CDAC

CARNEGIE / DOE ALLIANCE CENTER:

A Center of Excellence for
High Pressure Science and Technology

Russell J. Hemley

SSAA Program Symposium
Carnegie Institution
Jan. 20-22, 2010

CARNEGIE INSTITUTION FOR SCIENCE

NNSA

OUTLINE

CDAC

I. Overview of Center

MOTIVATION

TECHNIQUES

EDUCATION, TRAINING, OUTREACH

II. Selected Science

NEW METALS PHYSICS

NOVEL COMPOUNDS

LIQUIDS/AMORPH.

CHEMISTRY

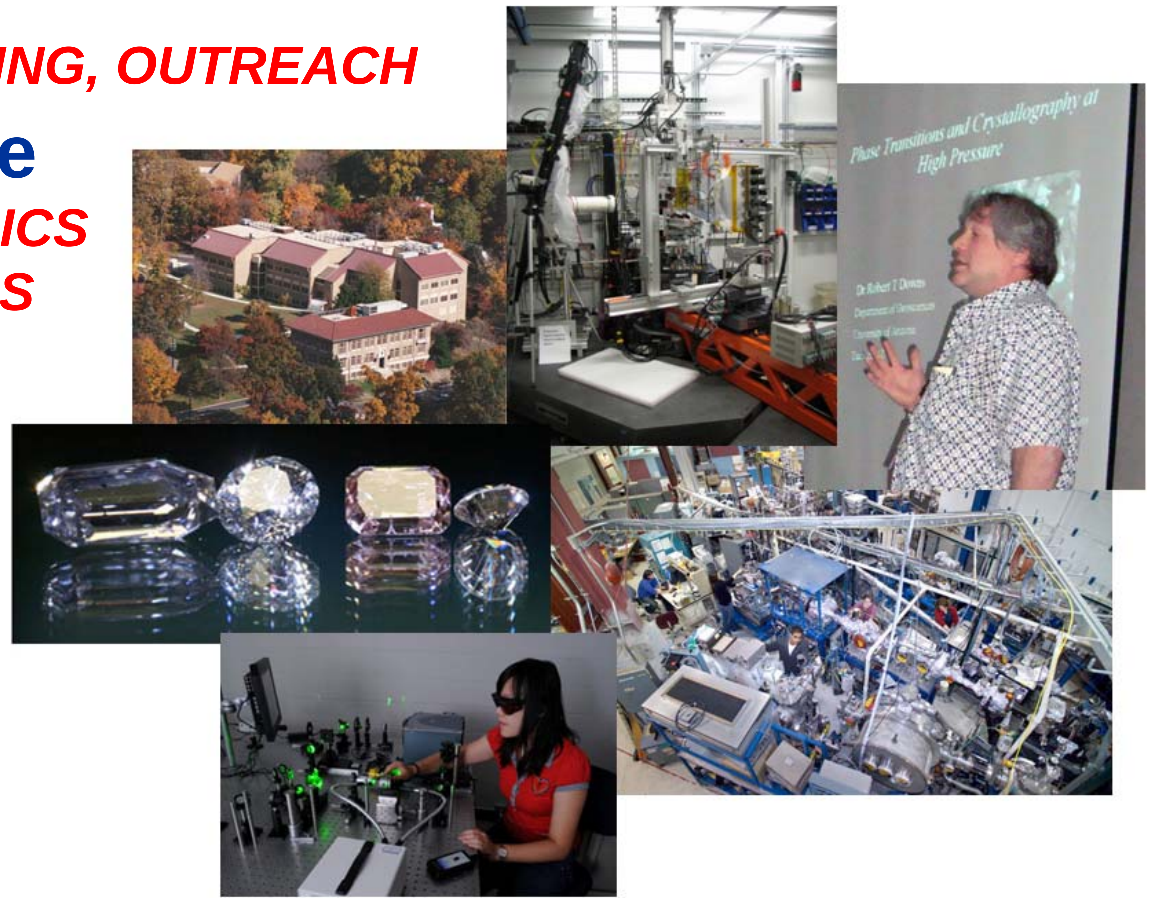
LOW-Z SYSTEMS

III. Technical Developments

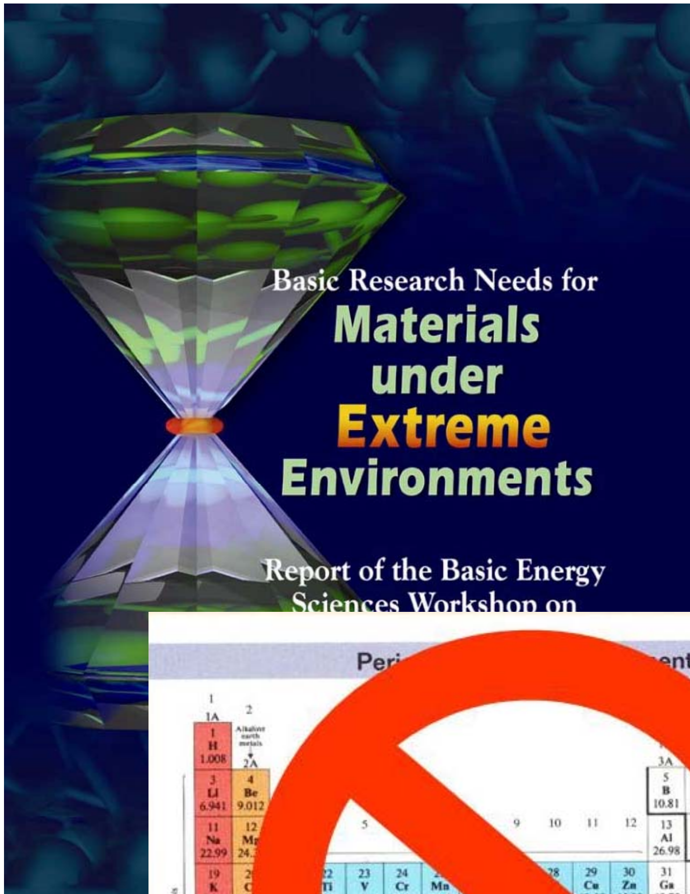
INSTRUMENTATION

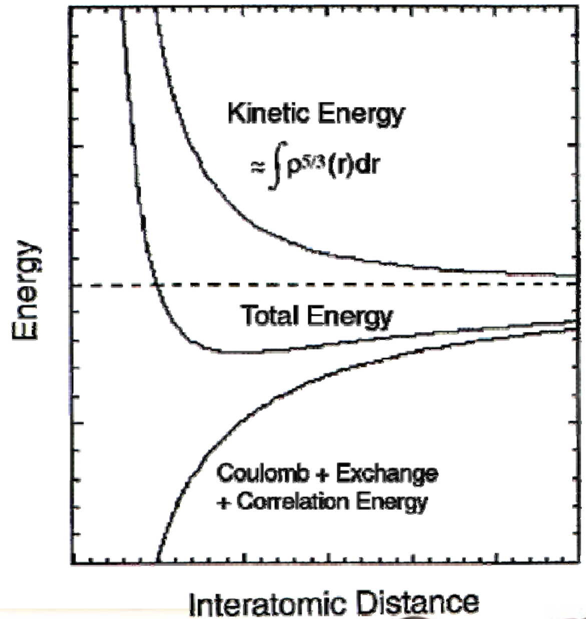
FACILITIES

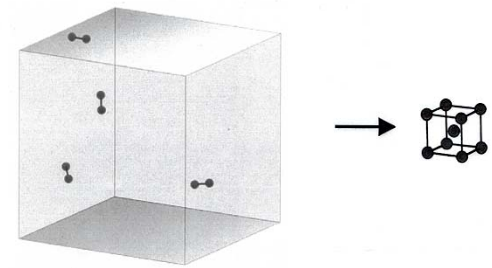
IV. Conclusions

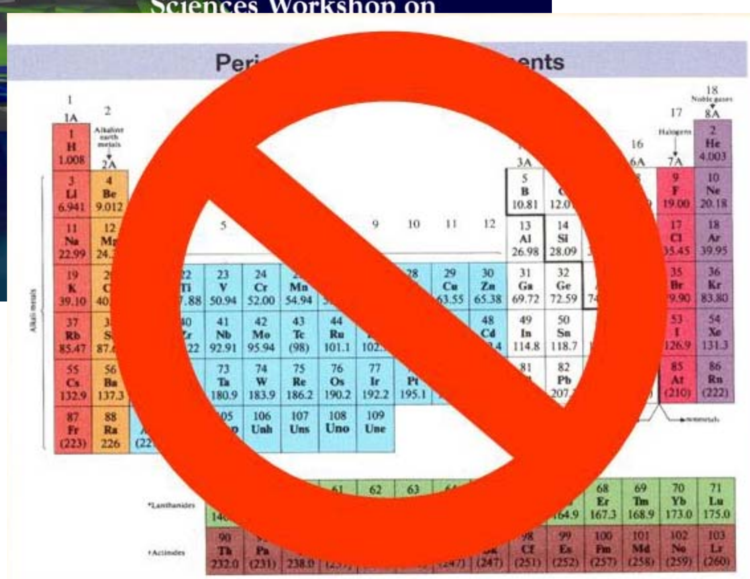


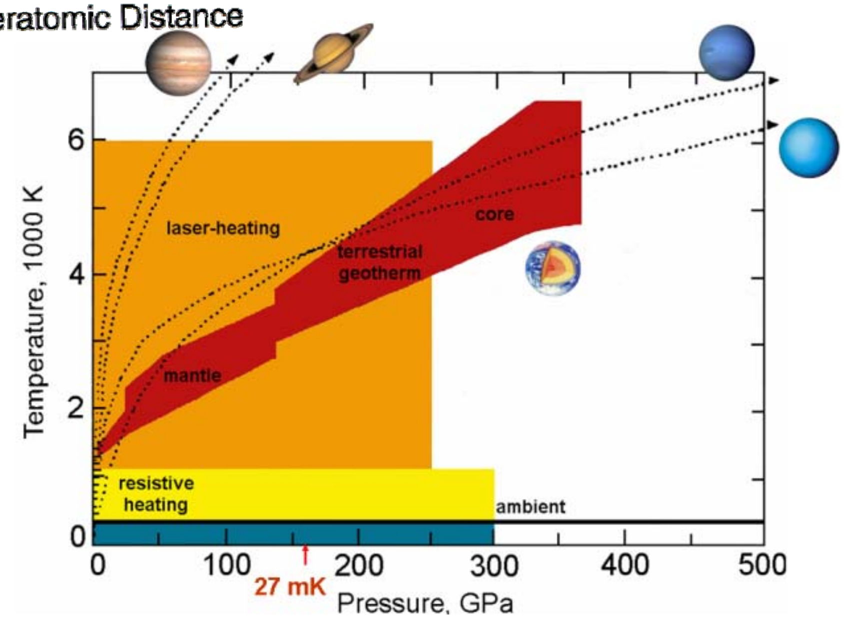
Studies of extreme environments are opening up a new world of materials behavior





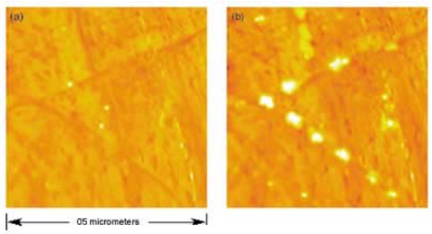




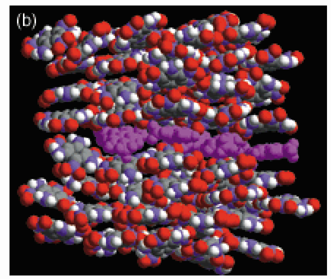


Understanding materials under extreme environments is central to the NNSA science mission

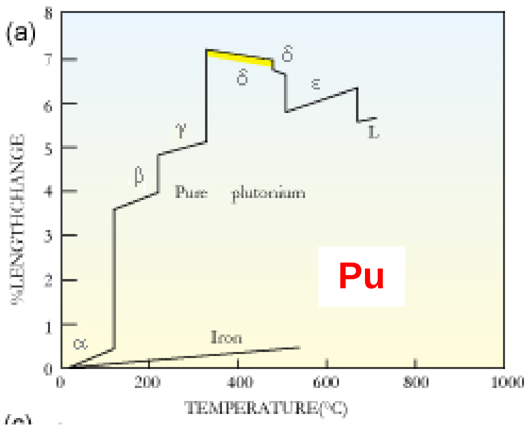
CDAC

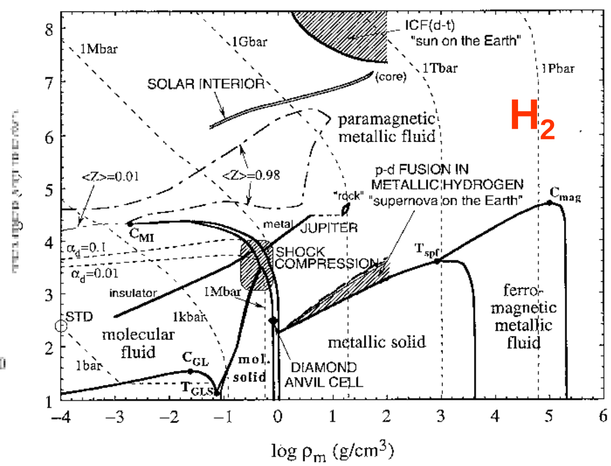


Hydriding reactions



TATB





Mission of CDAC

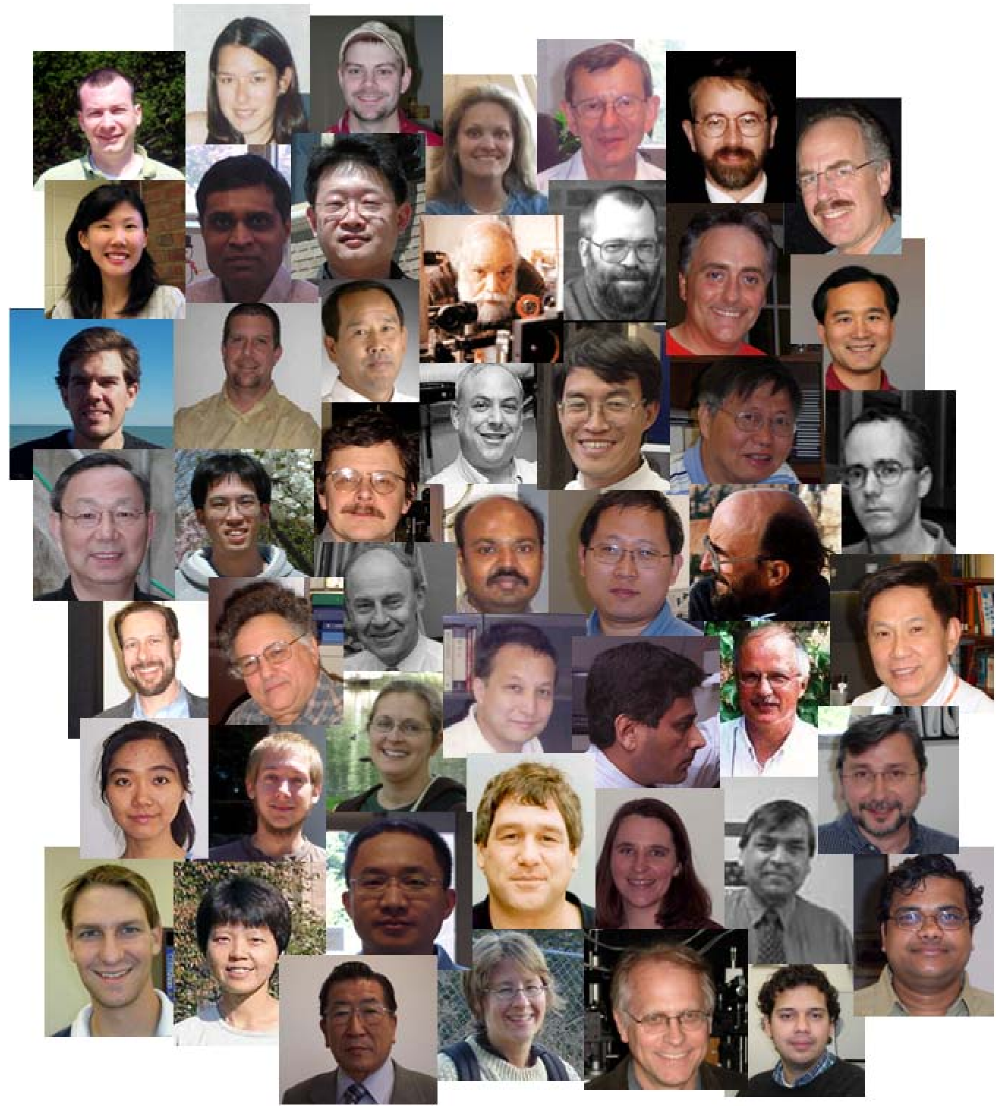
Develop techniques and training to examine the full complement of high *P-T* materials problems essential for stewardship science.

Components of the Center

CDAC

Academic Partners

CARNEGIE INST. (Hemley, H. K. Mao)
UNIV. ALABAMA - BIRMINGHAM (Vohra)
UNIV. CALIF. - BERKELEY (Wenk & Jeanloz)
UNIV. CHICAGO (Heinz)
UNIV. ILLINOIS (Dlott & Li)
CALTECH (Fultz)
PRINCETON UNIV. (Duffy)
NEW MEXICO STATE/YALE UNIV. (Lee)
FLORIDA INTERNATIONAL UNIV. (Saxena)
TEXAS TECH (Ma)
UNIV. NEVADA - RENO (Chandra)
ARIZONA STATE UNIV. (Yarger)
UCLA (Kavner)
NORTHWESTERN UNIV. (Jacobsen)
OHIO STATE UNIV. (Panero)
WASHINGTON UNIV. ST. LOUIS (Schilling)
UNIV. ARIZONA (Downs)
STANFORD UNIV. (W. Mao)



Academic Collaborators

FACILITY USERS

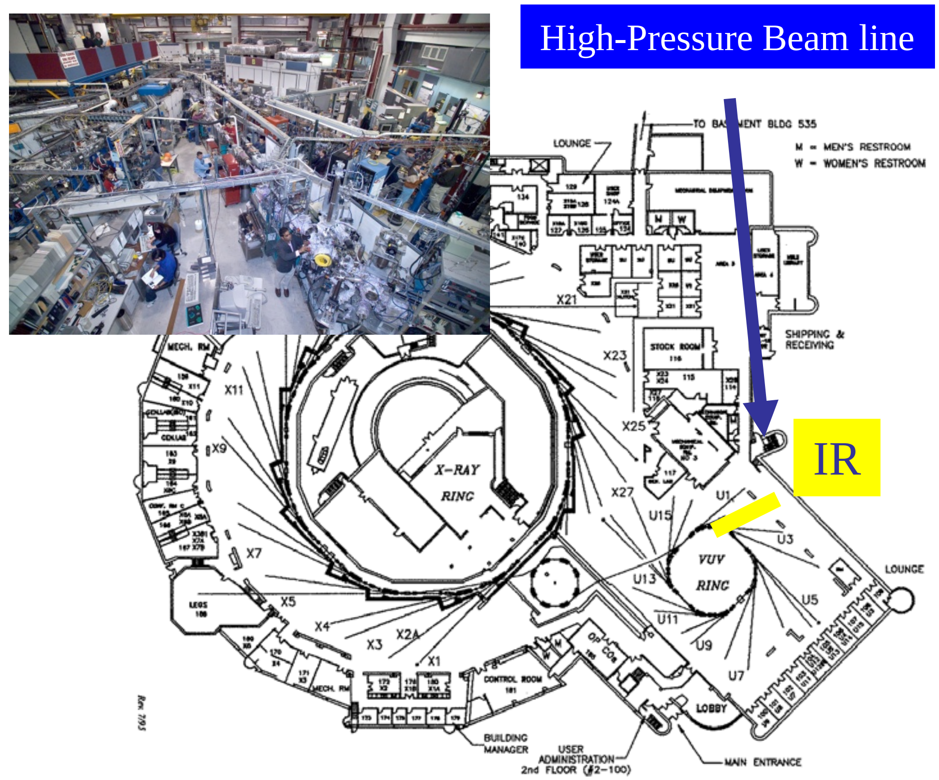
NNSA Laboratory Partners

ALL HIGH *P-T* GROUPS AT **LLNL, LANL, SNL**

CDAC manages and coordinates activities at major facilities for high *P-T* research

CDAC

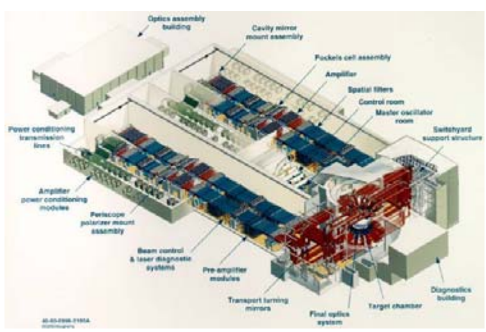
- Carnegie/Partner facilities:
  - ***High P-T technology***
  - ***Spectroscopy labs***
  - ***Diffraction and microanalysis***
  - ***Computational resources***
  - ***CVD diamond growth***



- Technique development/support for unique facilities at NNSA Labs

High P-T neutron scattering at LANSCE

Science campaigns at NIF



- Dedicated high-pressure synchrotron infrared beamline at the NSLS (U2A)

NNSA

CDAC supports high *P-T* facilities and activities at the Advanced Photon Source

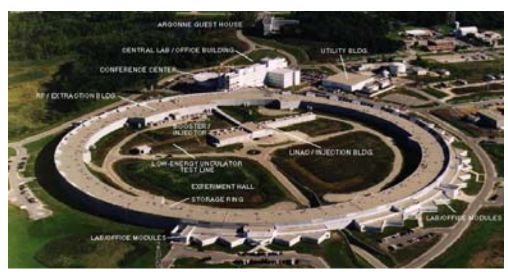
High-Pressure Collaborative Access Team (HPCAT)

Carnegie Inst./Livermore Nat. Lab./ Univ. Nevada Las Vegas/Univ. Hawaii

CDAC (Lab and Academic) is a 30% Member

- 9 hutches
- 4 independently operating
- support lab

DOE NNSA/SC Partnership



CDAC

CDAC supports high *P-T* facilities and activities at the Advanced Photon Source

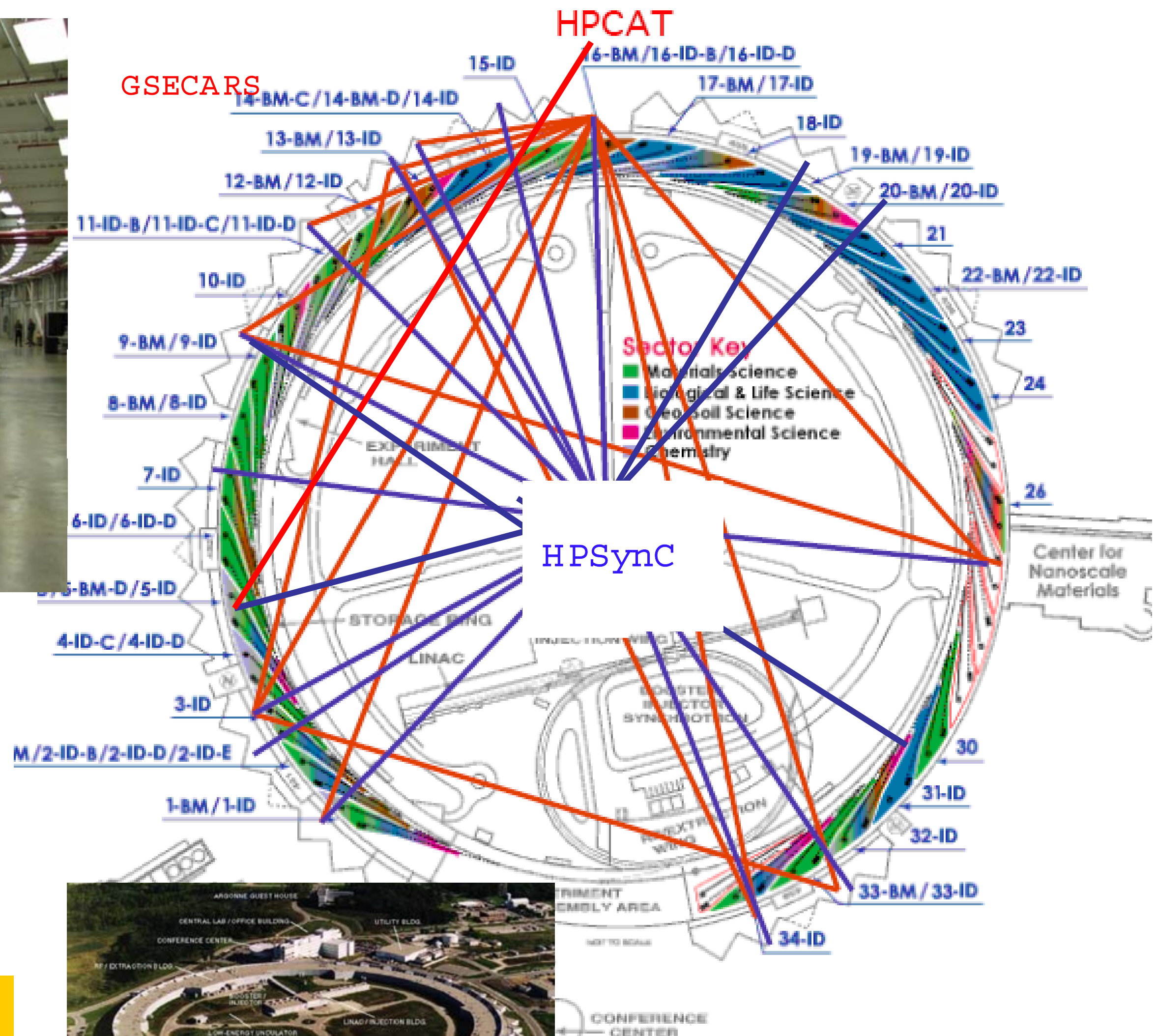
High-Pressure Collaborative Access Team (HPCAT)

Carnegie Inst./Livermore Nat. Lab./ Univ. Nevada Las Vegas/Univ. Hawaii

CDAC (Lab and Academic) is a 30% Member

- 9 hutches
- 4 independently operating
- support lab

DOE NNSA/SC Partnership



CDAC HIGHLIGHTS 2009:
Education, training and outreach

CDAC

- ***Growth of users at HPCAT (475+ to date)***
- ***Expanded collaborations with all NNSA Labs***
- ***CDAC supported 26 Ph.D. students***
- ***6 undergraduate/high school interns***
- ***Student Winter Workshop held Feb. 2009***
- ***Growing number of CDAC/HPCAT collaborations***
  - ***735 outside collaborators***
  - ***240 institutions***
- ***Presentations at major national meetings***
  - ***APS March – 23 abstracts***
  - ***AIRAPT – 38 abstracts & presentations***
  - ***Fall AGU – 56 abstracts & presentations (3 invited talks), including graduate session chair***

CDAC HIGHLIGHTS 2009:
Education, training and outreach

CDAC

• ***2009 CDAC Winter Workshop at APS Feb. 27-28, 2009***


- ***40 student attendees***
- ***46 posters presented***
- ***8 talks by CDAC students***
- ***9 talks by CDAC partners/ collaborators***

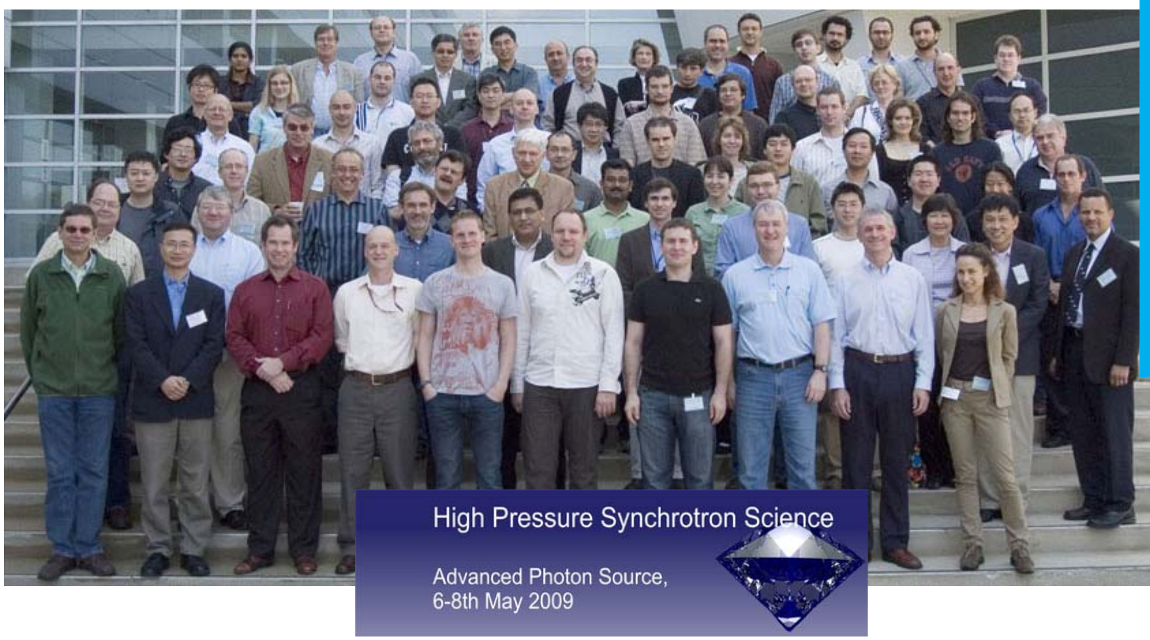


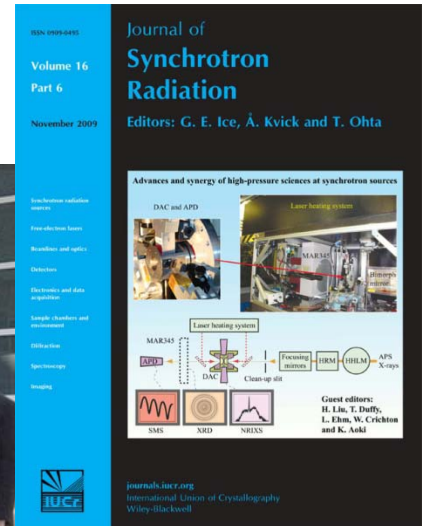
NNSA

CDAC HIGHLIGHTS 2009:
Education, training and outreach

CDAC

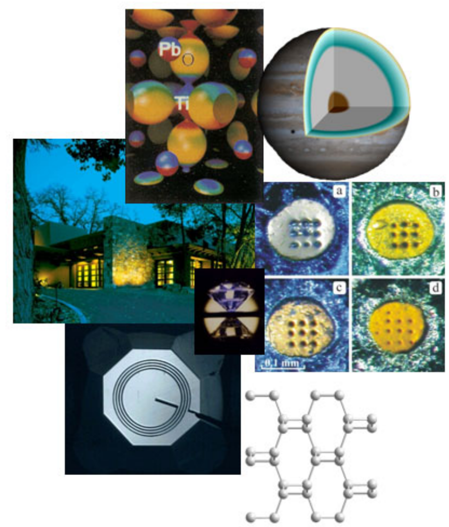
- ***High Pressure Synchrotron Science Workshop, APS May 6-8, 2009***
  - ***12 Scientific & Technical Sessions,***
  - ***10 talks by CDAC scientists***





- ***Advances in High Pressure Science Using Synchrotron X-rays, Oct. 4, 2008***

- ***21st Century Needs and Challenges in Compression Science Workshop***
  Santa Fe, Sept. 23-25, 2009



CDAC also support research by undergraduate and high-school summer scholars

CDAC

2009 Carnegie Summer Scholars

N. Foley (Carleton Coll.)
Fractionation of Sulfur Isotopes in the Formation of Mars

Z. Liang (Lehigh Univ.)
Crystallization of Periodic Mesoporous Organosilicas

A. Savello (Emory Univ.)
Measurement of the Thermal Conductivity of $(MgFe)SiO_3$ Perovskite at High P and T

A. Schad (Univ. Notre Dame)
High Pressure Raman Studies of Ferroelectric Perovskites

2009 Summer Scholars Z. Liang, A. Schad and A. Savello present their work at the Summer Scholars Research Symposium.

2009 High School Summer Scholars

C. Barkett (Good Counsel High School, Olney, MD)
Low-Temperature Synthesis of Fe-Bearing Solid Solutions

E. Sandford (Glenelg Country School, Ellicott City, MD)
High-Pressure Brillouin Spectroscopy of Polymers

CARNEGIE INSTITUTION FOR SCIENCE

NNSA

A broad range of fundamental problems in high *P-T* science is being investigated

CDAC

- *STRUCTURES AND PHASE RELATIONS*
- *EQUATIONS OF STATE*
- *ELASTICITY, RHEOLOGY, STRENGTH*
- *ELECTRON AND PHONON DYNAMICS*
- *TRANSPORT PROPERTIES*
- *EXTREME CONDITION CHEMISTRY*

SELECTED SYSTEMS

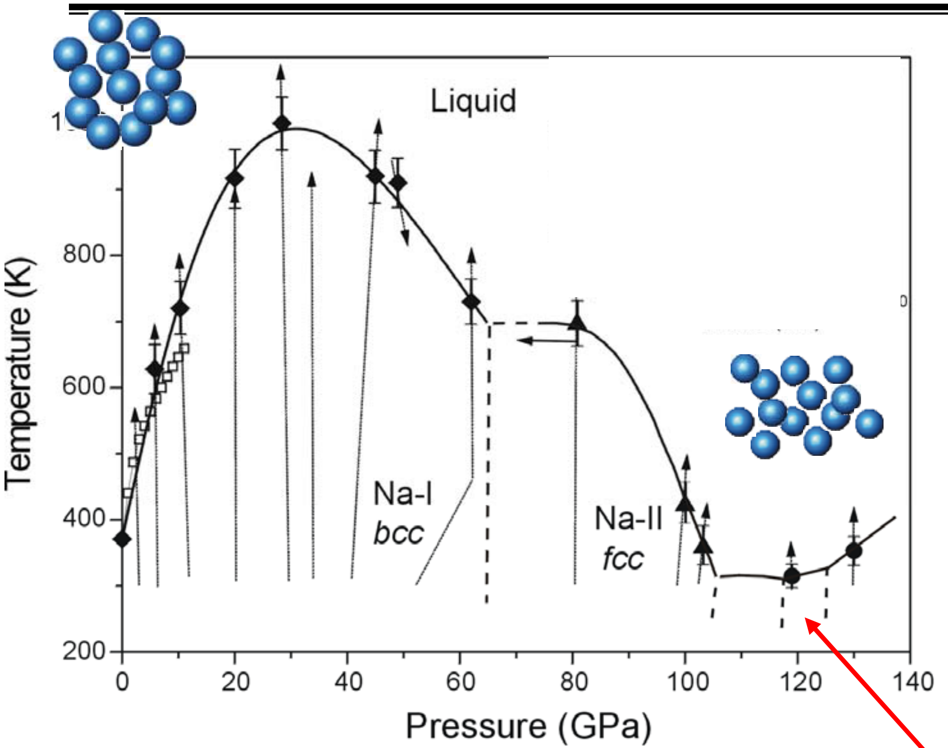
Metals physics
Novel compounds
Liquids/Amorphous Materials
Chemistry
Low-Z systems

2009: 129 Publications
(10 Phys. Rev. Letts., 4 Nature, 1 Science, 7 PNAS)

TO DATE: 750+ Publications
(50 Phys. Rev. Letts., 27 Nature, 12 Science, 38 PNAS)

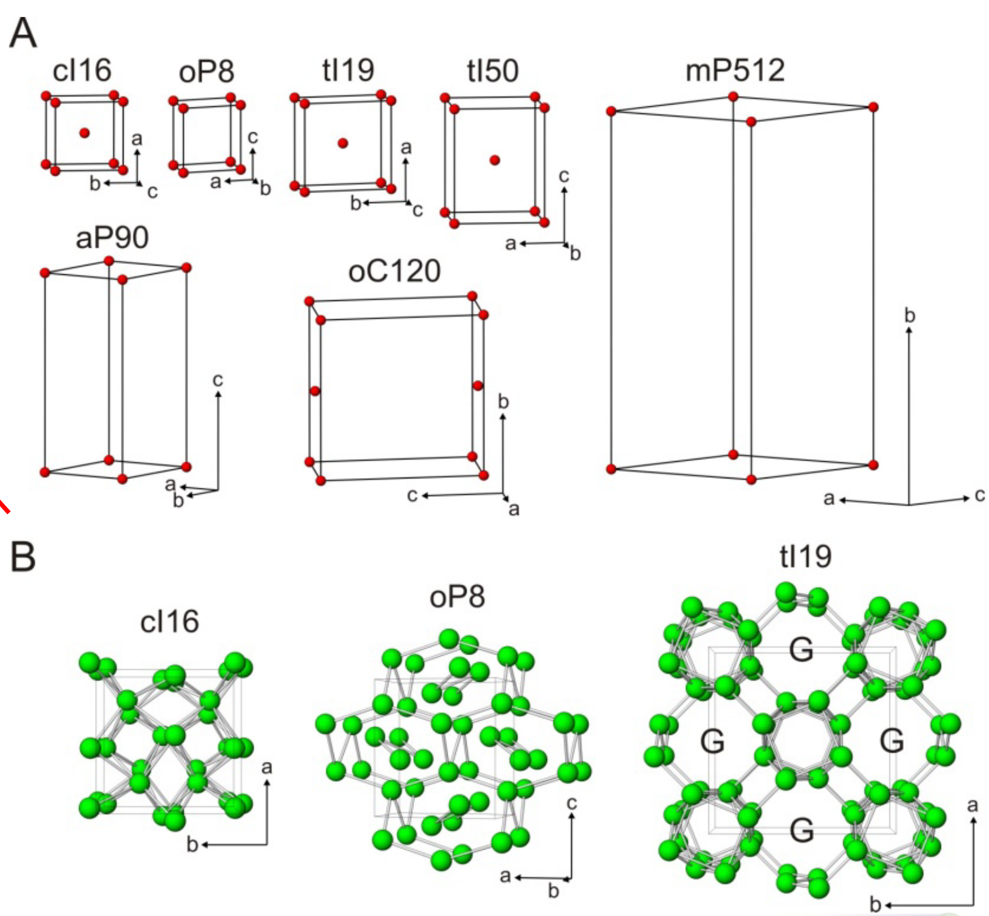
Unexpected phase behavior and complexity in 'simple' metals

CDAC



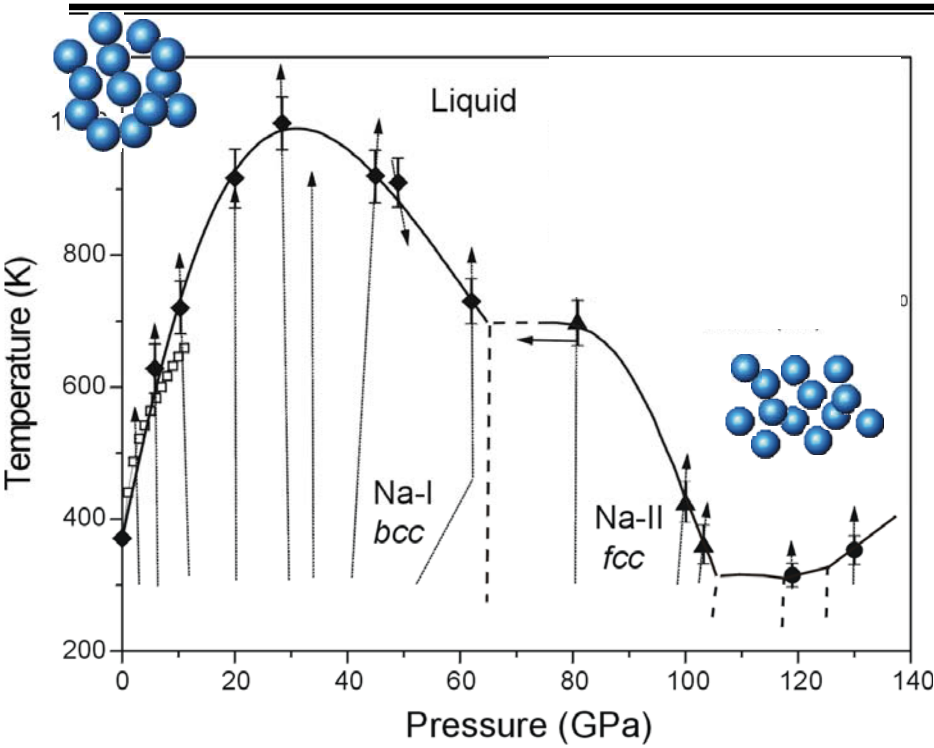
[Gregoryanz *et al*. *Phys. Rev. Lett.*. (2005)]

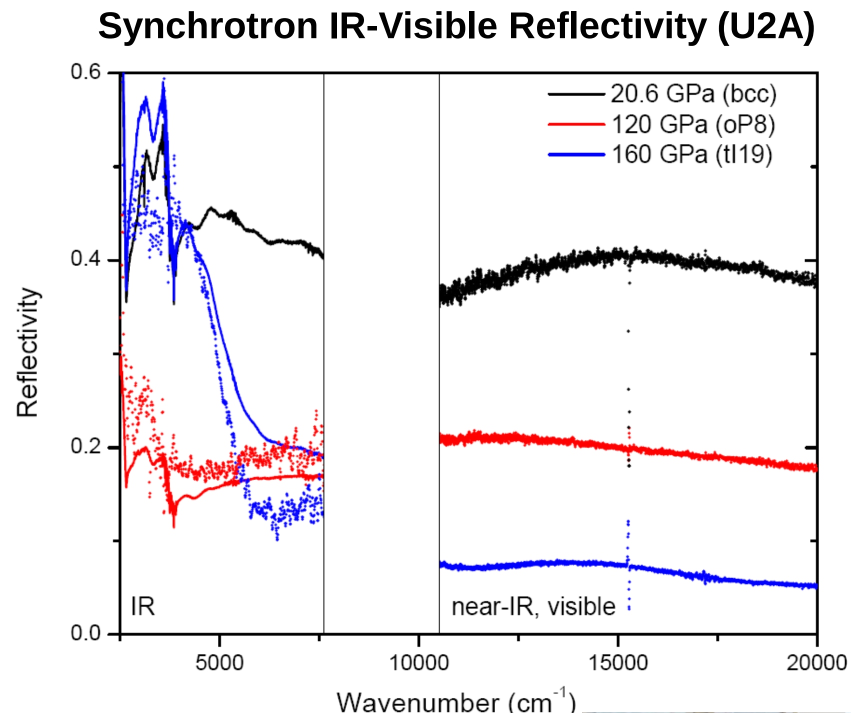
[Gregoryanz et al., *Science* (2008)]



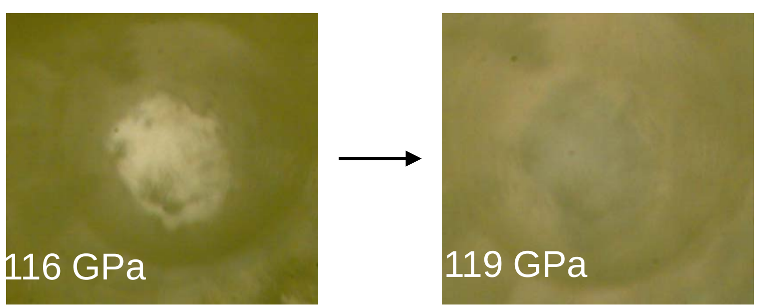
Sodium undergoes a metal to insulator transition at multimegabar pressures

CDAC





[Gregoryanz *et al*. *Phys. Rev. Lett.*. (2005)]



Reflectivity measurements and first-principles calcuations indicate a sudden decrease in free electron metallic behavior across the cI16-oP* transition

A. Lazicki *(Carnegie postdoc)*

CARNEGIE INSTITUTION FOR SCIENCE

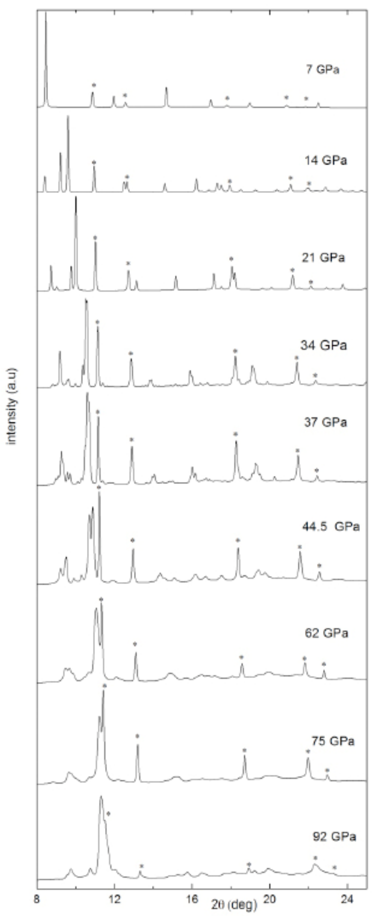
[Lazicki *et al., PNAS* (2009)]
[see also, Ma et al., *Nature* (2009)]

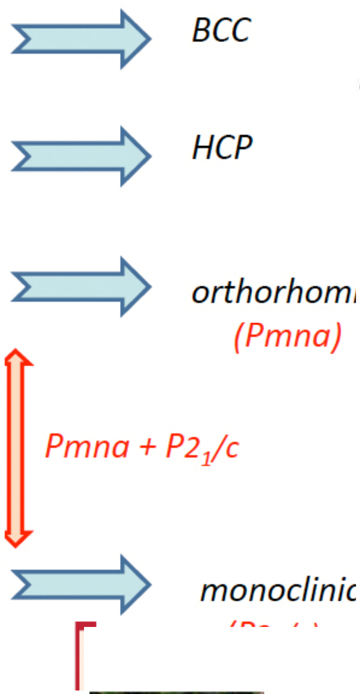
Continued studies of phase transformations and *P-V-T* EOS of elemental metals

2. SCIENCE

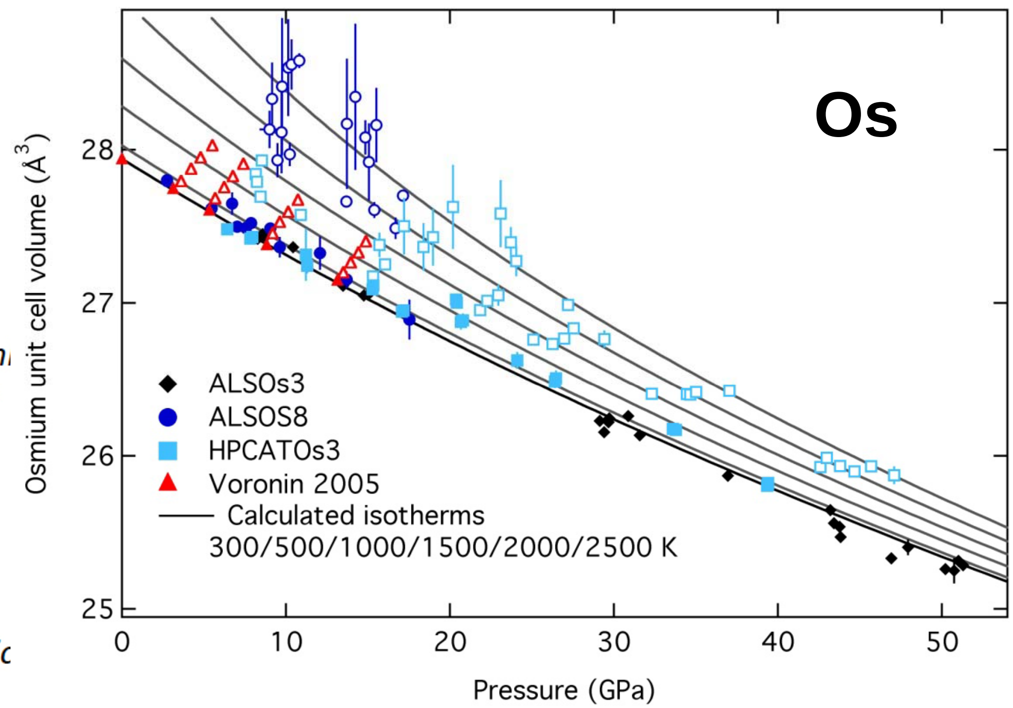
CDAC

- ***Eu is the 'newest' elemental superconductor***





W. Bi *(CDAC graduate student, Washington Univ.)*



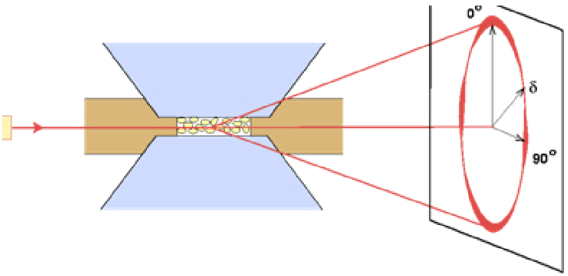
- ***High strength and incompressibility***
- ***P-V-T EOS of interest for metals systematics***

Matt Armentrout *(CDAC graduate student. UCLA)*

NNSA

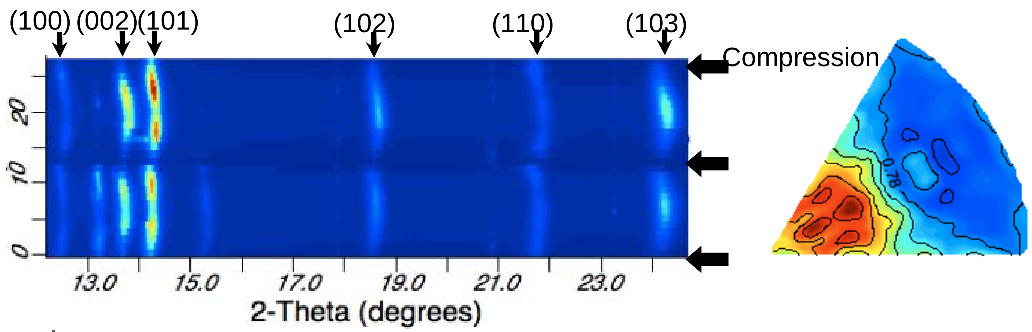
Twinning is a significant deformation mechanism in hexagonal metals at high pressure

CDAC

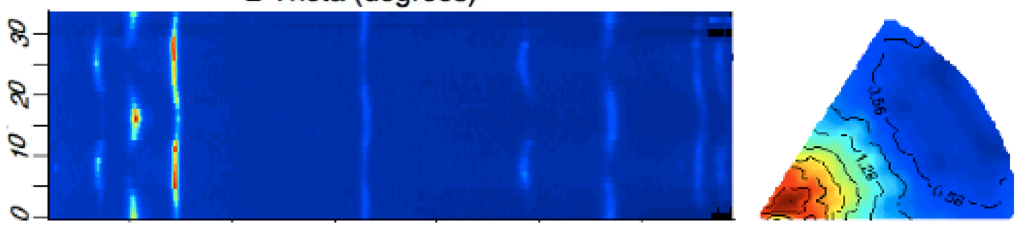


DAC in radial diffraction geometry to impose stress and pressure on pure osmium and zinc, inducing elastic and plastic deformations. The two hcp metals behave very differently.

Os
at 24 GPa
(2.0 m.r.d.)



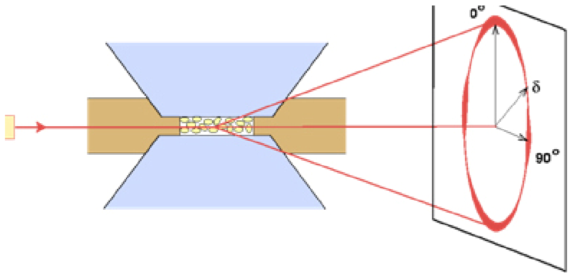
Zn
at 34 GPa
(3.1 m.r.d.)



W. Kanitpanyacharoen
P. Kaecher, CDAC graduate students (UC Berkeley)

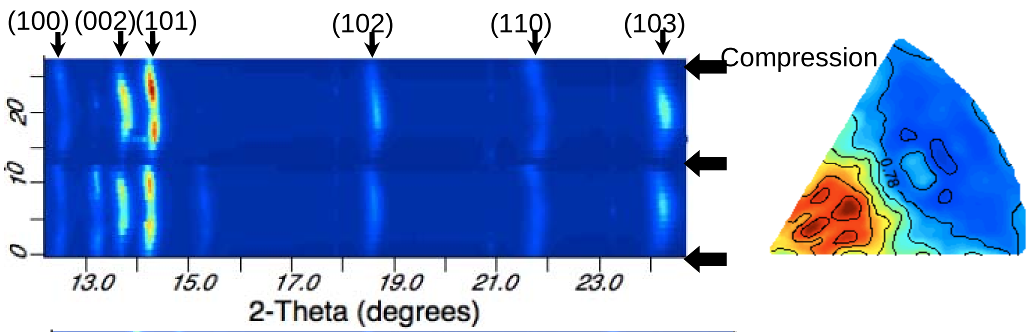
Twinning is a significant deformation mechanism in hexagonal metals at high pressure

CDAC

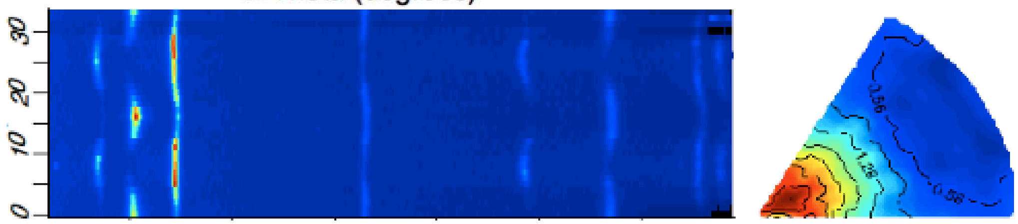


DAC in radial diffraction geometry to impose stress and pressure on pure osmium and zinc, inducing elastic and plastic deformations. The two hcp metals behave very differently.

Os
at 24 GPa
(2.0 m.r.d.)

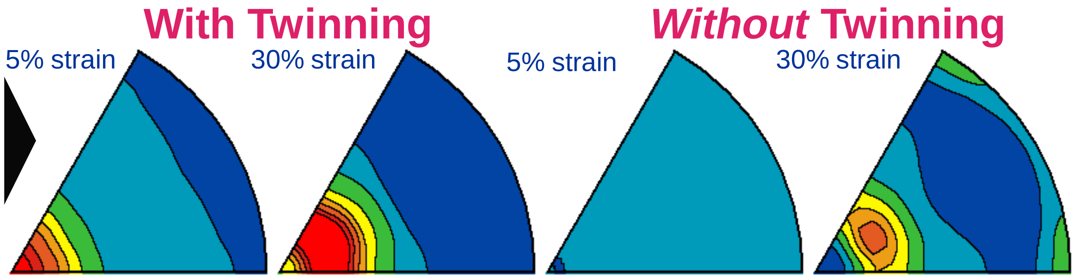


Zn
at 34 GPa
(3.1 m.r.d.)



W. Kanitpanyacharoen
P. Kaecher, CDAC graduate students (UC Berkeley)

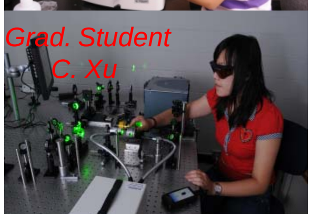
The visco-plastic self-consistent (VPSC) polycrystal model is used to provide insight into which slip systems and twinning modes are active under a given set of conditions.

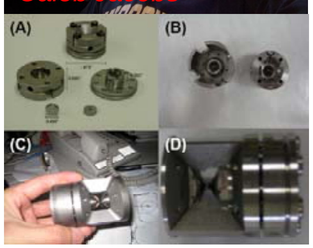


NNSA

Carnegie/DOE Alliance Center

Lattice dynamics of iron is directly measured at extreme *P-T* by inelastic x-ray scattering (IXS)

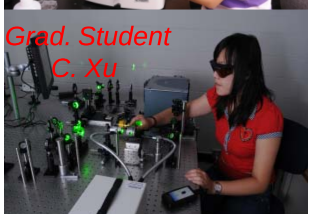


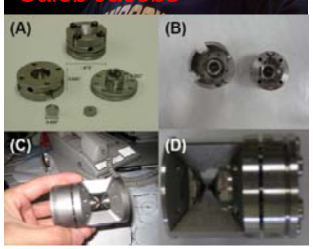


Lattice dynamics of iron is directly measured at extreme *P-T* by inelastic x-ray scattering (IXS)

2. SCIENCE

CDAC



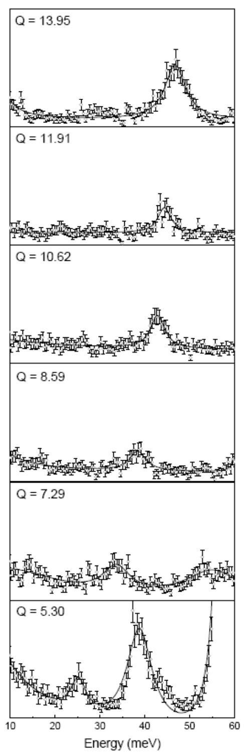


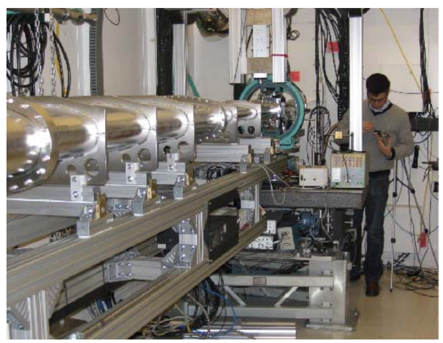
HERIXS on Hot Dense Fe

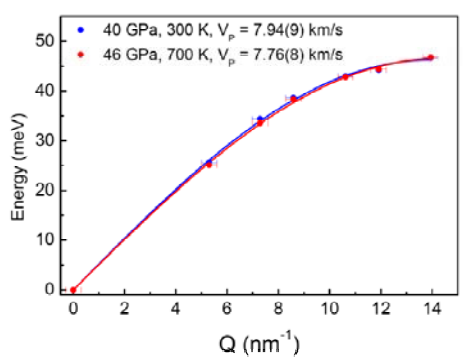
High energy resonant IXS (resolution of ~2 meV and beamsize of 25 μm at XOR3, LA phonon dispersions of hcp-Fe. HT has a strong effect on the Vp.

Phonon Dispersions 46GPa/700K

System setup at XOR3, APS





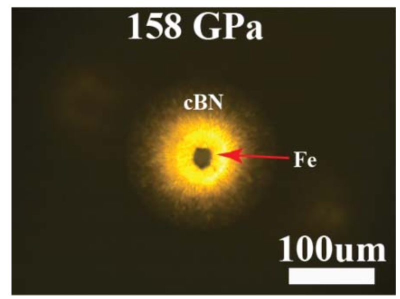


Z. Mao, J. F. Lin, G. Xu, A. Alatas, Compressional wave velocity of hcp-Fe at high pressures and temperatures, in prep., 2010.

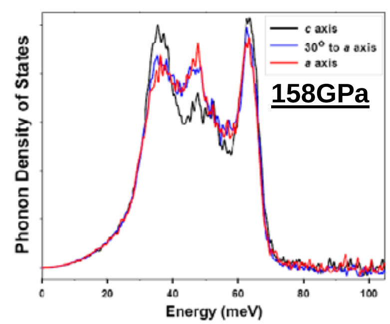
NRIXS on Textured hcp-Fe

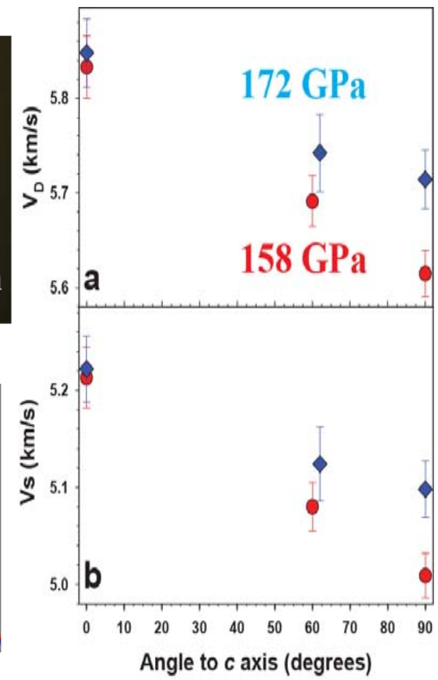
Nuclear Resonant IXS Vs is 4.1 % faster along the c relative to a axis giving elastic, vibrational, and thermodynamic parameters.

Hcp-Fe in cubic BN/Be gasket



Phonon Density of States





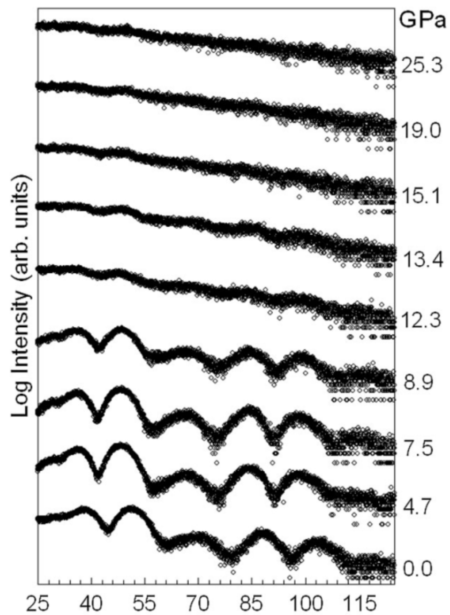
J. F. Lin, Z. Mao, H. Yavas, J. Zhao, and L. Dubrovinsky, Shear wave anisotropy of textured hcp-Fe in Earth's inner core, in submission, 2010.

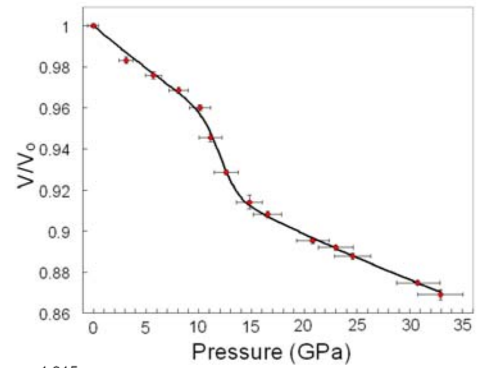
Carnegie/DOE Alliance Center

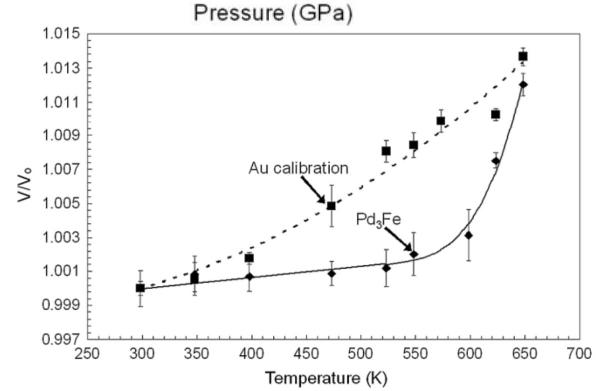
Pressure-induced Invar effect has been discovered in Pd_3Fe

CDAC

- It is possible to tune Invar behavior with pressure, rather than composition.
- The electronic structure at the Invar transition is the same for either composition-tuned or pressure-tuned Invar.







PRL **102,** 237202 (2009) PHYSICAL REVIEW LETTERS week ending 12 JUNE 2009

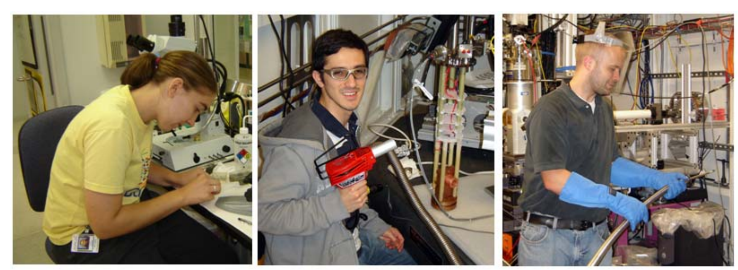
Pressure-Induced Invar Behavior in Pd_3Fe

M. L. Winterrose,[1] M. S. Lucas,[1] A. F. Yue,[1] I. Halevy,[1] L. Mauger,[1] J. A. Muñoz,[1] Jingzhu Hu,[2] M. Lerche,[3] and B. Fultz[1]

[1]*California Institute of Technology, W. M. Keck Laboratory 138-78, Pasadena, California 91125, USA*
[2]*National Synchrotron Light Source, University of Chicago, Upton, New York 11973, USA*
[3]*HPSynC, Carnegie Institution of Washington, Argonne, Illinois 60439, USA*
(Received 24 February 2008; published 10 June 2009)

Synchrotron x-ray diffraction (XRD) measurements, nuclear forward scattering (NFS) measurements, and density functional theory (DFT) calculations were performed on $L1_2$-ordered Pd_3Fe. Measurements were performed at 300 K at pressures up to 33 GPa, and at 7 GPa at temperatures up to 650 K. The NFS revealed a collapse of the ^{57}Fe magnetic moment between 8.9 and 12.3 GPa at 300 K, coinciding with a transition in bulk modulus found by XRD. Heating the sample under a pressure of 7 GPa showed negligible thermal expansion from 300 to 523 K, demonstrating Invar behavior. Zero-temperature DFT calculations identified a ferromagnetic ground state and showed several antiferromagnetic states had comparable energies at pressures above 20 GPa.

DOI: 10.1103/PhysRevLett.102.237202 PACS numbers: 75.50.Bb, 62.50.−p, 71.20.Be, 76.80.+y

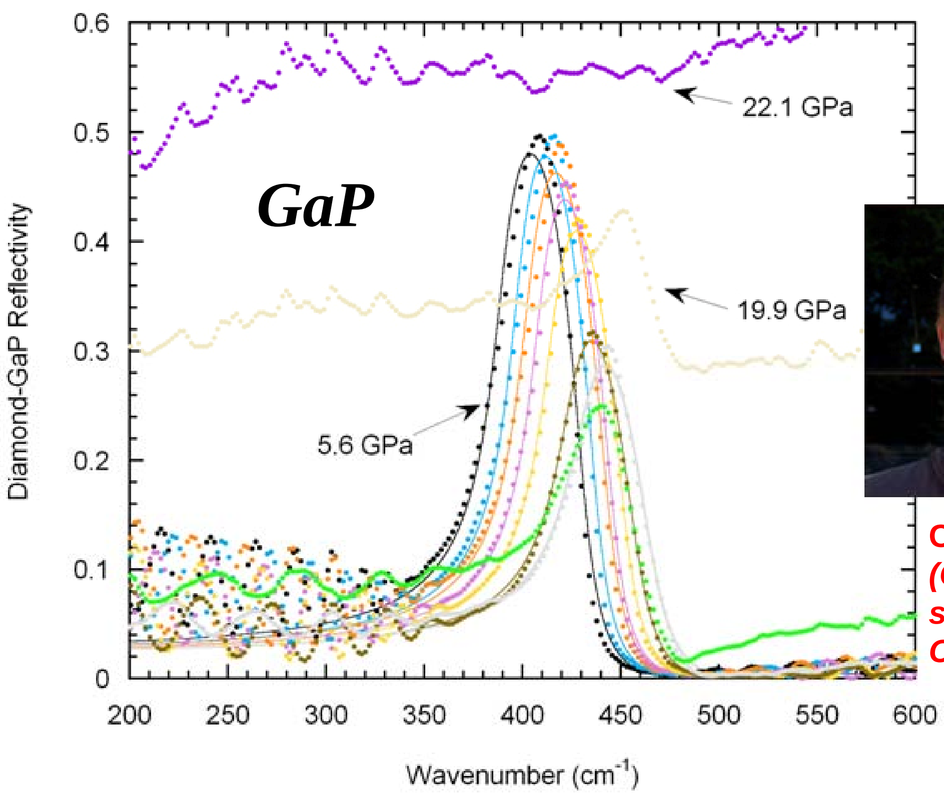


L. Mauger J. Munoz M. Winterrose
(CDAC graduate students, Caltech)

Infrared reflectivity of studies of pressure-induced insulator-metal transitions

CDAC

Far-IR Reflectivity U2A at NSLS



C. Seagle *(CDAC grad. student, Chicago)*

Reflectivity of the diamond-GaP interface at high pressure. The main peak in the spectrum is due to the TO phonon mode which shifts to higher wavenumber and decreases in intensity as pressure is increased. The disappearance of the phonon mode and sharp rise in the magnitude of the reflectivity are associated with the metallization of GaP at 20 GPa.

Far IR of FeO under pressure

[Seagle *et al., Phys. Rev. B* (2009)]

CARNEGIE INSTITUTION FOR SCIENCE

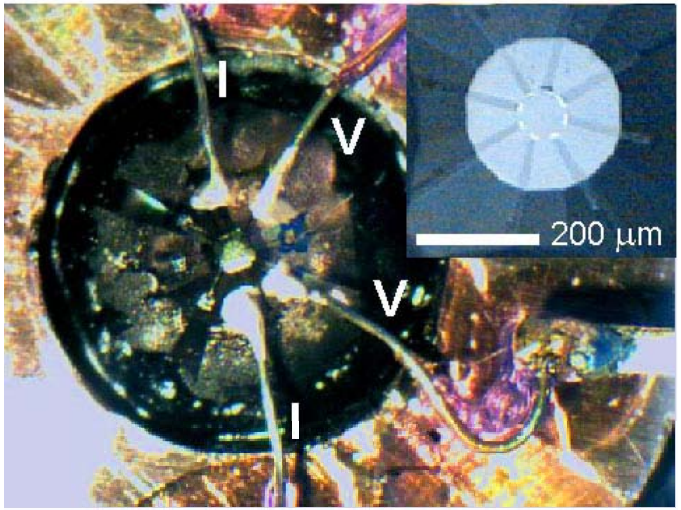
NNSA

Structural and magnetic phase transitions in NdCoAsO

CDAC

- **Iron-based layered compound $SmFeAsO_{1-x}F_x$ is known to exhibit superconductivity at 55 K**

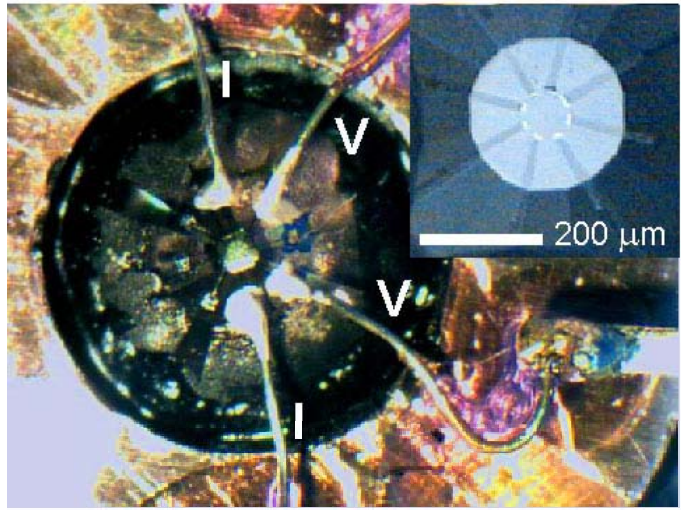
- **NdCoAsO is isostructural to layered superconductors**



Designer diamond anvil for electrical studies at high pressures and low temperatures

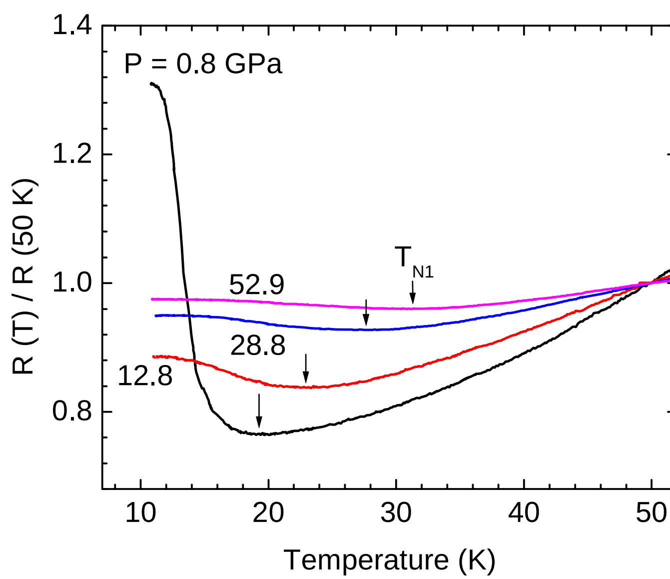
Structural and magnetic phase transitions in NdCoAsO

- **Iron-based layered compound $SmFeAsO_{1-x}F_x$ is known to exhibit superconductivity at 55 K**
- **NdCoAsO is isostructural to layered superconductors**
- **Magnetic ordering and superconducting transitions are detected by four probe electrical resistance measurements**



Designer diamond anvil for electrical studies at high pressures and low temperatures

W. Uhoya
(CDAC grad. student, UAB)

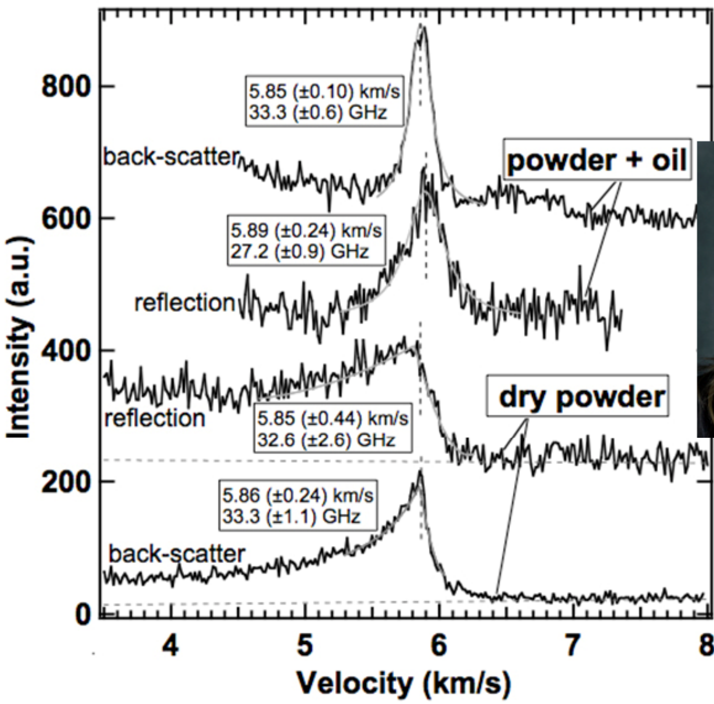


Material shows anti-ferromagnetic behavior to 53 GPa

EOS, phase transitions, and 'polyamorphism' of liquids and amorphous solids

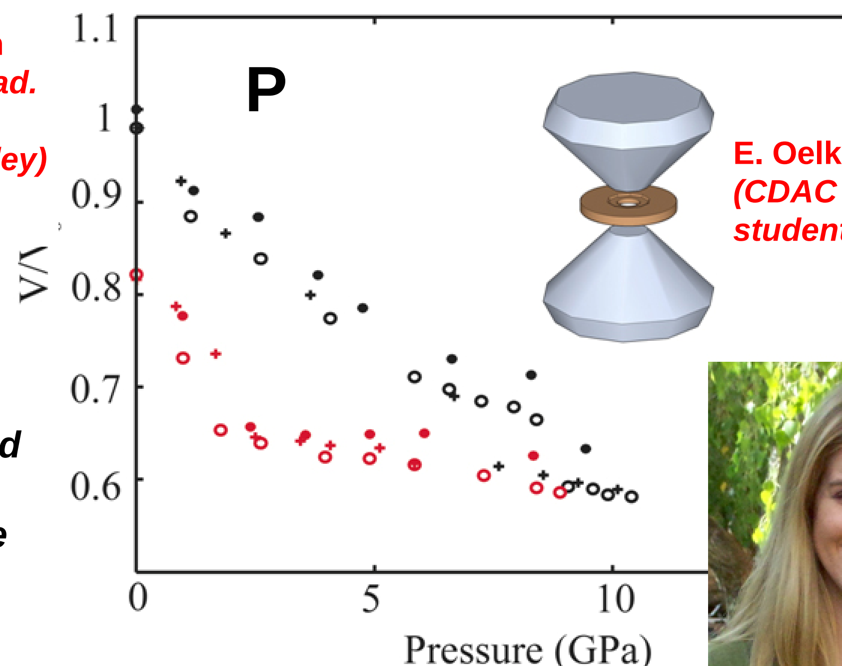
CDAC

Brillouin spectroscopy, ultrasonic, and diffraction techniques



A Gleason
(CDAC grad. student, UC Berkeley)

Brillouin spectra of soda-lime glass powder at ambient conditions (P = 0 GPa, T = 290 K) in back-scatter (top and bottom spectra: θ = 180˚) and reflection geometries (middle two spectra: θ' = 110˚),



E. Oelker
(CDAC graduate student, ASU)

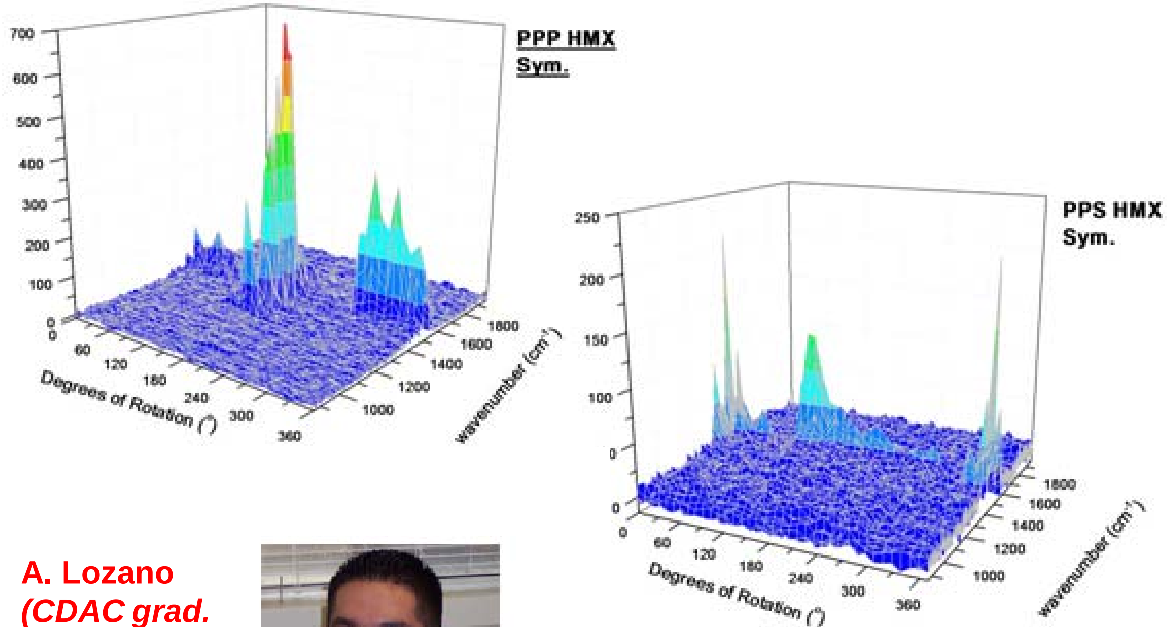
Measured DAC EOS for amorphous red phosphorus. The three sets of symbols represent separate runs. The compression data is in black and the decompression data is in red. Inset:

Surface chemistry and spectroscopy under extreme conditions

2. SCIENCE

CDAC

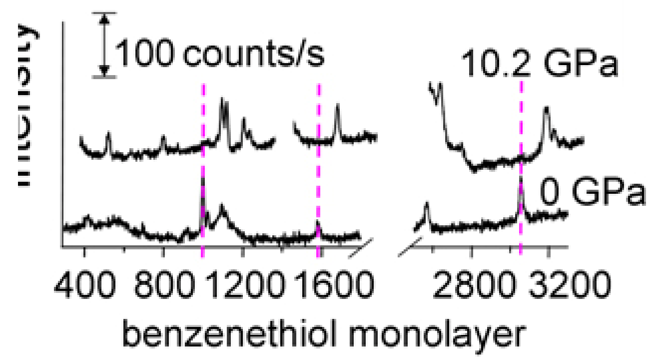
Sum Frequency Generation (SFG)



A. Lozano
(CDAC grad. student (UIUC)

SFG spectra of HMX of surface nitro groups in two polarization conditions (SFG, vis, IR) as the crystal is rotated. Spectra such as these should determine the orientation of surface nitro groups.

Raman spectrum of benzenethiol monolayer on photonic substrate in the DAC at 10.2 GPa.



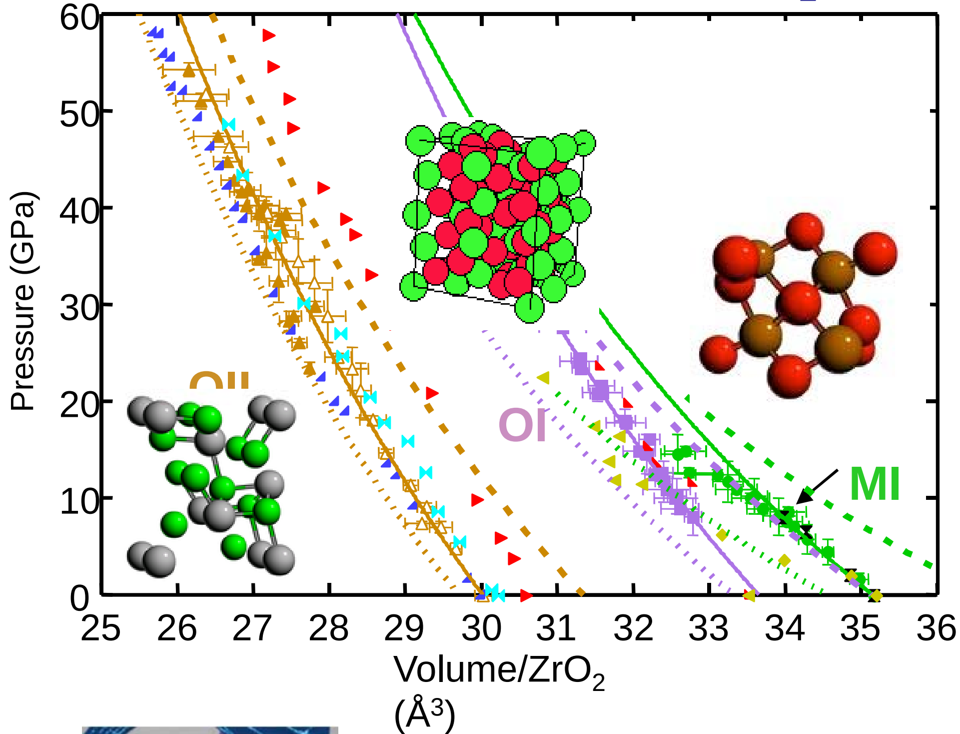
K. Brown
(CDAC grad. student (UIUC)

NNSA

There are new findings in high-pressure strength and toughness

CDAC

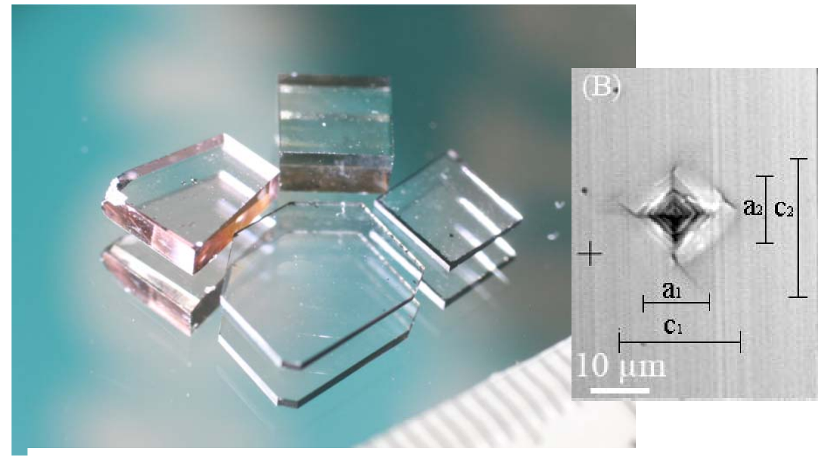
Hardness from EOS of ZrO_2

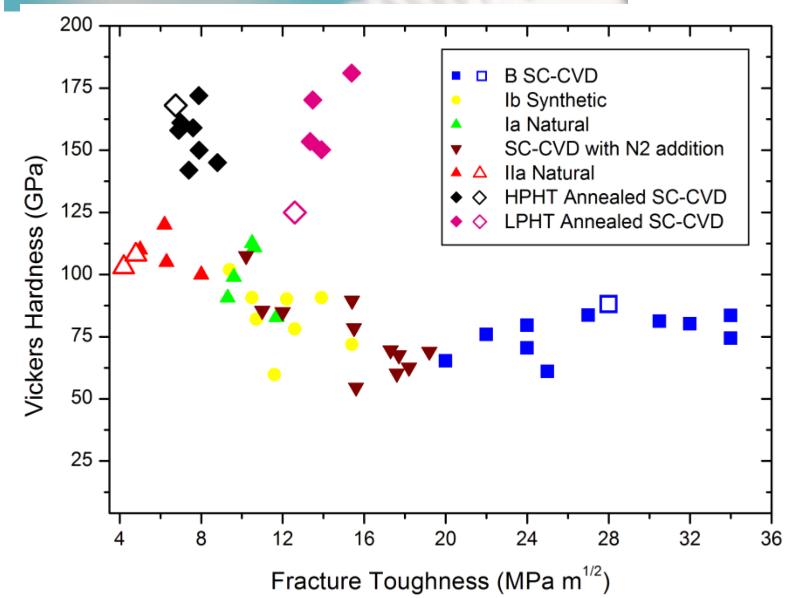


H(OII) < *H*(MI) < *H*(OI)
G(OII) < *G*(MI) < *G*(OI)
K(OII) > K(OI) > K(MI)
For all phases, *H* ~ 10 GPa

Y. Al-Khatatbeh (CDAC Grad. student, NMSU)

Ultratough CVD Diamond





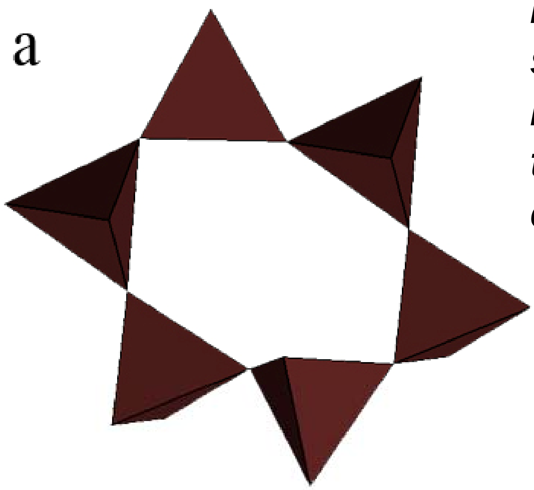
[Liang *et al*., *J. Phys. Cond. Matter*. (2009)]

Understanding the behavior of hydrogen in materials under pressure is fundamental

CDAC

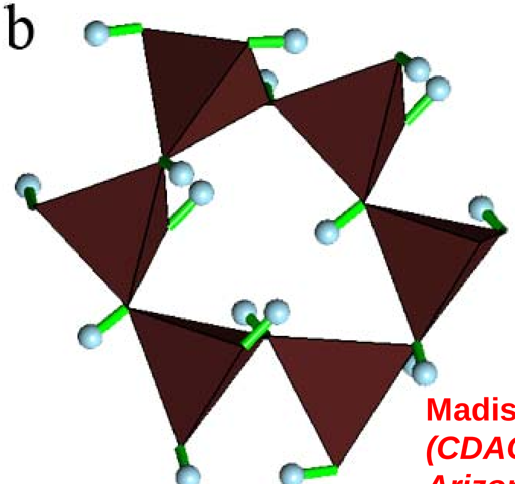
$Be(OH)_2$

a



Polyhedral image of the six-membered ring of silicate tetrahedra in cristobalite

b

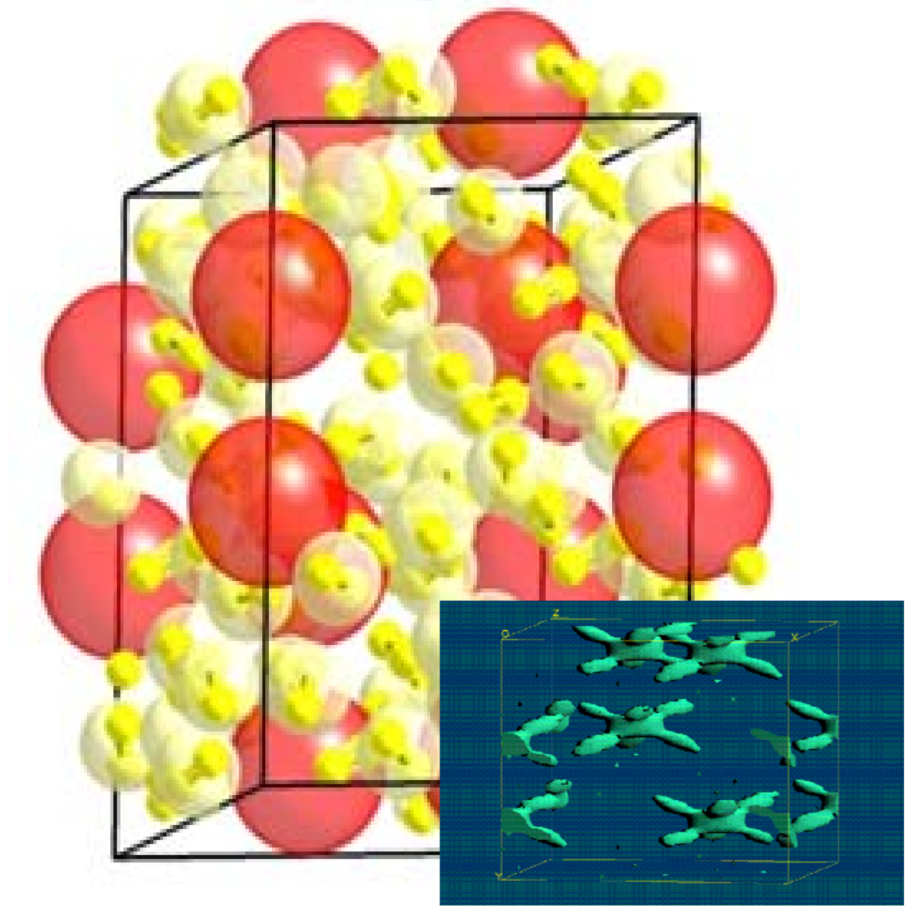


Equivalent ring of $Be(OH)_4$ tetrahedra in behoite

SCIENCE

Madison Barkley *(CDAC grad. student, Univ. Arizona)*

$Xe(H_2)_7$



- **Novel dimer structure**
- **Highest mole percent hydrogen**
- **Pressure-induced covalency**

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

NNSA

Novel intermolecular interactions in high-pressure van der Waals compounds

CDAC

- **SiH_4 is a metal/ superconductor at 100 GPa**

- **Discovery of $SiH_4(H_2)_2$**

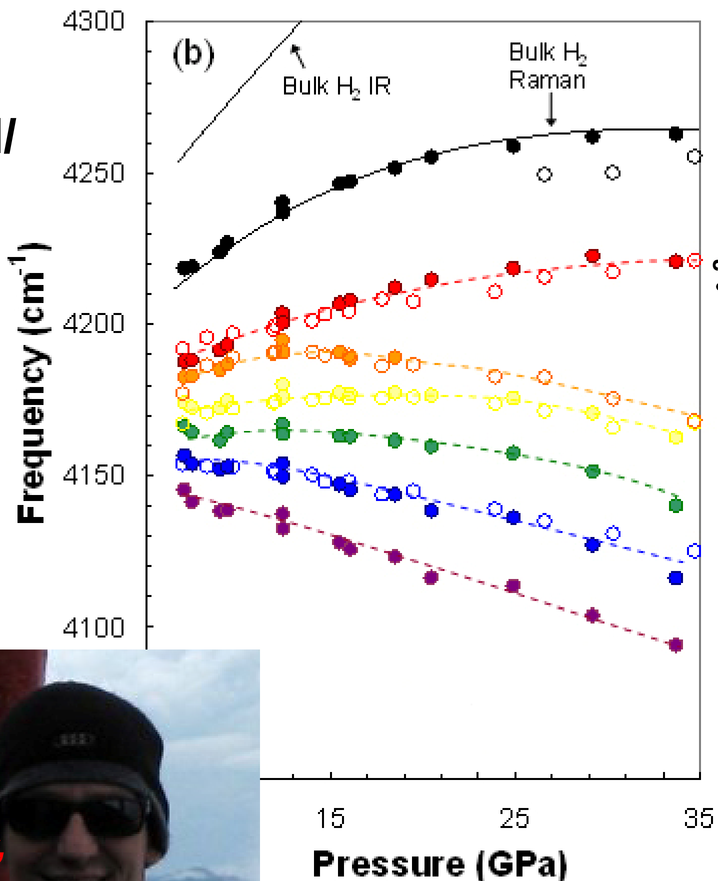
Novel intermolecular interactions in high-pressure van der Waals compounds

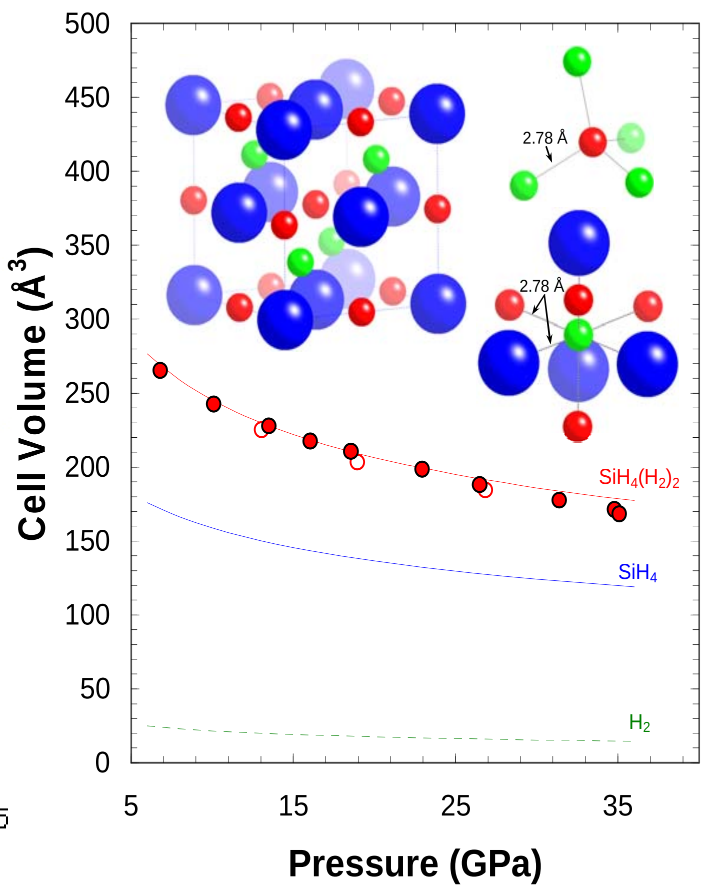
2. SCIENCE

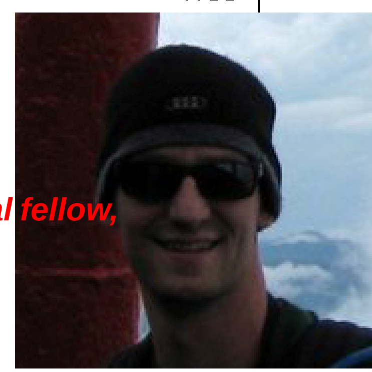
CDAC

- SiH_4 is a metal/ superconductor at 100 GPa

- Discovery of $SiH_4(H_2)_2$







Tim Strobel *(postdoctoral fellow, Carnegie)*

- **Intramolecular H-H bond weakens significantly**
- **Pathway for dissociation/metallization of H_2**

[Strobel et al., *Phys. Rev. Lett.* (2009)]

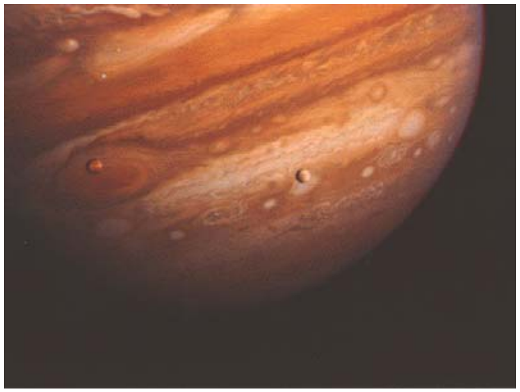
CARNEGIE INSTITUTION FOR SCIENCE

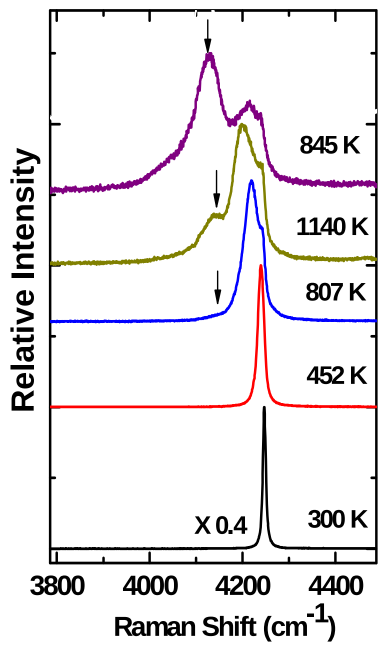
NNSA

New high *P-T* Raman measurements constrain the phase diagram of hydrogen

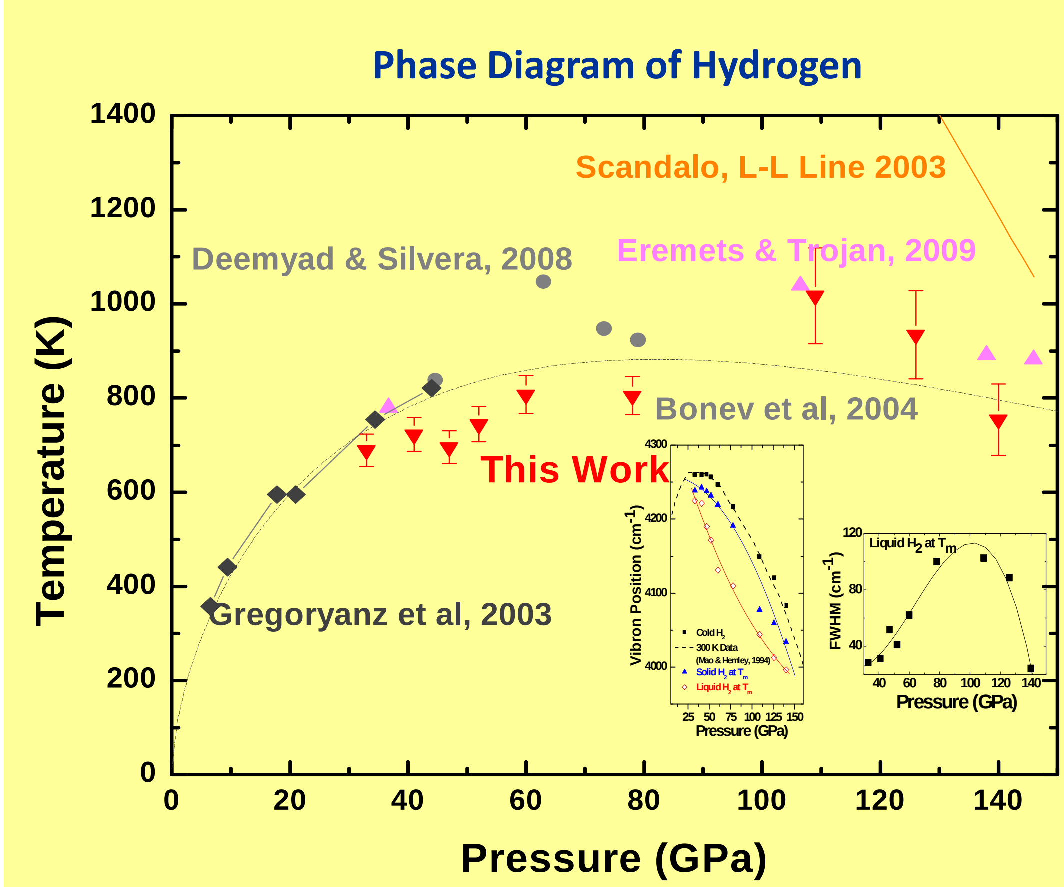
2. SCIENCE

CDAC





High P-T Raman
60 GPa

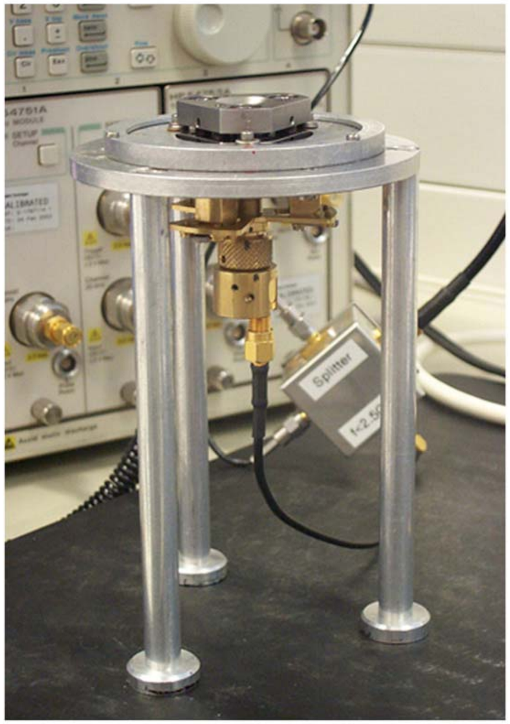


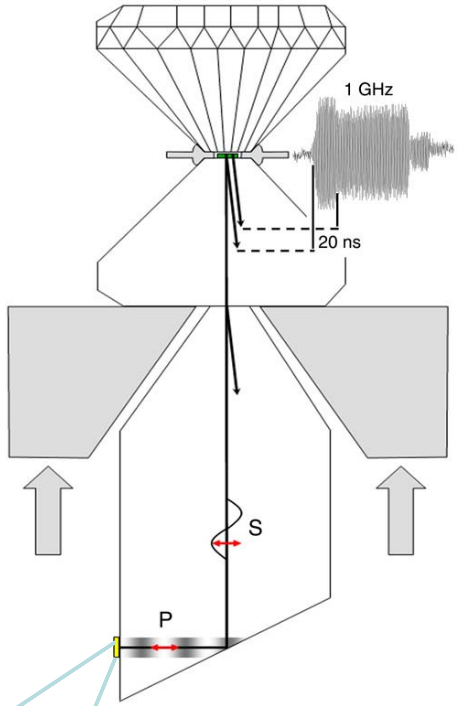
- Melting behavior studied to 110 GPa from observation of vibron discontinuity
- Possibility of a high temperature solid-solid transition above 110 GPa ?

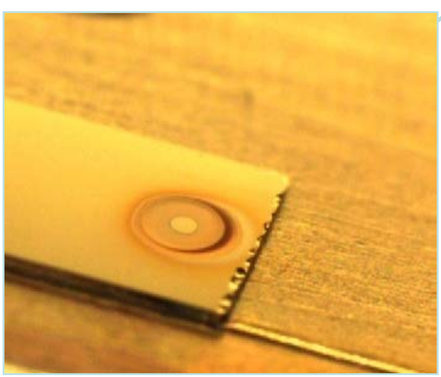
N. Subramanian (CDAC postdoc, Carnegie)

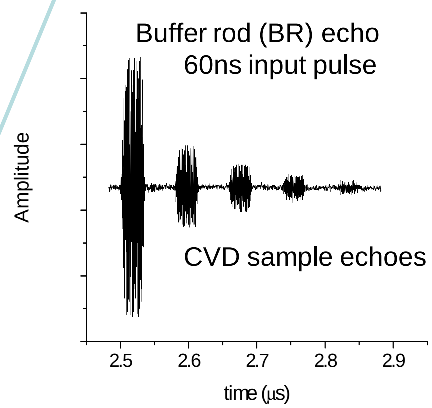
Gigahertz-ultrasonic interferometry elastic properties of superhard materials

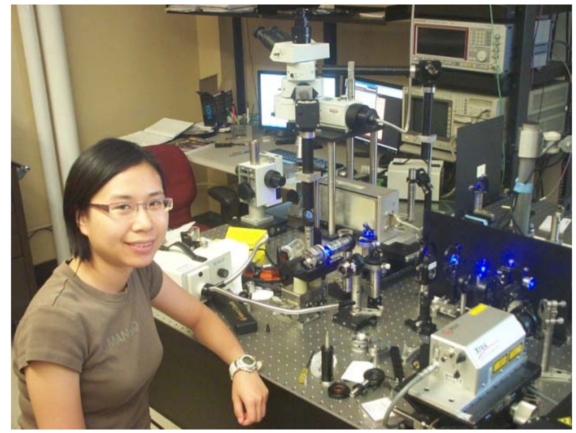
CDAC





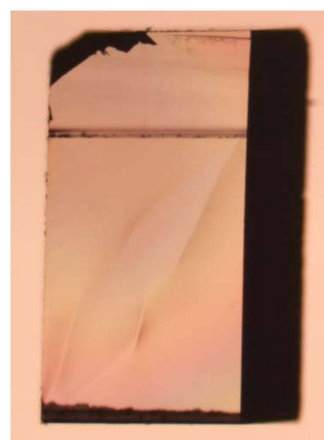






Y. Chang
(CDAC grad. student, Northwestern)

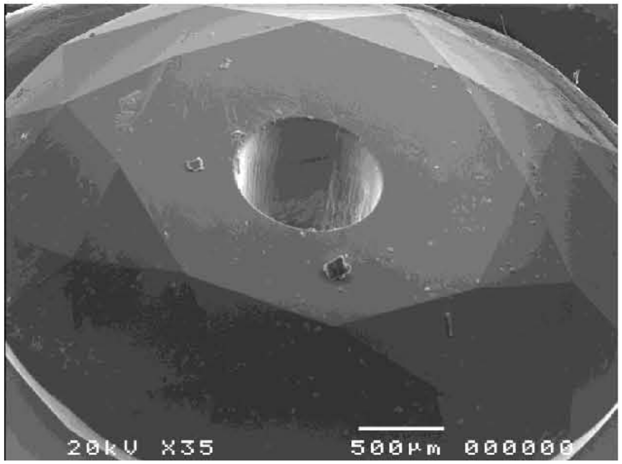
Application to CVD diamond: benchmark for elasticity studies

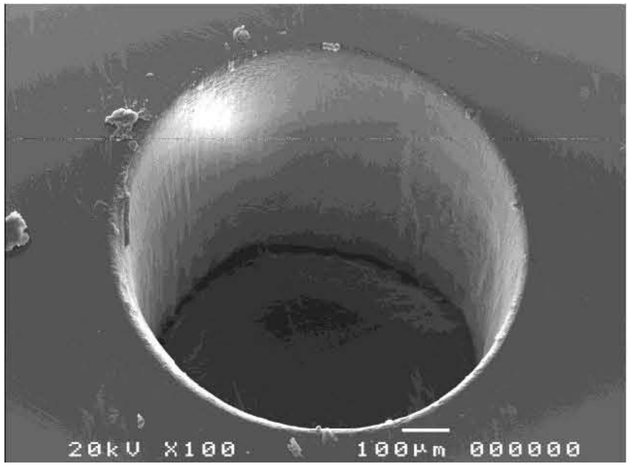


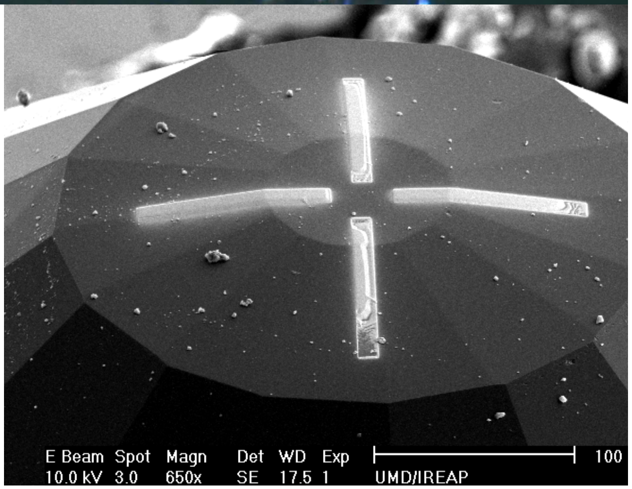
Acoustic wavelengths are <20µm at GHz-frequencies. Accurate C_{ij} can be obtained on transparent or opaque single-crystal and glassy materials as thin as 20µm, as well as at high P-T inside diamond-anvil cells for application to equations of state.

CVD single crystal diamond for a new generation of anvils

CDAC





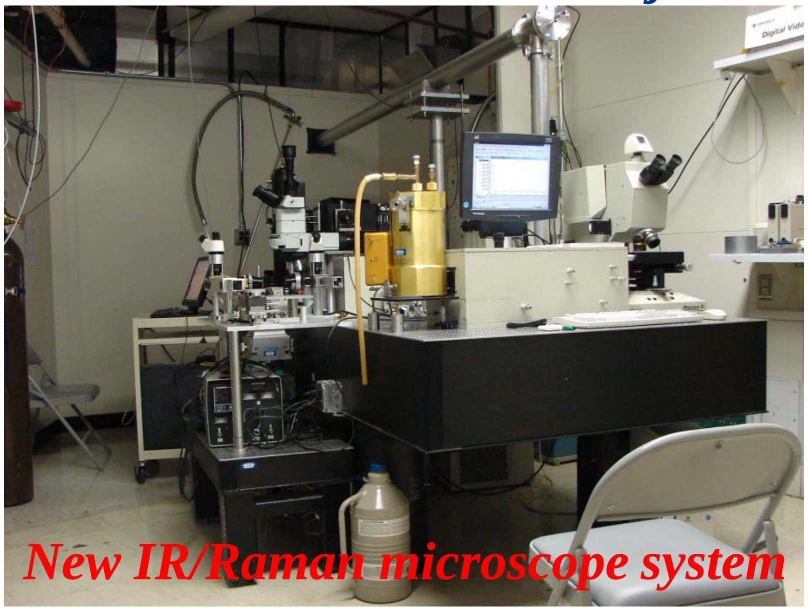


Major upgrade of the U2A beamline for spectroscopic studies under extreme conditions

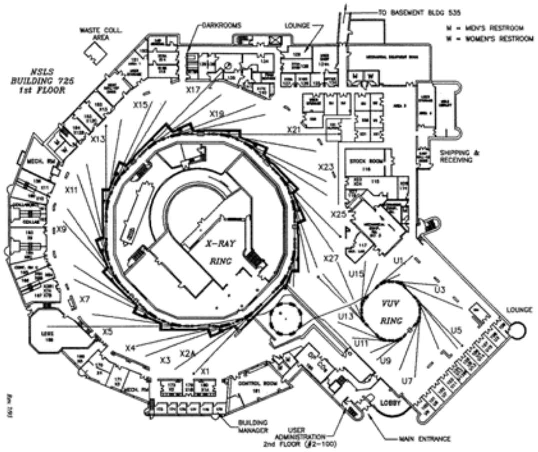
3. NEW TECHNIQUES

CDAC

Major Beamline Upgrades



- ***New capability: far-IR reflection***
- ***Routine high pressure experiments in the range of 10-1000 K***
- ***Extended side station to achieve ideal performance in terms of diffraction limited resolution***
- ***Path to NSLS II***

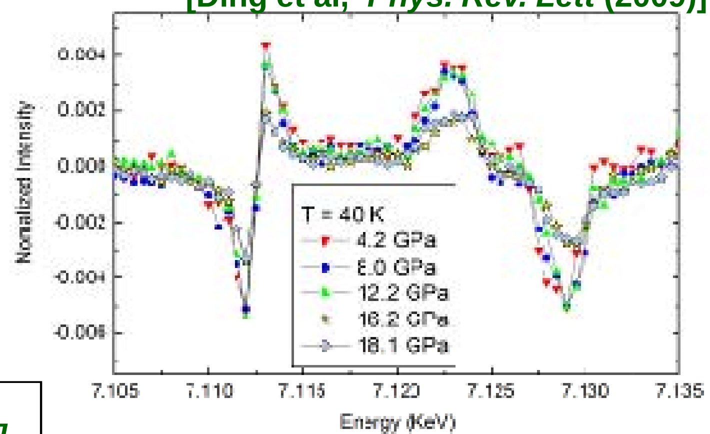


Many new tools are coming on line at HPCAT and HPSynC

CDAC

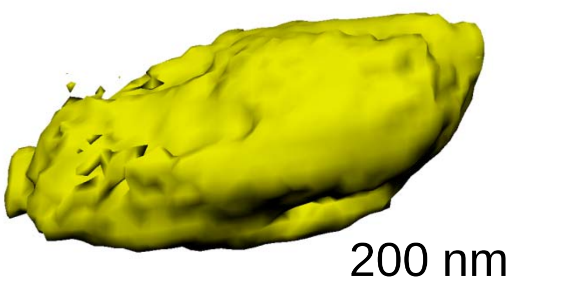
- *Nano imaging (TXM), diffraction*
- *Coherent diffraction imaging (CDI)*
- *High energy scattering (PDF)*
- *High energy resolution:*
- *HERIX and MERIX*
- *Time resolved: shock wave, XPCS*
- *Magnetic circular dichroism (XMCD)*

Spin transition of Fe_3O_4 discovered by XMCD technique
[Ding et al, *Phys. Rev. Lett* (2009)]



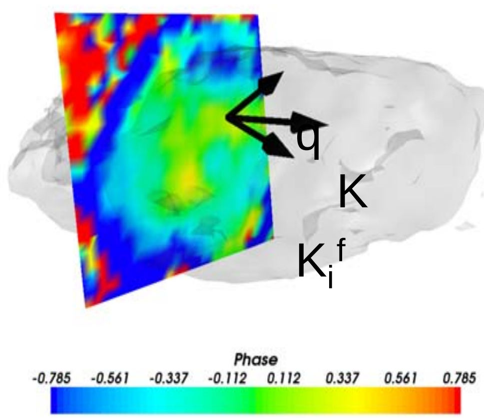
Coherent diffraction imaging
3D reconstruction from a single crystal of Au at 6 GPa

[Yang et al, *to be published*]

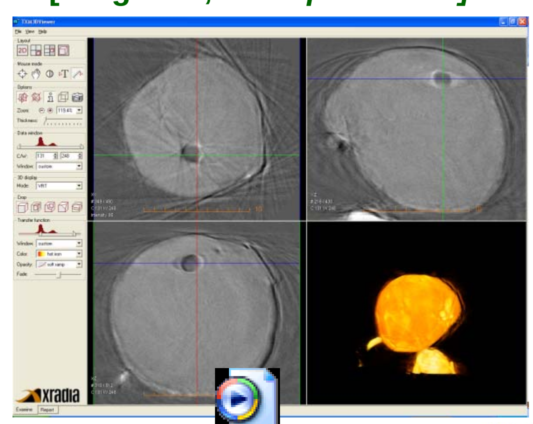


Magnitude reconstruction

Phase reconstruction



3d full field imaging (TXM)
30 nm spatial resolution
[Ding et al, *to be published*]



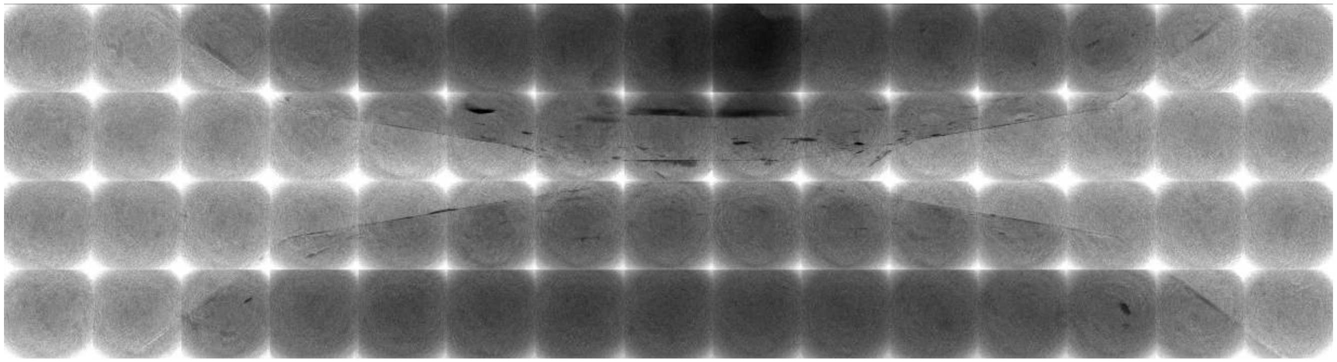
Tin_TXM_tomo.mpg

CARNEGIE INSTITUTION FOR SCIENCE

NNSA

Using nanoscopes and nanobeams to measure anvil strains to maximize pressure

CDAC



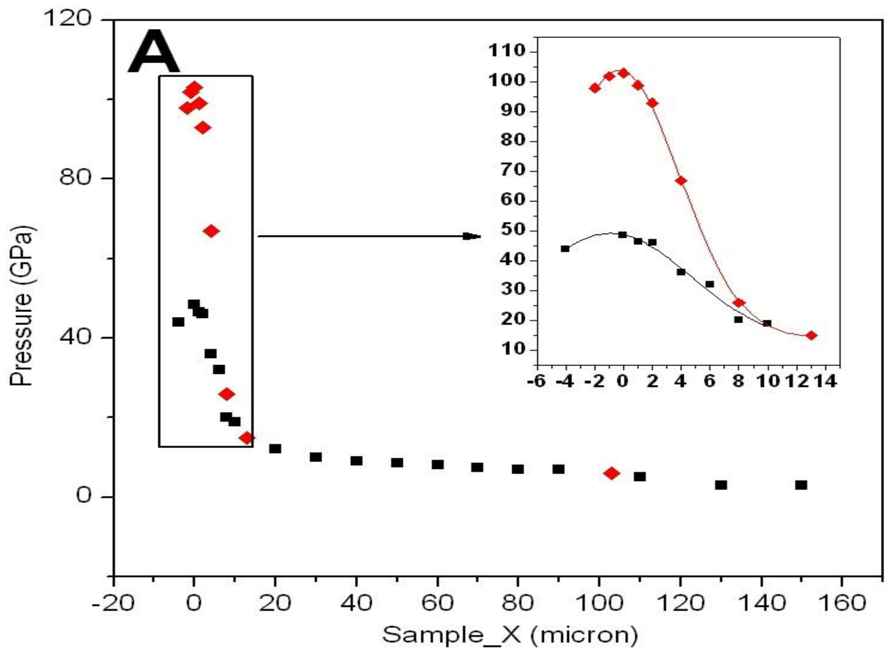
30 nm resolution radiography

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

Xradia nanoscope

Nanodiffraction (< 200 nm beams) mulitimegabar pressures measures the pressure gradient

[Wang *et al. PNAS* (2010)]



CARNEGIE INSTITUTION FOR SCIENCE

A new generation of large facilities are coming on line

CDAC

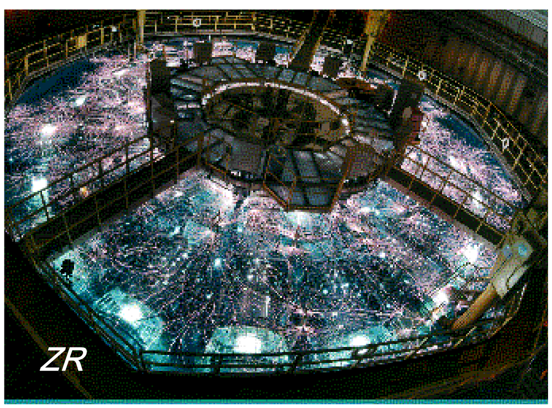
X-ray Sources

- *Higher brightness synch.*
- *Dynamic compression*
- *Energy Recovery Linacs*
- *Fourth Gen. Sources (LCLS).*

Neutron Sources

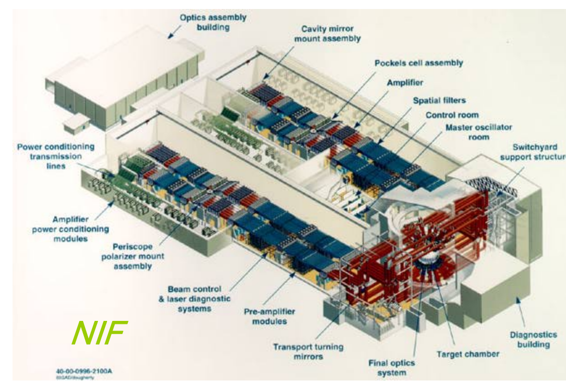
- *Dedicated beamlines*
- *>100 GPa neutron scattering*

Pulsed Power



- *Ultrahigh P-T conditions*
- *Larger samples*
- *Static/dynamic*

Laser Sources

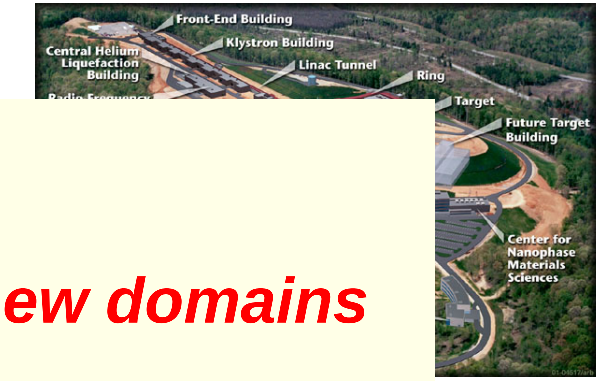


- *Still higher P-T conditions*
- *New diagnostics*
- *Static/dynamic*

A new generation of large facilities are coming on line

CDAC

X-ra
Sourc



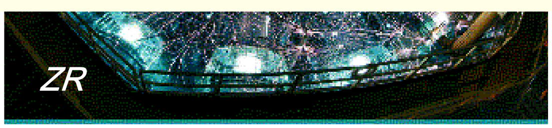
GRAND CHALLENGES

- *New inelastic scattering in new domains*
- *Time dependent (<ps-scale) diffraction/imaging*
- *Heterogeneous/complex assemblages: nm-diffraction*
- *Interfaces/grain boundaries*
- *New domains of P-T-t*

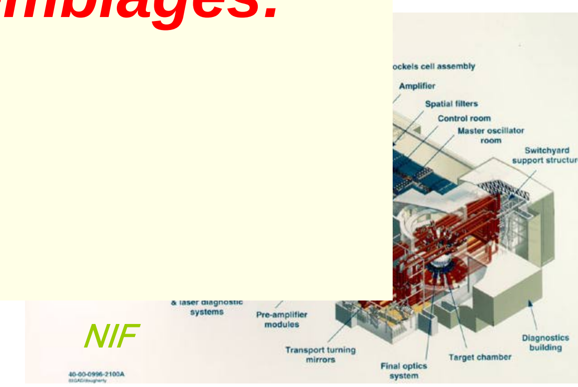
-
-
-
-

ring

Pul
Po



- ***Ultrahigh P-T conditions***
- ***Larger samples***
- ***Static/dynamic***

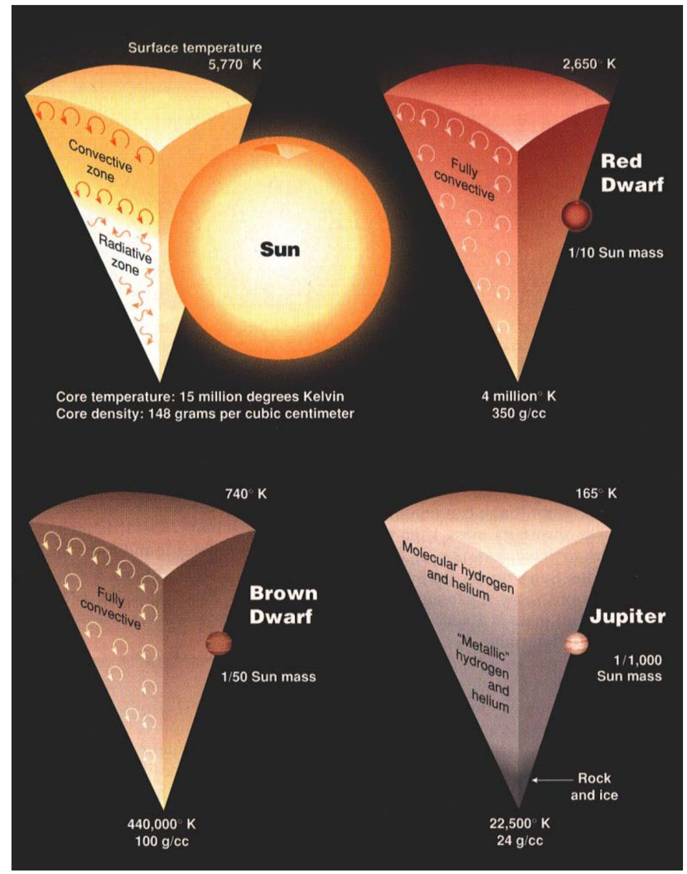


- ***Still higher P-T conditions***
- ***New diagnostics***
- ***Static/dynamic***

CDAC is supporting studies with ultrastrong shocks and isentropic compression techniques

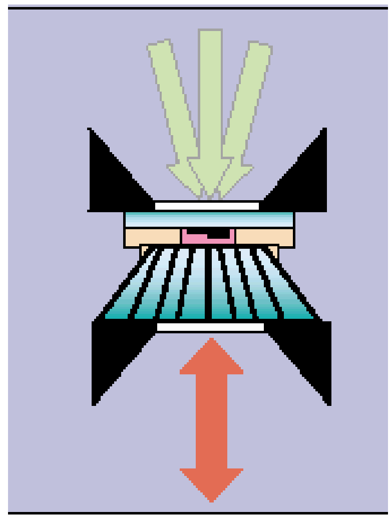
CDAC

- Hydrogen and helium at TPa pressures
- Fast ramp wave loading
- Chemistry at ultraextreme conditions
- Rigidity and plasticity
- Going beyond the EOS
- Wave-velocities in super-giant planets
- Rigidity of material properties
- Gigabar pressures
- Support of ICF



- Combined static/ dynamic compression
- Ultra-fast diagnostics

NIF Planetary Interiors Science Team



CONCLUSIONS AND OUTLOOK

CDAC

1. Education and Training

- **Expanded student program with increased partners**
- **High-pressure summer school/workshops**
- **Continued increase in number of CDAC collaborators**

2. Science Program

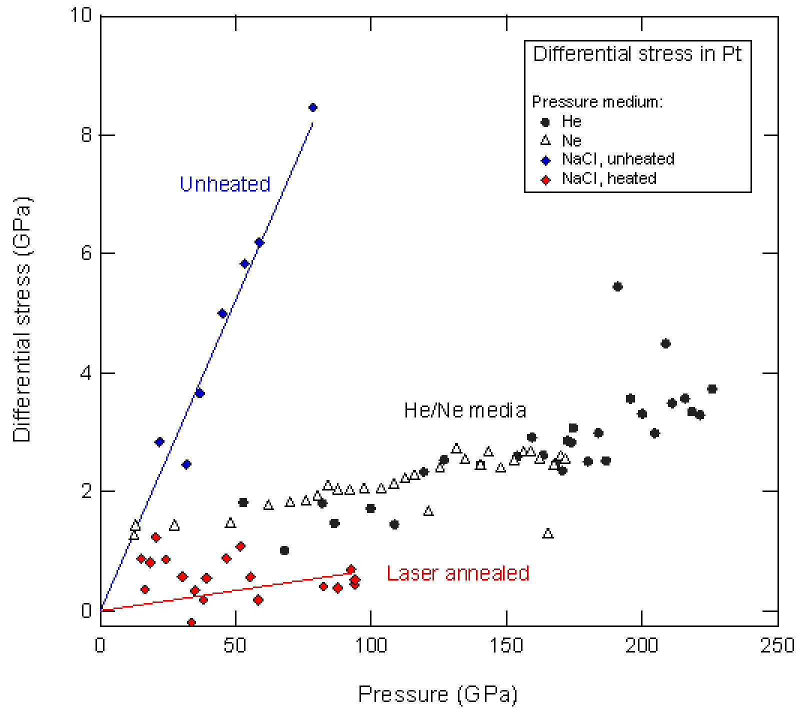
- **Growing number of publications**
- **Novel phenomena over a broad range of extreme conditions**
- **Many new opportunities, including time resolved methods**

3. Technique Development

- **New x-ray techniques (<100 nm beams, time-resolved)**
- **New developments in neutron methods**
- **Continued need for high *P-T* device developments**
- **Many new opportunities for combined static/dynamic compression**

Improved measurements of stress and strain at multimegabar pressures

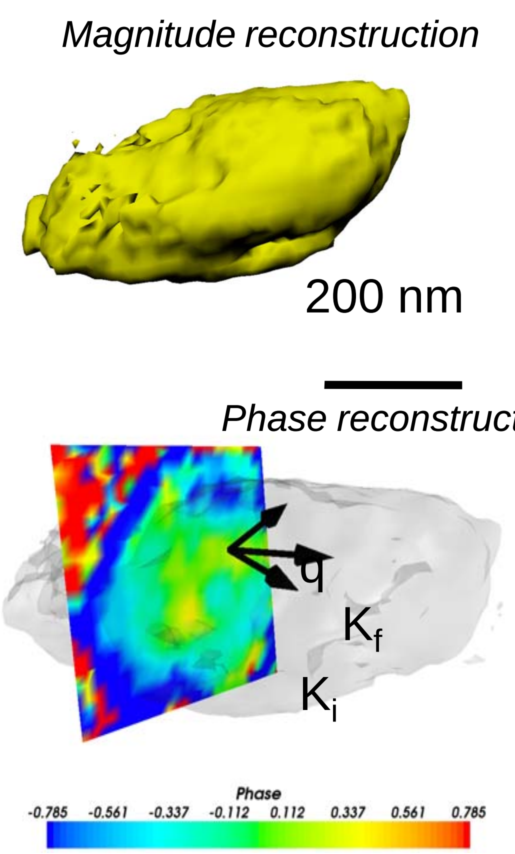
CDAC



S. Dorfman (*CDAC graduate student, Princeton*)

Measurements of differential stress in a platinum sample for various pressure media.

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



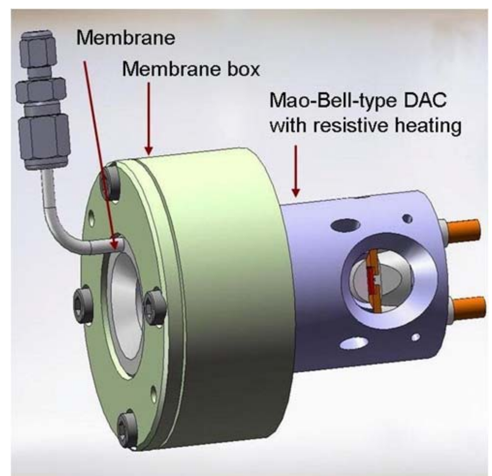
[Yang et al, *to be published*]

There have been major technical advances at HPCAT/HPSynC

CDAC

A second undulator installed to enhance brightness

New diamond anvil cell techniques



17-element analyzer array commissioned in June 2009

Microfocused X-Ray Diffraction Symmetric DAC in gearbox assembly

Carnegie Institution for Science

NNSA