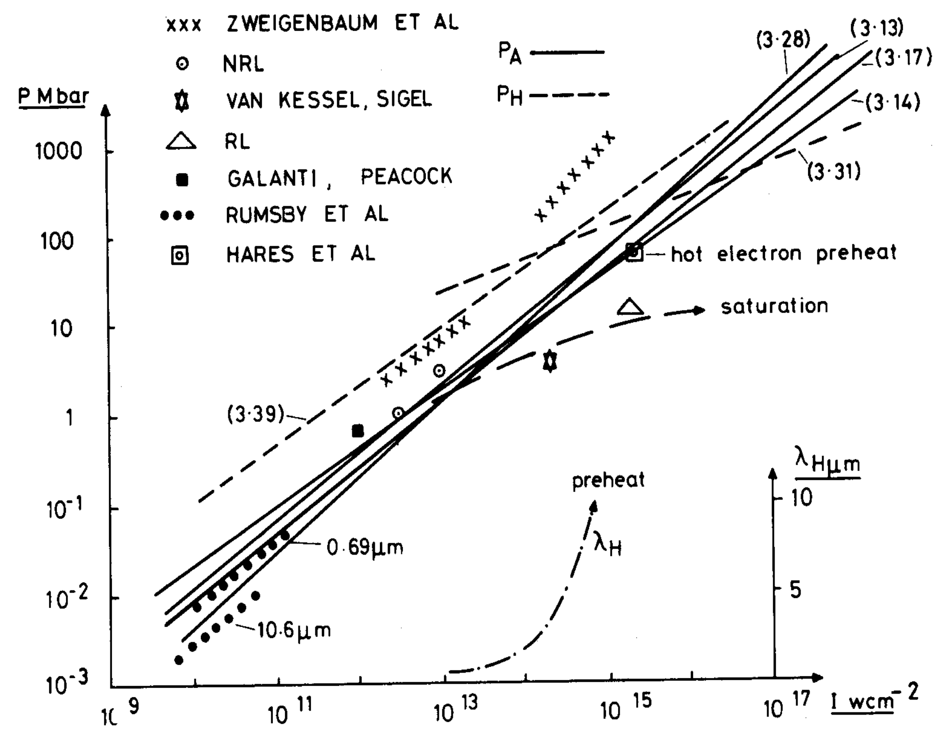
A VERY simple model would say a good fraction of the irradiance, I, flows down the temperature gradient to produce more plasma at the ablation surface. In steady state this produces a kinetic energy flow at the critical surface. Assume Mach 1 at critical surface

$$I \approx \frac{1}{2}\rho_c u_c^3 \approx \frac{\rho_c}{2}\left(\frac{P_c}{\rho_c}\right)^{3/2}$$

(note this equation must be wrong by about a factor of two, as there is thermal energy at the critical surface - we should really talk in terms of enthalpy flow)

$$P_c \approx \rho_c^{1/3} I^{2/3}$$

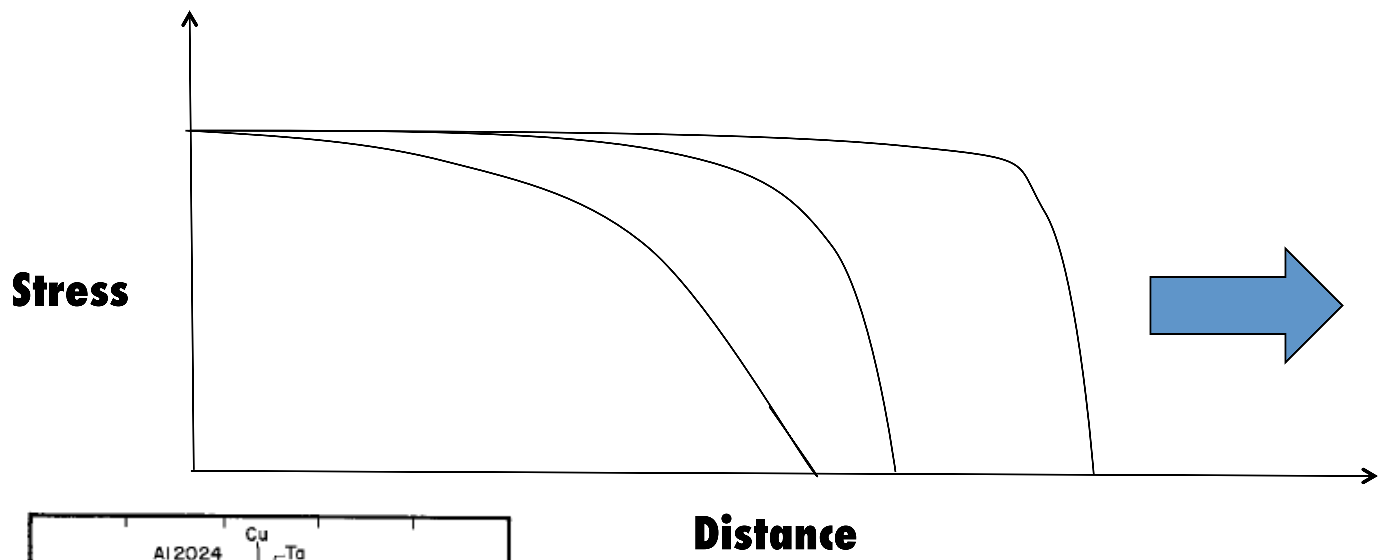
$$P_a = 3\times 10^{-9} \lambda_{\mu m}^{-2/3} I_{Wcm^{-2}}^{2/3} \ \text{Mbar}$$

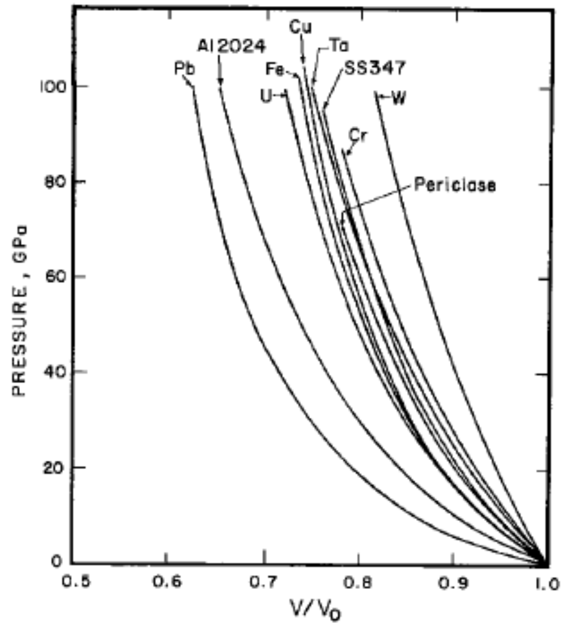


High Pressure Research with Lasers

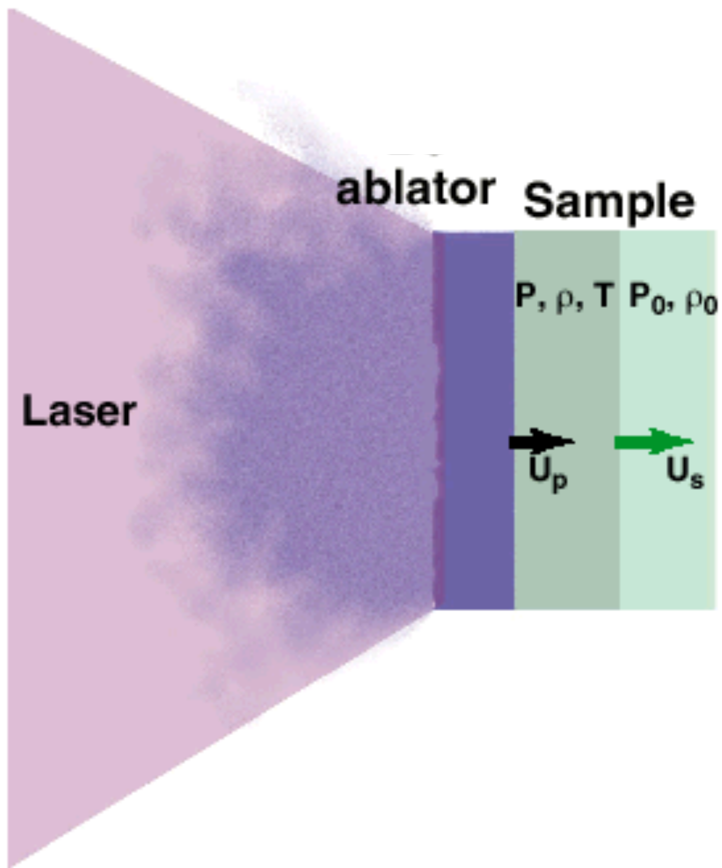
- We have seen that nanosecond lasers can create multi-megabar pressures.
- Ways of applying that pressure:
  - Shock Compression
  - 'Quasi' Isentropic Compression (slow - but how slow?)
- Applications:
  - Basic shock physics:
  - Plastic flow
  - Shock Induced Phase Transitions
  - Equations of State
  - X-ray diffraction to observe the above at the lattice level

Shock Compression





As the speed of sound generally increases with compression, a strong compression wave will steepen into a shock, where there is a discontinuity in density, temperature, and energy across the shock front.



$$\rho_0\left(Us\right) = \rho\left(Us - Up\right)$$

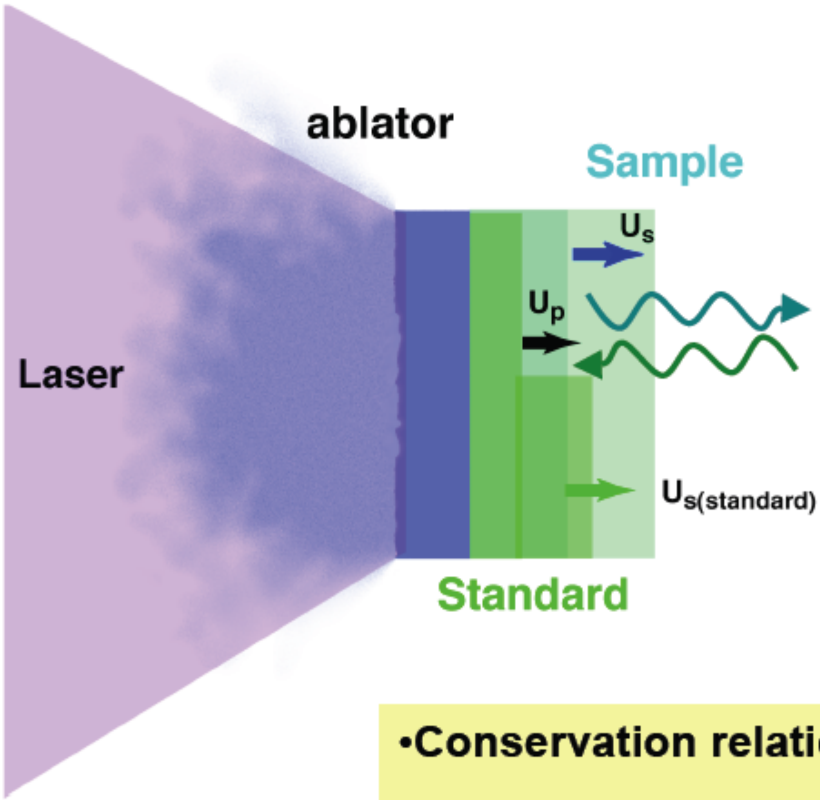
$$P = \rho_0 Us Up$$

$$E = \tfrac{1}{2} P\left(V_0 - V\right)$$

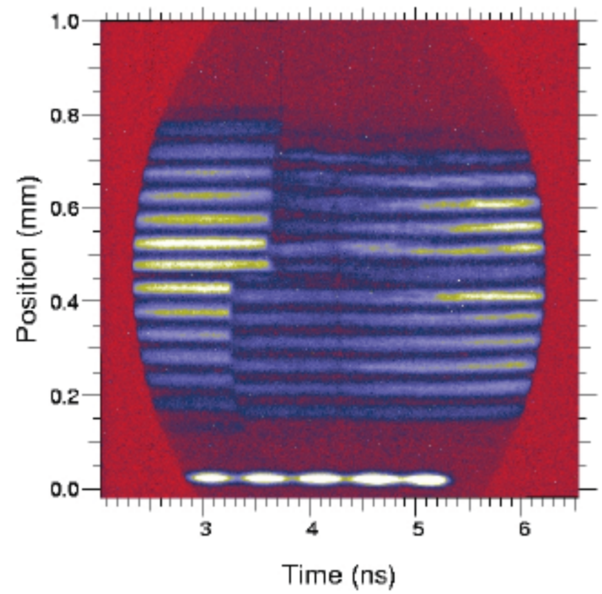
3 equations, 5 unknowns (*Us, Up, P, ρ, E*).

Measure two of these, the others can be calculated.

How do we measure the equation of state and transport properties



VISAR measures velocity and reflectance



- Conservation relations => $P = \rho_0 U_s U_p$

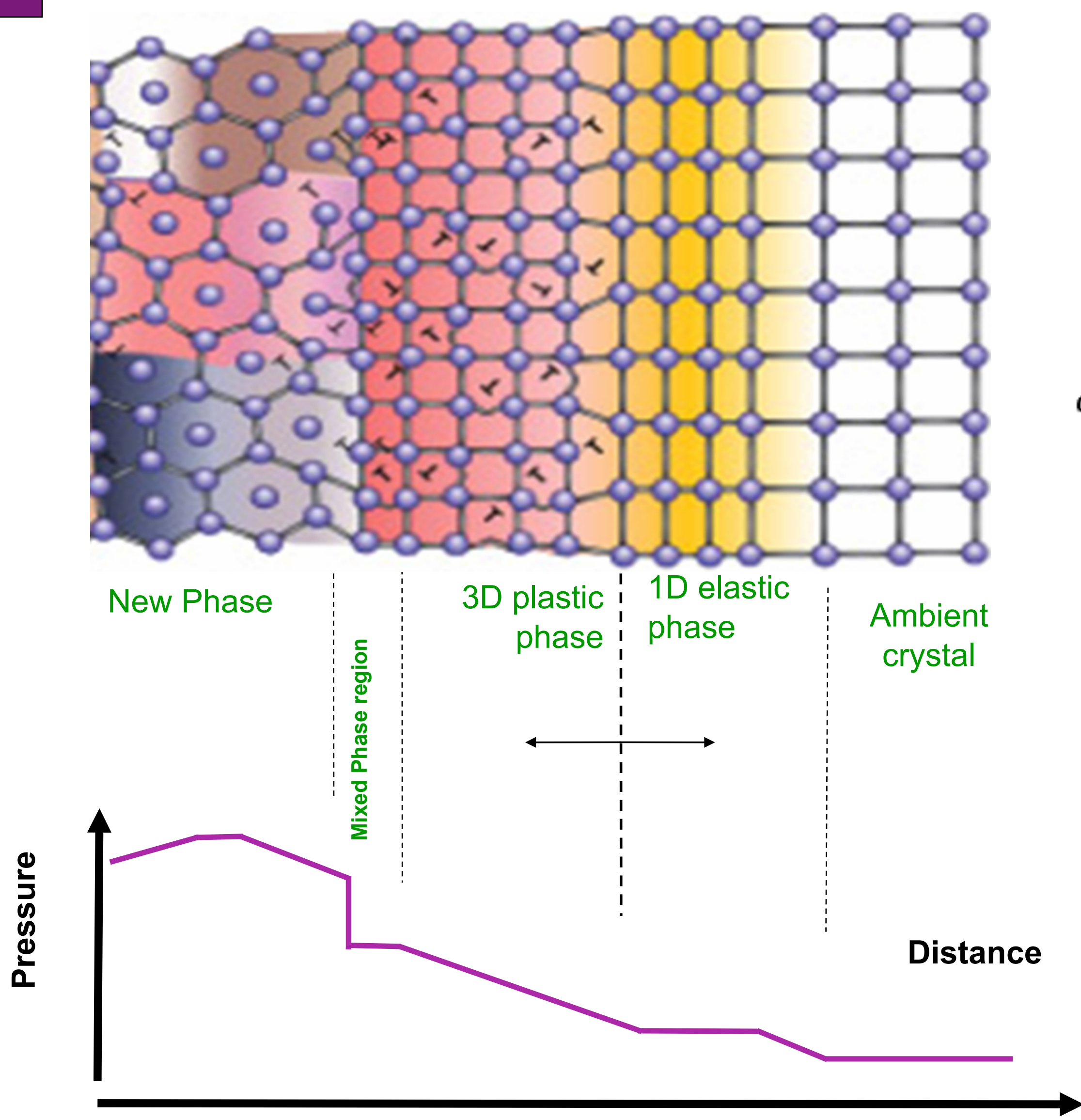
  $\rho/\rho_o = 1/(1-U_p/U_s)$

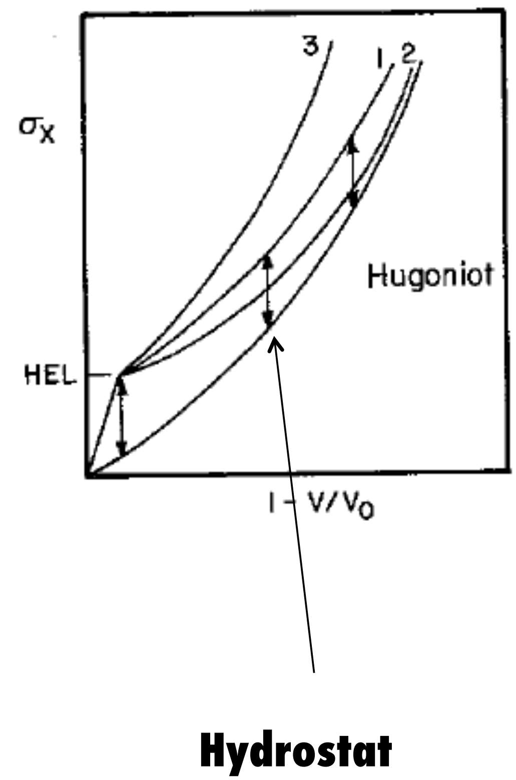
- Temperature needs to be measured separately

Slide from Rip Collins

Schematic Diagram of Shock

Motivation





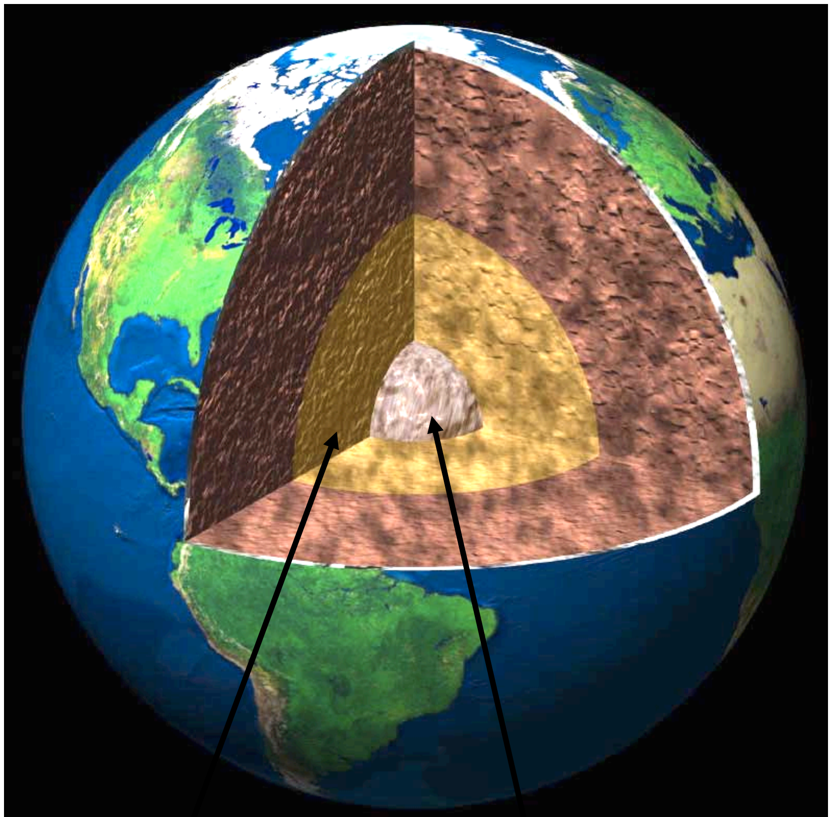
Where does Omega fit in?

- **Major problems in shock physics:**
  - How do solid materials 'flow' like a liquid (hydrostatic compression)?
  - Where do the defects come from (and where do they go)?
  - Interplay between defects/twinning and other deformation mechanisms.
  - How quickly can various phase transitions take place?
  - How well do we understand the equation of state at ultra-high pressures?

- **All of these issues necessitate, or greatly benefit from, a knowledge of what is happening at the lattice level.**
- **Answer: Ultra-short-pulse X-ray diffraction during the laser-driven shock**
- **Three Geometries:**
  - "Diverging Beam" (monochromatic X-rays, single crystals, large range of angles – tells us lattice spacings (strains) and new phase (if single crystal).
  - "Debye-Scherrer", monochromatic collimated X-rays, polycrystalline material, tells us lattice spacings (strains) and phases, and information on response of grains with varying orientation.
  - "White Light Laue", polychromatic collimated X-rays, single crystal, tells us about defects, elastic strain, new phases.

Motivation

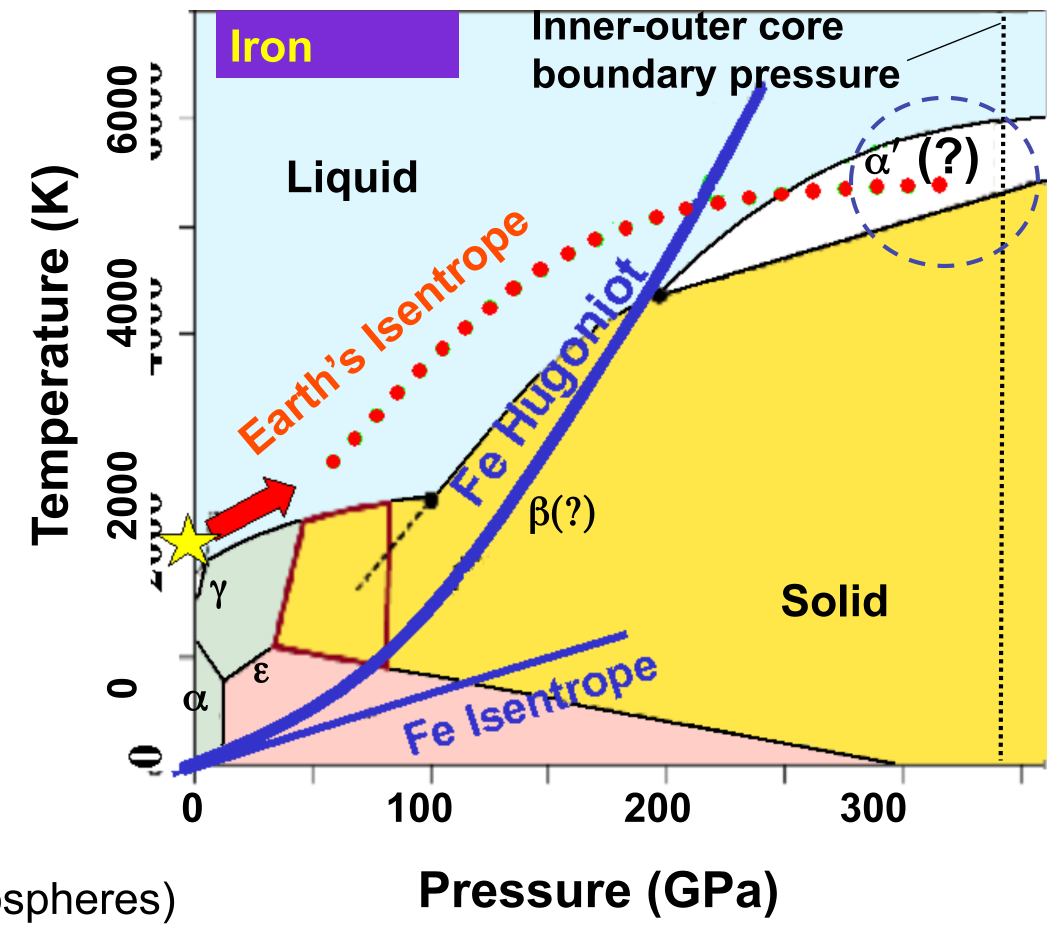
View Phase Transition in Iron



Outer liquid core

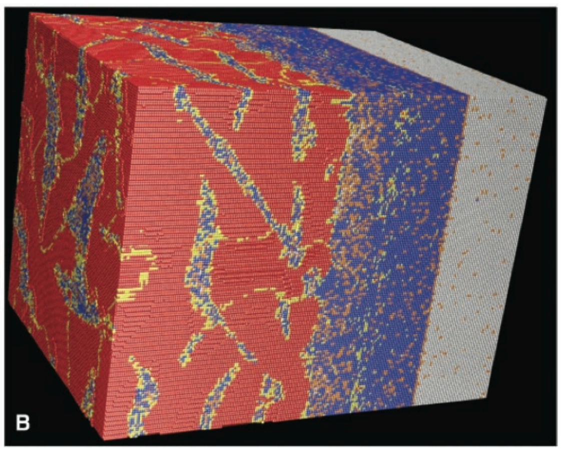
Inner solid core
(350 GPa = 3.5x10[6] atmospheres)

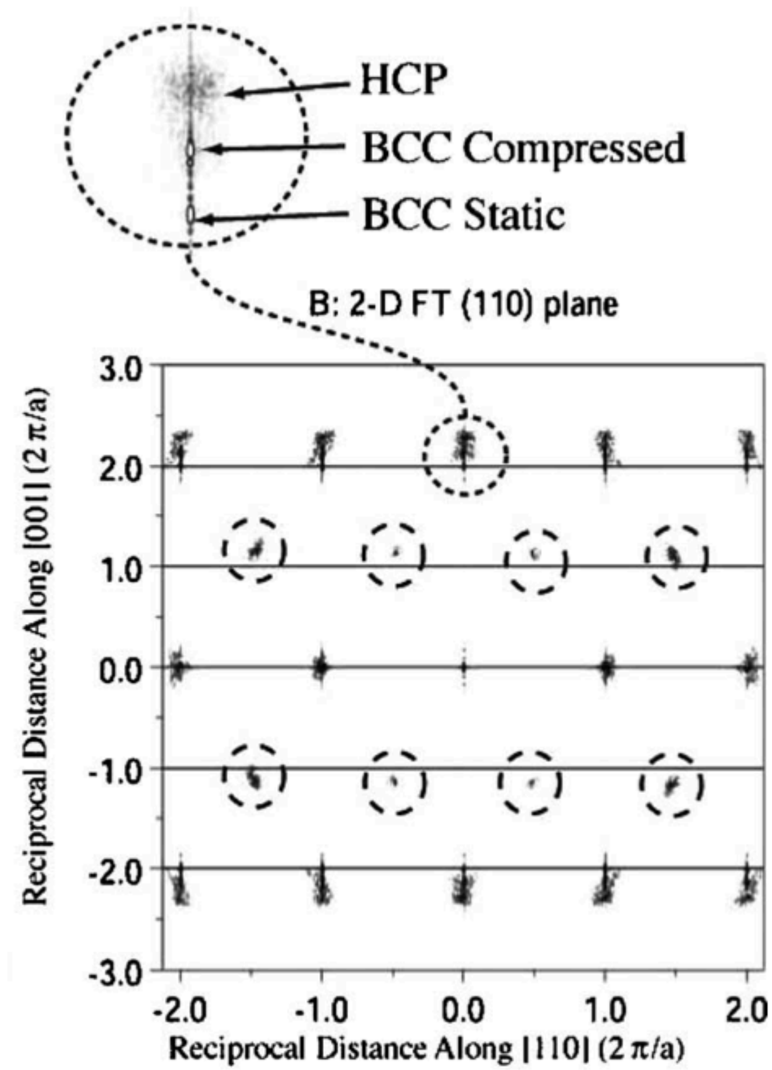
NB Ramp compression along the Earth's Isentrope may resolve existence of α' phase



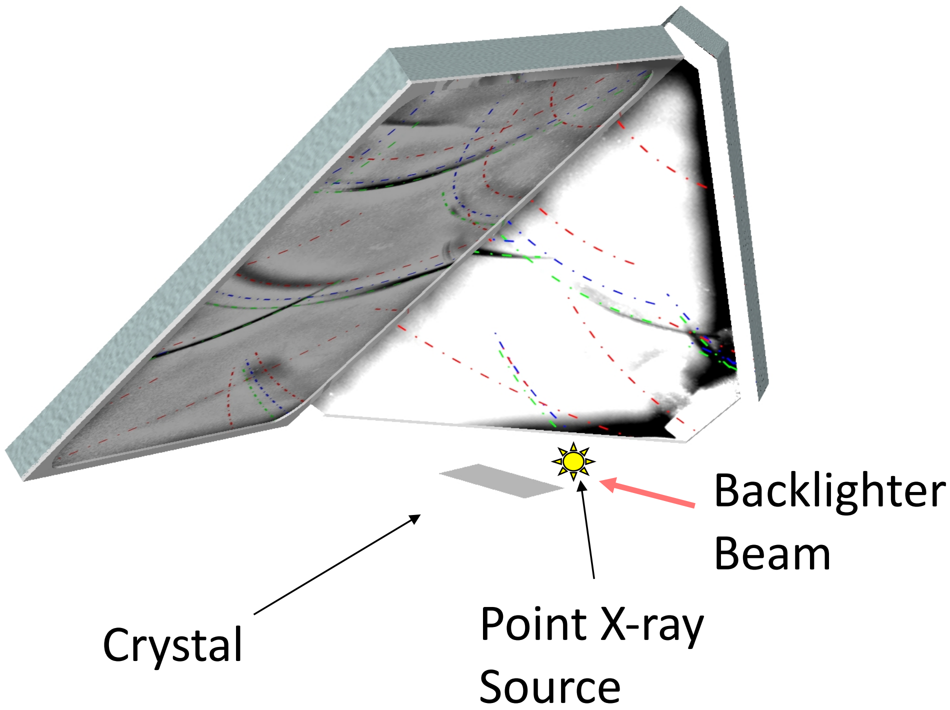
X-ray Diffraction

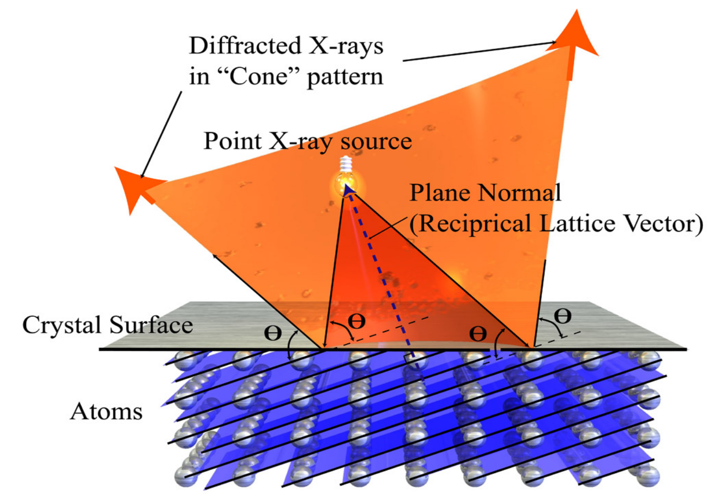
$$A \propto \sum_{r} f e^{-i\mathbf{G}.\mathbf{r}}$$





Multi-Plane X-ray Diffraction





Single crystal target

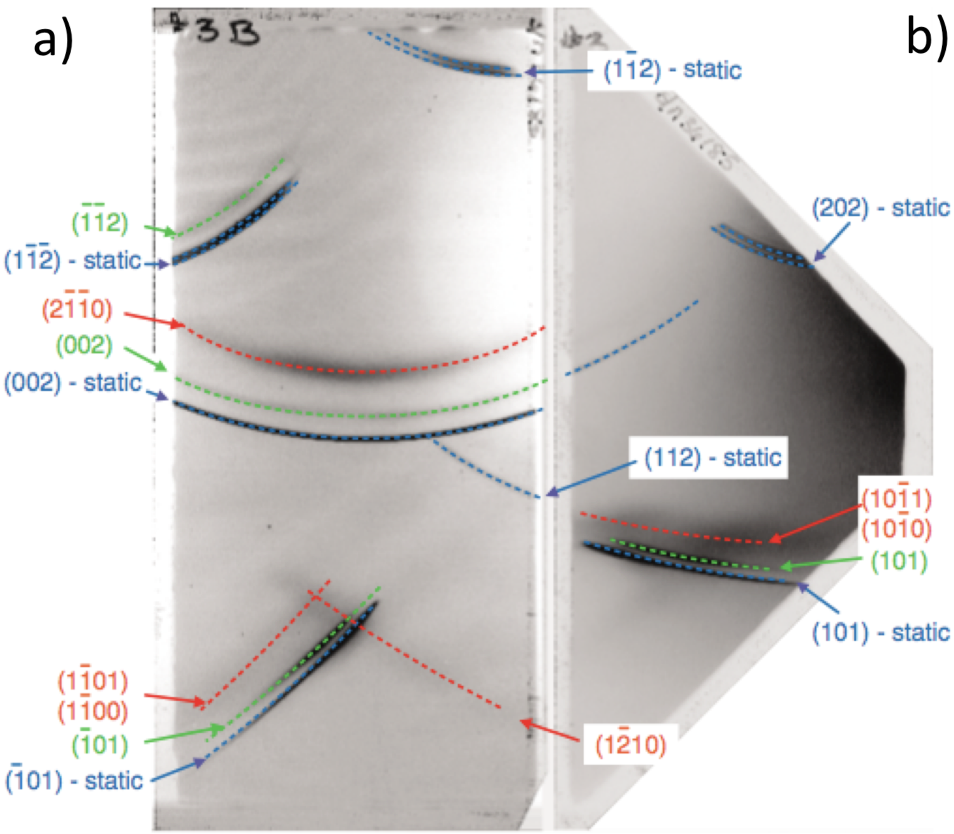
Divergent, monochromatic X-ray beam

Multi-Plane X-ray Diffraction

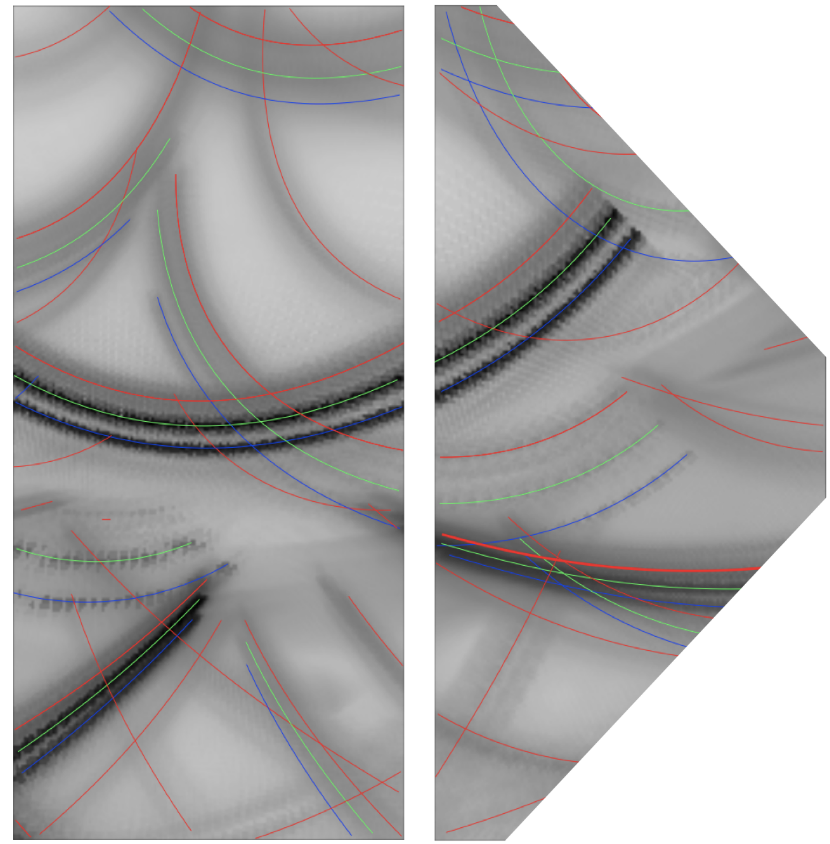
Experiment

Post-processed from MD Simulation
(Kimminau et al J. Phys. Condens. Matter 20, 505203 (2008))

a)

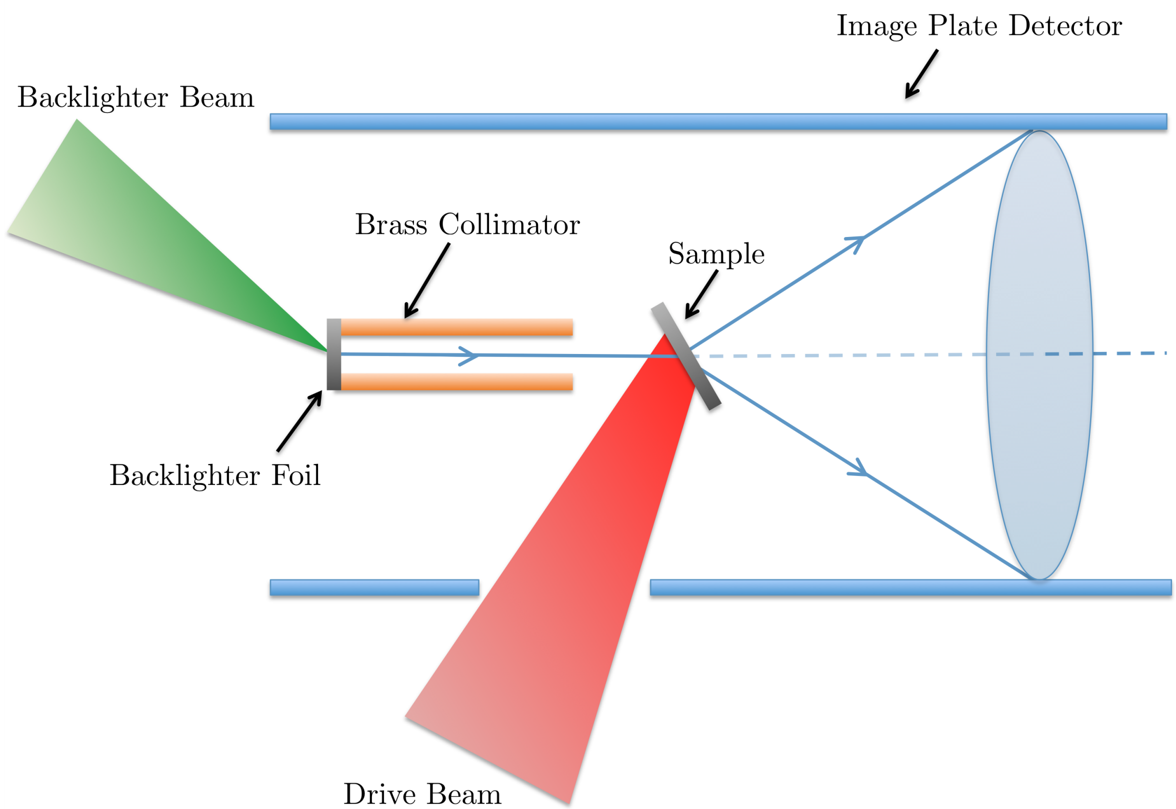


b)



Single crystal FE (001) target shocked to ~ 20GPa. Nsec Diiffraction
Divergent, monochromatic X-ray beam

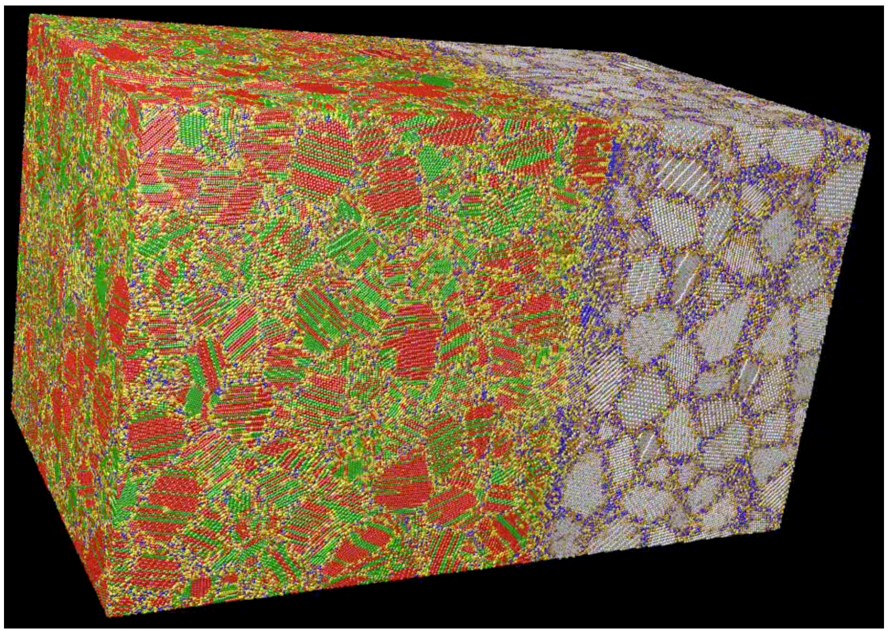
Diffraction from Polycrystalline Materials

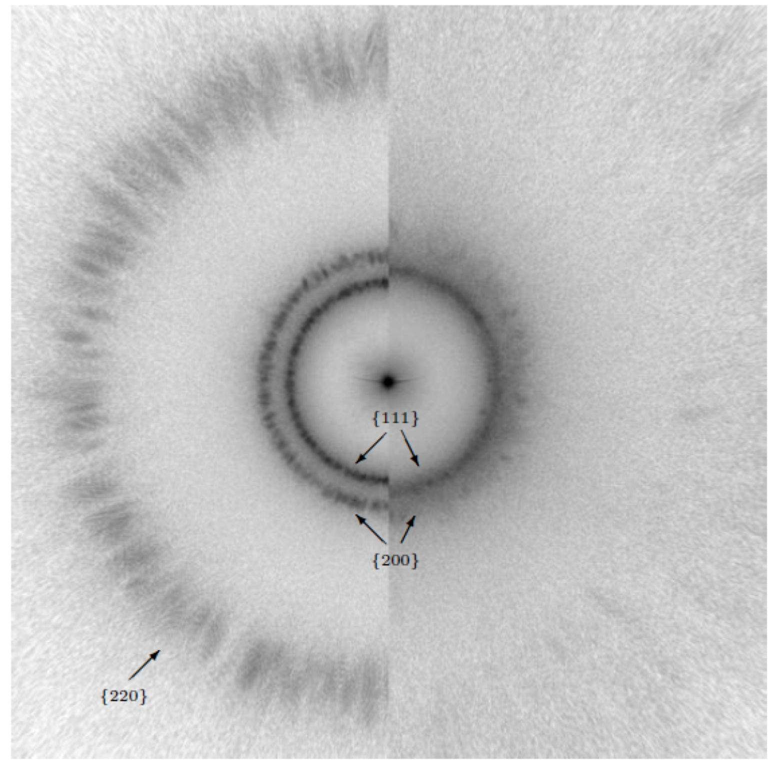


Polycrystalline target

Collimated, monochromatic X-ray beam

1st LCLS Experiments will use Nanocrystalline Samples



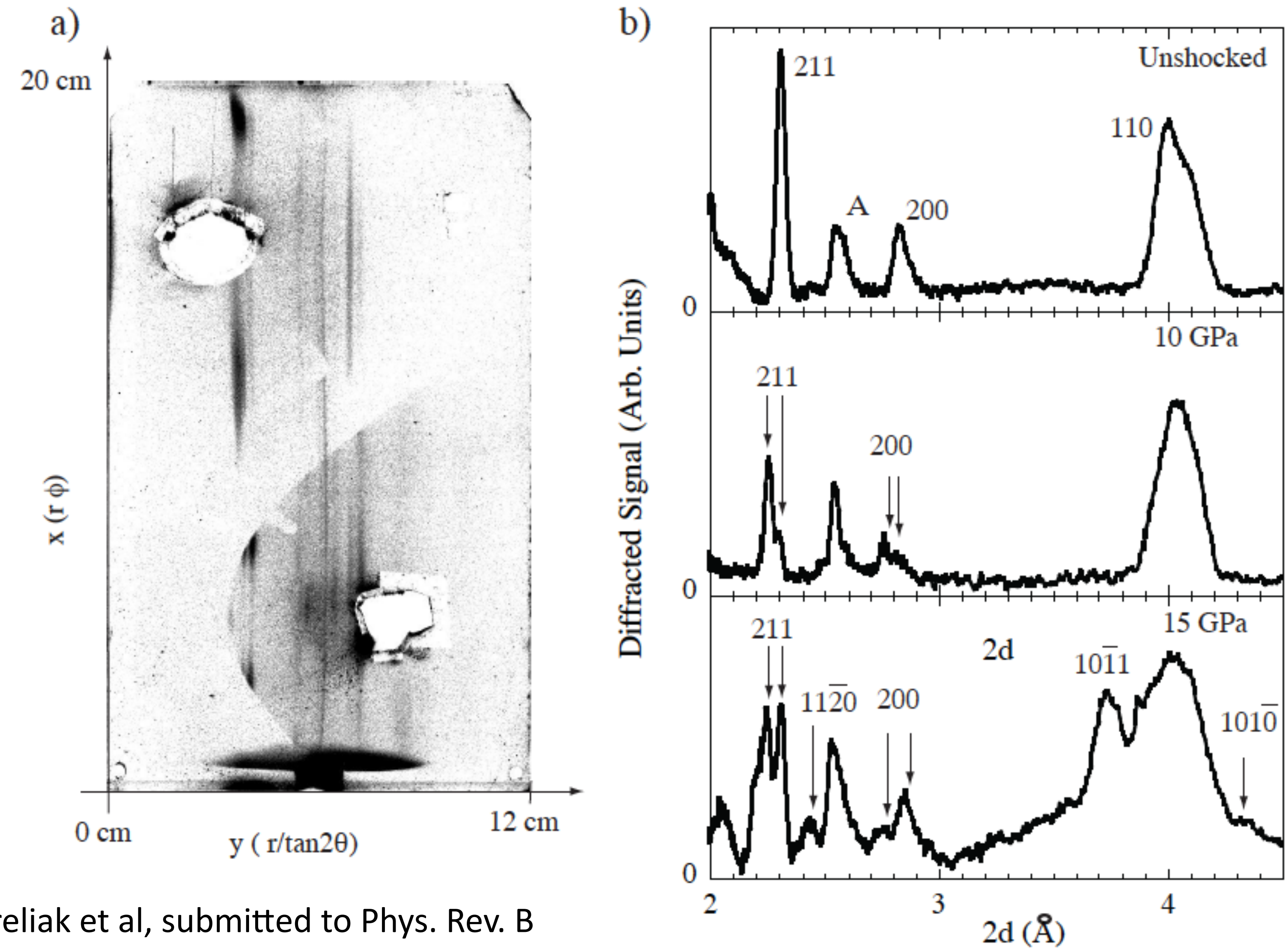


Unshocked Shocked

Polycrystalline target

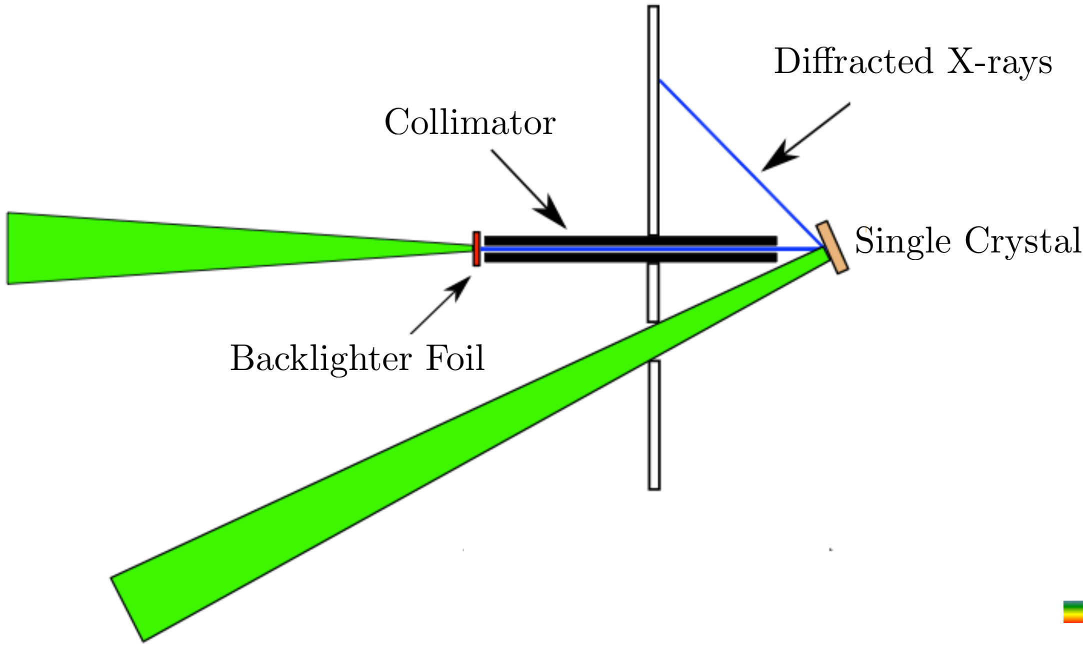
Collimated, monochromatic X-ray beam

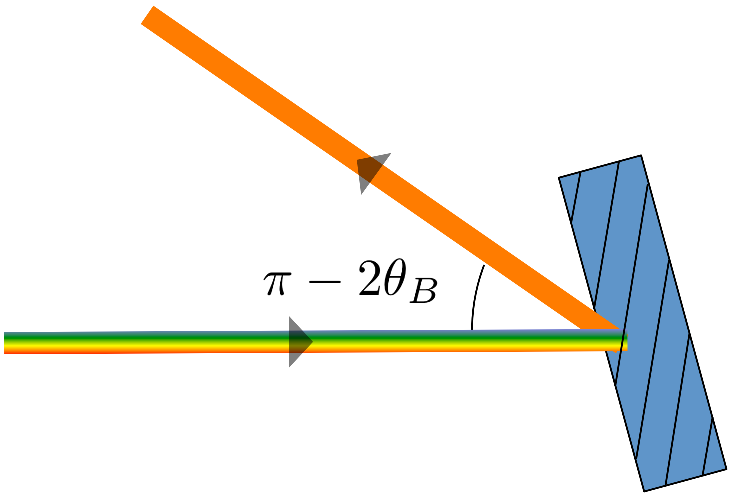
Diffraction from Shocked Polycrystalline Iron



Hawreliak et al, submitted to Phys. Rev. B

White Light Laue



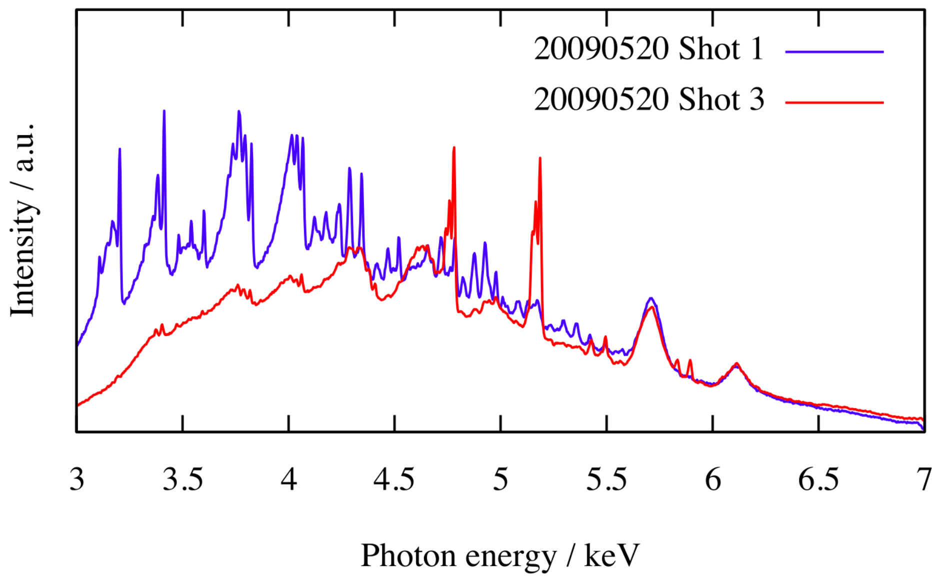


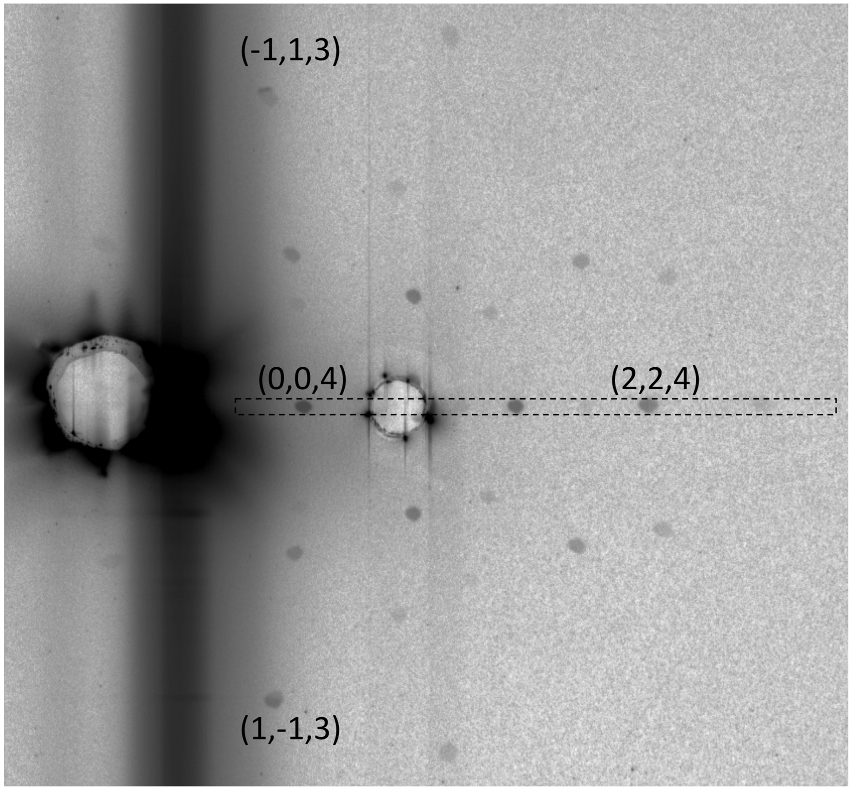
Single crystal target

Collimated, polychromatic, X-ray beam

White Light Laue Demonstrated

M. Suggit et al, Review Sci. Instrum., to be published



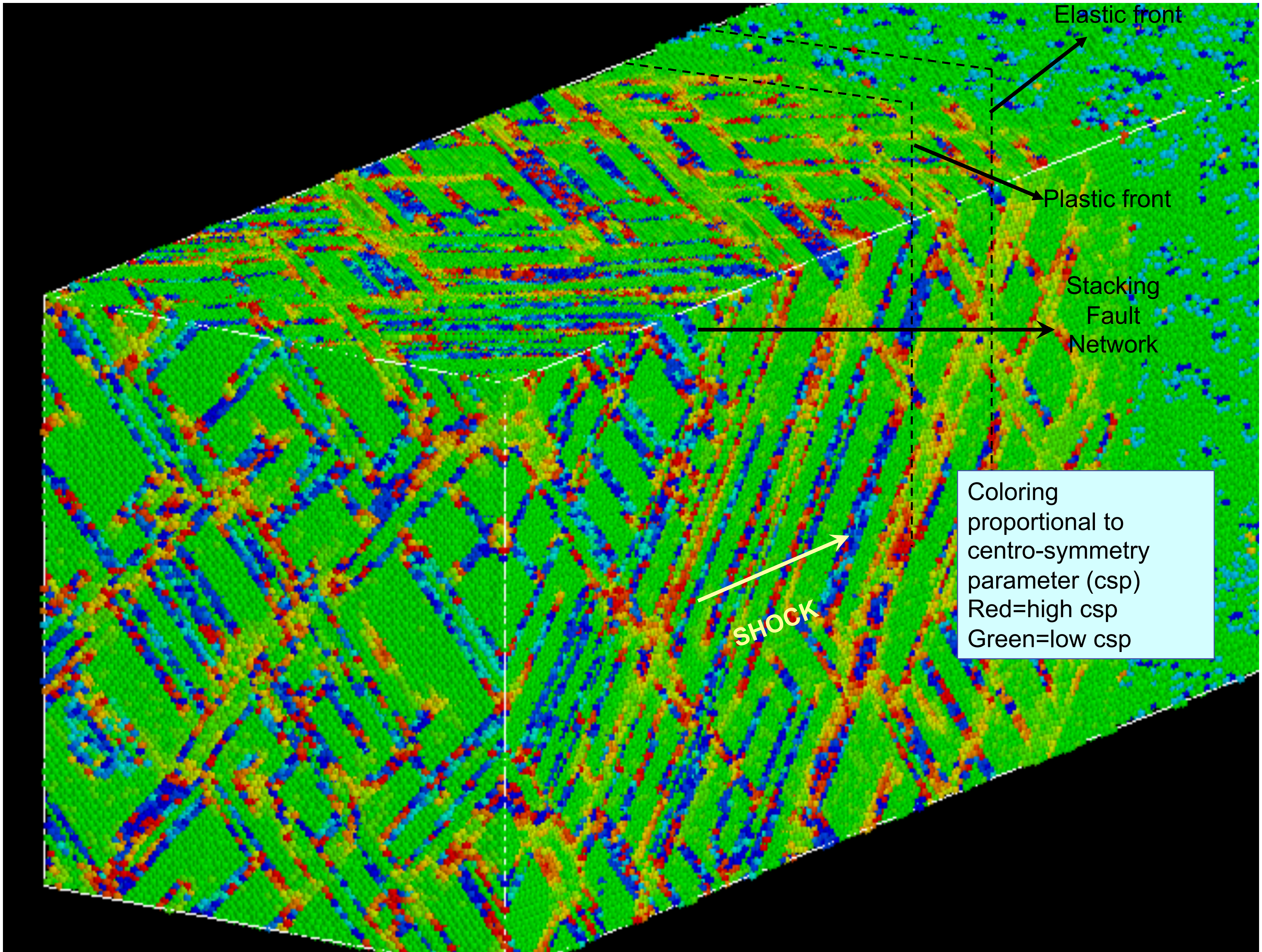


1-nsec pulse of ‘white light’ X-rays created by laser heating of a ‘cocktail’ target on Janus.
On Omega higher white light energies are formed at the peak of a capsule implosion.

Single crystal silicon target

Collimated, polychromatic, X-ray beam

Copper (001) Mishin MD, Shocked to 50 GPa



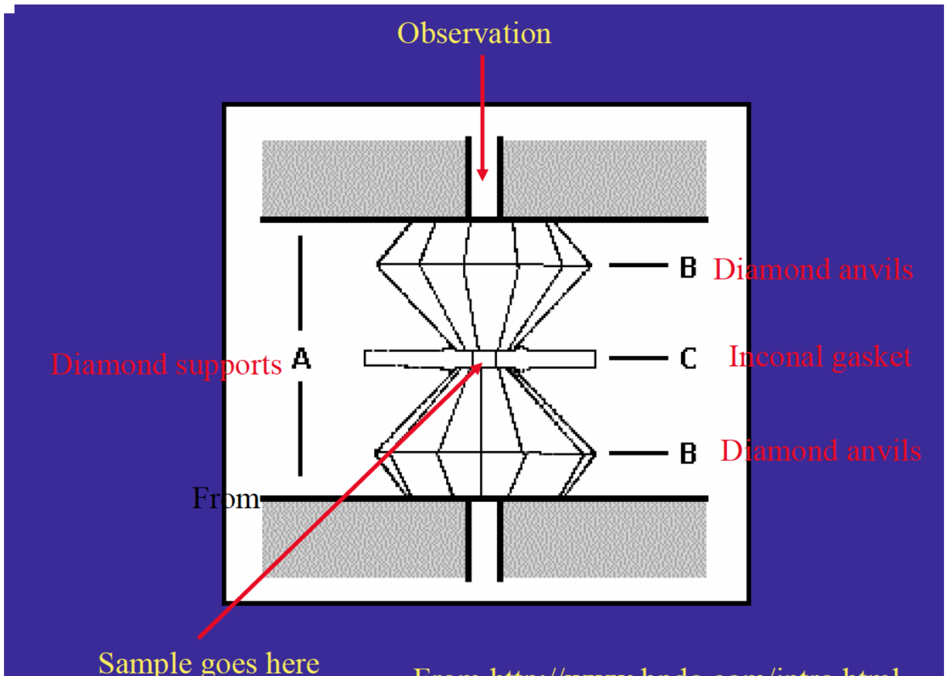
Shock Compression: Pros and Cons

- A steady shock is a relatively simple way to compress materials to high densities.
- An accurate point on the PV diagram can be located if shock and particle velocity can be measured.

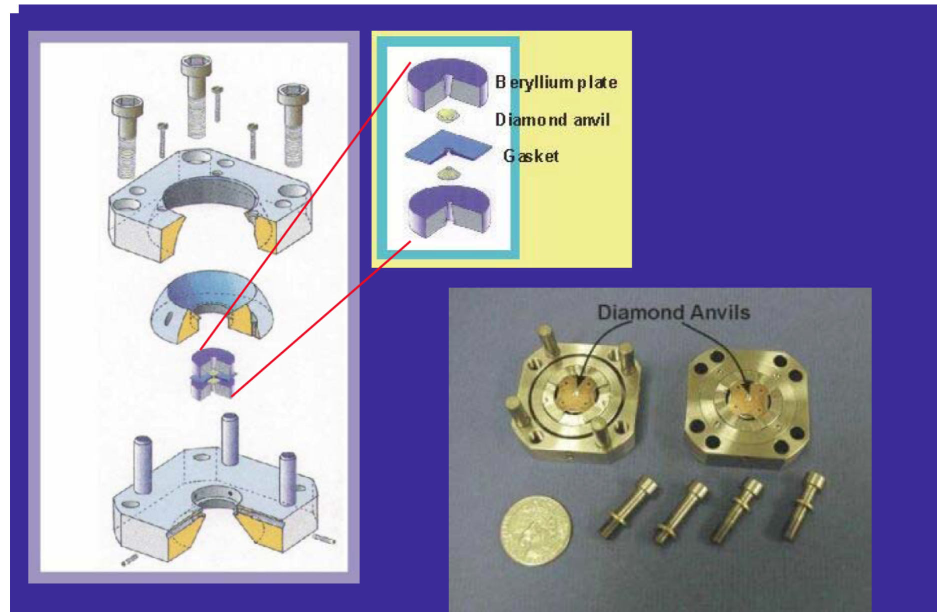
- Only get a point on the 'Hugoniot' - a single line in PV space - that is very limited EOS information.
- Shocks are irreversible, highly entropic events. The sample is heated to very high temperatures.
- Typical metals will melt under shock compression at pressures of order 1 -2 Mbar (note a diamond anvil cell keeps matter solid, and up to 3 Mbar).
- Planetary cores at high pressure are much cooler (probably solid) than the conditions we reach on the Hugoniot.

- CONCLUSION: We also wish to compress matter without the shock heating - for this we need to compress it more slowly.

The ‘Standard’ Technique: DAC



From http://www.hpdo.com/intro.html



Inside of a diamond anvil cell
(Virginia Tech Crystallography Laboratory, USA)

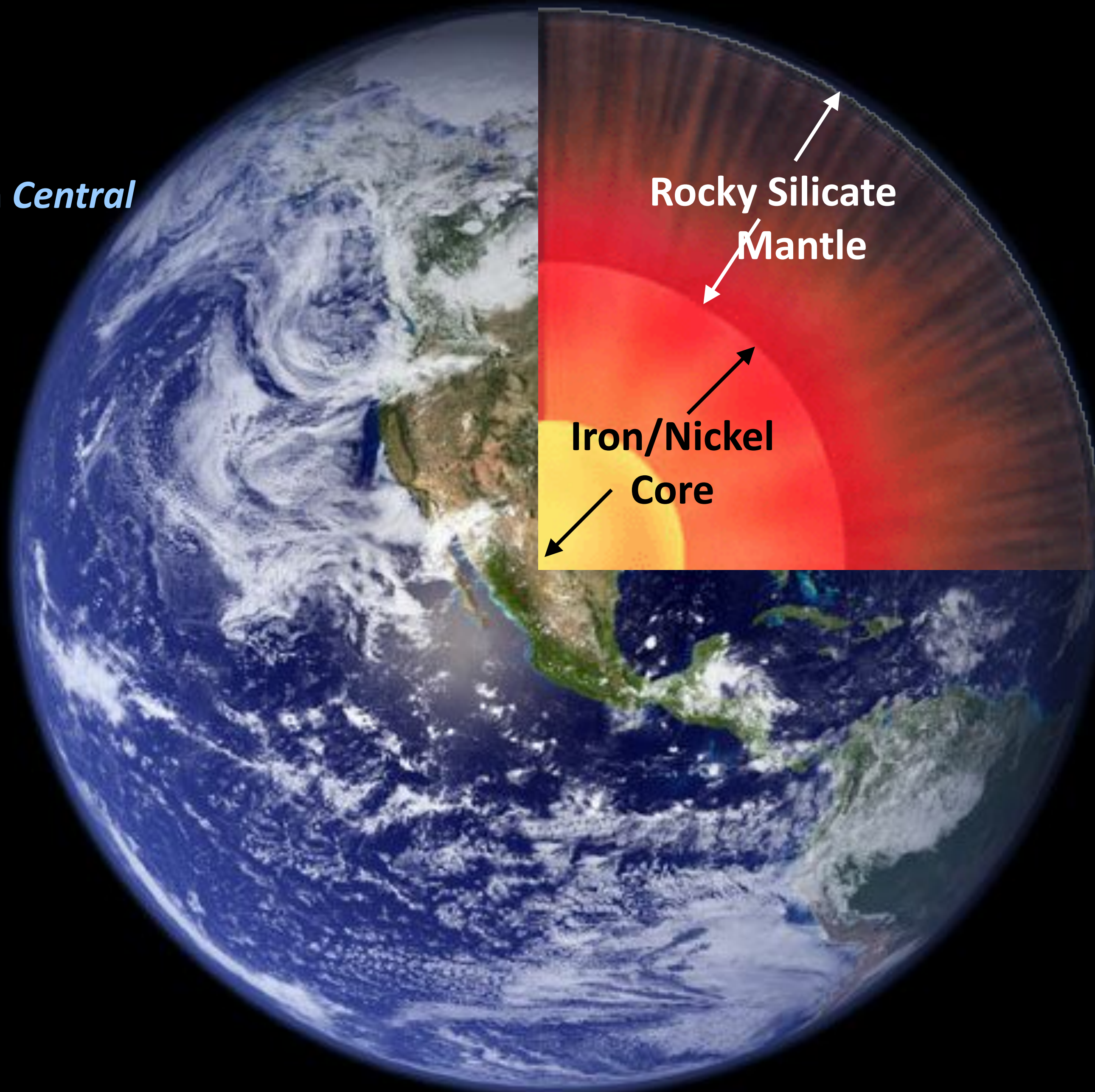
In Diamond Anvil Cells matter can be statically compressed to a few (~3)Mbars

Matter at P>>100 GPa (1 Mbar) is quite common

Earth

Central Pressure: 360 GPa *Central Temperature:* 6000 K

Saturn



When is a compression wave a shock?

- **With plastic flow, shock waves have finite thickness (due to an effective 'viscosity').**
- **The Swegle-Grady relation states that the strain-rate at the shock is proportional to the 4th power of the peak stress.**

$$\frac{d\varepsilon}{dt} = A\sigma^4$$

- **Note the constant of proportionality is different for different materials.**
- **The SG relation is <u>not fully understood</u>, and is an area of active research.**
- **However, it does imply that to keep a given material close to an isentrope (and thus cooler), we must apply the pressure more slowly than in the shock (for a given peak stress).**
- **This can be achieved by**
  - **Pulse-shaping.**
  - **"Smart" targets.**

Swegle-Grady 4th Power Law

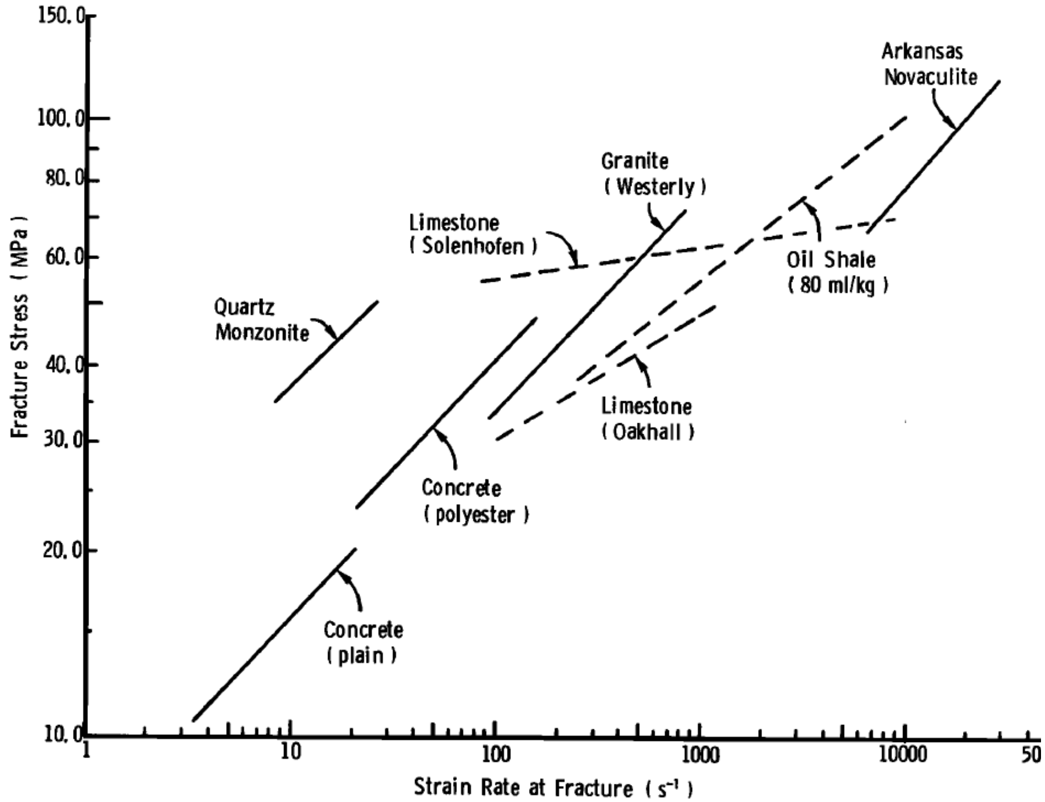
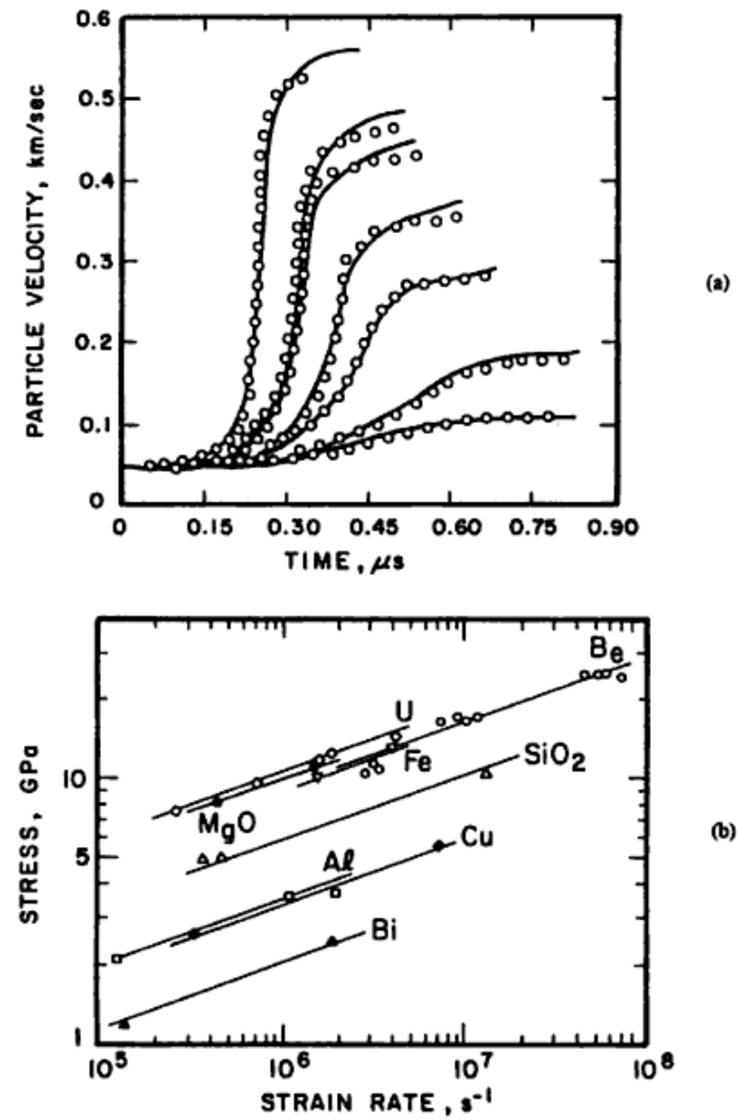
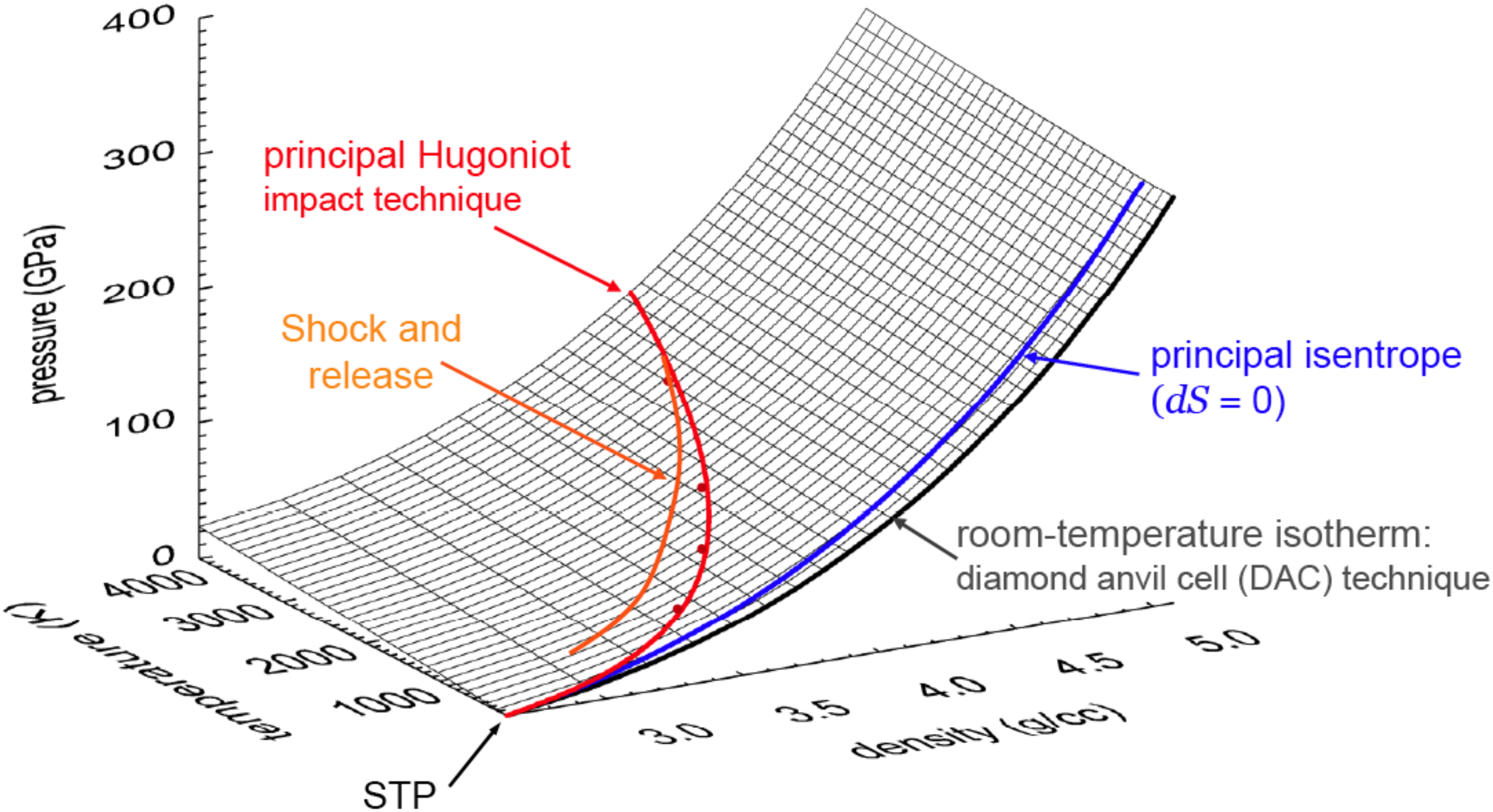


Fig. 1. Strain rate dependence of fracture stress.

Grady & Lipkin, Geophys. Res. Lett., 7, 255 (1980).

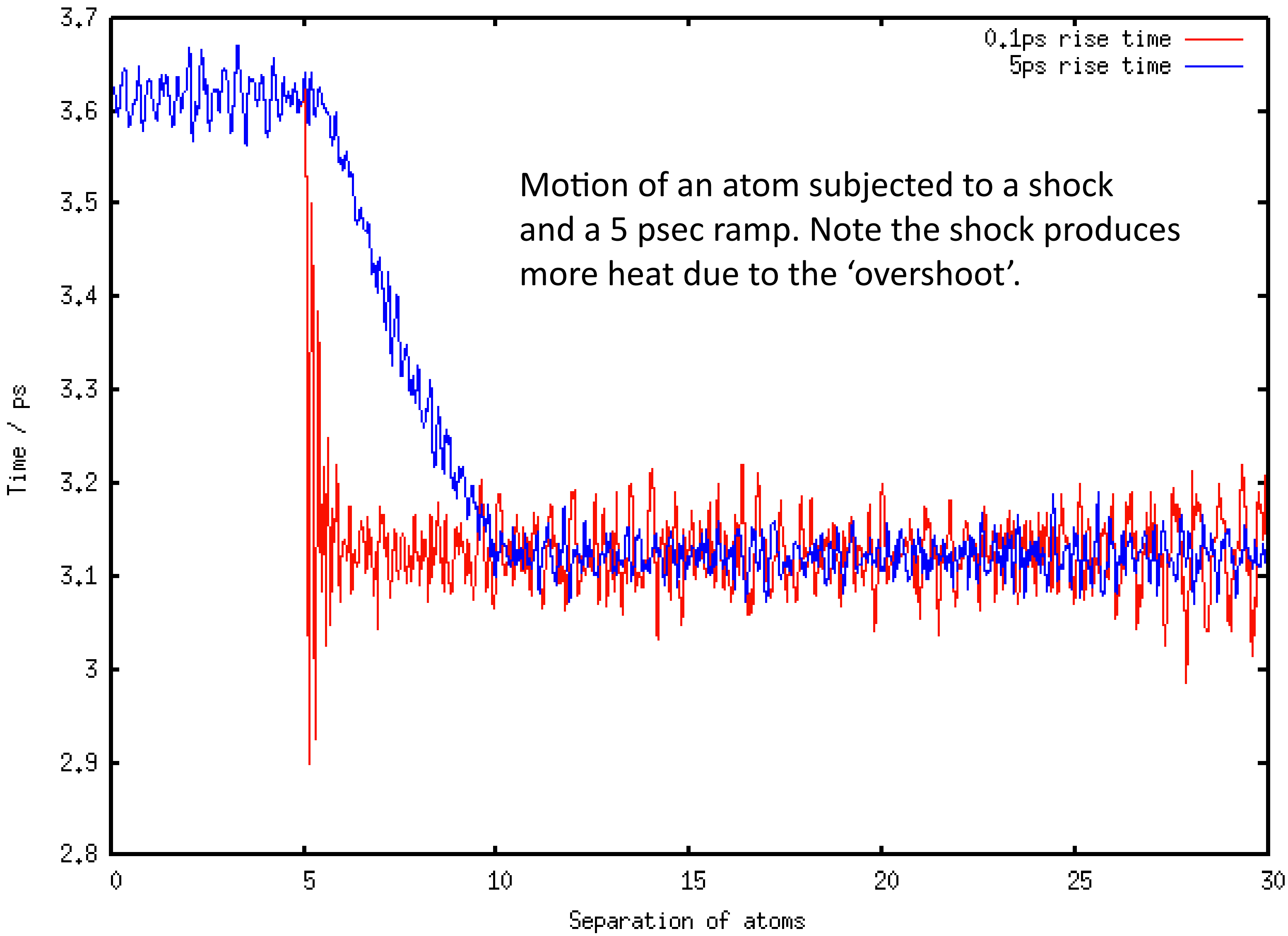


“Dynamic Behavior of Materials” Marc Meyers



principal Hugoniot
impact technique
Shock and
release
principal isentrope
(dS = 0)
room-temperature isotherm:
diamond anvil cell (DAC) technique
STP
pressure (GPa)
400
300
200
100
0
temperature (K)
4000
3000
2000
1000
density (g/cc)
3.0
3.5
4.0
4.5
5.0

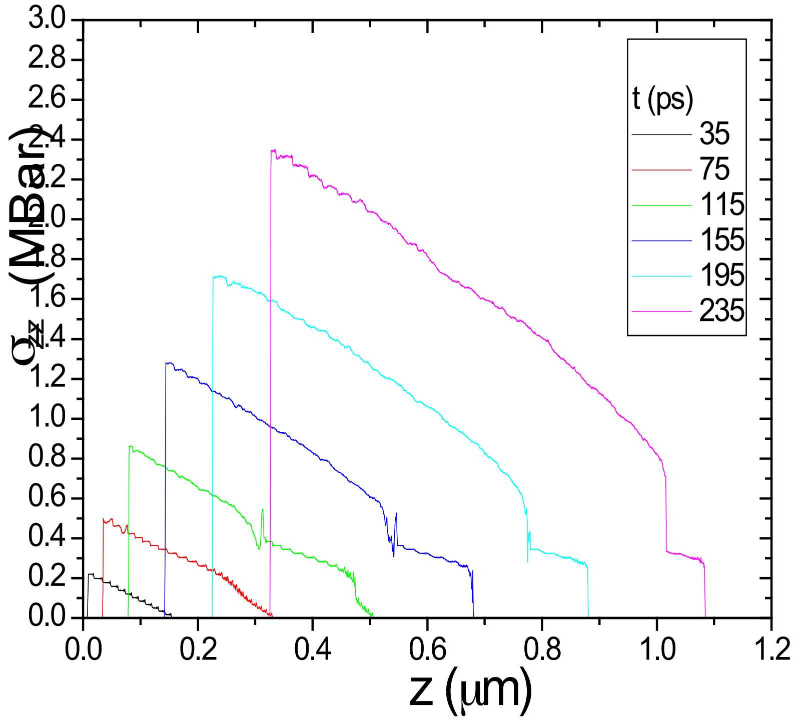
1-D Elastic Shock/Ramp

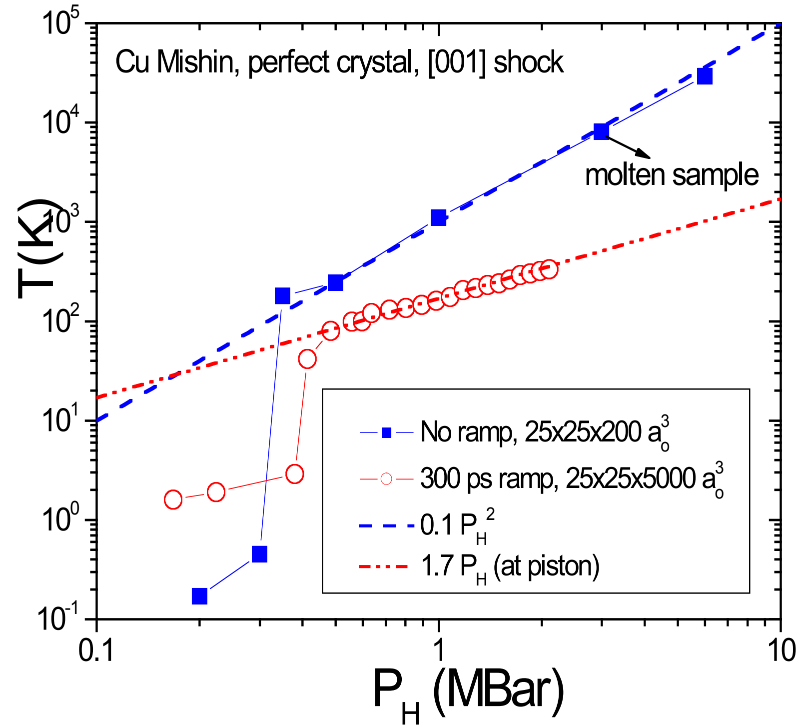


Motion of an atom subjected to a shock and a 5 psec ramp. Note the shock produces more heat due to the 'overshoot'.

MD simulations: ramp vs shock

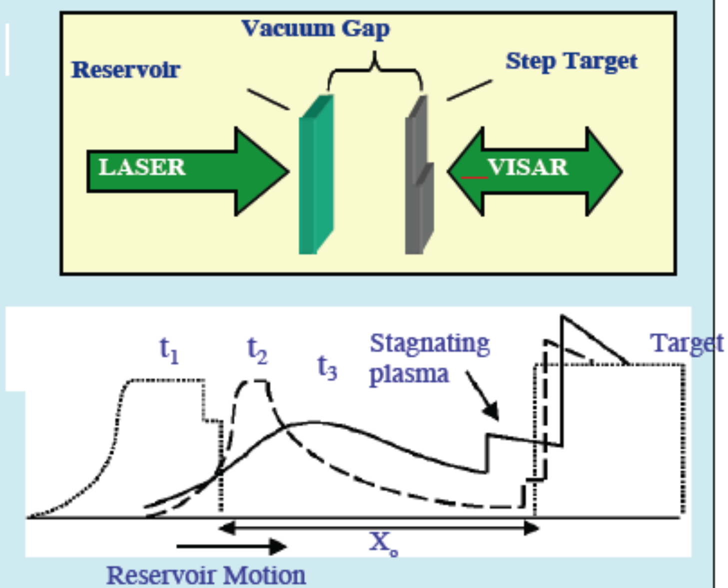
Cu Mishin [001], 25x25x5000 fcc cells (1.8 μm), 300 ps ramp, $U_{p\text{-}max}$=3.5 km/s ➔P~2.5 Mbar





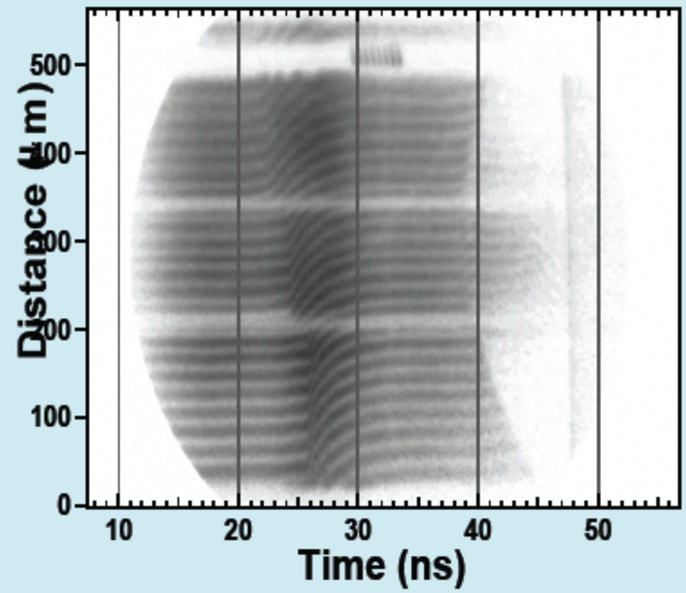
Laser produced isentrope is generated by a stagnating plasma and measured with line VISAR

Target design



•Design based on that of Edwards and Lorenz (PRL 04)

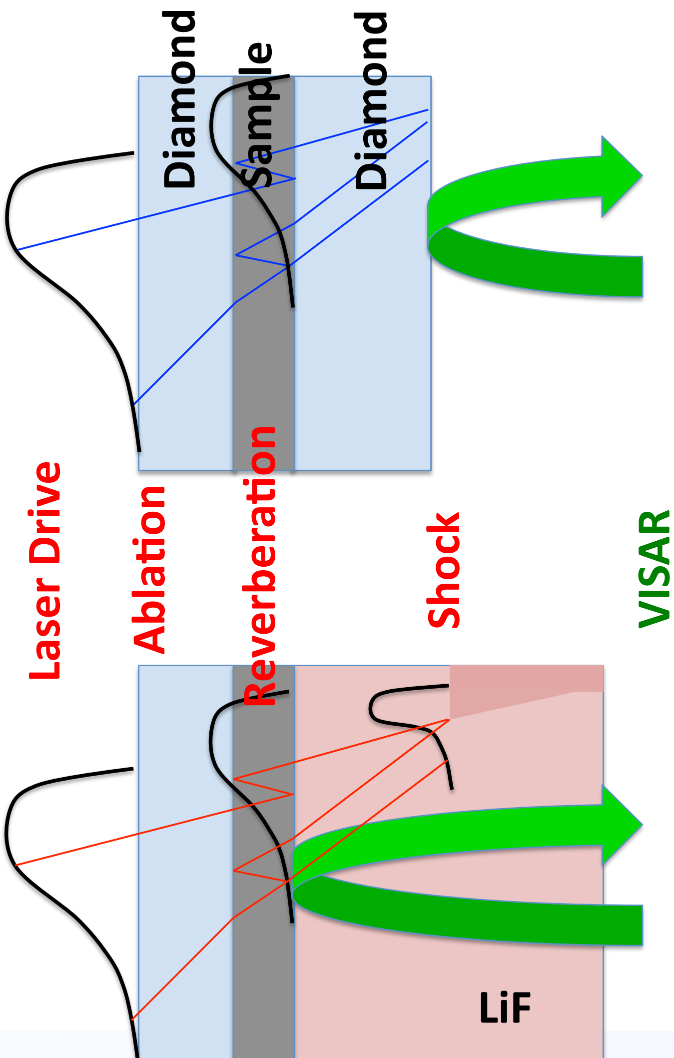
VISAR image



•Current direct drive design has ~ 800 μm planar region

Smith *et al.*, APS DPP, 2004

Sandwich Ramp-Compression



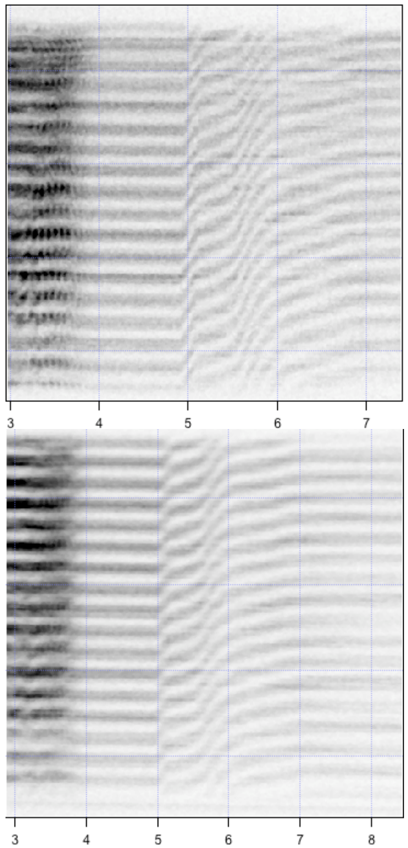
the LiF or Diamond interfacial pressure is the same as in sample

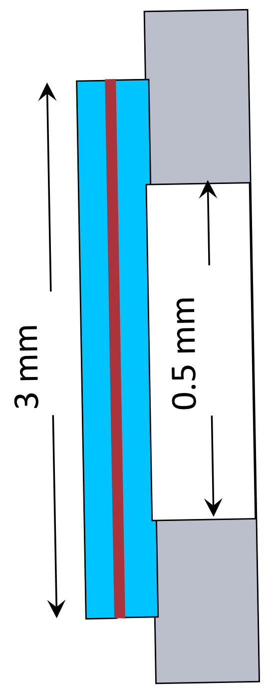
If we know the EOS of LiF or Diamond we can find the Pressure in the sample using the VISAR diagnostic

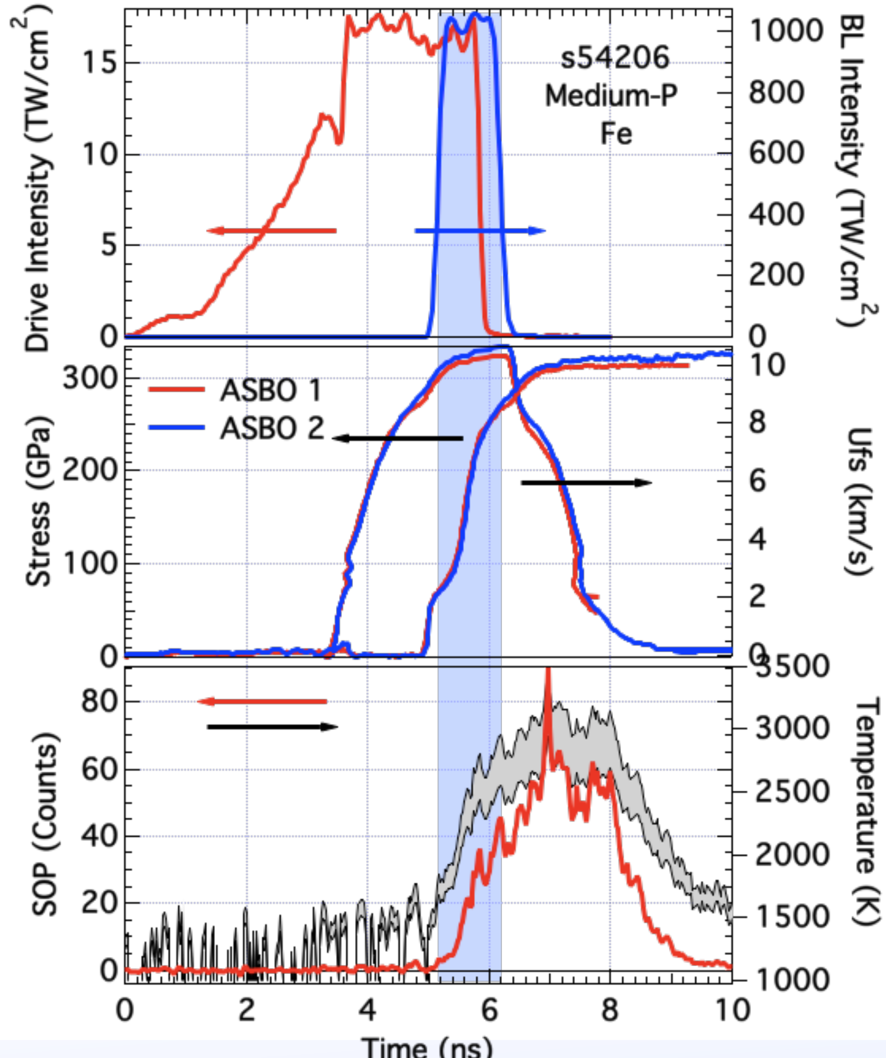
Using this target design, we believe we can ramp compress samples to ~30 Mbar, Hold the state for several ns, Determine the pressure, and Make a measurement.

XRD, XAFS, XANES, Reflectivity, ... Temperature remains the most important parameter that we do not know how to measure.

s54206, Fe X-ray Diffraction

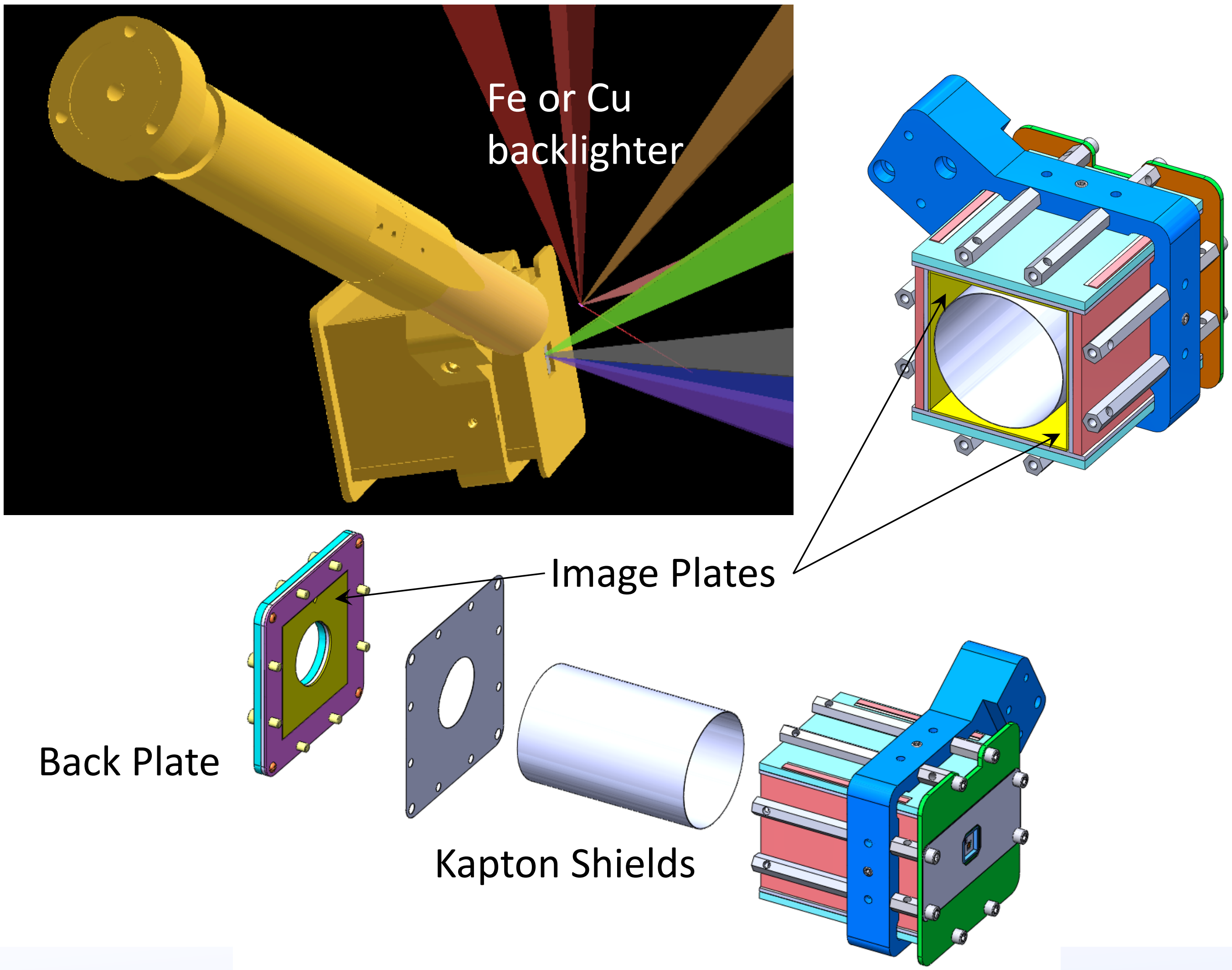






Strain rate is very high, ~10^8 s^{-1}.
Looks like temperature is low.
What does diffraction look like?

X-Ray Diffraction at Omega Laser



Future Work

- **Shock Physics:**
  - Understanding plasticity in body-centred-cubic materials (twinning).
  - Fundamentals of plasticity as a function of strain rate (shock pressure).
  - Phase transitions - What are the transition times?
- **High Pressure Isentropic Compression.**
  - N.B. - Completely new regime:
  - Can we produce and recover a new phase of Carbon?
  - New material properties as core electrons overlap?
  - Can we recreate and understand giant-planet and super-earth core conditions?
  - Various platforms (Janus/Omega/NIF) all have their role to play…