OVERVIEW

• Center Mission and Cluster Tasks
• Recent Scientific Achievements
• Current & Future Developments
Established in 1998, HiPSEC was first funded through DOE/NV00 as a university-based teaching and research center of excellence to support NNSA’s Stockpile Stewardship Program.

Currently funded on a competitive basis, UNLV/HiPSEC has built a strong research program in high-pressure studies and we are aspiring to be the best among DOE/NNSA Centers of Excellence.

— advancing materials science at pressures, temperatures, and strain rates needed to interpret legacy nuclear test data and to verify design codes for stockpile stewardship;

— preparing the future scientists and engineers for DOE/NNSA to assure effectiveness, safety, and security of the stockpile without requiring nuclear explosion tests;

— involving high pressure community in general as well as UNLV physics, chemistry, Earth and materials sciences faculties in research related to critical SSP, DOE Labs, NSTech interests.
NNSA Mission and UNLV Vision

NNSA Labs

HiPSEC

Equation of state, constitutive property, and phase relations

Physics of strongly correlated d- and f- electron materials system

Chemistry of energetic and radioactive materials system

APS/HPCAT

Advanced materials design, modeling, synthesis, and characterizations

Interdisciplinary scientific advancements
Integrated technological developments
Education and training for next generation scientists

Materials researches under extreme pressure temperature, and strain rate conditions for DOE/NNSA Stockpile Stewardship Sciences
High pressure diffraction on FeSe at RT and LT.

Pressure-induced transition behavior of FeSe at RT is different from LT.
In summary we have investigated the high pressure effect on Fe spin in the FeSe superconducting compound at ambient and low temperatures (8 K) up to 16 GPa. We identify a pressure induced high spin–low spin transition under pressure. Our results indicate that Fe local spin changes may play a vital role in altering the superconducting properties in addition to structural and electronic properties in the FeSe compounds.

FIG. 4. (Color online) (a) Unit cell of tetragonal FeSe. (b) Top view of AFM phase in cmma FeSe. The black square represents one unit cell. (c)–(e) and (f)–(h) The calculated spin moment per Fe, lattice parameters, and Se anion height with respect to Fe layer by GGA and LDA.
Pressure induced high spin-low spin transition in FeSe superconductor studied by x-ray emission spectroscopy and ab initio calculations

Ravhi S. Kumar, Yi Zhang, Yuming Xiao, Jason Baker, Andrew Cornelius, Sathishkumar Veeramalai, Paul Chow, Changfeng Chen, and Yusheng Zhao

Fig. 1. (Color online) X-ray emission spectra collected for FeSe at RT at various pressures up to 16 GPa. The normalized XES intensity is plotted as a function of pressure. The inset shows expanded view of the satellite peak.

Fig. 2. (Color online) Low temperature XES spectra at selected pressures up to 8 GPa collected at 8 K.
Striking correlation between anion height and superconductivity in FeSe and LaFeAsO

Ravhi S. Kumar et al., in preparation

LaFeAsO --- anion height at HP-LT

Magnetic ordering vanishes completely under pressure above 20 GPa

Striking correlation between anion height and superconductivity in FeSe and LaFeAsO

Ravhi S. Kumar et al., in preparation
Pressure pushes the magnetic moment and superconducting transitions to higher temperatures for CeFe$_{0.9}$Co$_{0.1}$AsO.

The inset shows the variation of $T_c$ onset as a function of pressure.

---

(a) Variation of key bond lengths as a function of pressure.
(b) Pressure versus volume plot for CFCAO compound. The solid squares represent the volume at RT, the open squares are the LT data and the open circles represent the volume data of EuFe$_2$As$_2$ from ref.16. The solid line is the P-V fit.
(c) The Ce-O and Fe (Co)-As layers in the CeFeAsO.

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Pressure induced $T_c$ enhancement in electron doped CeFeAsO

R. S. Kumar, D. Antonio, M. Kanagaraj, S. Arumugam, J. Prakash, S. Sinogeiken, G. S. Thakur, A.K Ganguly, A. Cornelius, Y. Zhao
Pressure induced phase transition in Co doped CeFeAsO

Pressure induced valence change of Yb in YbMn$_2$Ge$_2$ to a Monoclinic phase above 35 GPa

Experiments plus theoretical calculation
Research highlight: High-pressure phase transitions of Eu

PHYSICAL REVIEW B 83, 104106 (2011)

Pressure-induced structural transitions in europium to 92 GPa

W. Bi, Y. Meng, R. S. Kumar, A. L. Cornelius, W. W. Tipton, R. G. Hennig, Y. Zhang, C. Chen, and J. S. Schilling

1 Department of Physics, Washington University, CB 1105, One Brookings Dr., St. Louis, Missouri 63130, USA
2 HPCAT, Carnegie Institution of Washington, 9700 S. Cass Ave., Argonne, Illinois 60439, USA
3 Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA
4 Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA

(Received 16 December 2010; published 18 March 2011)

Top: Calculated Eu phase diagram.

Right: Measured x-ray diffraction patterns of Eu up to 92 Gpa.
Research highlight: Anomalous lattice dynamics of PbTe

Anomalous Lattice Dynamics near the Ferroelectric Instability in PbTe

Yi Zhang,1 Xuezhi Ke,2,1 Paul R. C. Kent,3 Jihui Yang,4 and Changfeng Chen1
1Department of Physics and HiPSEC, University of Nevada, Las Vegas, Nevada 89154, USA
2Department of Physics, East China Normal University, Shanghai 200062, China
3Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
4Materials Science and Engineering Department, University of Washington, Seattle, Washington 98195, USA
(Received 1 July 2011; published 17 October 2011)

The pair distribution function (PDF) of PbTe in the temperature range 50-500 K.

The phonon dispersion, density and vibration modes of PbTe.
Research highlight: Band engineering by nanodopants

Nanodopant-Induced Band Modulation in AgPb\textsubscript{m}SbTe\textsubscript{2+m}-Type Thermoelectrics

Yi Zhang,\textsuperscript{1} Xuezhi Ke,\textsuperscript{2,1} Changfeng Chen,\textsuperscript{1} Jihui Yang,\textsuperscript{3} and Paul R. C. Kent\textsuperscript{4}

\textsuperscript{1}Department of Physics and HiPSEC, University of Nevada, Las Vegas, Nevada 89154, USA
\textsuperscript{2}Department of Physics, East China Normal University, Shanghai 200062, China
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(Received 29 December 2010; published 20 May 2011)

The crystal and electronic structure of the LAST nanocomposite.

The thermoelectric properties of the LAST nanocomposite.
in situ synchrotron experiments on high explosives PETN and TATB to study radiation damage due to “white” focused x-ray irradiation

\[ n(NH_3BH_3) + h\nu \rightarrow (H_2NBH_2)_n + nH_2 \rightarrow (HNBH)_n + 2nH_2 \]

Hard x-ray induced decomposition

Successful loading of molecular H\(_2\) and O\(_2\)

\[ 2KClO_3 + h\nu \rightarrow 2KCl + O_2 \]

Studies of FOX-7 (DADNE) under extreme pressure and radiation (far-/near- infrared) conditions.


The single crystal technique is shown to be very useful in high pressure synthesis.

Fe$_4$O$_5$: a new iron oxide

Fe$^{2+}$: Fe$^{3+} = 50:50$

Stability of Fe$_4$O$_5$ in comparison with its breakdown products from first-principle calculations.

PNAS | October 18, 2011 | vol. 108 | no. 42 | 17281-17285

Photomicrograph of a single crystal synthesized in DAC after laser heating.

Single crystal diffraction

Recovered to Ambient

10.5 GPa

Powder pattern (further synthesis)
Technology Development

Analysis of structure factors in synchrotron micro-Laue diffraction at P > 20 GPa

<table>
<thead>
<tr>
<th>Challenges</th>
<th>Solutions</th>
</tr>
</thead>
<tbody>
<tr>
<td>limited reciprocal space access</td>
<td>wide opening DAC, multiple crystal orientation</td>
</tr>
<tr>
<td>DAC absorption and scattering</td>
<td>high energy collimated beam, collimated detector</td>
</tr>
<tr>
<td>Diamond diffraction attenuation</td>
<td>collection of multiple oscillation</td>
</tr>
<tr>
<td>Drifting of the crystal in the beam upon rotation</td>
<td>empirical correction, rastering oscillations</td>
</tr>
</tbody>
</table>

Schematic view of the experiment geometry

High quality structural analysis has obtained and result in the Fe₄O₅ discovery!

The diamond anvil cell is maintained at low temperature by means of a cryostat at 16IDB (HPCAT)

Variation of intensity with rotation

Variation of intensity with rotation

Variation of the X-ray flux on a microcrystal upon oscillation in a synchrotron μ-beam
Synchrotron Lang topography of shock-recovered materials:

*A novel technique for quantitative analysis of defects in shocked materials*

O. Tschauner (UNLV), P. Burnley (UNLV), S.N. Luo (LANL), S. Sinogeikin (CIW)

Lang topography probes bulk sample to study strain-induced modulation of Bragg signal so as to illustrate Shock-induced dislocations, disclinations, point defects

α-U type Cerium (DAC experiment in neon medium)

O. Tschauner (UNLV), N. Velisavljevic (LANL), J. Cooley (LANL), P. Dera (UChi), S. Sinogeikin (CIW)

1st SXD (in-situ growth) analysis (hydrostatic 4.8 GPa)

Structural relation to fcc via the bct-type

fcc $\rightarrow$ bct $\rightarrow$ Fmmm $\rightarrow$ α-U

*First two steps*: Only cell deformation, no structural distortion

*Last step*: Softmode at X, structural distortion
Aggregate rheological behavior depends on the population size and spatial relationship between hard and soft grains!

In-situ high pressure synchrotron x-ray diffraction measures elastic strain in the polycrystalline sample.

Burnley, 2011
Effect of strain on transformation kinetics

- ultra high pressure deformation in DAC
- white beam micro-Laue to observe deformation
Soft Bond-Deformation Paths in Superhard γ-Boron

Wei Zhou,1 Hong Sun,1,2,* and Changfeng Chen2,†

1Department of Physics, Shanghai Jiao Tong University and Key Laboratory of Artificial Structures and Quantum Control, Ministry of Education, Shanghai 200240, China
2Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA
(Received 16 May 2010; published 17 November 2010)

Top: Stress-strain relation of g-B28 under tensile loading.
Right: The corresponding charge distribution.
Research highlight: New carbon polymorph under compression

Low-Temperature Phase Transformation from Graphite to $sp^3$ Orthorhombic Carbon

Jian-Tao Wang,1,2,* Changfeng Chen,2 and Yoshiyuki Kawazoe3

1Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

2Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA

3Institute for Materials Research, Tohoku University, Sendai, 980-8577, Japan

(Received 17 November 2010; published 16 February 2011)

(a) Structure, (b) enthalpy, (c) electronic and (d) phonon dispersion of the new W-carbon.

The x-ray diffraction of W-carbon.

The kinetic barrier for various carbon polymorphs at high pressure.
Research highlight: The graphite-to-diamond transition

PHYSICAL REVIEW B 84, 012102 (2011)

Mechanism for direct conversion of graphite to diamond

Jian-Tao Wang,1,2,* Changfeng Chen,2 and Yoshiyuki Kawazoe3

1Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
2Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, Nevada 89154, USA
3Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan
(Received 12 April 2011; revised manuscript received 25 June 2011; published 27 July 2011)

Left: The kinetic barriers for the phase transitions from graphite to various diamond phases.

Right: A newly identified phase (12R) of diamond and its x-ray diffraction pattern in comparison with other known diamond phases.
Introduction to Mineral Physics

"Mineral Physics 101"

Prof. Pamela Burley (UNLV/HiPSEC)

a web lecture

COMPRES Graduate Course 2012 – Attendees

- Name: Joshua Towse
  - Affiliation: Northwestern University
  - Advisor: Dr. Steven B. Jacobsen

- Name: Asha Clark
  - Affiliation: University of California, Davis
  - Advisor: Dr. Charles L. Leber

- Name: Xiuling Xiao
  - Affiliation: University of Wisconsin-Madison
  - Advisor: Dr. Charles Rasor

- Name: Jordan Bower
  - Affiliation: Indiana University South Bend
  - Advisor: Dr. Ron L. Scott

- Name: Wendi Bi, Postdoctoral Researcher
  - Affiliation: University of Illinois at Urbana-Champaign/Argonne National Lab
  - Advisors: Dr. Jay Bass & Dr. Eran Alp

I am currently working on characterizing the hydration potential of silicate post-perovskite via synchrotron-XAS and first-principles calculations.

I am currently working on developing the fluid's composition and density to eliminate the effect of these properties' element mobility.

Current Project: Experimental Determination of C-water Diffusivity in Spinel at 1 bar

W-Diffusivity in Diopsid at 1 bar

Crystal Structure Refinement of High-Pressure Synthetic Pyroxenes

- Name: Emily A. Ford
  - Affiliation: Department of Geosciences, University of Arizona
  - Advisors: Dr. Michael D. Gaudry & Dr. Robert Stewart

- Name: Esteban Caceres
  - Affiliation: University of California, Davis
  - Advisor: Dr. Charles Rasor

- Name: Shengli Xiao
  - Affiliation: University of Wisconsin-Madison
  - Advisor: Dr. Pamela Basky

- Name: Edna Emanuelli
  - Affiliation: University of Nevada Las Vegas
  - Advisor: Dr. Michael D. Gaudry

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Current Project: Structural Compressibility Measurements at 1 bar

Structural Compressibility Measurements at 1 bar

My Ph.D. project focuses on the mobility of trace elements in aqueous fluids at the PT conditions found during melt-sediment dehydration. We have developed an in-situ experimental technique that utilizes a hydrothermal diamond cell and synchrotron X-ray fluorescence to quantify element concentrations in aqueous fluids. The technique allows us to use the properties of the fluid (composition and density) to eliminate the effect of these properties' element mobility.

I am currently working on developing the fluid's composition and density to eliminate the effect of these properties' element mobility.

Current Project: Investigation of phase transition behavior and transformation mechanisms of Na-TA topology minerals

Major current studies: Characteristics of changes in porosity, pore distribution and grain surface roughness of geological materials e.g., sedimentary rocks that undergo some metamorphic processes; where traditional metamorphic methods are limited to the length scales that small-angle scattering techniques can probe (~1 to 100 Å). The focus is to measure structures in many geologic materials control the evolution of fluids and their chemical reactions during metamorphism and/or hydrothermal processes.

- Name: Yong Hui Chen, Postdoctoral Researcher
  - Affiliation: University of Nevada Las Vegas
  - Advisors: Dr. Pamela Basky & Dr. Oliver Tackman

- Name: Gang Xia
  - Affiliation: Department of Geosciences, University of California, Riverside
  - Advisor: Dr. Harry W. Green

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Current Project: Research in experimental studies of metal and ceramic deformation as a function of strain

- Name: Young Chul Kim, Postdoctoral Researcher
  - Affiliation: University of California, Davis
  - Advisor: Dr. Charles Rasor

- Name: Alex Dube, Postdoctoral Researcher
  - Affiliation: University of California, Davis
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Current Project: Geobiology studies

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**Introduction to Mineral Physics**

"Mineral Physics 101"

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### On-line readings

1. **Ruby Pressure Scale**

   Measuring the shift of ruby fluorescence lines is one of the most commonly used means of determining the pressure in a DAC. Therefore it is important to have a sense of how accurate the ruby pressure scale is. In this assignment we will compute the most commonly used ruby scale (Mao et al., 1986) with a more recent refinement by Holzapfel (2003).

   First read the both articles:


   @: can be downloaded from http://phytaxonomy.uchicago.edu/sig/h-bae/1bb636fbb-121.pdf

   1. Create an excel spreadsheet or write a program in a language of your choice that calculates the pressure from the shift in the ruby R1 line for Mao et al. (1986) and for

### Homework Sets

- The lattice response to force
  - Pressure (isotropic forces)
  - Volume change
  - Stress (anisotropic forces)
  - Thermal expansion
  - Elastic deformation

- Visiting Crystal Structures

**Stereonet of your favorite mineral**

Stereonets are a very valuable tool for visualizing the positions of lattice planes. There are a number of programs that will plot stereonets and allow you to manipulate them. However, making one by hand is probably the best way to really appreciate how stereonets work. Therefore, I want you to plot up the poles to planes for your favorite non-cubic mineral for values of h, k, and l up to 5. For sanity’s sake I will not question anyone if it turns out that their favorite mineral is not monoclinic or triclinic.

1. If you don't own a Wulff net, you can make one by printing out the last page and sticking it on a piece of cardboard. Put a thumb tack through the central point (pointing up at you). Draw your stereonet on tracing paper, velum or an acetate placed onto the tack such that it is centered over the stereonet. This will allow you to rotate the stereonet over the Wulff net graph paper as needed.

2. Look carefully at how the stereonet is constructed.
DOE-NNSA Cooperative Agreement DE-FC52-06NA26274
**Diffraction**

- Images (a), (b), and (c) show diffraction patterns with different temperatures:
  - (a) 2420±40K
  - (b) 2540±55K
  - (c) 2650±35K

- Graph showing intensity vs. 2θ degrees for NaCl-B2 γ-Fe:
  - Peaks at 5, 10, 15, 20, 25 degrees.

**Imaging the domain wall in single crystal**

- Diagram of experimental setup:
  - Undulator X-ray source
  - Double-crystal Si(111) monochromator
  - Beam stopper
  - Pin hole
  - Diamond anvil cell with xyz translations and rotations

**DAC Synchrotron Techniques**

- High Pressure - Inelastic X-ray Scattering – Superhard Graphite

- **Carbon K-edge**
  - Normalized total intensity vs. energy loss (eV)
  - Samples at 2.4 GPa, 7.5 GPa, 10.0 GPa, 14.5 GPa, 15.7 GPa, 20.5 GPa, 23.2 GPa, 23.8 GPa

- At approximately 17 GPa, half of the π-bonds between graphite layers convert to σ-bonds while the other half remain as π-bonds in the high-pressure form.

**Inelastic Scattering**

- Graph showing intensity vs. 2θ for Mao et al. (2003)
  - Peaks at 5, 7.2, 11, 12 degrees

- Graph showing intensity vs. pressure for Be, Ga, Lu:
  - Pressure values: 1.0 GPa, 13.7 GPa, 18.4 GPa, 23.9 GPa

**Stress & Elasticity**

- Diagram of stress and strain in a material with diamond anvil

**Radiography**

- Diagram showing radiographic imaging with a x-ray beam passing through a diamond anvil.
Phonon Dynamics

DAC Synchrotron Techniques

Study single crystal diffraction in powder sample at high-P

Laue - single crystal

5 μm beam

0.5 μm beam
HPCAT: A dedicated high pressure research facility in which multiple x-ray techniques, as well as complementary optical and electromagnetic probes, have been developed, addressing scientific problems in multidisciplinary fields.

Established: 1998
1st experiment: 2002
HPCAT Established Capabilities

**HP x-ray diffraction**    **HP x-ray imaging**
Amorphous – (Nano-)Crystalline – Micro-structure
Measuring structures of materials at various scales in space and time

**HP x-ray spectroscopy**
Phonon dynamics
Charge dynamics
Bonding
Spin transition

> 500 person-visits per year
> 60% are graduate students and postdocs
> 1.5 per week peer-reviewed papers
> 23% appear in “high-profile” journals
HPCAT Key features:

- **Four** simultaneously operational beamlines
- Probing x-ray **beam size** suitable for high pressure equipment
- **Tunable x-ray energies** for various x-ray measurements
- **High energy resolution** (1eV-1meV) for x-ray scattering and spectroscopy
- Precise collimation systems for optimal S/N ratio
- User friendly operation

**HP Spectroscopy**
- HP x-ray absorption (XANES, XAFS, PFY)
- HP x-ray emission (XES, RXES)

**HP Inelastic Scattering**
- HP inelastic x-ray scattering (x-ray Raman, 1eV)
- HP nuclear resonant IXS (NRIXS, 2meV)
- HP nuclear forward scattering (Mossbauer)

**HP Diffraction**
- μ-XRD integrated with laser heating, cryostats
- μ-XRD integrated with XAS
- Single crystal XRD
- HP PDF (for amorphous and liquid materials)

**HP Support Equipment**
- Double sided laser heating
- Various cryostats
- Paris-Edinburgh cell
- A numbers of on-line and off-line systems
- Software
Science at HPCAT

• Materials Science
  – *Structures, New materials, Properties*

• Fundamental Physics
  – *Molecular, atomic, and electronic interactions, Phonons*

• Fundamental Chemistry
  – *New bonding, New reactions, HP periodic table*

• Earth and Planetary Sciences
  – *Mineral physics, Geophysics, Geochemistry*

• Special Focuses
  – *NNSA mission related science, Stockpile stewardship*
Users at HPCAT

- **Member users**
  - CDAC, LLNL, UNLV, Carnegie
- **General users**
- >600 individual users since 2003;
  >2500 person-visits
- >60% are students and post-docs

![User Group Pie Chart]

- Student (41%)
- DOE Laboratory Scientist (29%)
- Others (<1%)
- Univ. Faculty (14%)
- Post-doctoral Scientist (16%)
Recent Development: mini-XES

A factor of ~50 increase in efficiency
Xiao, Paul, with U. Washington (Seidler) and LLNL (Pacold, Bradley)
Recent Development – multiple analyzers

Mao et al, PRL (2011)

17 element analyzer for HP IXS

Mao et al, PRL (2011)
Recent Development – improved laser heating system

• Larger and more uniform heating
• More precise alignment
• Improved stability

Meng, Smith, with CIW (R. Boehler)
Recent Development – pressure controls

- Automated pressure control
- Undisturbed alignment

Compression of SC NaCl+Au with gearbox

- Gear box
- Universal diaphragm
- Diaphragm control
- Sinogeikin, Rod, Kenney-Benson

Graph:
- Gold pressure, GPa vs. DAC screw rotation (deg)
- Compression of SC NaCl+Au with gearbox
- 2 hours

Data points: 0, 5, 10, 15, 20, 25, 30, 35 GPa at various DAC screw rotations.

2 hours compression time.
Recent Development
– Paris Edinburgh cell

- **Liquid / Melt properties**
  Structure – XRD
  Density – XAS
  Viscosity – imaging
  Sound velocity – ultrasonic
  Conductivity – XRD and imaging

Park, Kono, Kenney-Benson, with U. Chiacgo (Y. Wang) and UNLV (Kumar)
Recent Development – HP imaging

- Imaging resolution of 30 nm
- $\Delta e/e \sim 10^{-2}$
- $\Delta e/e < 10^{-3}$

GeO$_2$ glass at 10 GPa

In collaboration with HPSynC

Xrdia machine in 16ID-E

30 nm resolution
Recent Development – time resolved

Pulsed laser heating

- Single pulse: down to sub-\(\mu\)s
- Multiple events: \(\mu\)s-ms

With R. Boehler

With C-s Yoo
Yoo et al RSI 2011
HPCAT upgrade

**Source brilliance** (newly available undulators)

**Source preservation** (position, distribution, coherence)

**On-sample flux** (advanced optics)

**Beamsize reduction** (down to sub-μm probes)

**Spatial and temporal resolution**

**Resolution in energy and d-spacing**

**Counting efficiency**

- > S/N (depth resolution)
- > advanced detecting systems

Newly installed canted undulators
Next generation static experiments

- More extreme P-T conditions
- More precise determination
- Sub-micron single crystal work
- Grain boundaries
- Combinatorial studies
- Composite materials...

The diagram shows a region of high pressure (P) and temperature (T) conditions. The probe sizes indicated are:

- ~50 µm probe
- ~5 µm probe
- 0.1-0.5 µm probe

An image of a current probe of 5 µm is also shown.
APS Upgrade

- Higher brilliance
- More stable beams
- More advanced x-ray techniques
- Coordinated research areas
- Better detectors
- Better infrastructure (software, support equipment)

- Mastering hierarchical structures through imaging
- Real materials under real conditions in real time