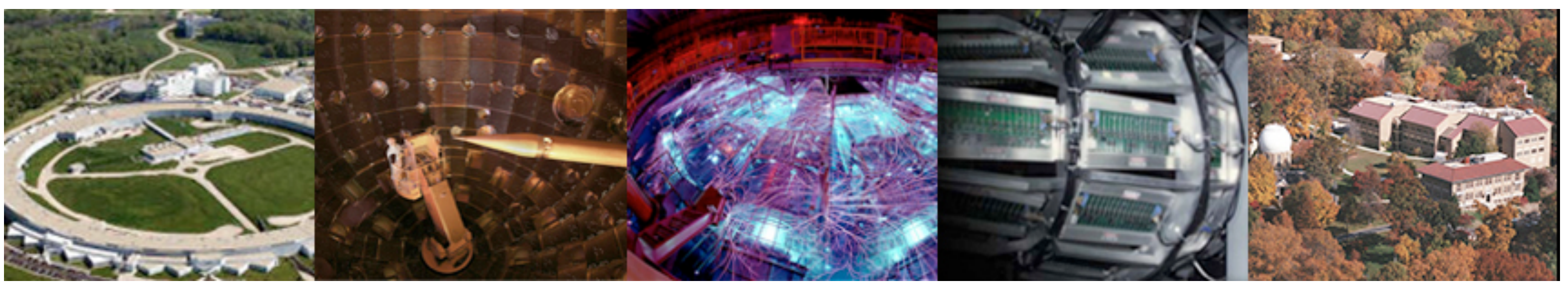
CDAC

CARNEGIE / DOE ALLIANCE CENTER:

A Center of Excellence for High Pressure Science and Technology



Russell J. Hemley

Stephen A. Gramsch

CARNEGIE INSTITUTION FOR SCIENCE

SSAP Symposium

Santa Fe, NM

March 11-12, 2015

NNSA

OUTLINE

CDAC

I. Overview of Center

MISSION

PARTNERS

FACILITIES

II. Selected Highlights

EDUCATION

TRAINING

OUTREACH

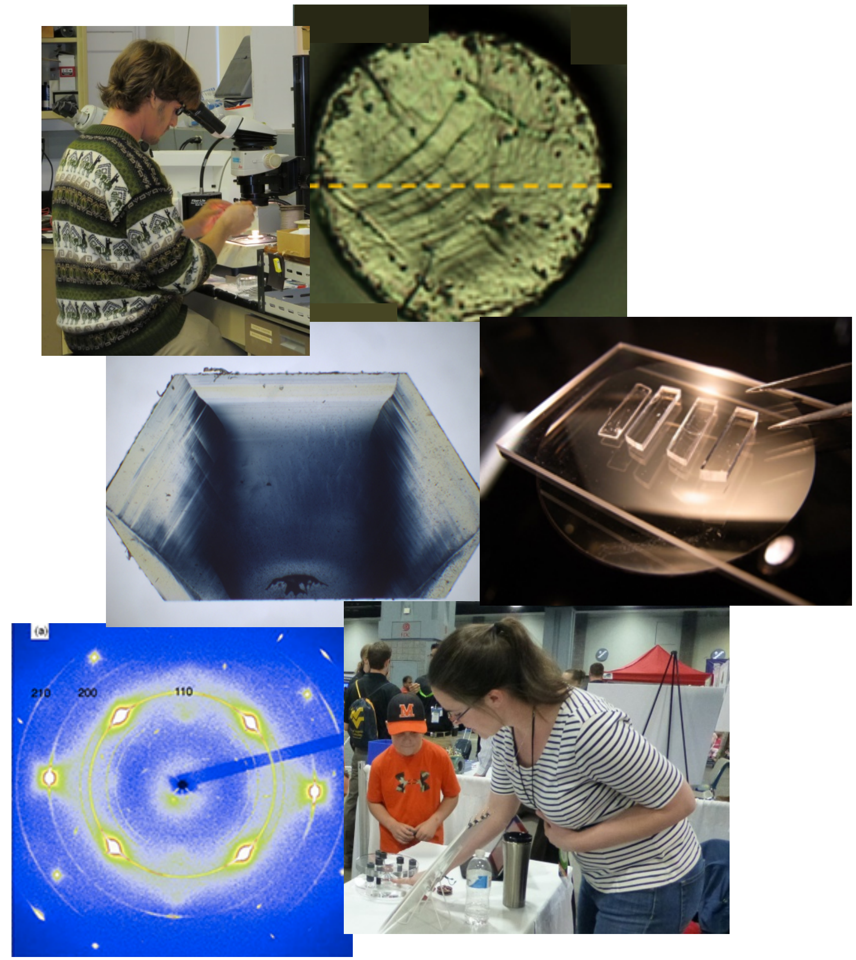
SCIENCE

TECHNIQUES

III. Future Outlook

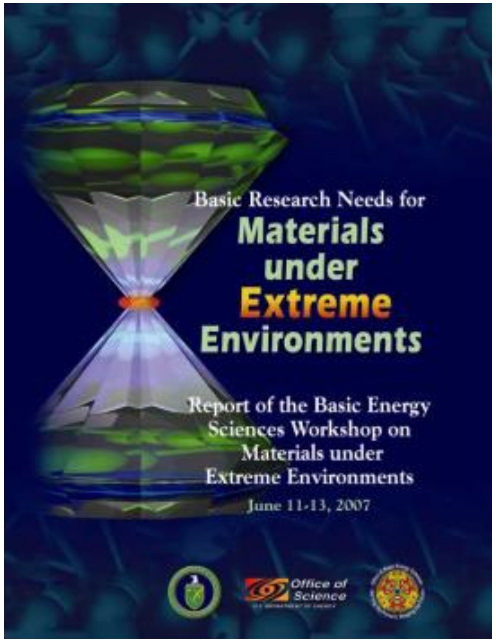
NNSA OPPORTUNITIES

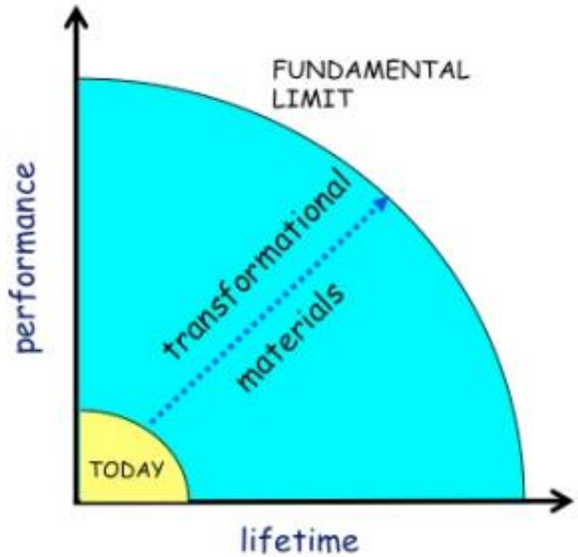
NEW PARTNERSHIPS

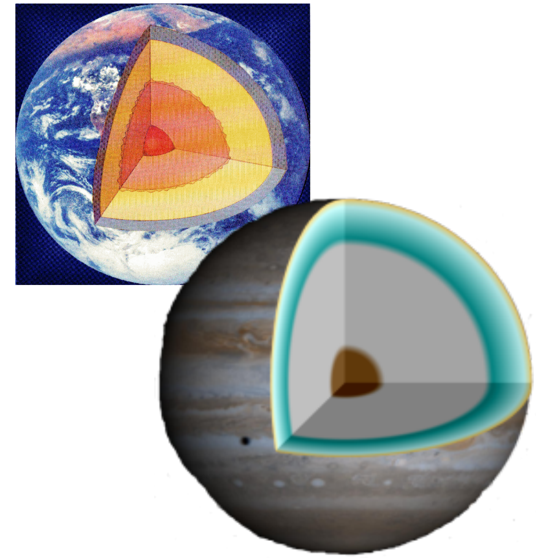


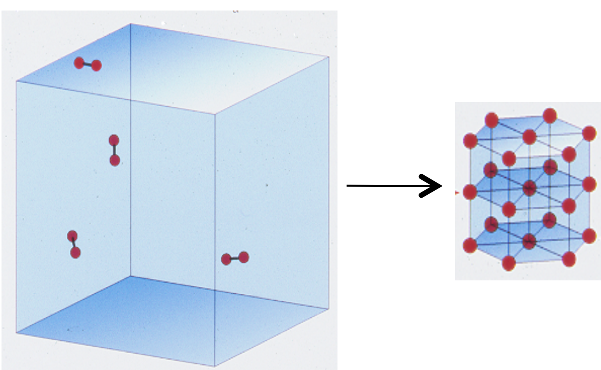
Studies of extreme environments have opened up a new world of materials

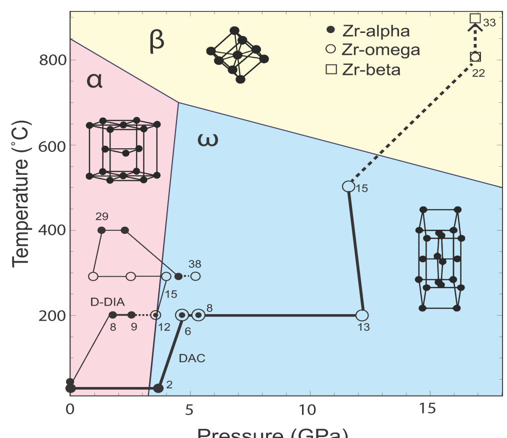
CDAC



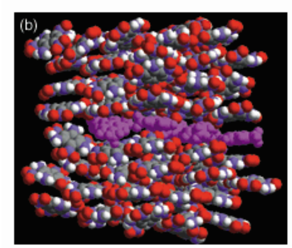








Zr



TATB

- *Physics*
- *Chemistry*
- *Materials*
- *Geoscience*
- *Planetology*
- *Astrophysics*

Components of the Center

CDAC

MISSION

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

Academic Partners

CARNEGIE INST. (Hemley)
ALABAMA - BIRMINGHAM (Vohra)
CALIF. - BERKELEY (Wenk&Jeanloz)
ILLINOIS (Dlott & Cahill)
CALTECH (Fultz)
YALE (Lee)
UCLA (Kavner)
NORTHWESTERN (Jacobsen)
WASHINGTON-ST. LOUIS (Schilling)
HAWAI'I (Dera)
WASHINGTON STATE (Yoo)
SUNY-UNIV AT BUFFALO (Zurek)
UTAH (Miyagi)

Academic Collaborators

FACILITY USERS

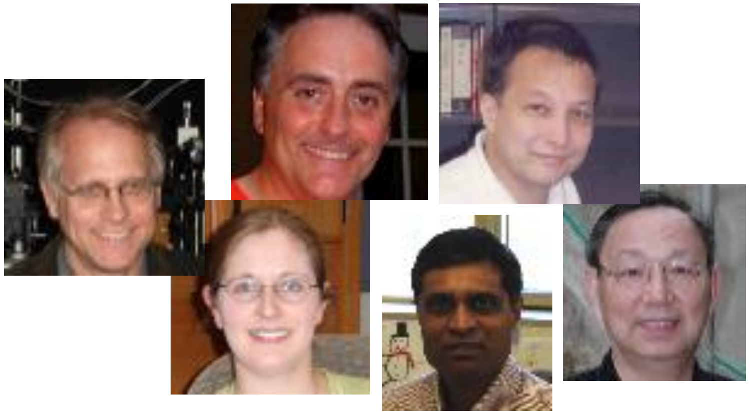
NNSA Laboratory Partners

ALL HIGH *P-T* GROUPS AT **LLNL, LANL, SNL**; STEERING/ADVISORY COMMITTEE MEMBERS

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

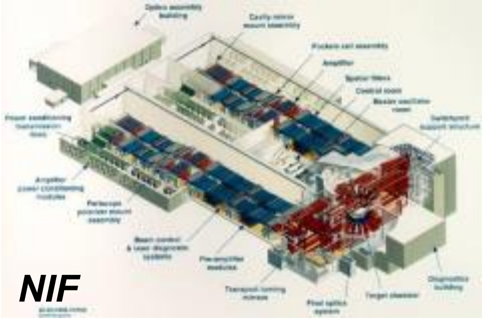
CDAC

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



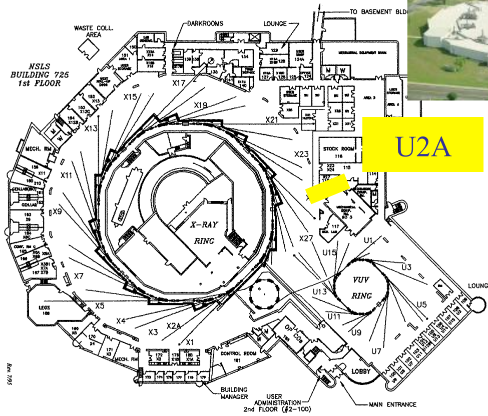
- **Technique development/training at unique facilities at NNSA Labs**

LANSCE



NIF

- **High *P-T* synchrotron IR beamline at NSLS**

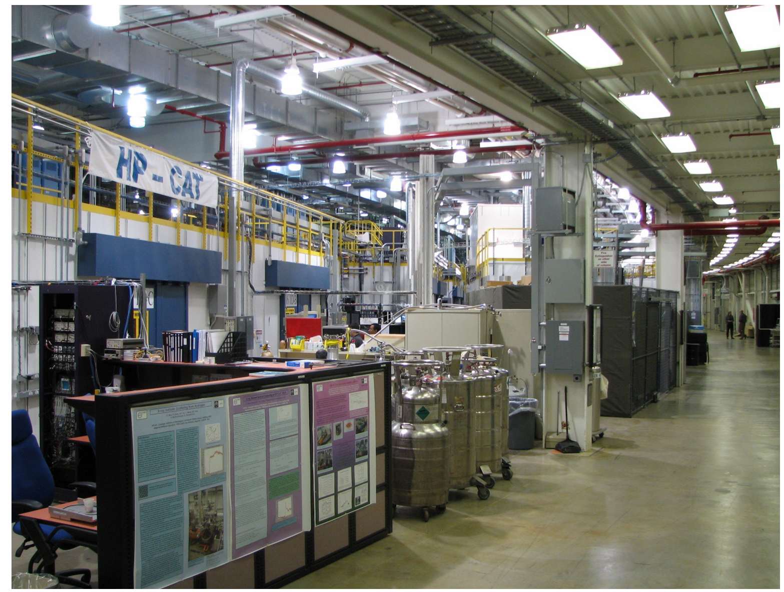


NNSA

Dedicated high *P-T* facilities at the Advanced Photon Source

- 1988 ANL/Chicago Workshop
- GSECARS (Sector 13)
  - High-pressure geoscience
- HPCAT (Sector 16) launched 1998
- Dedicated high-pressure facility
  - Physics, chemistry, materials
  - Advanced techniques
  - Programmatic work (NNSA Labs)
- > 5600 person visits (1/15)
- 843 peer reviewed publications
- Training and education
  - Approx. 60% users are students and post-docs
- Enhanced capabilities
- 2012 Trilab (LLNL, LANL, SNL)
- Upgrade APS-U and HPCAT-U

HPCAT HIGH PRESSURE COLLABORATIVE ACCESS TEAM
at the Advanced Photon Source
GEOPHYSICAL LABORATORY, Carnegie Institution of Washington



75% : CDAC/Carnegie, LLNL, UNLV
25%: DOE-BES

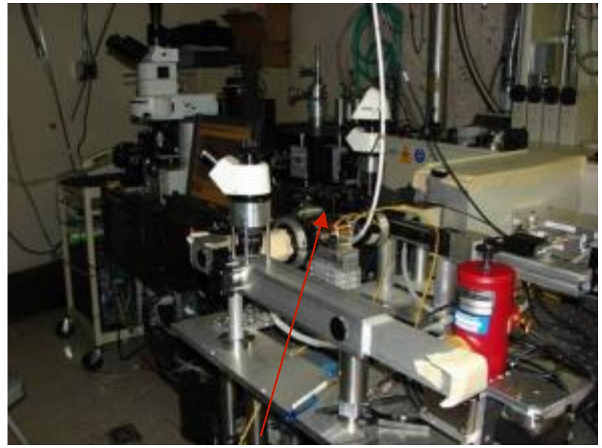
- 9 hutches
- 4 independently operating stations
- support laboratories

DOE NNSA/SC Partnership

High *P-T* IR synchrotron beamline NSLS-FIS is an important CDAC facility

CDAC

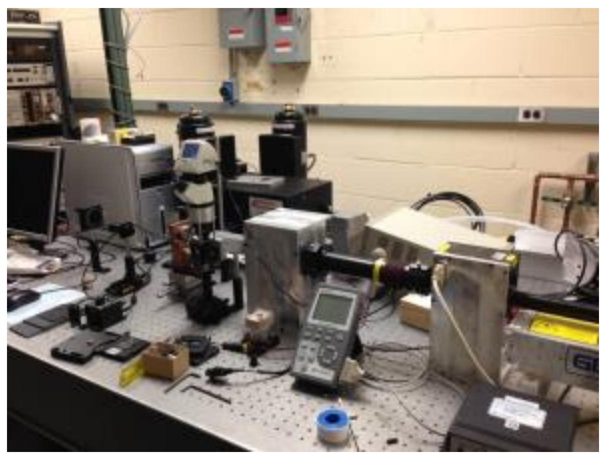
Fully upgraded U2A end station with new Raman systems



Hydrothermal DAC for high-P and high-T IR experiments

Standard symmetric DAC for high-P and low-T IR experiments

U2A side station with additional far-IR microscope



Off-line CO_2 laser heating system

Complete sample preparation facilities

The facilities will be moved to NSLS-II as one of the NxtGen beamlines

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CDAC HIGHLIGHTS 2014:
Education, training and outreach

CDAC

- ***Growth of users at HPCAT***
  - *(800+ to date)*
- ***CDAC supported 18 PhD students***
- ***42 PhDs awarded with CDAC support***
- ***14 Students/Postdocs to NNSA Labs***
- ***4 undergraduate/high school interns***
- ***Workshop/symposium sponsorship***
  - *Ferroelectrics 2014 (Carnegie)*
  - *Neutron and X-Ray Scattering School*
  - *Workshop on Time-Resolved Techniques*
- ***Presentations at national meetings***
  - *2014 APS March – 33 presentations*
  - *2014 Fall AGU – 47 presentations*

Katie Brown (LANL)

Nenad Velisavljevic, Raja Chellappa (LANL)

CDAC HIGHLIGHTS 2013-2014:

Education, training and outreach

CDAC

CDAC
CARNEGIE/DOE ALLIANCE CENTER
A Center of Excellence for High Pressure Science and Technology Supported by the Stewardship Science Academic Program of DOE/NNSA

CARNEGIE INSTITUTION FOR SCIENCE

About CDAC | Research Highlights | People | CDAC Publications | CDAC Abstracts | Students

RESEARCH

PREVIOUS PAUSE NEXT

Spectroscopic Steps to Stronger Steel
FEBRUARY 27TH, 2015

As iron is heated, the arrangement of the atoms in the solid changes several times before the iron finally melts. This unusual behavior is one reason why steel is so strong. The atomic-level details of how and why iron takes on so many different forms during heating remains a mystery, however. Recent work by Caltech CDAC scientists...

Novel Carbon Bonding at High Pressure
FEBRUARY 11TH, 2015

Only a small fraction of our planet's total carbon budget is found at the surface. In fact, Earth's mantle is thought to be the largest carbon reservoir. Carbonates, and in particular ferromagnesite ((Mg,Fe)CO3), are likely candidates for deep-Earth carbon storage and therefore play a key role in the deep carbon cycle. The behavior of...

People Highlights

- Carnegie Summer Scholars Program Now Accepting Applications
- CDAC at AGU 2014
- Jacobsen's Research Featured on BBC World News
- Hemley Presents Lectures at Berkeley and Buffalo
- Zurek Wins 2014 CMOA Award

See more »

Meetings and Symposia

- APRIL 6-10, 2015 SAN FRANCISCO, CA — MRS Spring Meeting
- MARCH 11-12, 2015 SANTA FE, NM — 2015 Stewardship Science Academic Program Meeting

- ***Student-Focused***
- ***Research Highlights***
- ***People News***
- ***Announcements***
- ***Resources***

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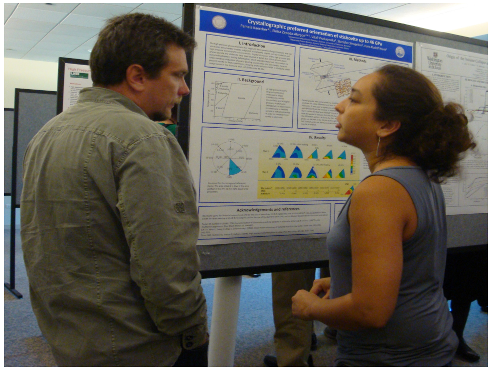
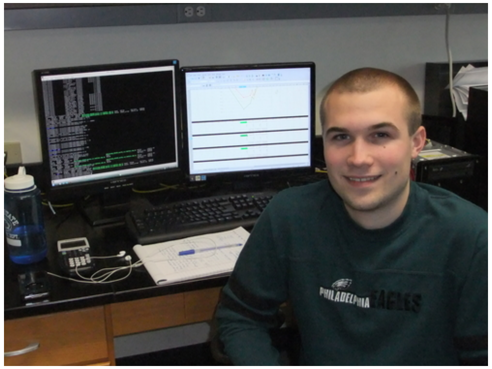
Summer Enrichment at NNSA Laboratories

CDAC

- **Eloísa Zepeda-Alarcón**
  UC-Berkeley
  Advisor: Hans-Rudolf Wenk
  LANL Sponsors: Ricardo Lebensohn, Carlos Tome
  ViscoPlastic Modeling of Two-Phase Materials: Periclase + Silicate Perovskite Aggregates



- **Andrew Shamp**
  University at Buffalo
  Advisor: Eva Zurek
  LLNL Sponsors: Sebastien Hamel, Tadashi Ogitsu
  Theoretical Predictions of the EOS of Boron Carbide Under Extreme Conditions



- **John Lazarz**
  Northwestern University
  Advisor: Steven Jacobsen
  LANL Sponsors: Cindy Bolme, Kyle Ramos, Dan Hooks
  Determination of the Elastic Tensor of Acetominophen, an RDX Analogue

Carnegie Institution for Science

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CDAC investigates a broad range of fundamental problems in high *P-T* science

CDAC

- ***STRUCTURES AND PHASE RELATIONS***
- ***EQUATIONS OF STATE***
- ***PHONONS AND ELASTICITY***
- ***RHEOLOGY AND STRENGTH***
- ***TRANSPORT PROPERTIES***
- ***EXTREME CONDITIONS CHEMISTRY***

18 POSTERS AT THIS MEETING

2014-: 136 Publications (including in press)

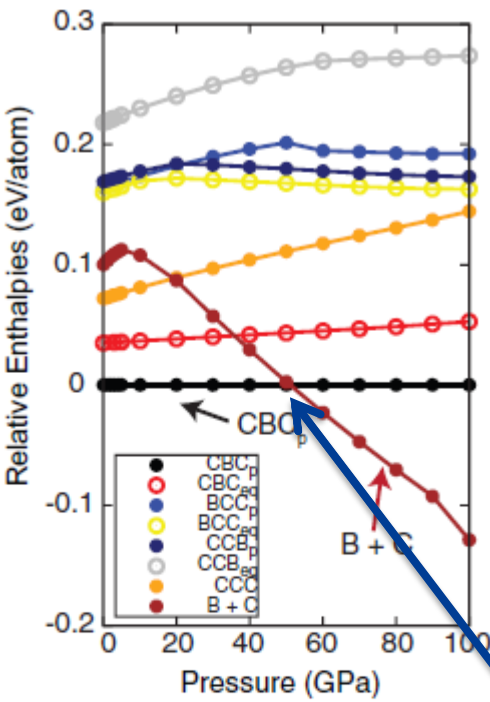
Since 2003: 1465+ Publications (200 Student Publications)
(128 Student First Author Papers)

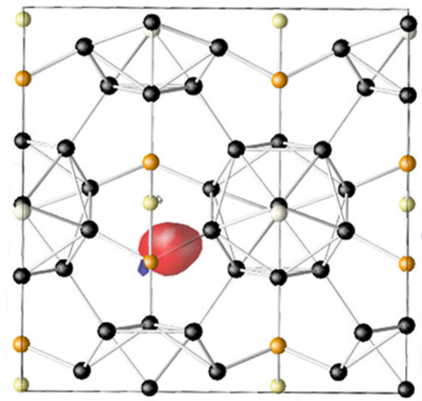
(92 Phys. Rev. Lett., 45 Nature, 22 Science, 88 PNAS)

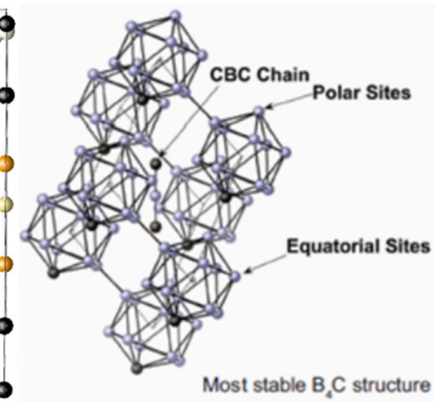
Boron Carbide Under Pressure

CDAC

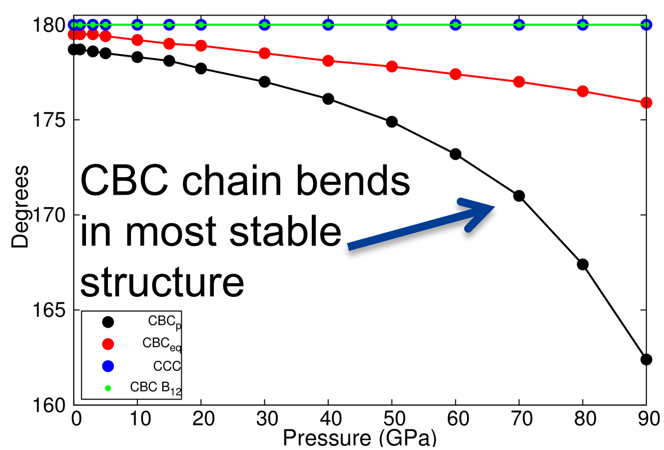
- **XtalOPt Evolutionary Algorithm**
- **CBC_p Dynamically Stable**
- **Thermodynamically Unstable**

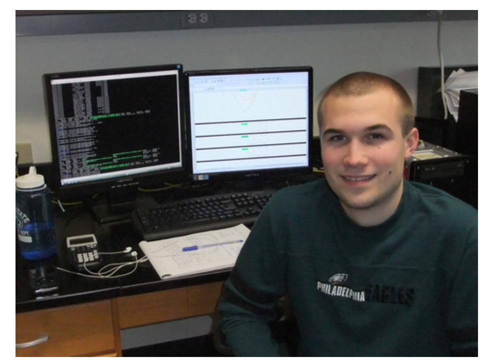






Most stable CBC_p structure





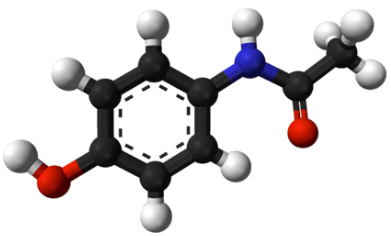
Andrew Shamp
University at Buffalo

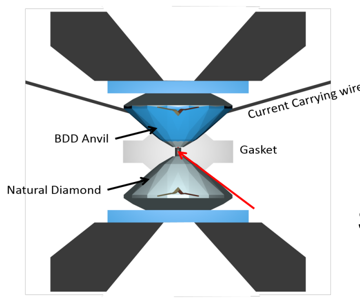
Unstable with respect to pure C and B for P > 50 GPa.

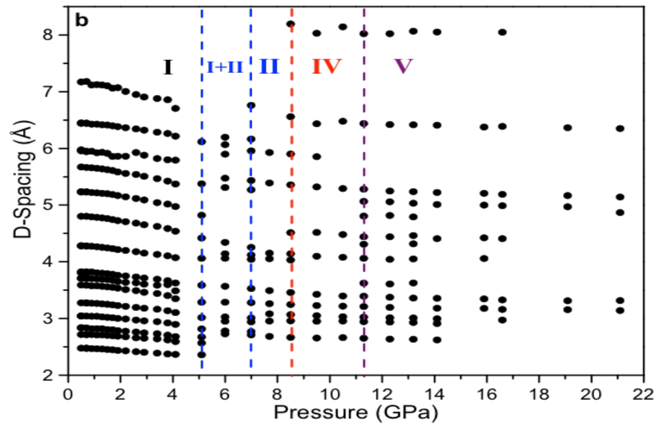
Small Molecules at Extreme Conditions

CDAC

- Paracetamol, $C_8H_9NO_2$
- Raman + Angle-dispersive XRD (HPCAT)
- Four phases below 15 GPa



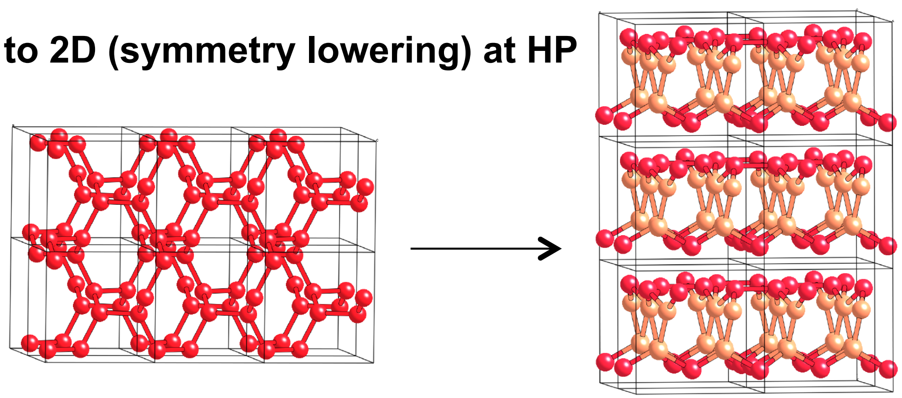




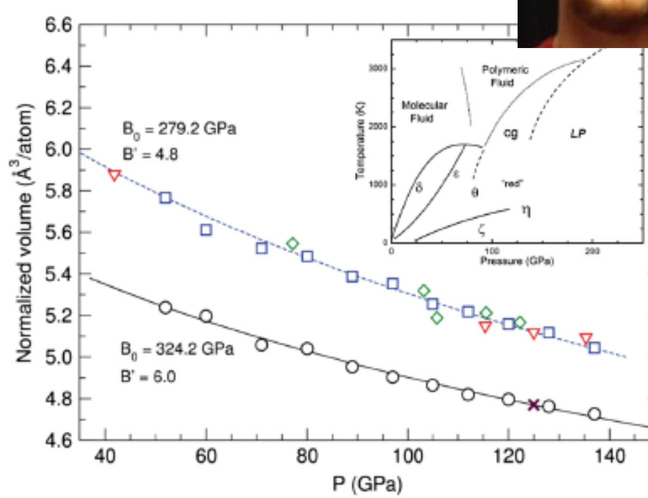
Spencer Smith
Alabama-Birmingham

S. Smith, et al. *J. Phys. Chem. A* **2014**, *118*, 6068.

- N2 in *I* 2_13 (cg) and *Pba*2 (LP)
- Laser heating + Raman spectroscopy
- 3D to 2D (symmetry lowering) at HP



Dane Tomasino, Washington State



D. Tomasino et al. *Phys. Rev. Lett.* **2014**, *113*, 205502.

Dehydration Melting in Earth's Mantle

CDAC

- $(Mg,Fe)_2SiO_4$ at 30 GPa, 1600 °C, 1% H_2O
- Laser heating, synchrotron IR spectroscopy (NSLS-U2A)
- Transformation to $(Mg,Fe)SiO_3$ + (Mg,Fe)O : Intergranular melt
- Dehydration melting consistent with seismic velocity decrease below 660 km
- Suggests hydration of a large part of the mantle, with H_2O trapped in transition zone

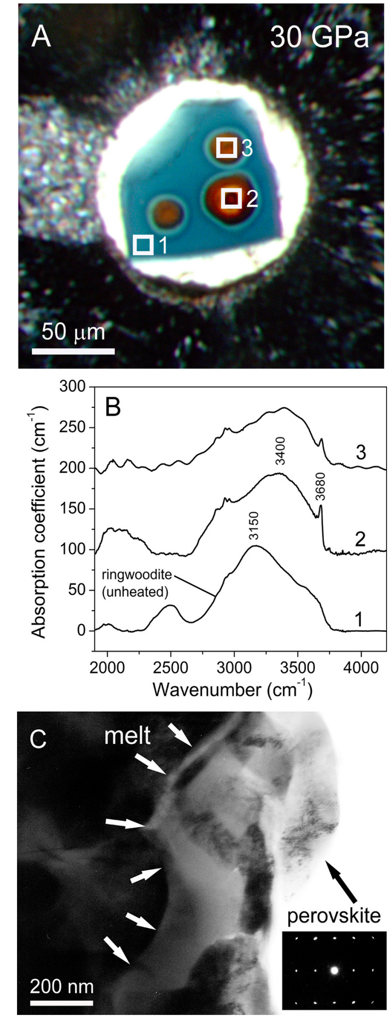
Steve Jacobsen, Northwestern

BBC NEWS

OH in quenched glass

Hydrous Ringwoodite

Intergranular melt



Schmandt, et al. *Science* **2014**, *344*, 1265.

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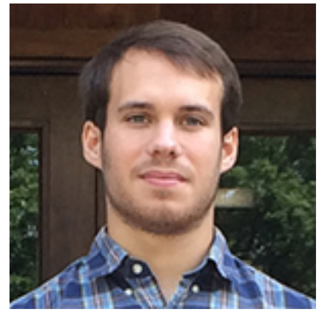
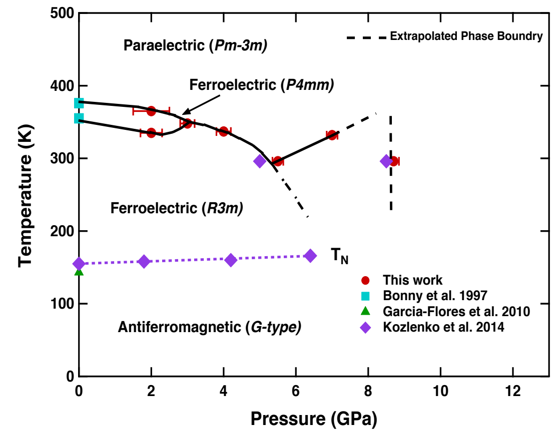
High Pressure Studies on Ferroelectrics

CDAC

- Polycrystalline $Pb(Fe_{0.5}Nb_{0.5})O_3$
- Raman scattering at high P and T
- Refined phase diagram

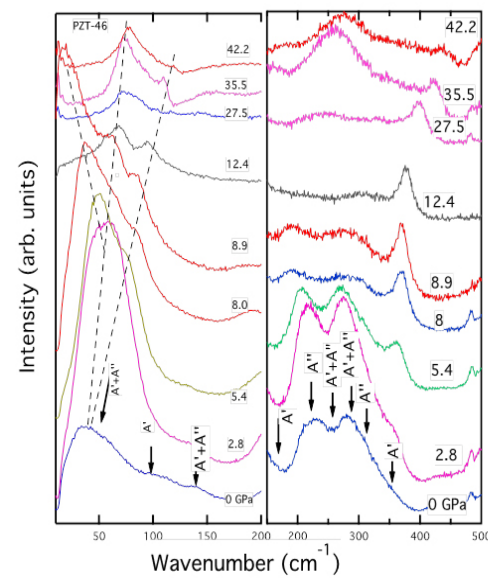


Brandon Wilfong
Washington College



- Single crystal $Pb(Mg_{0.33}Nb_{0.67})O_{3-x} – PbTiO_3$
- Raman scattering at high P and T
- XRD at HPCAT 16-BM-D (High Energy)
- Monoclinic-Rhombohedral at 3 GPa
  Octahedral tilting
- Soft optical phonon at 9 GPa
- Drastic changes at 27 GPa
  Orthorhombic or monoclinic?

Muhtar Ahart, Carnegie



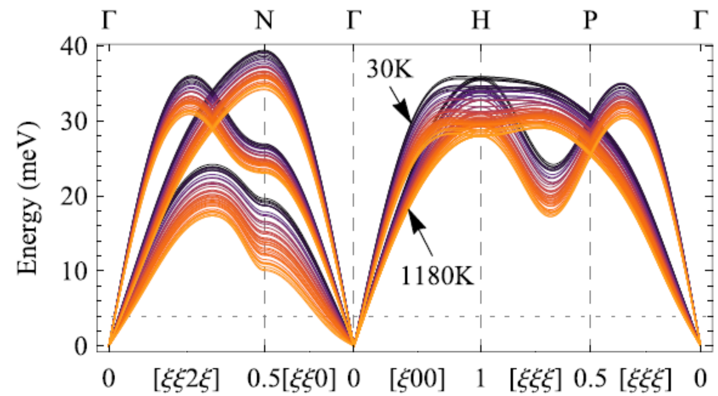
Ahart, et al. *Ferroelectrics* **2014**, *467*, 138.

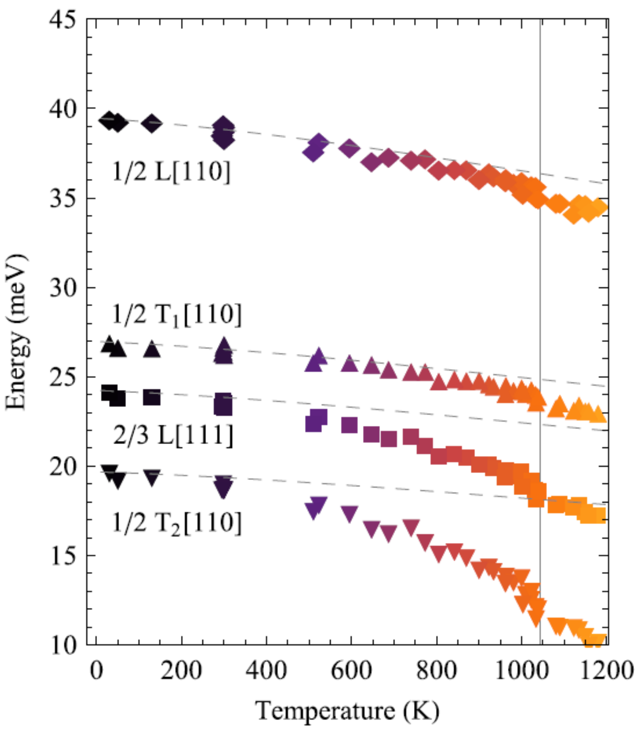
Carnegie Institution for Science

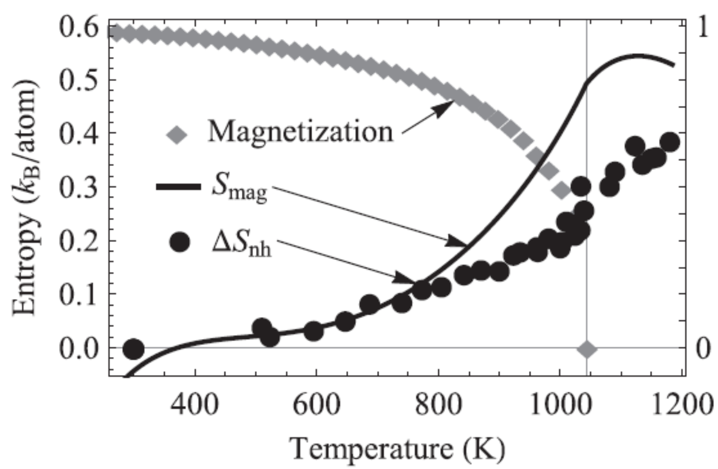
Magnon-Phonon Interactions in bcc-Fe

CDAC

- **Phonon dispersions from NRIXS**
- **Large non-harmonic phonon softening caused by magnon-phonon interactions**
- **Magnon-phonon vibrational entropy stabilizes bcc-Fe above T_C**







Lisa Mauger, Caltech

L. Mauger et al., *Phys. Rev. B* **90**, 064303 (2014).

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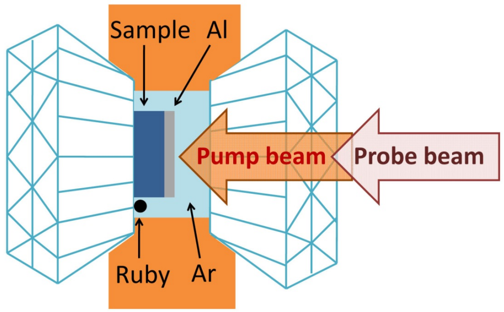
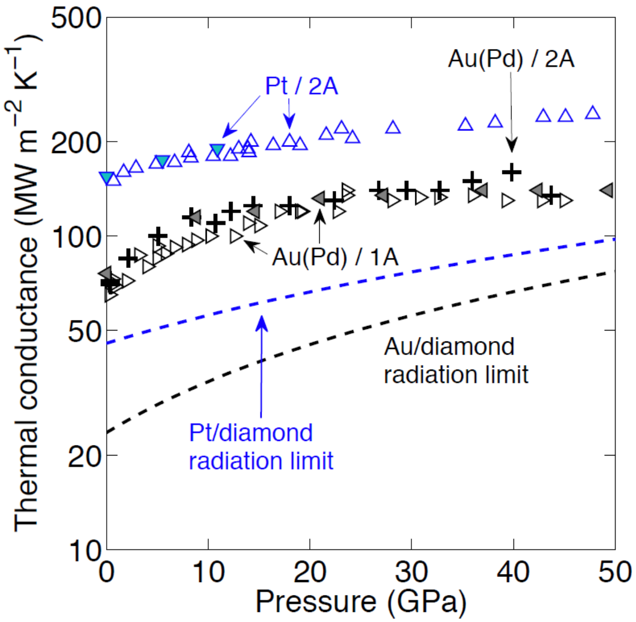
Thermal Transport at High Pressure

CDAC





G. Hohensee et al., *Nature Communications*, in press.

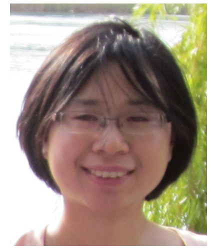
- **Extension of time-domain thermoreflectance measurements to high pressures**
- **Tests of theoretical models of thermal energy transport in materials and across interfaces.**
- **Pressure is used to systematically vary phonon and electron densities of states, and interface bonding.**
- **Measured thermal conductance is well above the phonon radiation limit.**
- **Unexpectedly high thermal conductance consistent with two high frequency diamond phonons interact with a low-frequency metal phonons.**

Greg Hohensee, Illinois

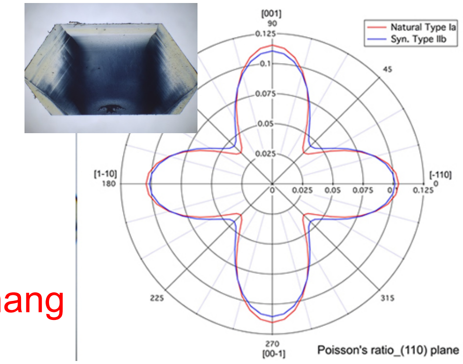
Defects and the Elastic Properties of Materials

CDAC

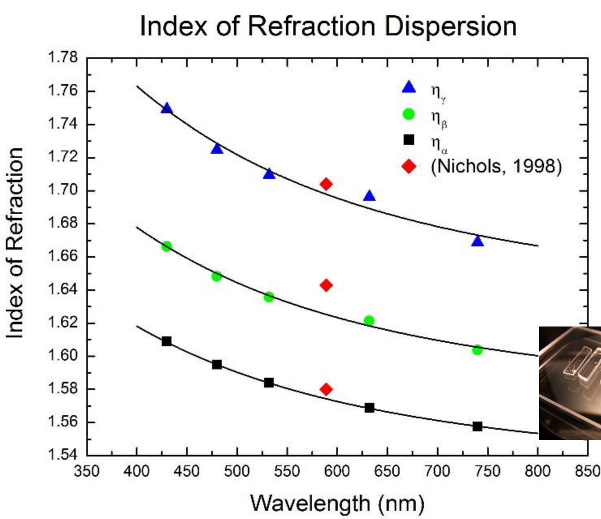
- **At Northwestern, GHz interferometry is used to determine the elastic properties of materials.**
- **Acetominophen (RDX analog), vitreous silica, B-doped diamond**



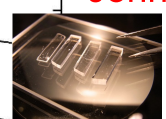
Yun-yuan Chang

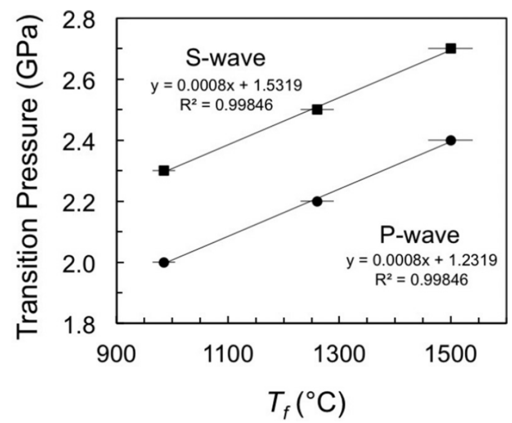


- Poisson's ratio from elastic tensor as measured by GHz Interferometry
- Boron reduces elastic Moduli and elastic anisotropy of diamond



John Lazarz





A. Clark et al., *Phys. Rev. B* 90, 174110 (2014).

Alisha Clark

- Complete optical indicatrix
- Completing elastic tensor (Brillouin + ultrasonics)
- Applied to modeling elastic properties of composites in energetic materials

- Anomalous compressibility in v-SiO_2
- HAD:LDA ratio set at T_f, fixed below permanent densification
- Compression behavior consistent with floppy modes in a mixture of LDA and HDA domains

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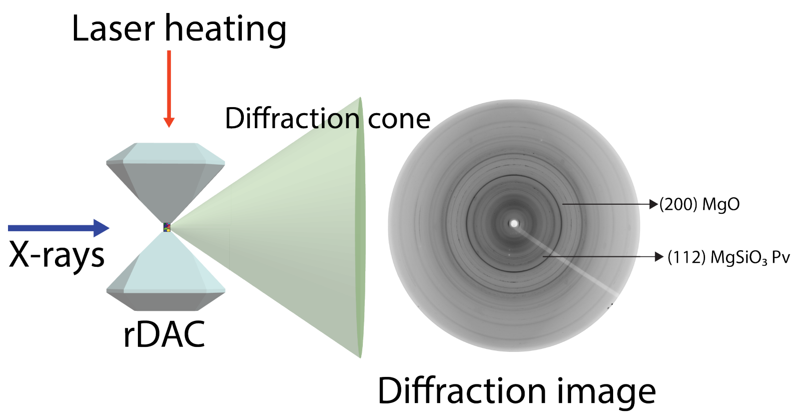
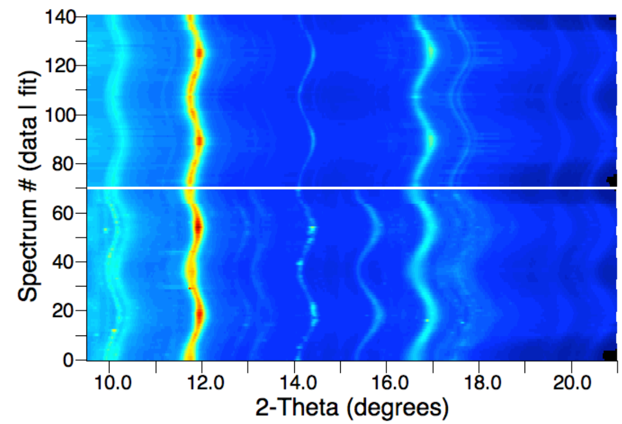
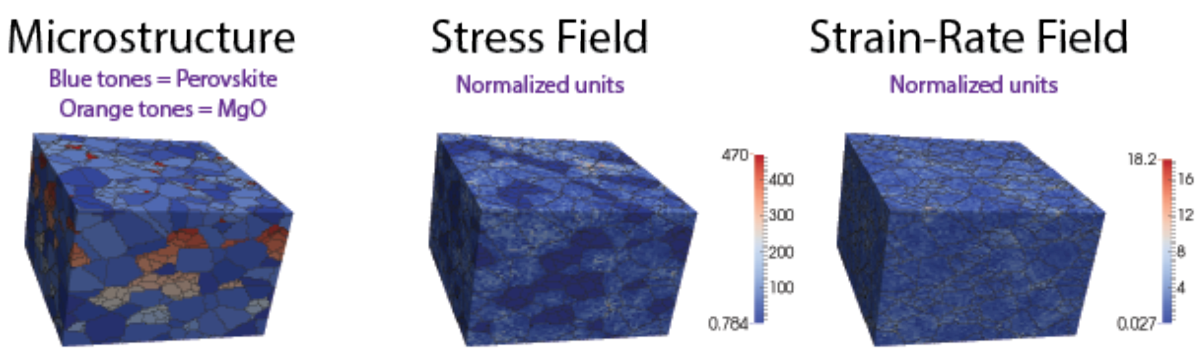
Deformation of Polyphase Samples at High Pressure

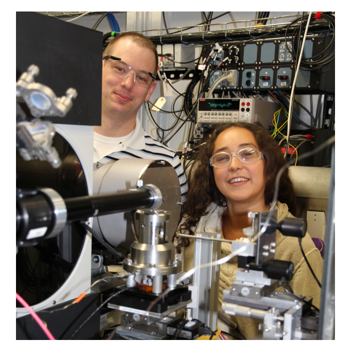
CDAC

- Studies of deformation in $MgSiO_3$ – MgO at high pressure allow interpretation of seismic anisotropy and infer flow patterns in the Earth's mantle.
- Collaboration with LANL on simulations with VPSC and VPFFT codes allows modeling of deformation microstructures including intersite interactions.









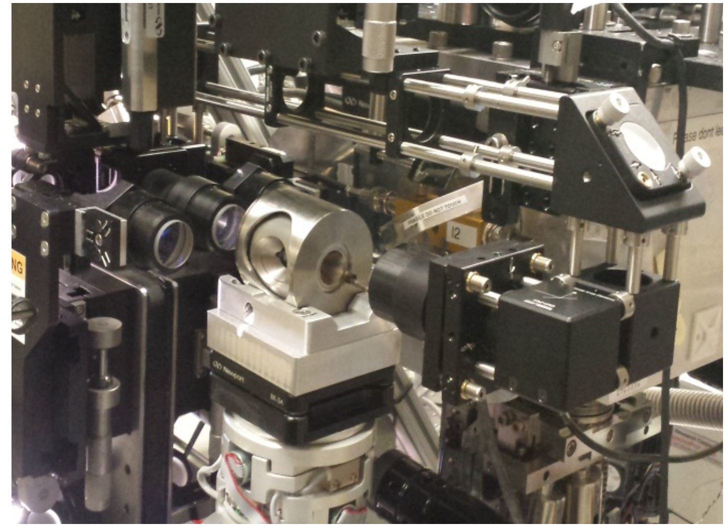
Jesse Smith, HPCAT and Eloísa Zepeda-Alarcón, Berkeley

Deformation of Polyphase Samples at High Pressure

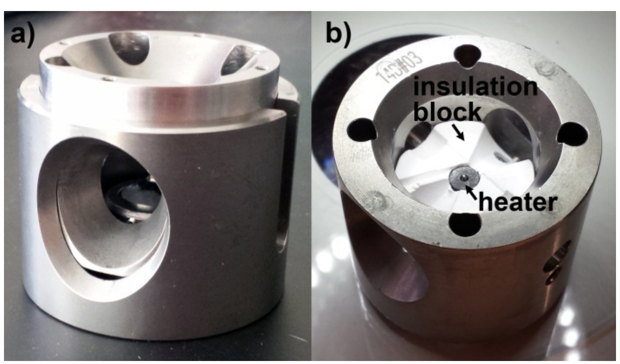
CDAC

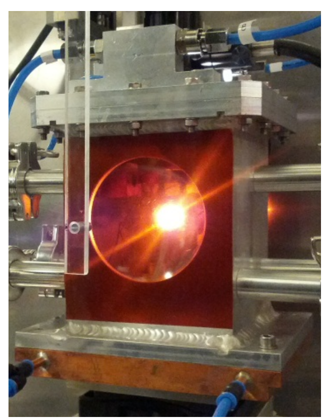
- B1 NaCl exhibits different textures as a pure phase under deformation as as compared to 75% NaCl-25% MgO.

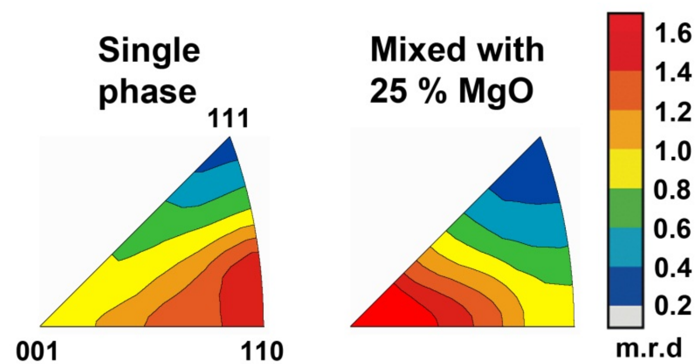

Mike Jugle and Max Gianetta, Utah



Laser heating in radial geometry
ALS 12.2.2



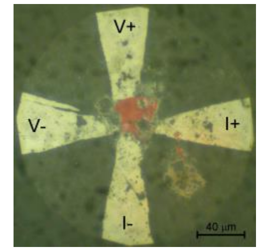


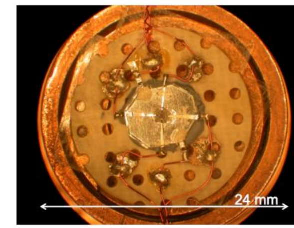


Magnetic Ordering in Rare Earth Metals: Dy

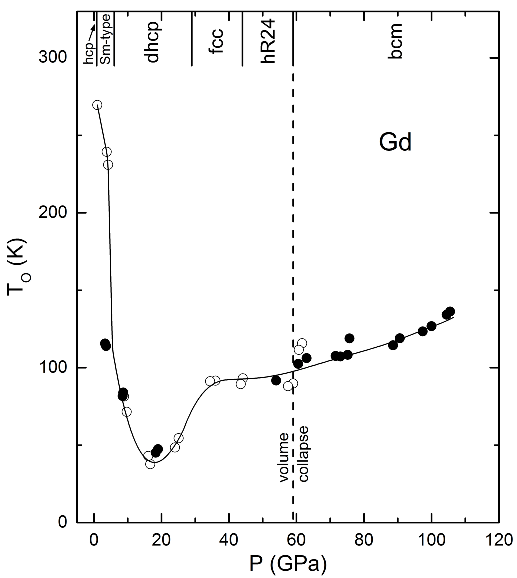
CDAC

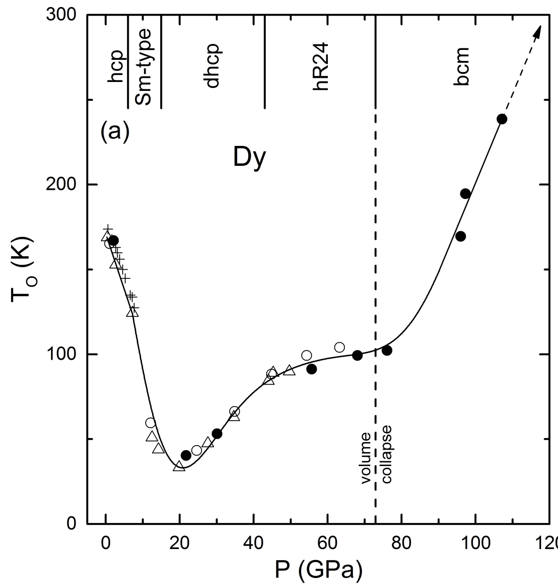
- T_o rises rapidly in Dy metal at P > 70 GPa reaching 400 K at 157 GPa.
- Surpasses T_o = 292 K at 0 GPa in Gd metal T_o rises slowly with pressure.
- Suggests that high ordering temperature in Dy metal is a highly correlated electron effect—pressure destabilizes the magnetic state.

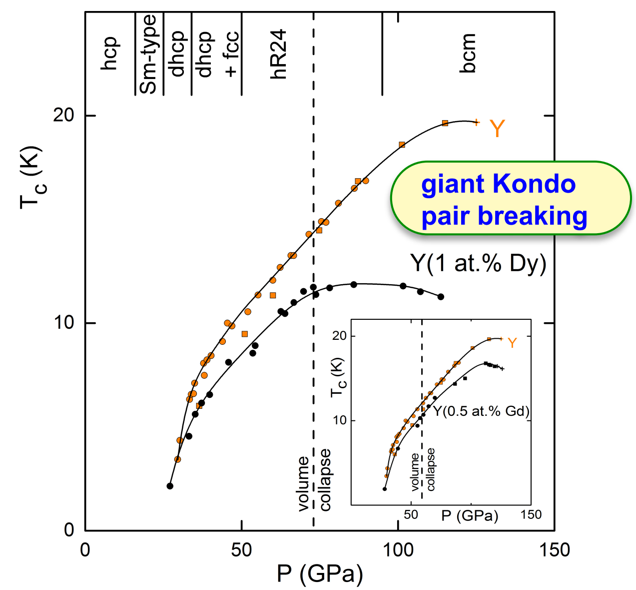




Jinhyuk Lim, Washington / St. Louis







J. Lim et al., *Phys. Rev. B* **91**, 045116 (2015)

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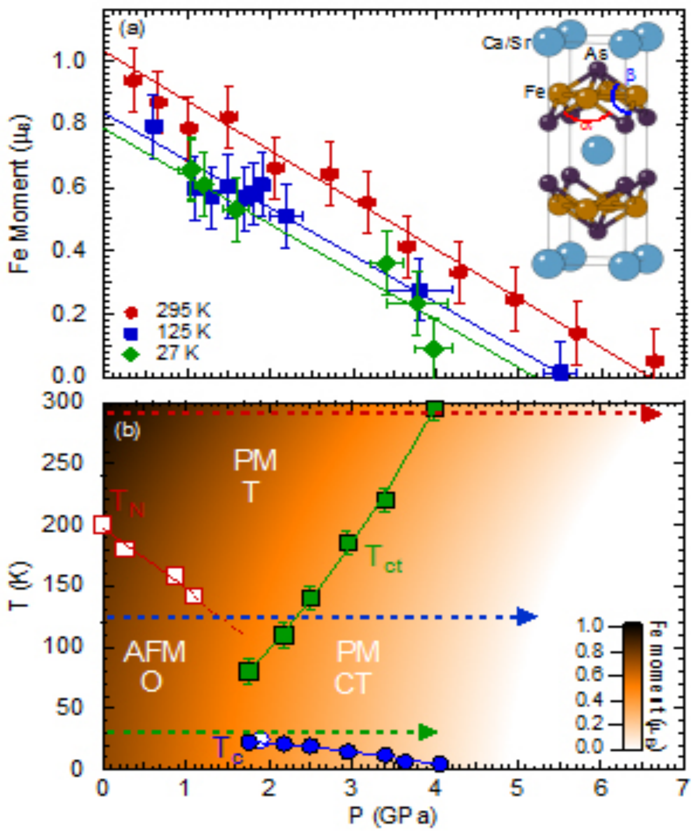
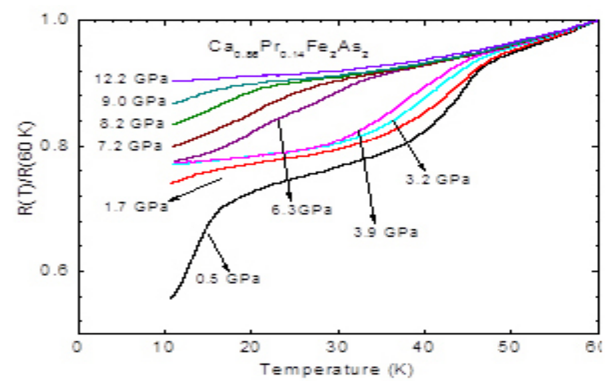
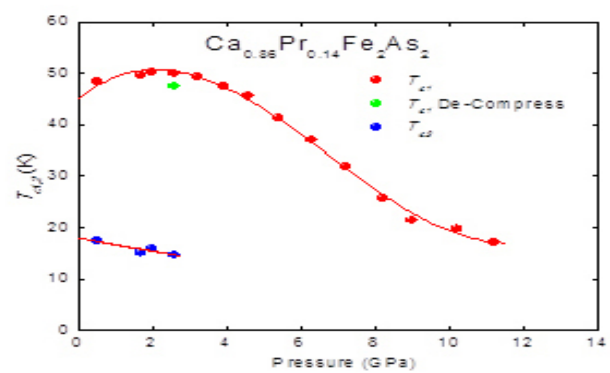
Superconductivity in the $CaFe_2As_2$ System

CDAC

- Sr substitution into $CaFe_2As_2$ decouples volume collapse from the Fe moment.
- Superconductivity develops out of the paramagnetic normal state.
- Pr substitution into $CaFe_2As_2$ yields T_c = 51 K at 1.9 GPa.
- Resistance measurements suggest two superconducting phases at 0.5 GPa.







J. Jeffries et al., Phys Rev. B 90, 144506 (2014).

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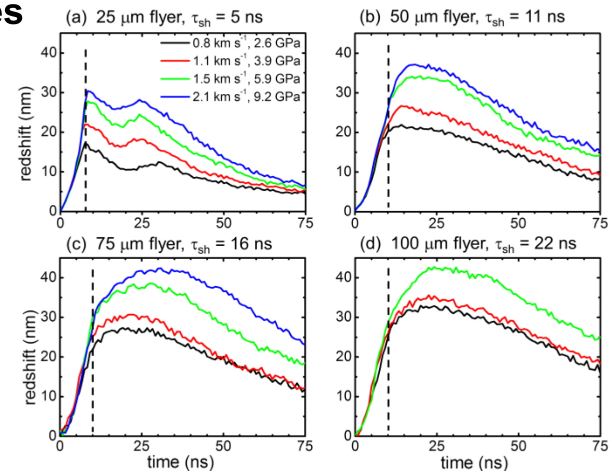
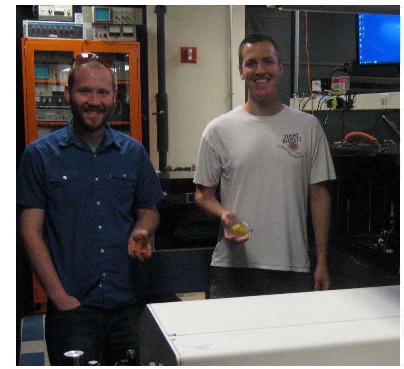
Shocked Polymers and Fluorescent Probes

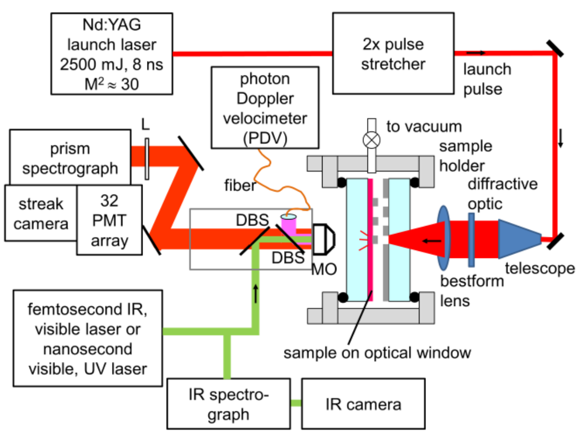
CDAC

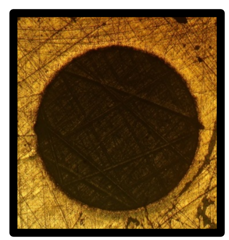
- Laser-launched cold, intact flyer plates
- Embedded dye + PMMA
- Time-resolved monitoring of dye emission spectrum: variation of red shift with time.
- At ~ 10 ns, change from elastic to viscous compression
- Next: materials that *absorb* shocks

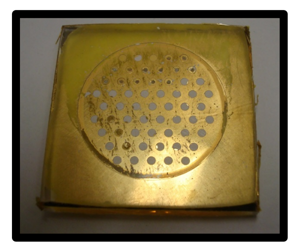


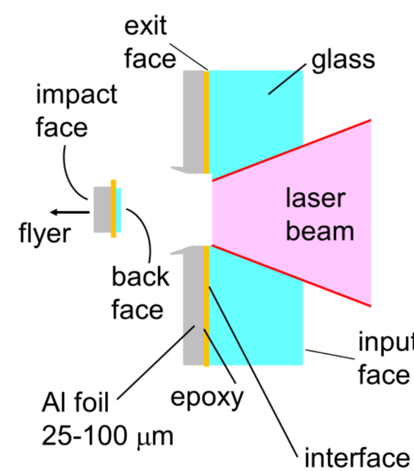


Will Bassett and Will Shaw
Illinois









Banishev, Shaw, and Dlott, *Appl. Phys. Lett.* **104**, 101914 (2014).

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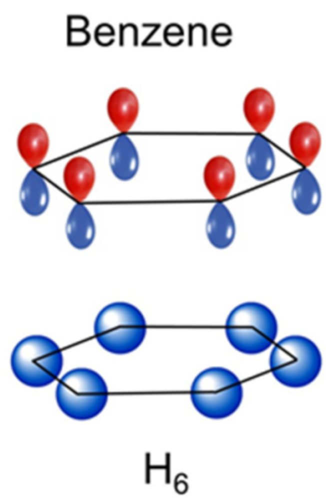
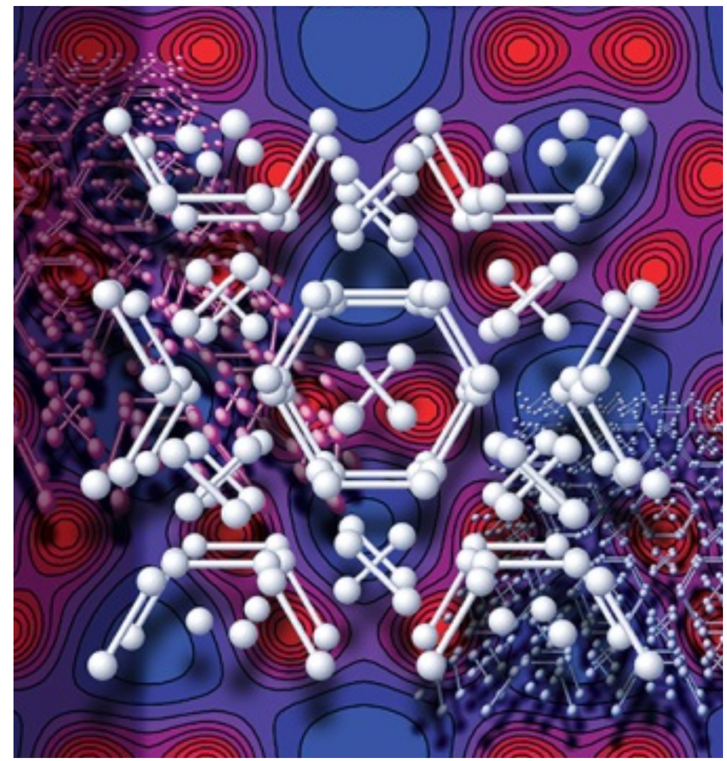
Aromaticity and Closed-Shell Effects in Hydrogen

- H_2 in molecular clusters, 2D and 3D crystals investigated using quantum chemical and solid state physics approaches.
- Stability of dense hydrogen structures at > 200 Gpa arises from the intrinsic stability of 6-membered rings with properties similar to carbon graphene.
- Atomic and electronic properties are controlled by closed-shell effects.
- Closed shell effects are critical to understanding how hydrogen becomes metallic.

Ivan Naumov, Carnegie





I. Naumov and R. Hemley,
Accts. Chem. Res. **47**, 3551 (2014).

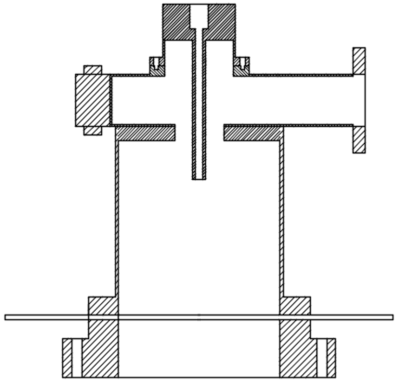
Nanodiamond Research at Carnegie

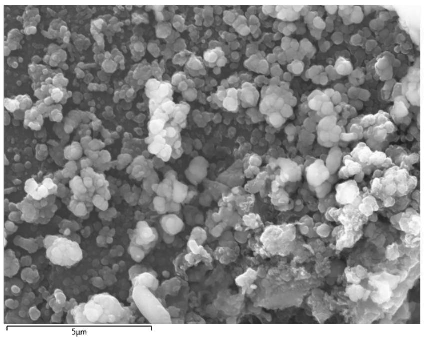
CDAC

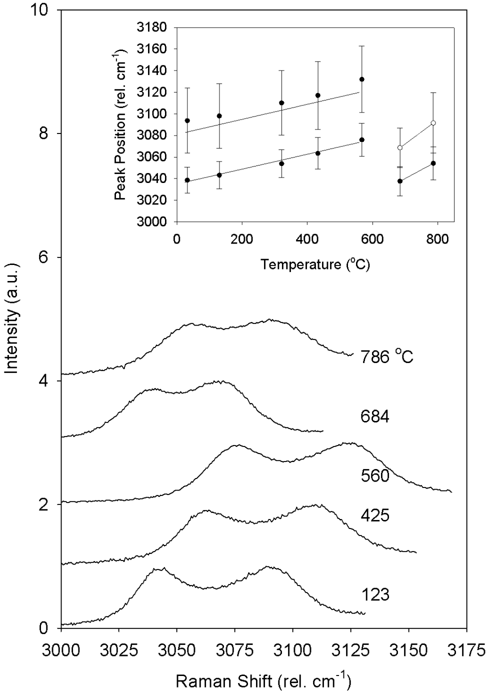
- **MPCVD process results in nanodiamond formation at atmospheric pressure (3 mm quartz tube in CVD chamber cavity).**
- **SEM, Raman measurements show a pure diamond phase.**
- **Adamantane at HP-HT conditions results in nanodiamond formation through dehydrogenation.**
- **Abrupt change at ~600 °C indicates loss of hydrogen.**
- **HRTEM shows developing periodicity.**

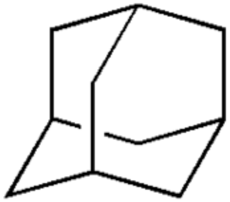
Kadek Hemawan
Carnegie

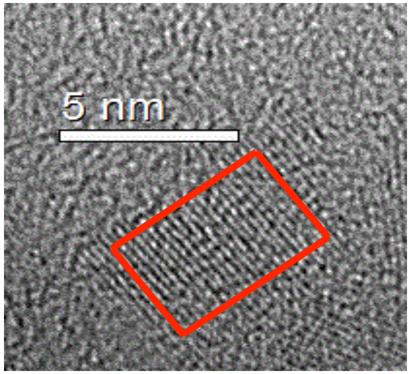
Todd Zapata
Texas A&M, Carnegie







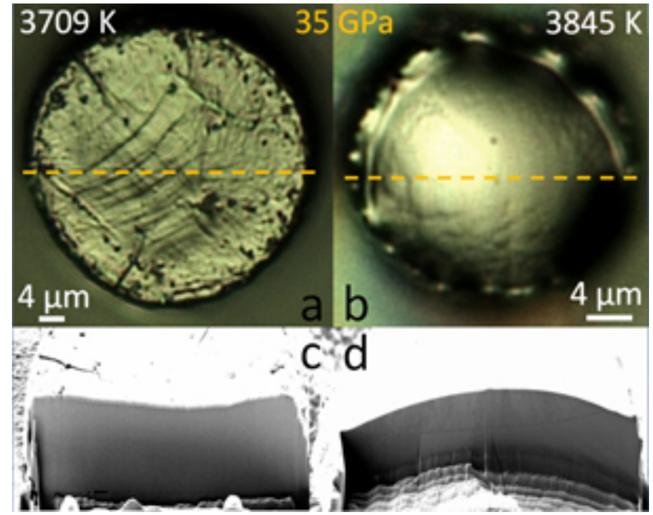


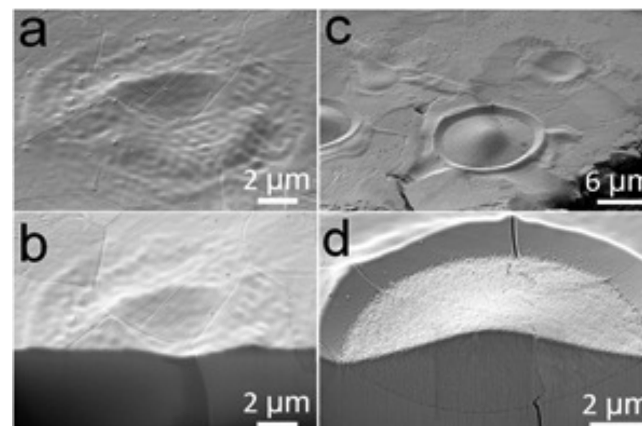


Flash Heating and the Melting of Refractory Transition Metals

CDAC

- Issues to overcome: chemical reactions, sample instability, thermal runaway
- 20 ms rectangular heating pulse, increase laser power to give 100 K increase in temperature for each new sample area—8-10 runs per sample loading
- SEM, EDS, FIB analysis of heated sample spots
- Re to 48 GPa, Mo to 45 GPa, melting curves reproduced well compared to other methods
- Ta to 85 GPa and 4320 K—discrepancies with previous methods are significant





Amol Karandikar
Carnegie

A. Karandikar and R. Boehler, submitted.

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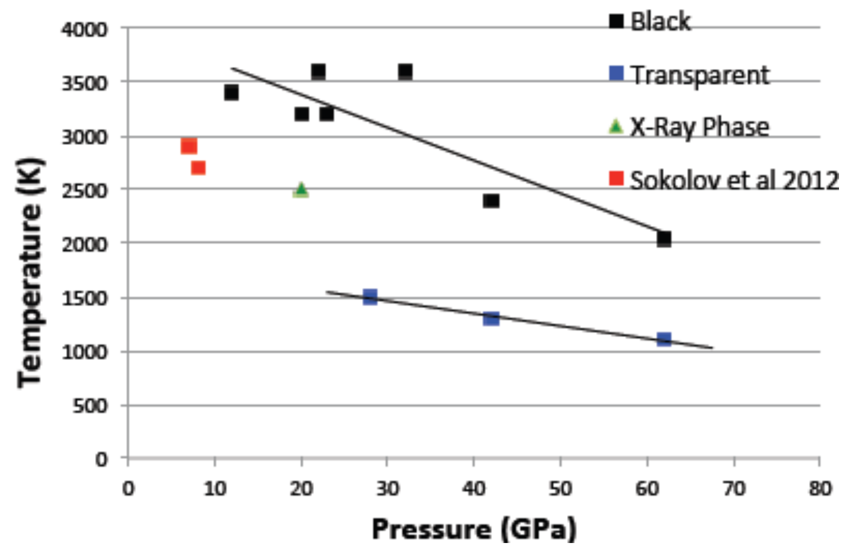
Temperature and Emissivity Mapping: Melting of SiC

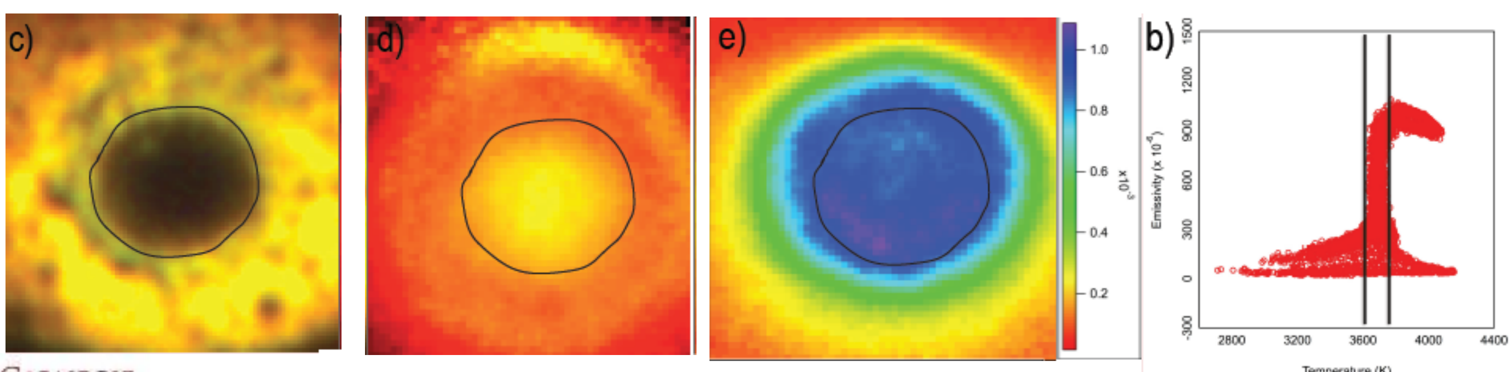
CDAC

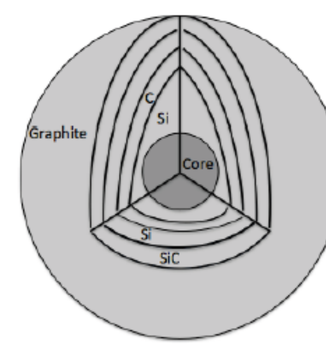
- Carbon-rich exoplanets: Interior Details?
- Flash heating, temperature, emissivity mapping
- SiC appears to decompose upon melting
- Suggests a mantle with alternating Si and C layers

Kierstin Daviau, Yale



β-SiC: 22 GPa   Temperature   Emissivity

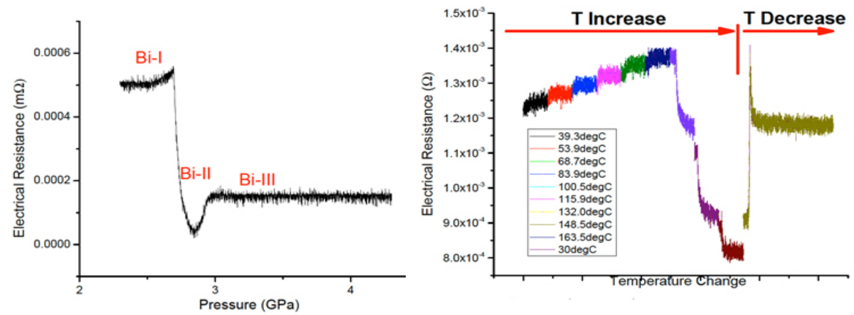




New Developments at HPCAT BM-B

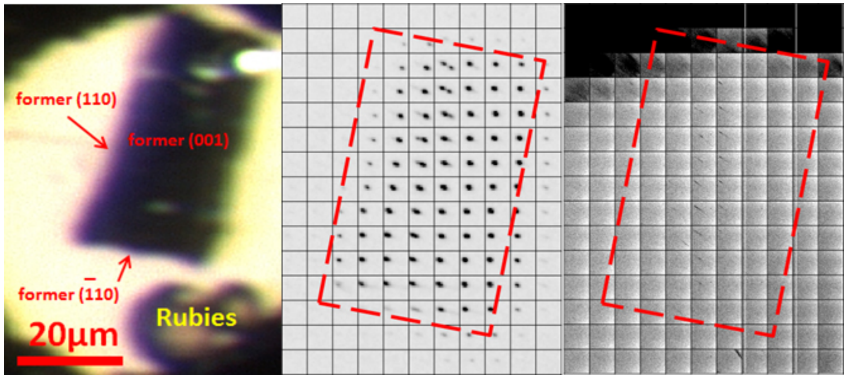
CDAC

- Simultaneous diffraction, radiography, resistance, and thermal measurements in the Paris-Edinburgh Cell
- Feasibility demonstrated to 6 GPa and 1000 °C
- White-beam Laue diffraction applied to spatially resolved strain mapping during α-β transition in Si
- Opens possibilities for studies of kinetics, mechanisms of phase transitions
- 2-3 orders of magnitude faster than with a monochromatic beam



Nenad Velisavljevic, LANL

α-Si (862)



Dimitry Popov, HPCAT

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Recent progress at CDAC presents new opportunities

CDAC

1. Education and Training

- Expanded student program with a large group of partners
- Continued placement of personnel in NNSA labs
- Summer schools/workshops and other outreach
- Student visits to NNSA Labs

2. Science Program

- Continued growth in number of high-profile publications
- Novel phenomena over a broad range of extreme conditions
- New opportunities for materials dynamics under extremes
- *Opportunities for the NNSA labs (beyond SSAA)*

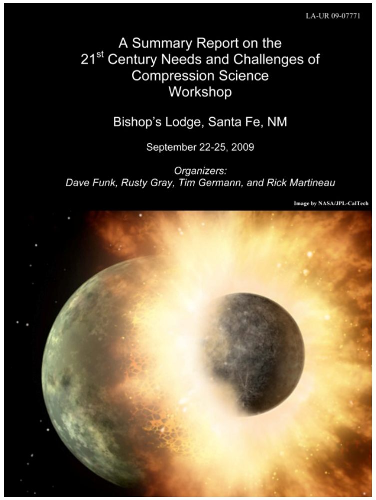
3. Technique Development

- Continued high *P-T* device developments
- New x-ray techniques (imaging, time-resolved, static/dynamic)
- Need to take advantage of APS upgrade

Broader Science Challenges

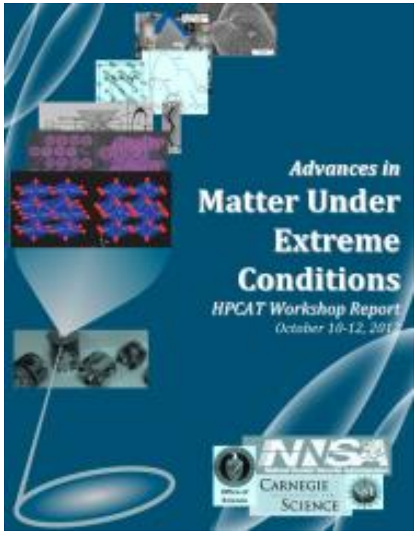
CDAC

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



Technical Challenges

1. Reaching 1 TPa and beyond
2. Multiprobe ‘intelligent’ devices
3. Stress-strain and P-T calibration
4. Advancing x-ray methods
5. Real time x-ray imaging with nm resolution
6. Filling the strain-rate gap: static to shock
7. Transport/constituitive properties
8. Liquids and amorphous materials
9. Thermochemical & magnetic measurements >100 GPa
10. Other techniques, including neutron scattering



FUTURE PERSPECTIVE

CDAC

1. Science Opportunities

There are numerous opportunities to address major scientific questions that both span the sciences and cut across static and dynamic compression research

2. Compression Science and the APS

Research at APS has led, and continues to lead, many of the advances in the field, and is poised to lead an integrated and coordinated program in materials in extreme environments for basic, applied, and programmatic science.

3. Role of CDAC

CDAC will serve as a bridge to help grow the academic and broader user communities.

Opportunity for a coordinated effort for extreme conditions science at APS

4. OUTLOOK

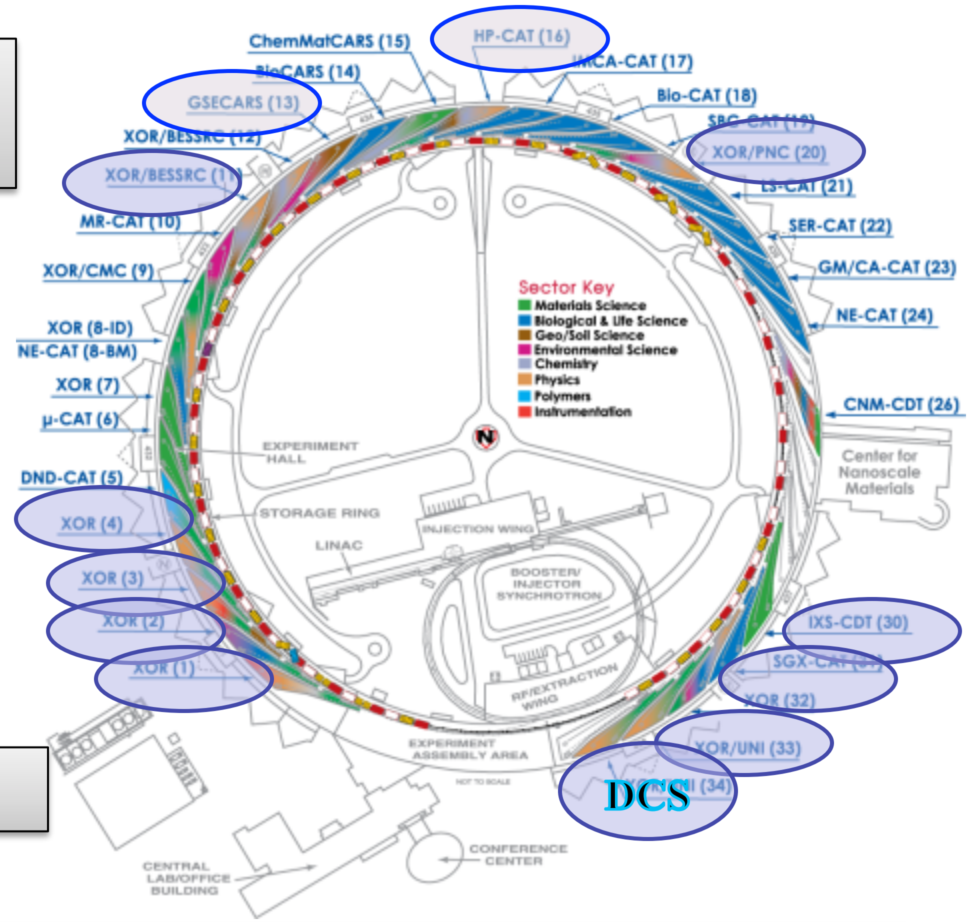
CDAC

APS beamlines being enhanced in the APS-U

HPCAT Upgrade

New DCS sector

Other sectors



Other facilities (LCLS, NSLS-II, Omega, NIF, MaRIE, …)

Opportunities for coordination at APS

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