Overview – *STATIC COMPRESSION*

- **Diverse accessible problems spanning the physical, engineering, and biological sciences**
- **Advantages and importance of static compression methods**
  - ***Multiple 'simultaneous' diagnostics and 'complete' characterization***
  - ***Accuracy and precision***
- **Addressing the 'DOE Grand Challenges'**
  - ***'observation to control'***
- **Strong synergy with dynamic compression and theory**

Scientific Discovery Challenges

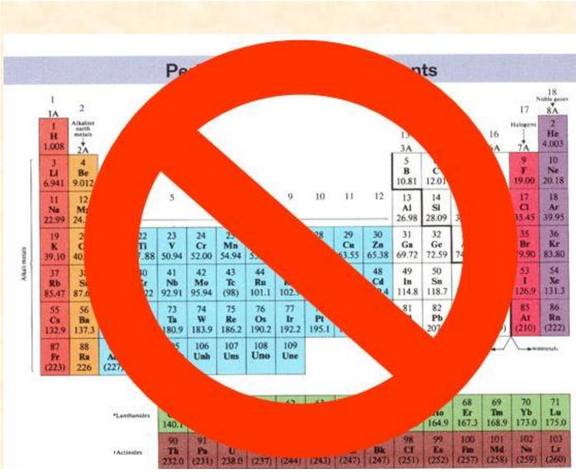
1. Structure and bonding at high compression
2. New physics in cold dense matter
3. Fundamental thermodynamics
4. Time-dependent transformations
5. High-pressure strength, plasticity, rheology
6. Optimized new materials
7. Synthetic chemistry frontier
8. Radiation-induced high-pressure chemistry
9. Earth science, planetary science and astrophysics
10. Life in extreme environments

Technical Grand Challenges

1. Reaching 1 TPa and beyond
2. Developing multiprobe ‘intelligent’ devices
3. Stress-strain states and P-T calibration
4. Advancing x-ray methods
5. Real time x-ray imaging with nm resolution
6. Neutron scattering to >100 GPa
7. Filling the strain rate gap: static to shock
8. Transport/constituitive properties
9. Challenge of liquids and amorphous materials
10. Thermochemical, magnetic measurements (e.g., to 100 GPa)

Scientific Discovery Challenge:
1. Structure and bonding at high compression

Premise: We have limited understanding of structure and bonding in condensed matter at high compressions.



Challenges:
1) Measurements with an accuracy and resolution equal ambient conditions (diffraction, scattering, spectroscopy,
2) Reaching higher pressures with larger sample volumes
3) Developing a predictive theory

Expected Result: A new paradigm for understanding condensed matter – the extension of the periodic table across the full range of pressure and temperature. Extending chemistry from valence to core electrons (e.g., 'kilovolt' chemistry).

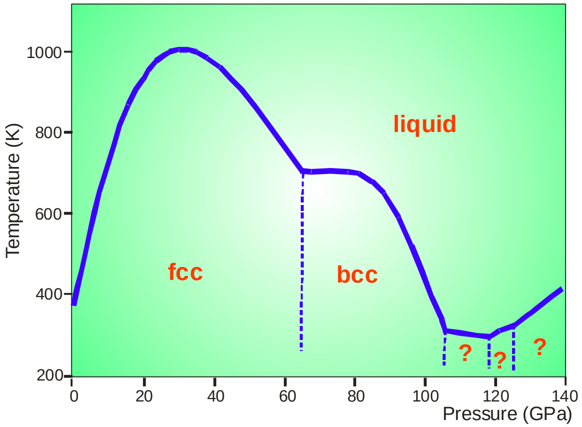
Possible other applications/fields: Materials science, planetary science, astrophysics.

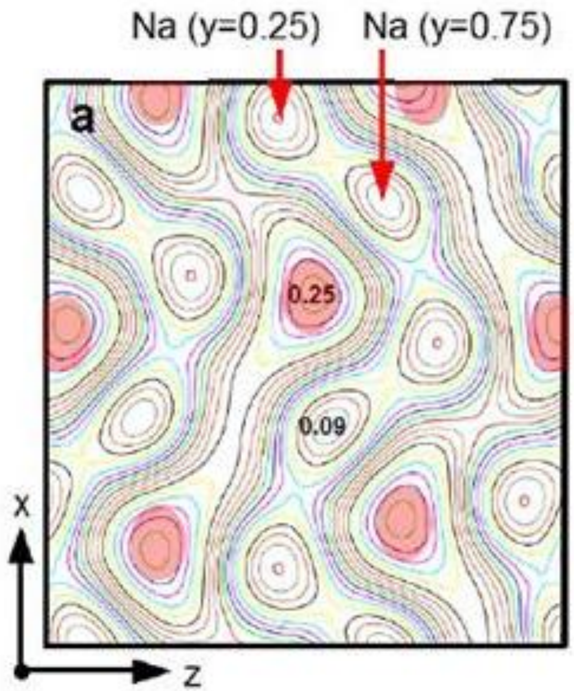
Scientific Discovery Challenge:
1. Structure and bonding at high compression

Present Status:

Sodium

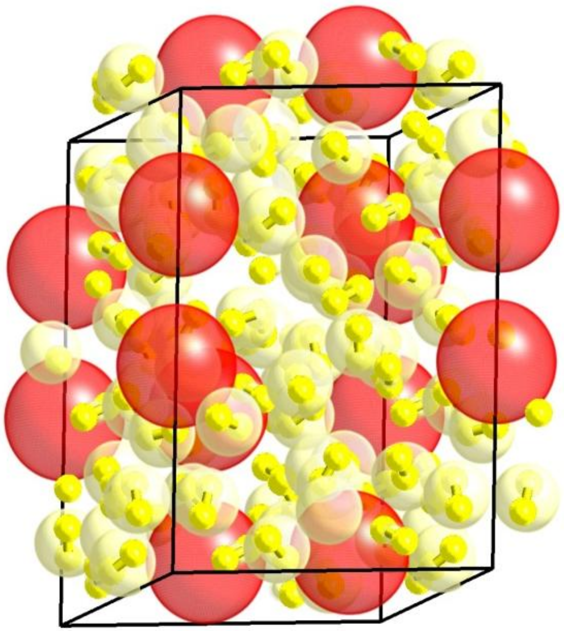
- **Unexpected polymorphism (11 phases)**
- **Anomalous melting**
- **Metal to insulator transition at 200 GPa**





[Gregoryanz et al., *PNAS* (2009); see also, Ma et al., *Nature* (2009)]

$Xe(H_2)_8$



[Somayazulu et al., *Nature Chem.* (2009)]

Future Prospects:
Understanding the origin of this behavior?
What happens from 300 GPa to 1 TPa and beyond?

2. New physics of cold dense matter

Premise: Theory suggests the existence of altogether new physics in simple materials at very high pressures (e.g., 0.5-1 TPa) and low temperatures. There are no experimental data in this regime.

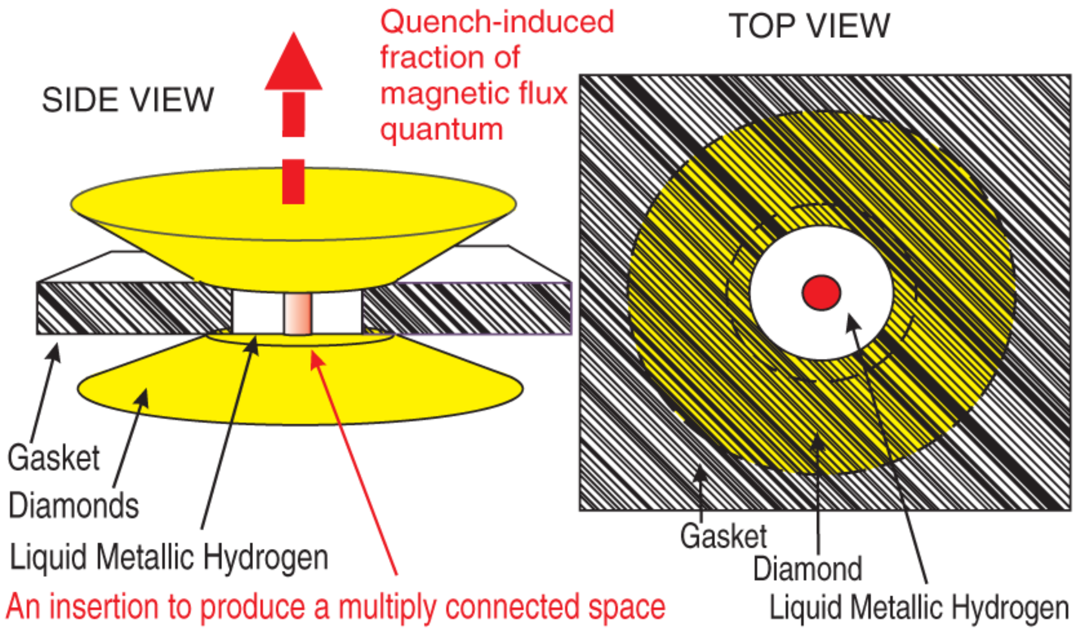
Challenges: 1) Reaching higher pressures and variable temperatures.
2) Combining with other extreme conditions (magnetic fields)
3) New diagnostics (e.g., imaging)

Expected Result: Deeper understanding of the nature of matter. New physics that will drive new theory. Mechanisms of magnetic and electronic order (e.g., superconductivity).

Possible other applications/fields: Energy, planetary science, astrophysics

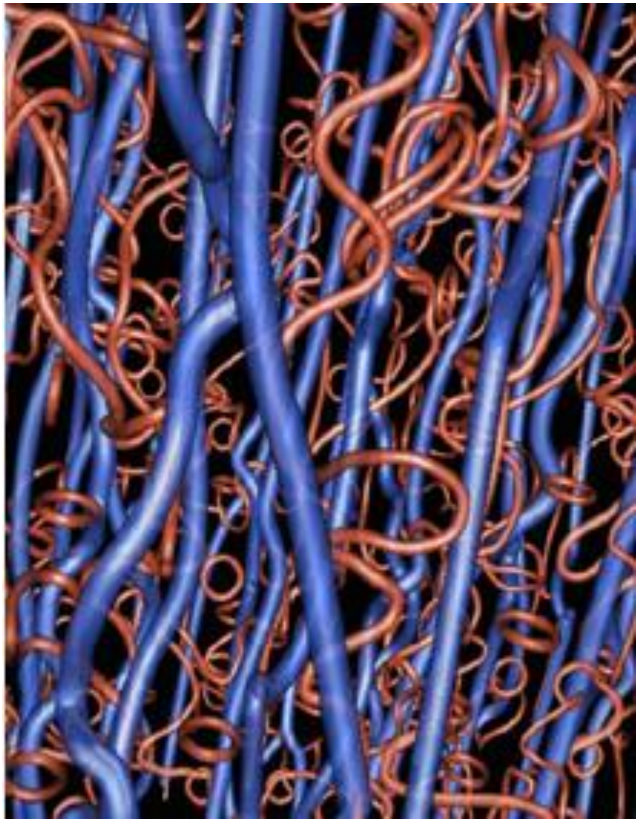
Scientific Discovery Challenge:
2. New physics of cold dense matter

Predicted metallic superfluid in ultradense hydrogen



[Babaev *et al., Phys. Rev. Lett.* (2008)]

- ***Combined P-T-H?***
- ***Can we create and image these structures?***



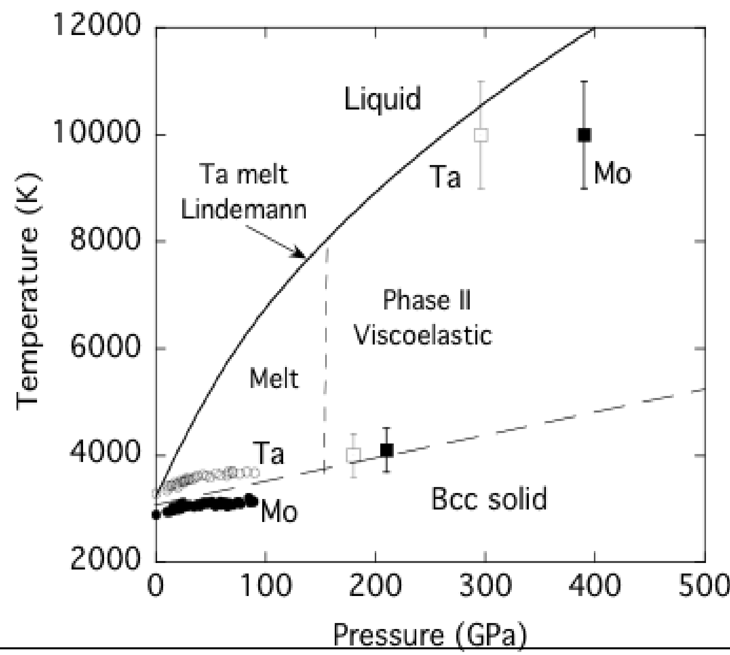
3. Fundamental thermodynamic properties

Premise: We have limited understanding of the basic phase diagrams of many systems. In some cases extremely large discrepancies in melting temperatures exist between static and shock compression. Is this evidence for new phenomena?

Challenges: 1) Bridging gap between static and dynamic experiments
2) Solving questions of mechanism, dynamics, structure
3) understanding general phase behavior at very high P-T (simple or complicated?)

Expected Result:
Accurate *P-V-T*-structure results at multimegabar pressures and at least 5000 K

Possible other applications/fields:
Planetary science, astrophysics.



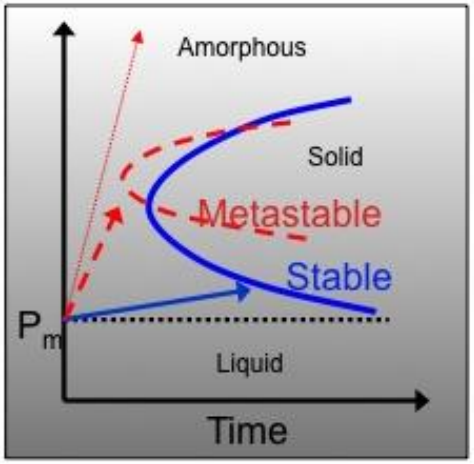
Scientific Discovery Challenge:
4. Time-dependent transformations

Premise: Equilibrium phase diagrams do not adequately describe the material behavior in dynamic processes. The compression-rate dependence of phase nucleation /growth /melt/microstructure are profoundly important to understanding/modeling dynamic events.

Approach: A broad range of time-resolved diagnostic probes (x-ray, neutron, laser) will selectively interrogate materials during pressure-induced transitions. We will make time-resolved measurements while retaining the high-fidelity character of static techniques.

Challenges:

Pressure-drives with broad range and precise control/tunability
Time-resolved probes with short duration (<ns) & adequate fluence
High-fidelity & high-speed detection systems
3D Time-resolved tomography of phase transformations.



Expected Result:

Deliver rate-dependent kinetic phase diagrams
Establish experimental basis for implementing predictive capability

Possible other applications/fields:

Identification of novel metastable materials with technological applications
geoscience (impacts)

Scientific Discovery Challenge:
5. High-pressure strength, plasticity, rheology

Premise: Material response at elevated pressure is a function of phase content, microstructure, defects, impurities, etc., as well as pressure and loading rate.

Approach: X-ray diffraction and nanoimaging in unique pressure devices with the ability to apply controlled and characterized uniaxial or shear strain in a well characterized environments.

Challenges:

- Quantify the complete stress state in materials exposed to high pressure.
- Quantify deformation mechanisms and flow stress as a function of:
  - strain rate at constant pressure
  - quantify the stress continuity across grain boundaries.

Expected Result:

Determination of stress tensor across a material microstructure as a function of hydrostatic and deviatoric stresses.

Possible other applications/fields:

Geoscience, astrophysics and planetary physics, input to theory, modeling, and simulation.

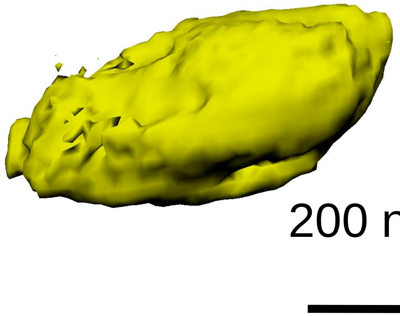
5. High-pressure strength, plasticity, rheology

Present status:
Most high pressure strength measurements rely on assumptions and do not take advantage of new developments (e.g., magic angle analysis, peak broadening).

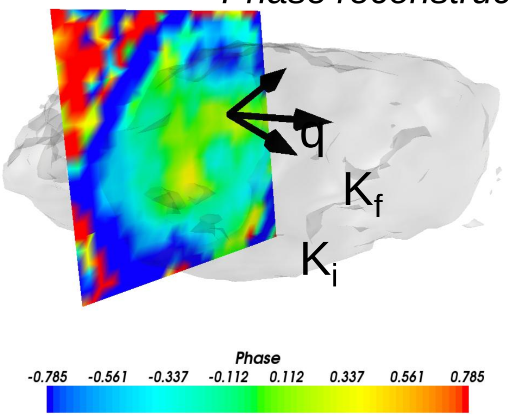
Future prospects:
- Advances in anvil cell design to permit pre-defined and controlled loading paths.
- Direct nanoimaging of the stress state with nanometer resolution at nanosecond time scales.
- 3D tomographic mapping of strain of grains in composite materials.
- Full definition of the stress state as a function of material, pressure, and loading rate.

3D reconstruction of coherent diffraction from a single crystal of Au at 6 GPa

Magnitude reconstruction



Phase reconstruction



Yang et al, to be published

6. Optimized new materials

Premise: High compression has the possibility of creating new, quenchable materials with enhanced properties and functionality.

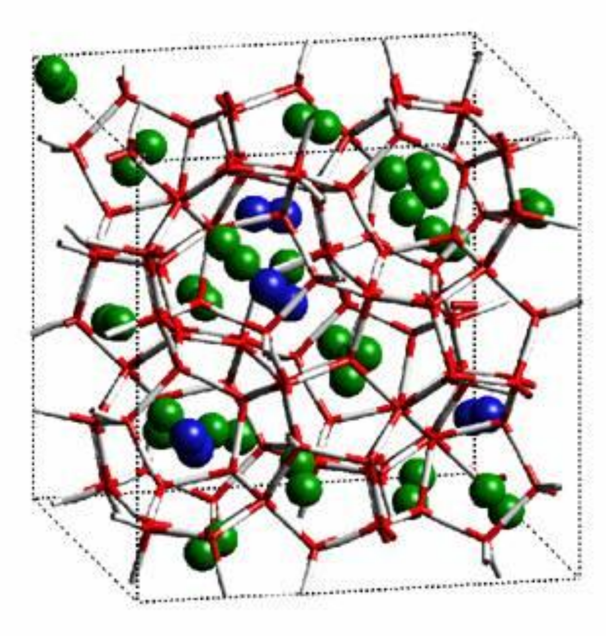
Challenges:
1) Using altered bonded stated to create new, useful materials
2) Recovering stabilized materials to ambient conditions.
3) Developing theory to predict material properties, suitable catalysts and recovery pathways

Expected Result: New materials with enhanced superconducting, magnetic, thermoelectric, hydrogen storage, solar and physical properties

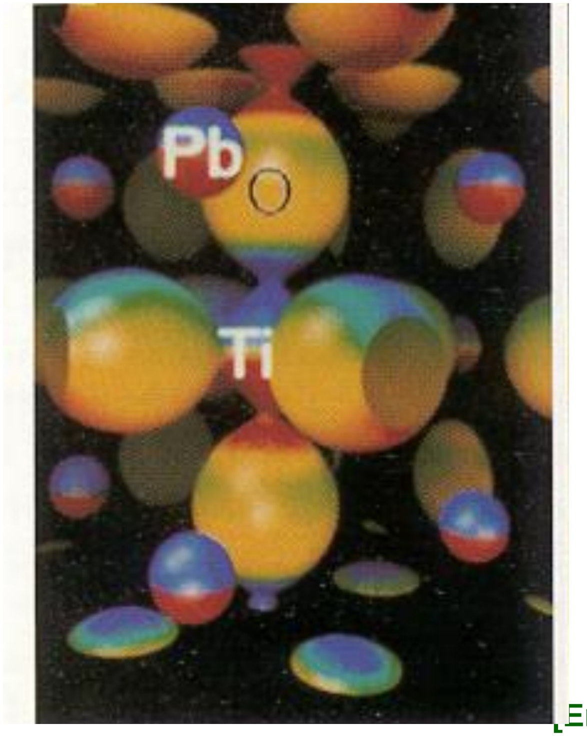
Possible other applications/fields: Materials science, energy science

Scientific Discovery Challenge:
6. Optimized new materials

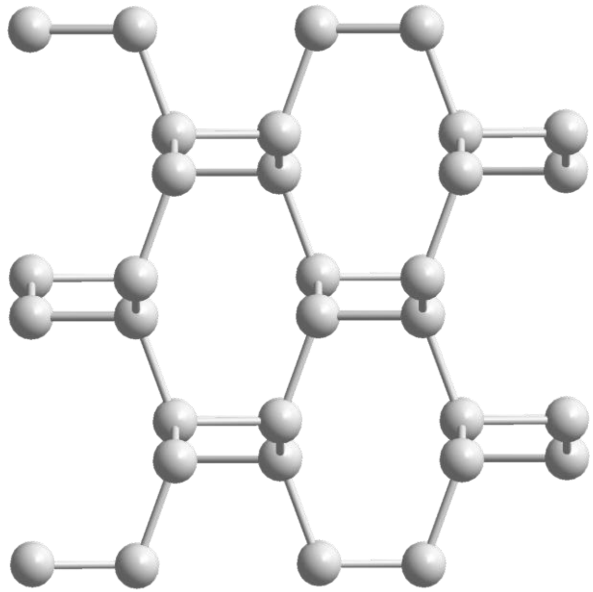
Present Status:



[W. Mao *et al. Science* (2002); Lokshin *et al. Phys. Rev. Lett*. (2004)]



[Wu and Cohen, *Phys. Rev. Lett*. (2005)]



[Eremets *et al.* , *Nature Mat.* (2004); *J. Chem. Phys*. (2005)]

Future Prospects:

Improved hydrogen storage and solar cell materials
Ultrahard materials with superior properties to diamond

Future prospects:

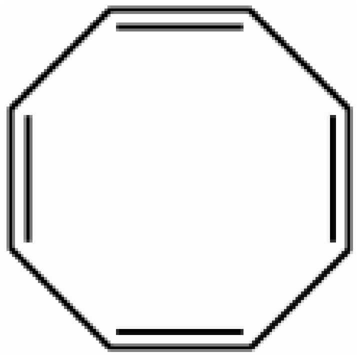
7. Synthetic chemistry frontier

Premise: Pressure can be utilized as a novel reactive variable in chemical synthesis.

Approach: Time resolved probes following compression event, x-ray diffraction and spectroscopies, recover samples and analysis (in situ and ex situ), dynamics/kinetics measurement

Challenges:

- Prediction of bond manipulation to synthesize desired product with a given functionality.
- Interrogation of intra- and inter- molecular bond character via x-ray and optical spectroscopies
- Development of feasible recovery schemes
- Elucidating and exploiting thermodynamic path dependencies



Novel material synthesized from COT at high pressure

Expected Result:

- Predict and control chemical reaction of novel materials
- Better understand the deeper intra- and inter- molecular interactions of electrons within the lattice under extreme conditions.

Possible other applications/fields: Drugs, defense science (novel energetic materials), structural components, polymer, electronic materials,energy storage

8. Radiation-induced high-pressure chemistry

Premise: Ionizing radiation (x-rays, visible light, neutrons, protons) can be utilized as a novel source of electronic rearrangement in chemical synthesis as well as a unwelcome mechanism of damage which must be quantified and calibrated.

Approach: Time resolved probes following compression, x-ray diffraction and spectroscopies, recover samples and analysis (in situ and ex situ), dynamics/kinetics measurement.

Challenges:

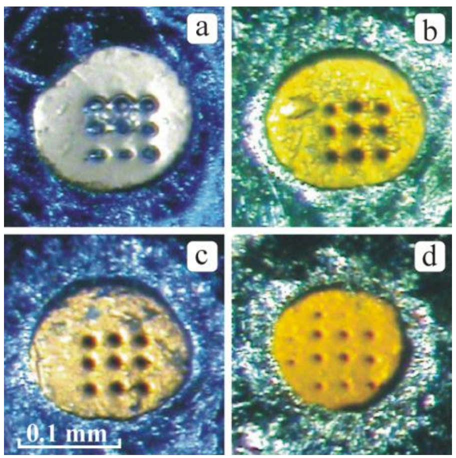
- Prediction of bond ionization to synthesize desired product with a given functionality.
- Interrogation of intra- and inter- molecular bond breaking via x-ray and optical spectroscopies.
- Development of feasible recovery schemes.
- Elucidating and exploiting thermodynamic path dependencies.
- Determining frequency and flux dependence of damage and/or synthesis.

8. Radiation-induced high-pressure chemistry

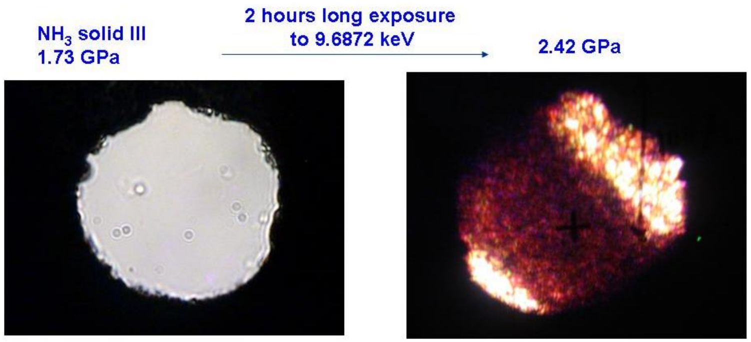
Expected Result:
Predict and control chemical reaction of novel materials, calibrate damage for more accurate x-ray studies.

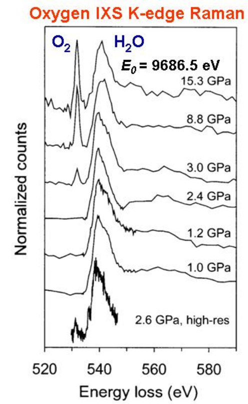
Possible other applications/fields: Drugs, defense science (novel energetic materials), structural components, polymer, electronic materials,energy storage

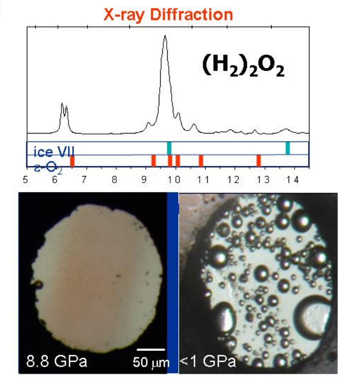
Present Status:



PETN damage spots at different pressures

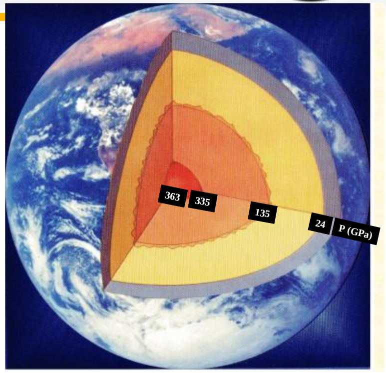






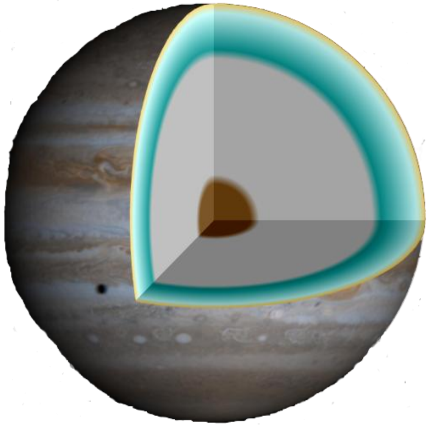
9. Earth science, planetary science, and astrophysics

The universe from Earth to beyond our solar system



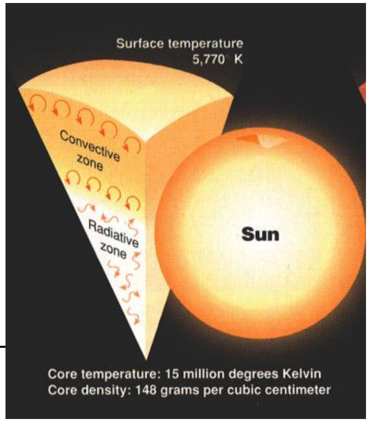
Premise: Advances in observational planetary science and astronomy have led to materials questions about bodies throughout the cosmos.

Challenges: Reaching higher pressures and temperatures and accurate determination of the physical and chemical properties of planetary materials.



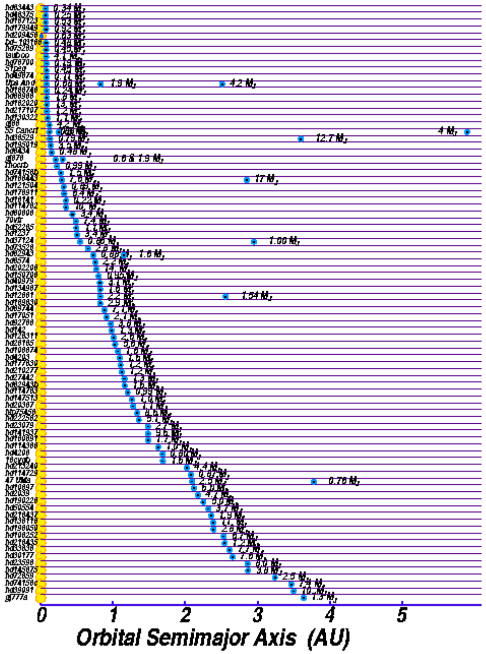
Expected Result: Determination of the structure, composition, dynamics, and evolution of the full range of planetary bodies and other astrophysical objects. An understanding of the evolution of solar systems. The possibility of life elsewhere in the universe.

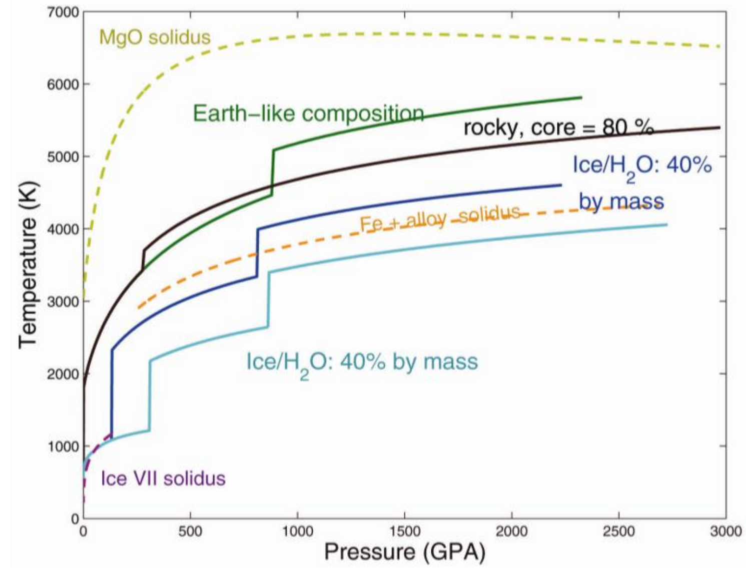
Possible other applications/fields: Fundamental physics, chemistry, materials science



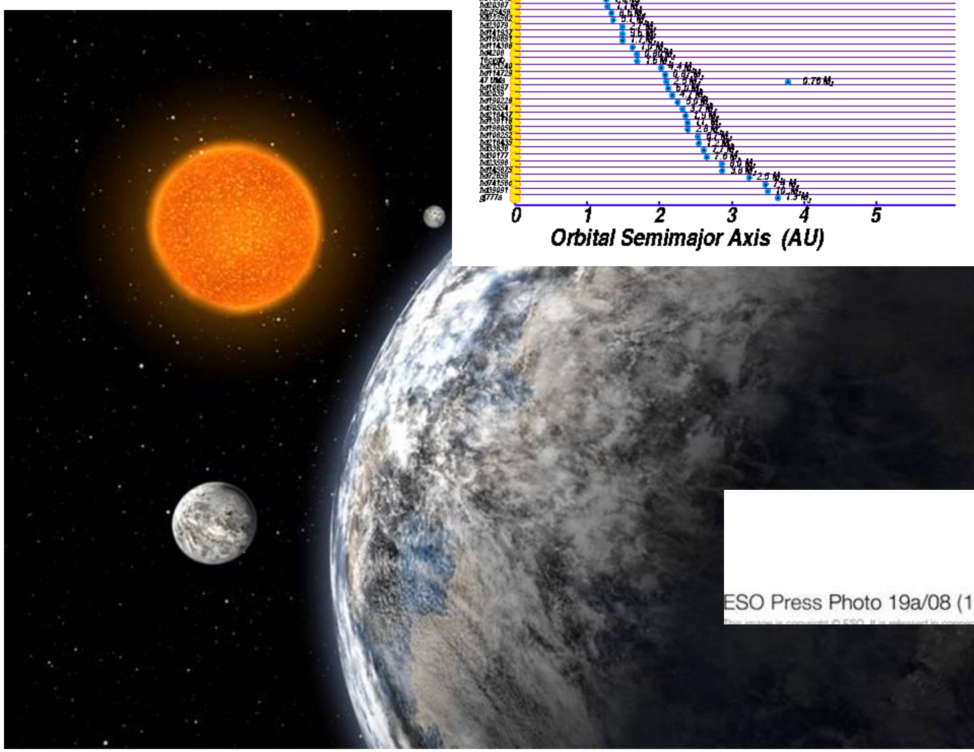
Present Status:

Extrasolar Planets





[Umemoto *et al.*, *Science* (2006)]
[Valencia *et al.*, *Icarus* (2006)]



A Trio of Super-Earths
(Artist's Impression)

ESO Press Photo 19a/08 (16 June 2008)

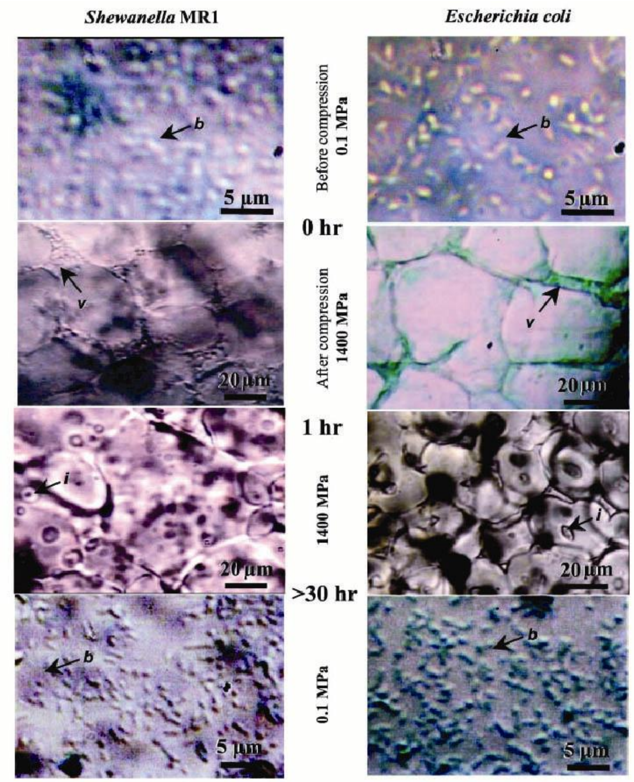
Scientific Discovery Challenge:
10. Life in extreme environments

Premise: We do not know the limits of life in extreme environments

Challenges: In situ measurements of structure-function of biological systems, from whole communities of organisms to component molecules

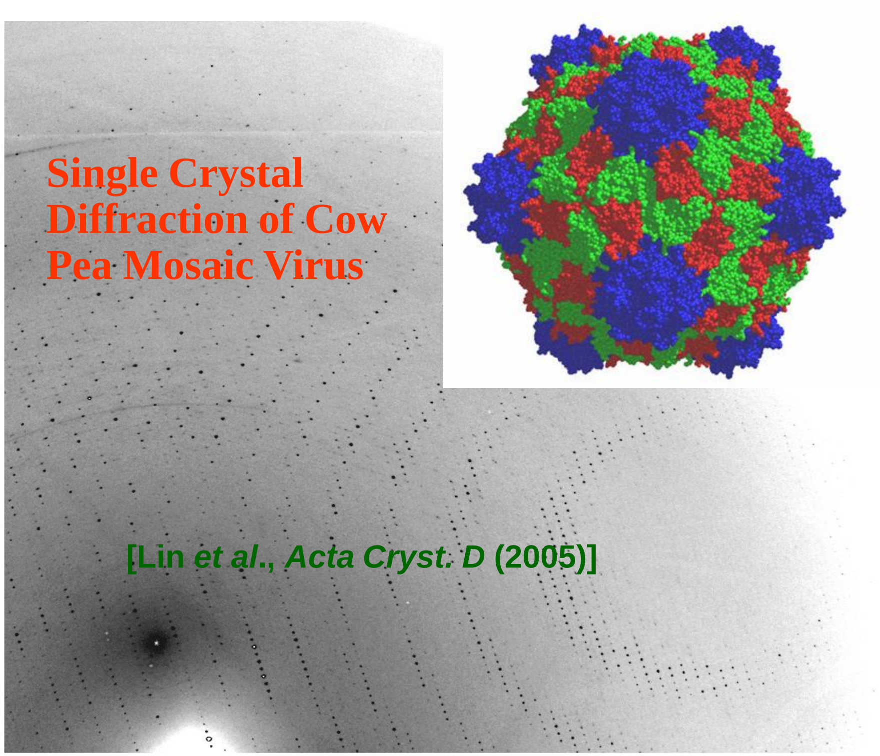
Expected Result: Defining the habitable zone in the cosmos, limits of life on Earth, possible origin of life, new methods for directed evolution, development of the new field of high-pressure genomics/proteomics

Possible other applications/fields: Biology, geology, planetary science.

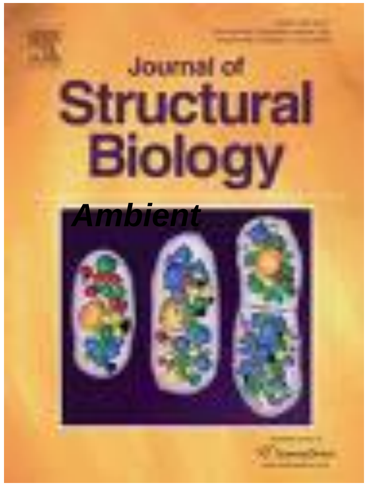


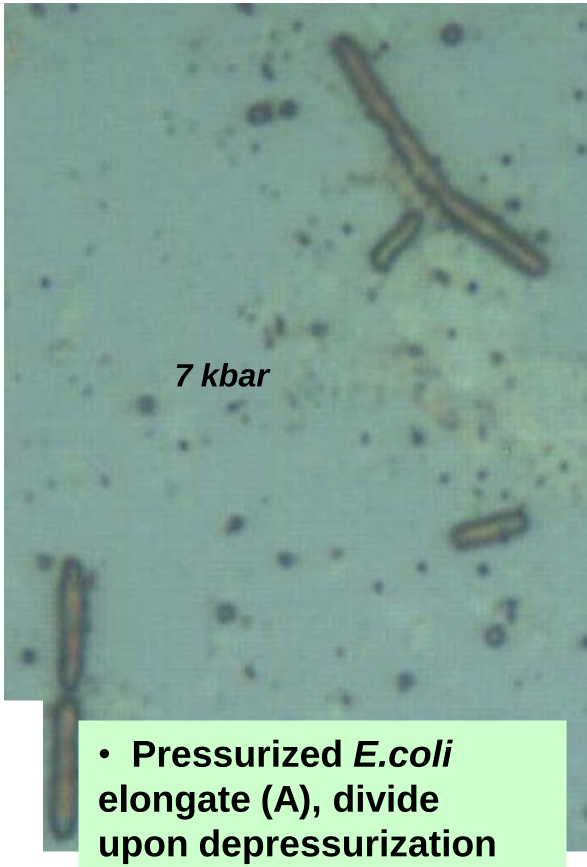
[Sharma *et al.*, *Science* (2002)]

Scientific Discovery Challenge:
10. Life in extreme environments



Future prospects:

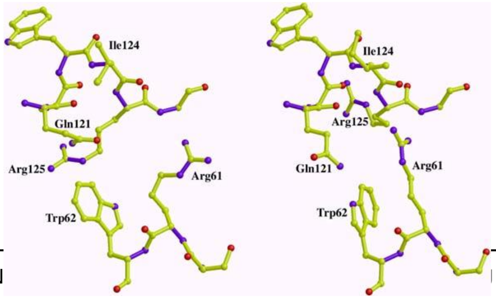




- **Pressurized *E.coli* elongate (A), divide upon depressurization (B) and finally return to normal size (C).**

3.5 kbar

Lysozyme



Time-resolved structures

- ***X-ray imaging of subcellular structure***

[Fourme *et al.* (2002)]

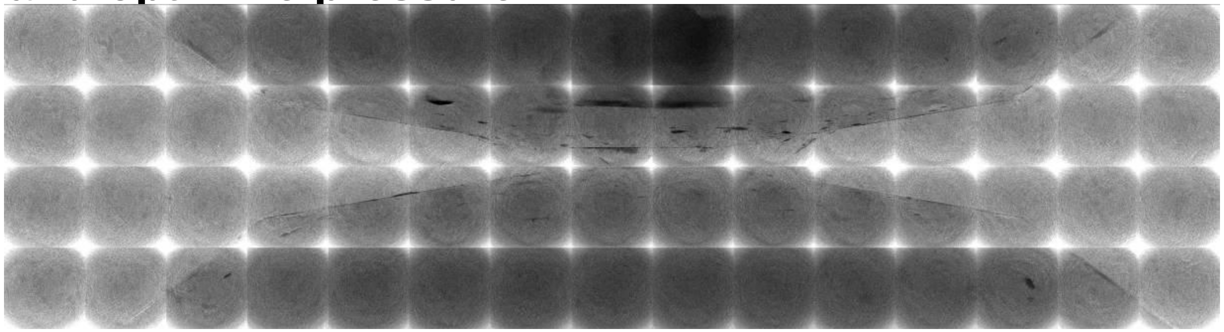
Technical Grand Challenges

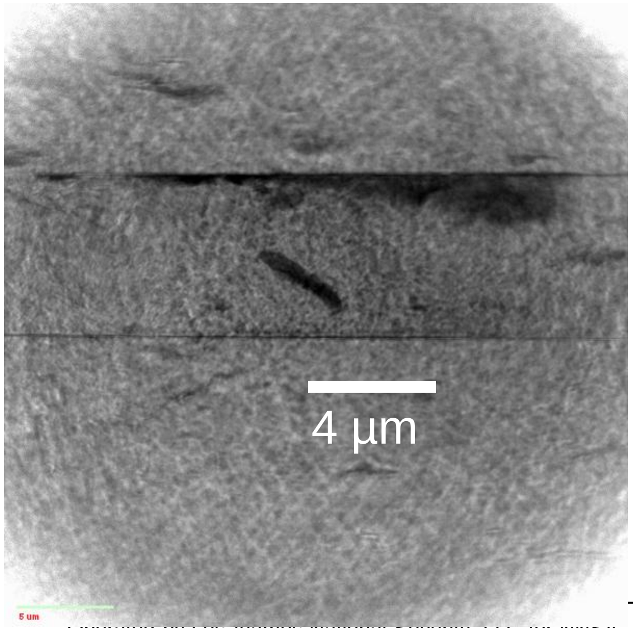
1. Reaching 1 TPa and beyond
2. Developing multiprobe ‘intelligent’ devices
3. Stress-strain states and P-T calibration
4. Advancing x-ray methods
5. Real time x-ray imaging with nm resolution
6. Neutron scattering to >100 GPa
7. Filling the strain-rate gap: static to shock
8. Transport/constituitive properties
9. Challenge of liquids and amorphous materials
10. Thermochemical & magnetic measurements (e.g., to 100 GPa)

Technique Grand Challenge:
Reaching terapascal pressures – Optimized designs

Present Status:

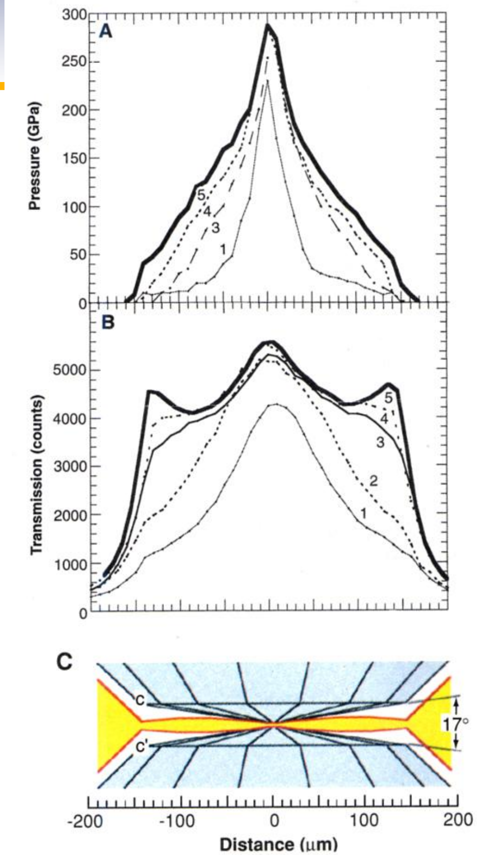
Using nanobeams to measure anvil nanostrains and optimize pressure





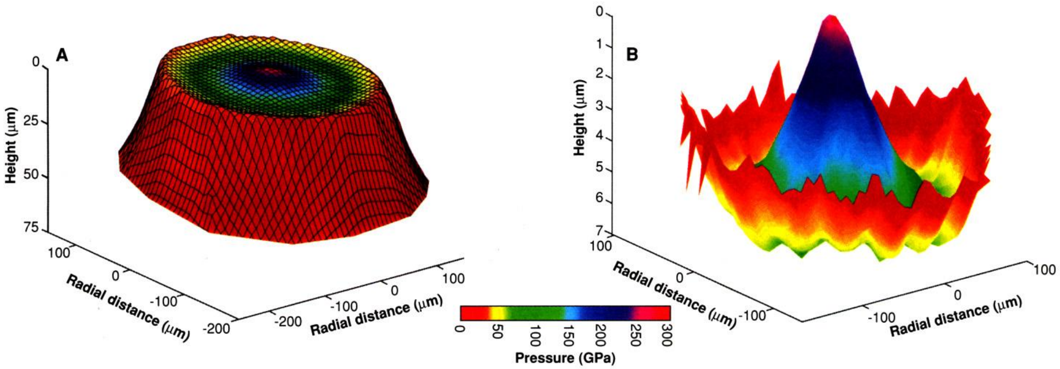
30 nm resolution

[W. Mao, et al. to be published]



[Hemley et al., *Science* (1997)]

5 µm resolution

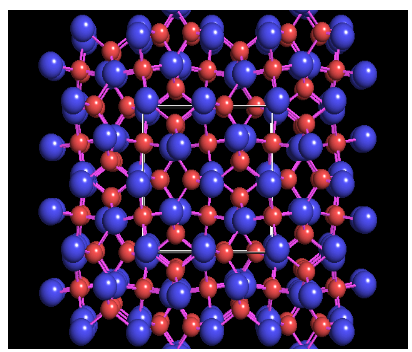


Xradia nanoscope with 30 nm resolution

Reaching terapascal pressures – New materials

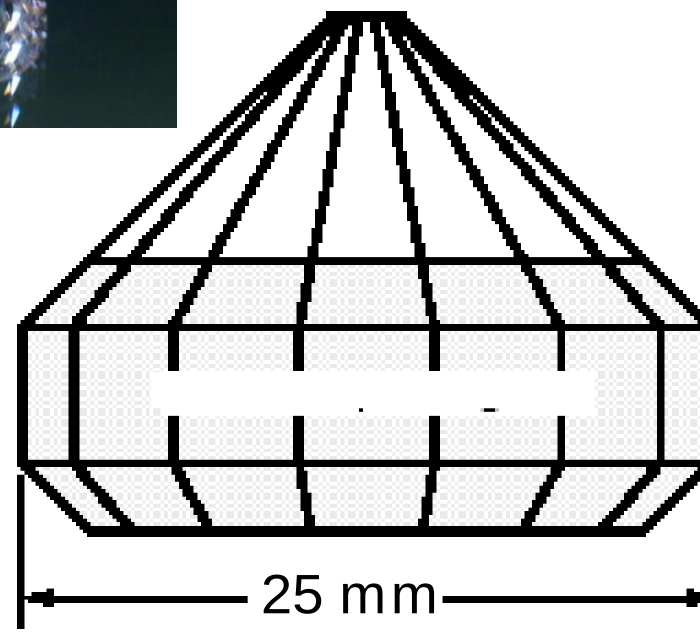
CVD diamond for high-pressure experimens

Future prospects:



C_3N_4 (theory)

[Teter & Hemley, *Science* (1996)]



100 ct

Technique Grand Challenge:
Intelligent anvils and multiple probes

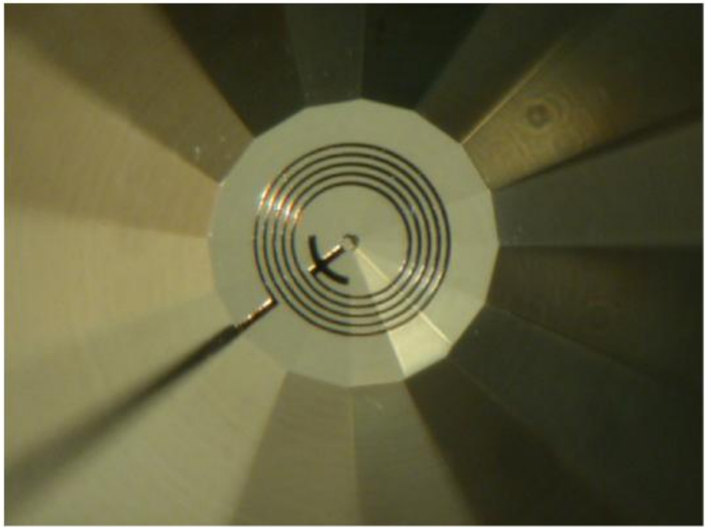
Premise: Dramatic improvements in high-pressure capabilities and extreme condition diagnostic capabilities will lead to important scientific advances

Approach: Novel high pressure apparatus design and materials (pcd) may extend pressures limits to >1TPa. Tailored anvils can measure new physical properties (electric transport, NMR,…). High-spatial resolution probes can make detailed mapping

Challenges:

Nano-scale manipulation and diagnostics

Sub-micron patterning and modification on anvils



Expected Result:

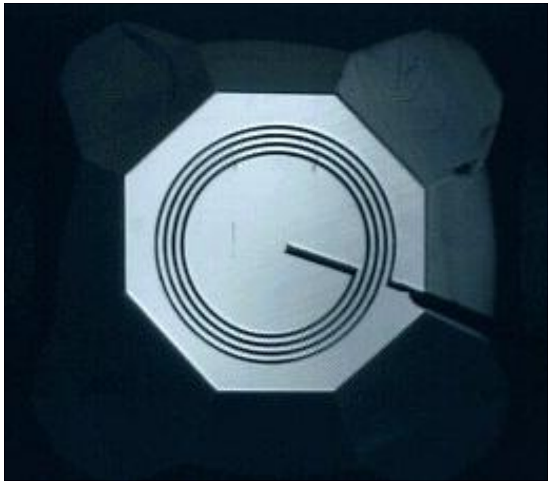
Dramatic extension of measurements possible for extreme environments

Possible other applications/fields:

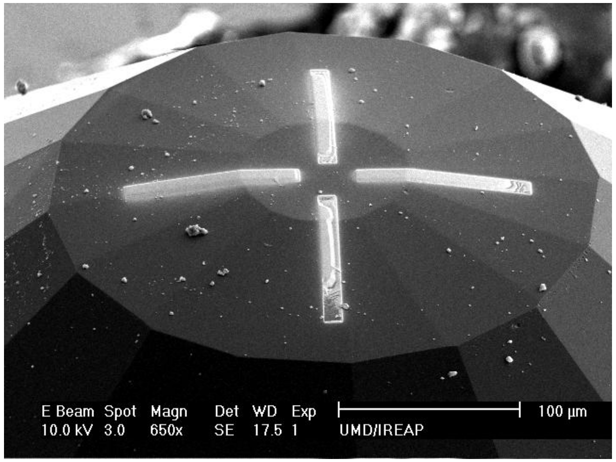
Sensor Technologies

Technique Grand Challenge:
Intelligent anvils and multiple probes

Smart diamond anvil devices

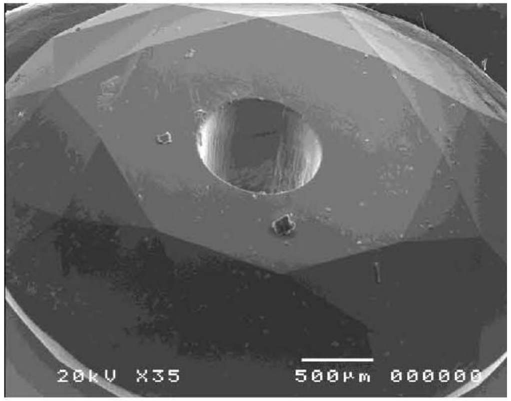


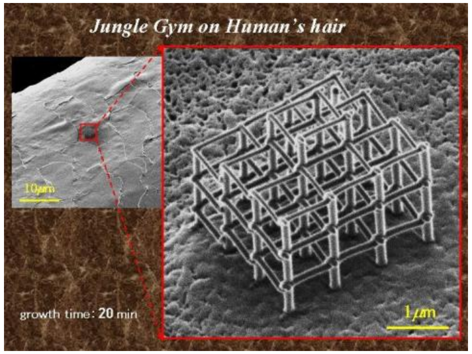
[Vohra and Weir (2002)]

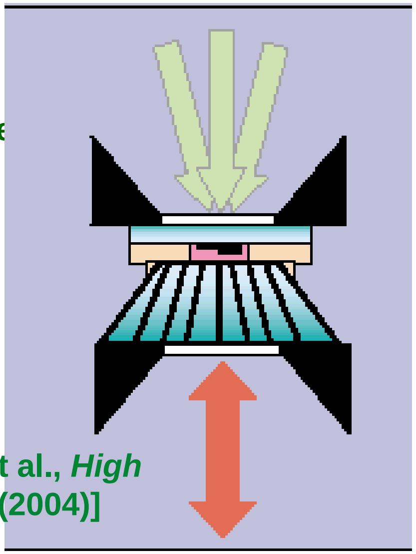


[Struzhkin, Cuk, Shen, Rotundu, Greene, to be published]

- **Combined static/ dynamic compression**
- **Ultrafast diagnostics**







[Loubeyre et al., *High Pres. Res.* (2004)]

Shinji MATSUI http://www.nanonet.go.jp/english/mailmag/2006/files/086a1.jpg

Technique Grand Challenge:
Bridging the strain-rate gap

Premise: Interesting and largely unexplored physics between the static and dynamic time scales at high pressure. Mode transitions as well as phase transformation kinetics are known to be strong functions of loading rate.

Approach: Develop high pressure cells with precisely controlled and calibrated loading rates capable of compression rates to 10e5, cycles at kHz, and single-shot rapid decompression. Develop detectors and probes systems consistent with experimental capabilities (sub-micron spatially, sub nano-second temporally)

Challenges:

Develop high-pressure cells capable of multi-Mbar pressures and are ultra-responsive to drive conditions

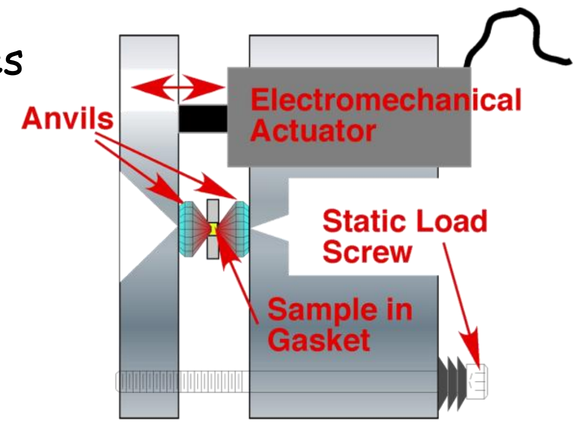
Elucidate the rate -dependent properties

Expected Result:

Cells capable of delivering controlled pressure drive and diagnostics

Possible other applications/fields:

New technological synthesis capability



Dynamic DAC

Advancing x-ray methods

Premise: Inelastic x-ray spectroscopies such as XRS, XAS, XES, EXAFS, NFS, and NRIXS will be harnessed to interrogate bonding changes and phonon density of states (DOS) determinations under extreme conditions.

Approach: (NRIXS, NFS) Via meV phonon modulation of Mossbauer nuclear energies, the phonon density of states can be determined. (XRS) Deep core-level electron bonding states are excited and explored via the x-ray Raman effect. (XAS, XES EXAFS) : Valence electronic states are probed by photo electron emission and absorption.

Challenges:

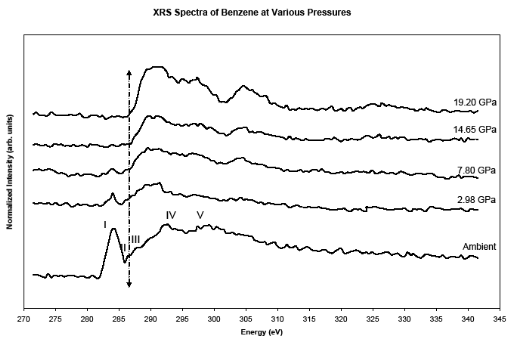
Long detection times required. Need to use Mossbauer-sensitive nuclei (NRIXS, NFS). Need to use Be gaskets to allow x-rays into and out of sample region. Sample decomposition with bombardment.

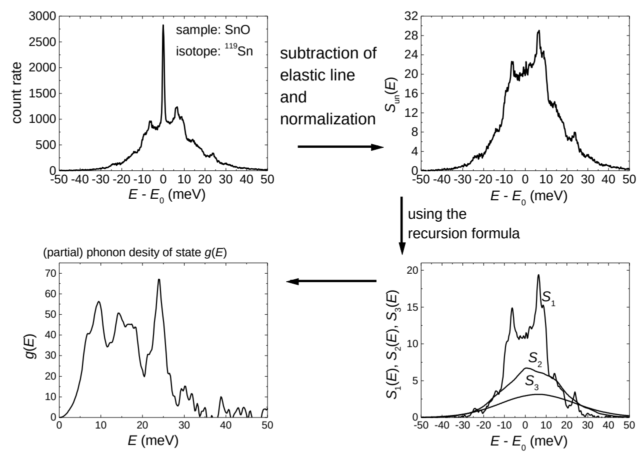
Expected Result:

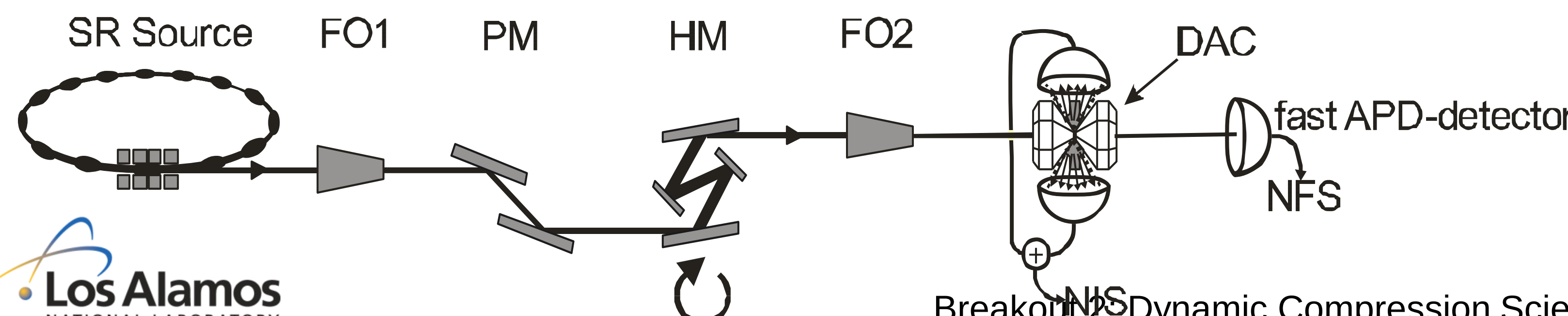
Obtain phonon DOS. Demonstration of bonding changes (e.g. hybridization alteration) under extreme conditions.

Present Status:

Possible other applications/fields: Lanthanides/actinide DOS, defense science (another method to interrogate energetic materials).



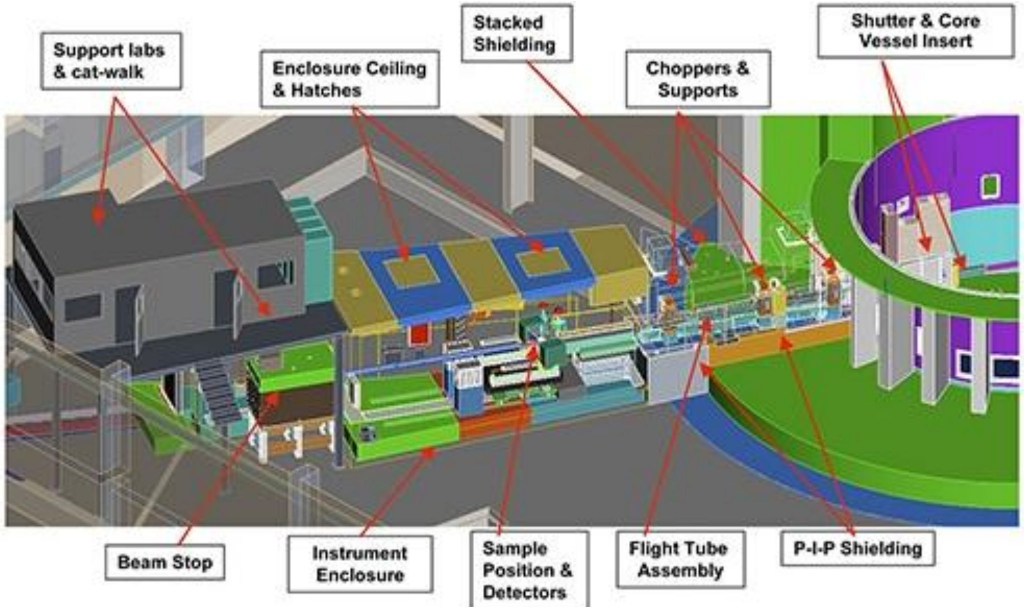




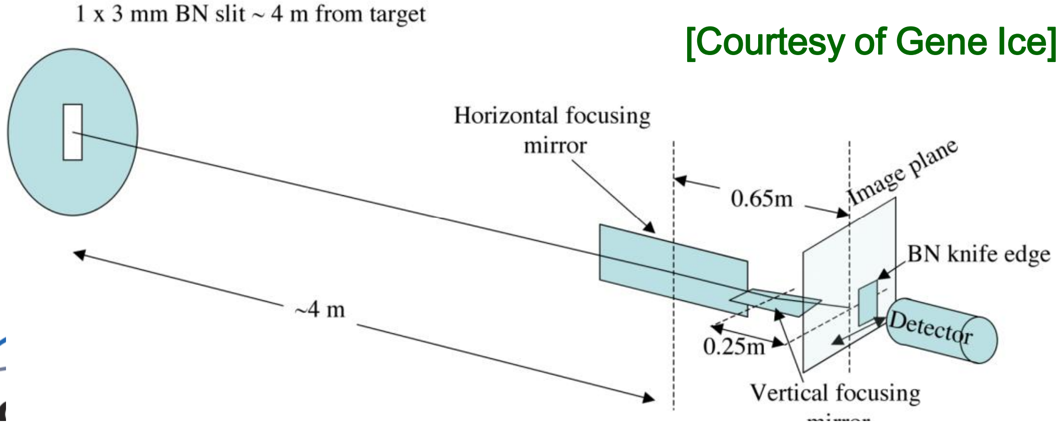
Breakout 2: Dynamic Compression Science

Technique Grand Challenge:
Neutron scattering at megabar pressures

Present Status:

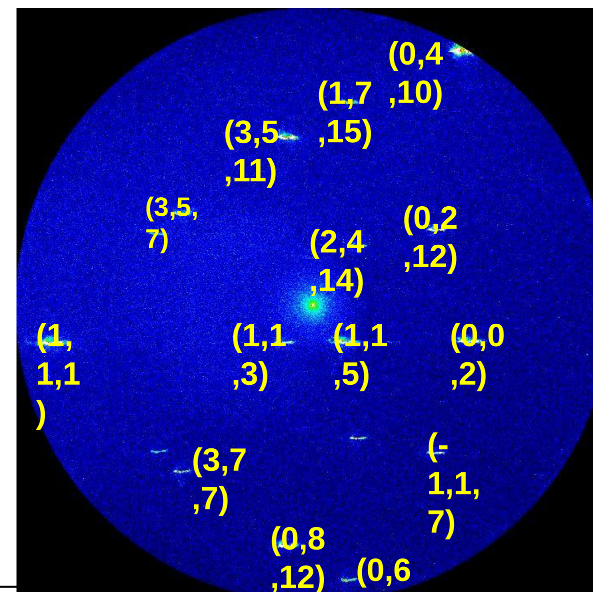


Fu



[Courtesy of Gene Ice]

Spallation Neutrons and Pressure (SNAP) beam line at the Spallation Neutron Source (SNS)



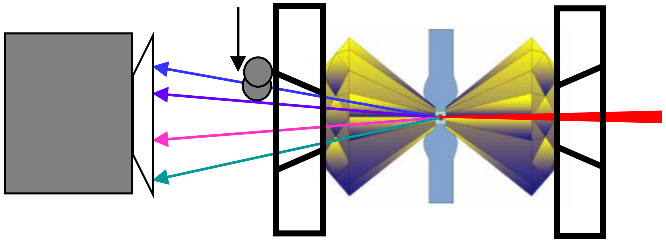
LAUE DIFFRACTION

- **100x gain with neutron K-B's**
- **Combine with 10x flux and >100x sample volume**

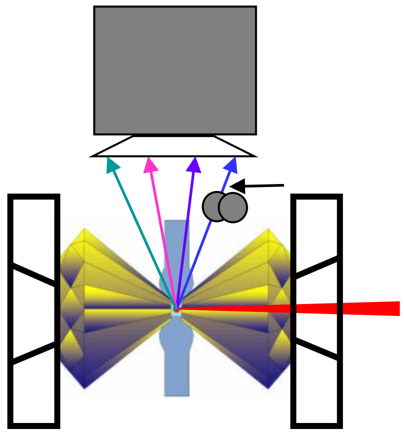
Technique Grand Challenge:
Nanoscale imaging of hetereogeneous materials

Present Status:

3d grain boundary mapping

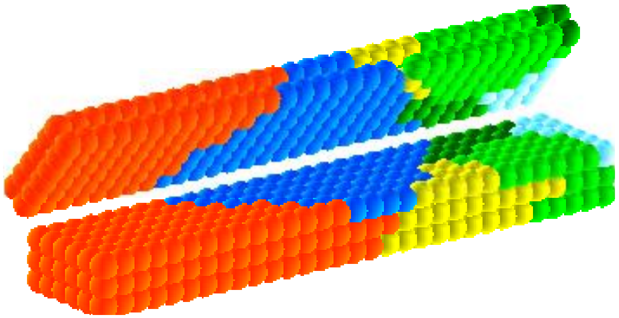


Forward x-ray diffraction with high energy x-ray beams



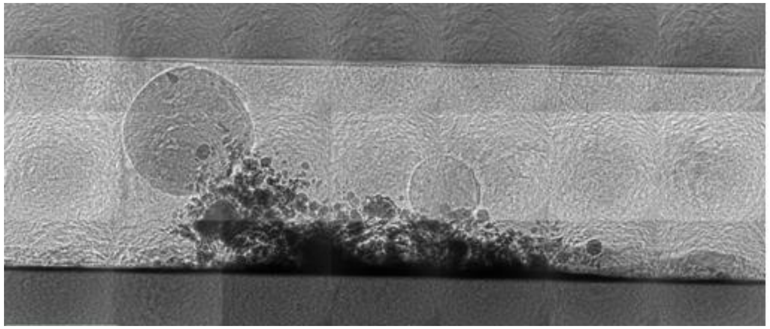
High resolution with medium energy x-ray beams

X1_Tomo_Movie_box_14um.mpg



Example of 3d grain boundary mapping at ambient condition

20 um

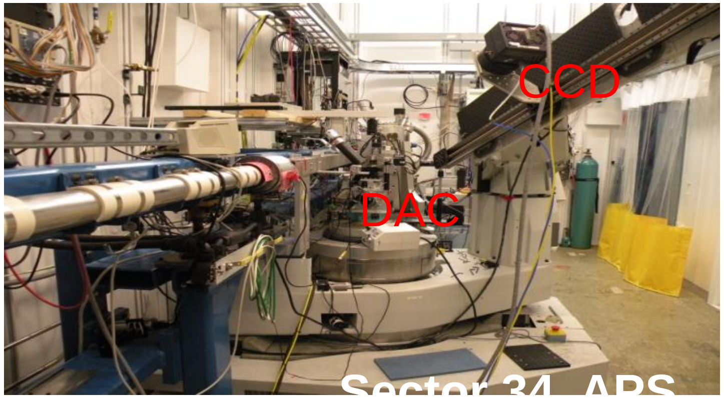


Nano-imaging (TXM)
- **30 nm in 3d**
- **Individual grains**
- **EoS of amorphous, liquid, crystals**
- **interaction under P**

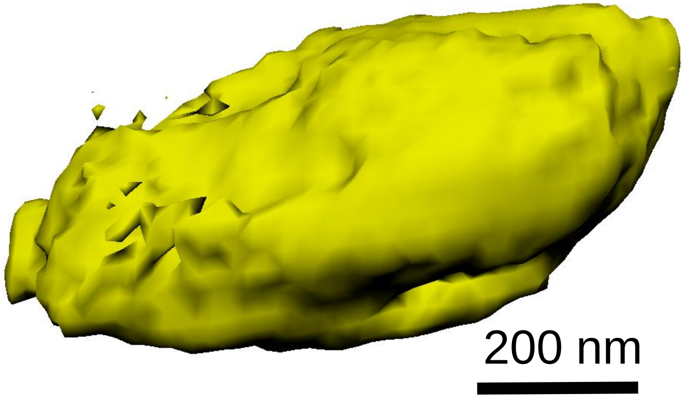
Present Status:

Coherent Diffraction Imaging (CDI)

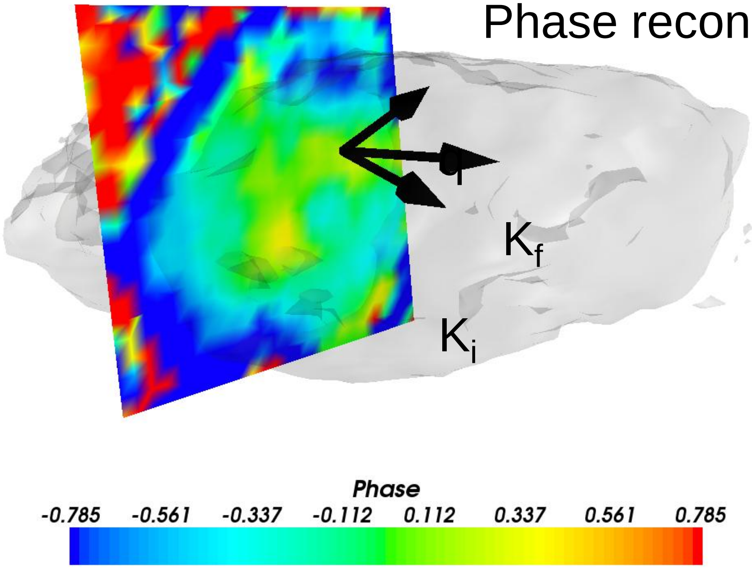
3D reconstruction of CDI data from a single crystal of Au at 6 GPa



Magnitude reconstruction



Phase reconstruction



Yang et al, to be published