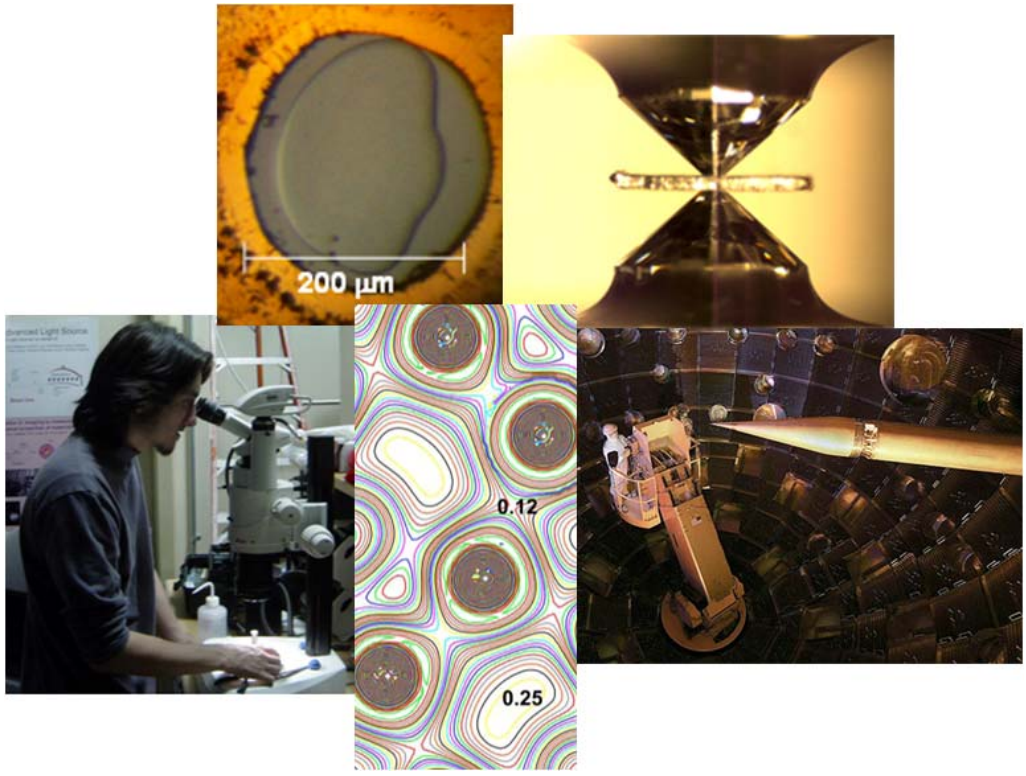
CDAC

CARNEGIE/DOE ALLIANCE CENTER

A Center of Excellence for
High Pressure Science and Technology
Supported by the Stewardship Science
Academic Alliances Program of DOE/NNSA



Year Six Annual Report

December 2009

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Ho-kwang Mao, *Associate Director*
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NNSA
CARNEGIE INSTITUTION FOR SCIENCE

Carnegie/DOE Alliance Center (CDAC):
A CENTER OF EXCELLENCE FOR HIGH PRESSURE SCIENCE AND TECHNOLOGY

YEAR SIX ANNUAL REPORT

On the Cover

Clockwise from top left: 1) Crystalline $SiH_4(H_2)_2$ formed from a mixture of SiH_4 and H_2 at in a diamond anvil cell and separated from the surrounding fluid at 7 GPa. In this high pressure material, the H_2 covalent bond weakens substantially, suggesting a pathway for dissociation and metallization of molecular hydrogen. 2) One of many types of diamond anvil cells in use at CDAC. Simple in design and powerful in application, such diamond-based devices allow measurements of structural, spectroscopic and transport properties of materials at extreme pressures up to several hundred gigapascals and temperatures close to 10^4 K.. 3) Target Chamber of the National Ignition Facility (NIF). CDAC personnel are participating the first materials science experiments carried out at NIF. Credit for this image is given to Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory, and the Department of Energy under whose auspices this work was performed. 4) Calculated electron density of the high-pressure, incommensurate tl19 phase of sodium metal prior to the formation of its recently discovered dense insulating state. 5) CDAC Graduate Student Lowell Miyagi examines a sample in a diamond anvil cell. Miyagi, who received his PhD from the University of California – Berkeley in 2009, investigated the deformation mechanisms of materials at high pressures and temperatures for his dissertation research with Academic Partner Hans-Rudolf Wenk.

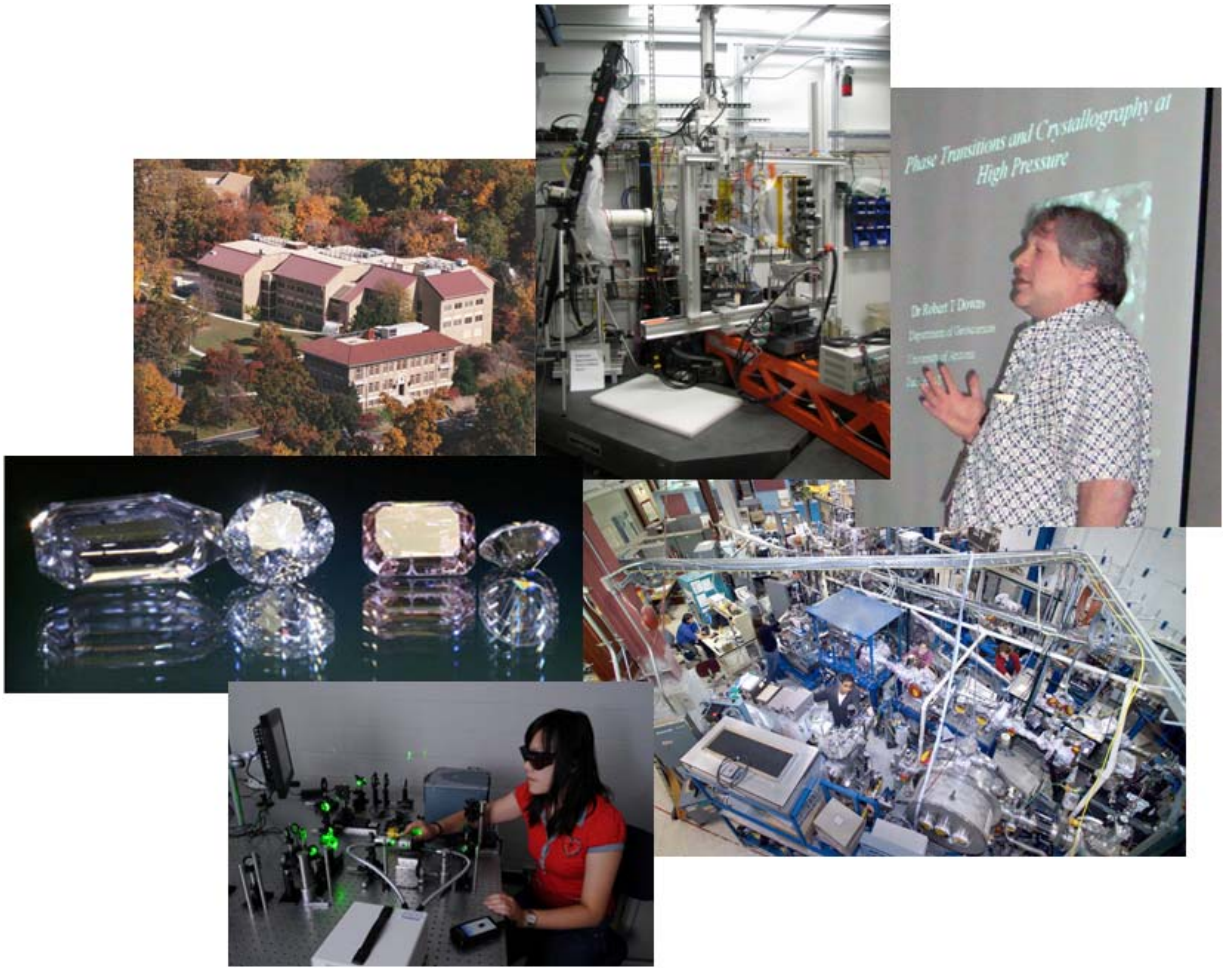
1. OVERVIEW

Science is the foundation of our Nation's security in the modern world. Indeed, the importance of science continues to grow with the numerous challenges we now face in maintaining the safety, security and reliability of our nuclear deterrent as the size of the stockpile is reduced. Moreover, that same fundamental knowledge is essential for nuclear forensics and the support of non-proliferation of nuclear weapons. In the absence of explosive nuclear testing, we must rely on accurate knowledge of the underlying physics, chemistry and materials science of the remarkable variety of components in the nuclear weapons complex. A key part of this broad scientific effort is an understanding of material behavior in extreme environments of pressure and temperature.

The Carnegie-DOE Alliance Center (CDAC) is a vibrant partner working in support of the national security effort, through our work with stewardship science campaigns in the Department of Energy (DOE)/National Nuclear Security Administration (NNSA). As a Center of Excellence within the Stewardship Science Academic Alliances (SSAA) program, the primary scientific work of CDAC is high *P-T* materials science of interest to DOE/NNSA. Here we highlight progress from the first year of our second five-year phase of funding as part of the SSAA program in an evolving era of stockpile stewardship.

1.1 CDAC in Year 6—New Advances and Opportunities

Since its founding, CDAC has been characterized by a remarkable diversity of scientific interests, and through our Center-like structure, CDAC continues to make a significant impact in scientific achievement, technique development, and student education and training. Academic



Partners in CDAC have been selcted from leading high-pressure programs in the United States representing chemistry, physics, materials science and geoscience departments, while CDAC Laboratory Partners come from the high-pressure groups at all three NNSA Labs. The scientific research carried out by CDAC groups is equally diverse, from investigating the equations of state, magnetic properties and phase transitions of rare earth and transition metals at high pressure and temperature to determining the high *P-T* vibrational properties of hydrogen and hydrogen-rich alloys and compounds. Increasingly important is chemical information at the atomic scale, and CDAC has made great strides in understanding how pressure affects chemical processes at interfaces and in bulk materials. Improved x-ray diffraction and analysis methods have enabled determinations of the elastic and rheological properties of a wide selection of polymeric materials and oxides, as well as the solution of structural models for polymers and bulk metallic glasses.

Advancements in a variety of x-ray spectrosopic techniques have likewise resulted in new information on phonon dynamics at high pressures, along with new views on the evolution of chemical bonding and magnetism in an extensive array of materials with pressure. This diversity in the CDAC experimental program provides an excellent framework for addressing the many multi-faceted issues in stewardship science, while interactions with theoretical groups in academia and the National Labs add an increasingly important compliment to the experimental work carried out within CDAC.

The Center is headquartered at **Carnegie** and managed by **Russell Hemley** (Director), **Ho-kwang Mao** (Associate Director), **Stephen Gramsch** (Coordinator) and **Morgan Phillips** (Administrative Assistant). In Year 6, CDAC consisted of 19 formal Academic Partners together with the **Carnegie** group: **Tom Duffy** ***(Princeton University)***, **Dion Heinz** ***(University of Chicago)***, **Dana Dlott** ***(University of Illinois)***, **Yogesh Vohra** ***(University of Alabama – Birmingham)***, **Hans-Rudolf Wenk** ***(University of California – Berkeley)***, **Brent Fultz** ***(California Institute of Technology)***, **Kanani Lee** ***(New Mexico State University/Yale University)***, **Surendra Saxena** ***(Florida International University)***, **Yanzhang Ma** ***(Texas Tech University)***, **Dhanesh Chandra** ***(University of Nevada – Reno)***, and **Jeffrey Yarger** ***(Arizona State University).*** The new Academic Partners joining the CDAC group in Year 6 brought an array of new experimental capabilities to CDAC, and have helped to maintain the ability to support stewardship science, as well as to define new areas of fundamental interest. New Academic Partners include **Abby Kavner** ***(University of California-Los Angeles)***, **Steven Jacobsen** ***(Northwestern University)***, **Jie Li** ***(University of Illinois)***, **Raymond Jeanloz** ***(University of California-Berkeley)***, **Wendy Panero** ***(Ohio State University)***, **James Schilling** ***(Washington University in St. Louis)***, **Robert Downs** ***(University of Arizona)***, and **Wendy Mao** ***(Stanford University)***.

In addition to facilitating the education of graduate students in high *P-T* materials science through our Academic Partners, CDAC fosters interactions with Laboratory Partners at each of the NNSA Labs, which adds to the outstanding scientific breadth of the CDAC effort. Through CDAC, Laboratory Partners have been able to initiate collaborations with Academic Partners, with staff at **Carnegie**, and with members of the broader academic high pressure research community, as well as to take advantage of cutting-edge technique developments and the availability of beam time at CDAC experimental facilities.

Addressing the key scientific problems associated with NNSA goals requires a continued effort to push forward the technical frontier of high *P-T* research into new pressure and temperature regimes and new levels of resolution (Fig. 1). This advancement can only take place at facilities specially geared toward high *P-T* work. In addition to ongoing work at **Carnegie**, **HPCAT**, the dedicated high-pressure synchrotron x-ray facility at the **Advanced Photon Source (APS)**, plays a leading role in pioneering developments in x-ray diffraction and spectroscopic techniques. Beamline U2A at the **National Synchrotron Light Source, Brookhaven National Laboratory (NSLS)** likewise provides key facilities and technique development in infrared spectroscopy. Both of these experimental facilities are supported by CDAC and managed by **Carnegie.** The **LANSCE** facility at **Los Alamos National Laboratory** also plays an important role in CDAC, with a number of groups actively engaged in the development of advanced experimental methods and analysis procedures in neutron scattering for high *P-T* research.

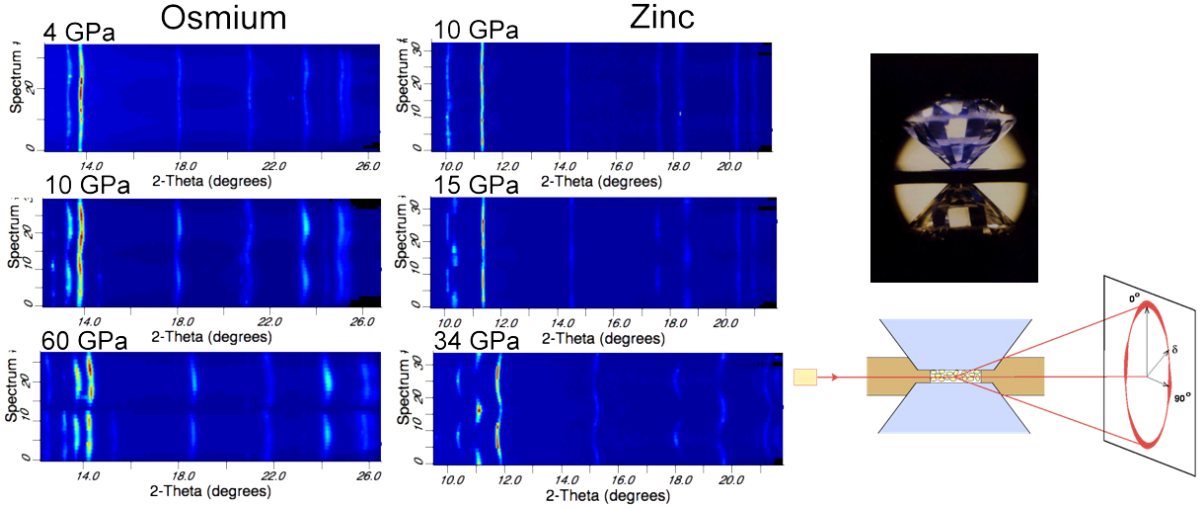


Figure 1. *Left) Intensity variations along Debye rings provide key information on texture development in metals at high pressure. The ability to carry out diffraction measurements in the radial geometry (right) at high pressure using the DAC is an important aspect of ongoing research in the group of CDAC Academic Partner* ***Hans-Rudolf Wenk*** *at* ***Berkeley****. The precision achieved in these experiments relies on the state-of-the-art diffraction capabilities available at HPCAT. Here, the data show distinct differences in texture development between hcp metals osmium and zinc at high pressure.*[77]

Managed by **Ho-kwang Mao** (Director) and **Guoyin Shen** (Project Manager), HPCAT (Fig. 2) was founded in 1997 to provide a facility dedicated to the development of spectroscopic and diffraction techniques critical to the advancement of the high *P-T* research frontier. The facility has reached the mature stage, with the original goal of four simultaneously operating beamlines having been realized. While new techniques are continuously under development at HPCAT and existing techniques are perfected, the facility now accepts General User Proposals (GUPs) for all four beamlines. At this point, more than 475 different users (*i.e.,* from National Labs and academia) have carried out experiments at HPCAT since its initial commissioning activities. Through its mission of promoting high pressure research at additional beamlines at the APS, the HPSynC initiative has after two years become an important resource for building the high pressure research community. Its dual program of technique development and scientific outreach has yielded a number of key collaborations and important new experimental methods that will be significant in addressing problems of relevance to the NNSA mission.

High-pressure neutron diffraction facilities at LANSCE, and U2A, the synchrotron infrared spectroscopy laboratory at the NSLS, provide additional venues where technical and scientific developments continue in support of high *P-T* materials science research, in addition to the specialized spectroscopy, diffraction, sample preparation and CVD diamond growth facilities

Figure 2. *The HPCAT Sector at the Advanced Photon Source is dedicated to advancing the state of the art in high P-T science and technology. With four separate beamlines and the capability to operate all four simultaneously around the clock, HPCAT provides critical resources for the high pressure research community. CDAC retains a 30% share in the available beam time, which is utilized by Academic Partners and their graduate students, and Laboratory Partners from the NNSA Labs. CDAC beam time is available to all Academic and Laboratory partners through a proposal review process, while Beamline Scientists at HPCAT provide experimental support for both new and experienced users.*

available at **Carnegie**, that have led to the recent breakthrough in ultratough diamond[1]. Research on material properties at extreme conditions continues to expand with the development of new methodologies, for example, in the overlap of static and dynamic compression experiments. The study of matter in transient, ultra high-density states is also of fundamental interest, and recently, a key goal of CDAC was realized when we were able to provide facilities at NSLS and HPCAT for the first synchrotron x-ray measurements of dynamic compression events, which have ushered in a new scientific frontier to complement ongoing developments within the NNSA Labs such as those at NIF and Z_R, CDAC seeks to facilitate the participation of the academic community in all of these areas, which will present important opportunities for NNSA research programs in the near future. With the potential of these and other facilities now in the planning stages, such as MaRIE at LANL, DC-CAT at APS, and NSLS-II at BNL, CDAC will continue to promote the integration of static and dynamic experiments for stewardship science.

This report covers activities from the CDAC Academic Partners, Laboratory Partners, and University Collaborators from July 2008 through July 2009. Research carried out by National Lab partners, but done outside of the CDAC facilities, is not included.

1.2 Highlights from Year 6

Outreach and Training

A primary goal of the CDAC program is the education and training of graduate students in high *P-T* materials science. Fully one-third of the CDAC budget each year is directed toward the support of graduate students in our Academic Partner groups. In addition, CDAC seeks to promote the growth of high *P-T* research through the support of relevant workshops and symposia. The following items provide highlights in this area from Year 6.

- In Year 6, CDAC supported the Ph.D. dissertation research of 26 graduate students at CDAC partner universities and **Carnegie**. Thus far, 18 graduate students from Academic Partner institutions have received the Ph.D. degree with CDAC support. Completing the Ph.D. degree this year were six students, including two students who had been completely supported by CDAC since the beginning of their graduate work.

- In association with the Year 6 Review, CDAC hosted its first Winter Workshop at the Advanced Photon Source February 27-March 1, 2009 (Fig. 3). This workshop provided an opportunity for

Academic Partners, Laboratory Partners and graduate students alike to present recent results and become familiar with the research taking place throughout the Center. More than 40 people attended the workshop, including the majority of CDAC graduate students.

- **Carnegie** hosted four undergraduate students and two high school students, who worked on projects related to high *P-T* materials science in our laboratories, with close supervision and guidance provided by the staff.

Figure 3. *The CDAC Winter Workshop, clockwise from top left. Students listen to the presentation of* ***Rip Collins (LLNL)*** *on laser shock compression; Academic Partner* ***Dana Dlott (Illinois)*** *presents his lecture "Laser-driven shock waves and molecular spectroscopy;" Laboratory Partner* ***Marcus Knudson (Sandia)*** *presented a tutorial on current research activities at* ***Sandia's*** *Z machine; students listen to the presentation of Academic Partner* ***Hans-Rudolf Wenk (Berkeley)*** *on texture development at high pressure; CDAC graduate student* ***Zhu Mao (Princeton)*** *discusses her poster with Professor Wenk.*

- CDAC continued its longstanding commitment to the support of the HPCAT sector at the Advanced Photon Source. Due in part to the substantial 30% share CDAC provides to the operations budget of HPCAT, the number of users of the facility continues to grow. As of the writing of this report, the number of individual users carrying out original research or technique development projects is now over 475.

- CDAC supported the High Pressure Sychrotron Science Symposium, which was held May 6-8, 2009 at the Advanced Photon Source. More than 100 people from around the world attended the meeting, which provided an overview of cutting-edge synchrotron science and technique development.

- In celebration of the retirement of **Jingzu Hu** and **Quanzhong Guo** from the NSLS after 18 years of service to the high pressure research community, the symposium "Advances in High

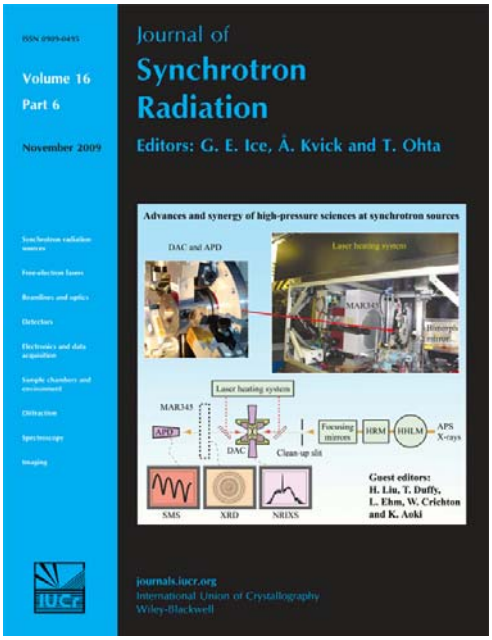


Figure 4. *Cover of the November 2009 issue of the* Journal of Synchrotron Radiation*, which contained invited papers presented at the symposium "Advances in High Pressure Science Using Synchrotron Radiation."*

Pressure Science Using Synchrotron Radiation" was convened October 4, 2008 at the NSLS. CDAC support allowed a number of graduate students to attend the event. The proceedings were published in a special issue of the *Journal of Synchrotron Radiation* (Fig 4).

Scientific Breakthroughs

An expansion in the number of Academic Partners, and increased interactions between academic nodes, Carnegie and NNSA Laboratory Partners, has yielded impressive scientific results across the spectrum of research areas in the CDAC program. To date, more than 750 papers have been published in the open literature, including an increasing number in high-impact journals. Through Year 6, 50 papers have appeared in *Physical Review Letters*, 12 in *Science*, 27 in the *Nature* magazines, and 38 in the *Proceedings of the National Academy of Sciences*. Virtually all the work reported in CDAC publications represents graduate student or postdoctoral training. These publications include work carried out by CDAC Academic and Laboratory Partner groups, as well as work at Carnegie supported by CDAC. In addition, work at HPCAT and U2A with CDAC support is also included. Scientific progress will be outlined in detail in Section 2.

- CDAC graduate student **Mike Winterrose** (**Caltech**, see photo, p. 2) used a combination of nuclear resonance spectroscopy and first principles computational methods to work out the microscopic causes of Invar behavior in iron-containing alloys.[2] The use of high pressure techniques along with the technical capabilities available at HPCAT were instrumental in resolving this long-standing problem in materials physics.

- Laboratory Partners **Neal Chesnut** and **Nenad Velisavjlevic** (**LANL**) showed that the pressure of the α-ω phase transformation in the group IV metals decreases with increasing temperature. Detection of the phase transformation in Ti by monitoring the electrical resistance of the sample with pressure was made possible by the use of "smart anvils."[3]

- CDAC Research Scientist **Maddury Somayazulu** (**Carnegie**) examined the behavior of the Xe- H_2 system at high pressure and temperature and discovered the compound $Xe(H_2)_7$, which has the highest mole percent hydrogen of any compound yet prepared. (Fig. 5) The results of this work open a new area of research on noble gas chemistry.[4]

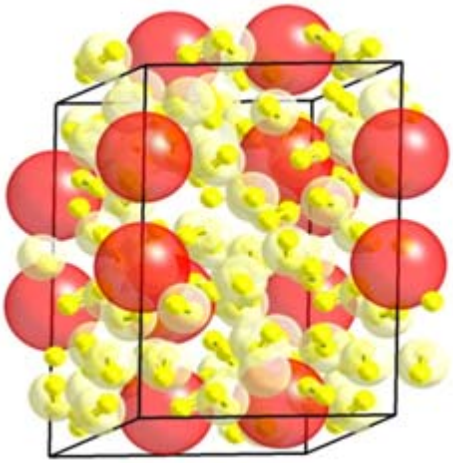


Figure 5. *The crystal structure of $Xe(H_2)_7$. Large pink spheres represent Xe atoms, and the small yellow spheres represent the rotationally averaged positions of the hydrogen molecules.*[4]

- CDAC graduate student **Arianna Gleason** (**Berkeley**) showed that is it possible to obtain reliable information on the elastic properties of materials as well as the equation of state using Brillouin spectroscopy on powder samples. Agreement between single crystal and powder results from Brillouin scattering and powder x-ray diffraction shows that

the technique is a viable method for equation of state (EOS) and elasticity determination at high pressure.

- CDAC Academic Partner **Hans-Rudolf Wenk** (**Berkeley**) used the HIPPO diffractometer at LANSCE to document grain growth patterns in pure uranium metal at high temperatures. Results indicate that a memory of the orthorhombic phase exists even after a phase transformation to the cubic bcc structure.[5]

- Working with the SiH_4-H_2 system, postdoctoral fellow **Tim Strobel** (**Carnegie**) prepared the compound $SiH_4(H_2)_2$ at 7 GPa (Fig 6). Raman spectroscopy shows that the intramolecular H-H bond weakens significantly at low pressure, suggesting a pathway for molecular dissociation of H_2.[6]

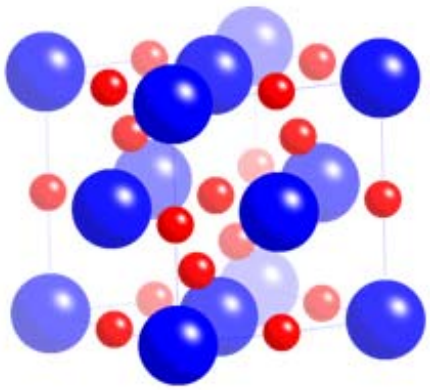


Figure 6. *Crystal structure of $SiH_4(H_2)_2$. Blue spheres represent the positions of the SiH_4 molecules on an fcc lattice, with the red spheres showing the rotationally averaged positions of H_2 molecules.*[6]

- Orientation-dependent SFG spectrscopy of surfaces is now possible in the laboratory of CDAC Academic Partner **Dana Dlott** at **Illinois**. Graduate student **Aaron Lozano** is using the technique to investigate the orientation of nitro groups on the surfaces of single crystal HMX and RDX.[7]

- At **Carnegie**, postdoctoral fellow **Yufei Meng** showed that microwave plasma annealing of CVD diamond at 2000 ºC and below atmospheric pressure is an effective method for removing defects in the material. Following annealing, diamond material that is originally yellow-brown becomes colorless or light pink.

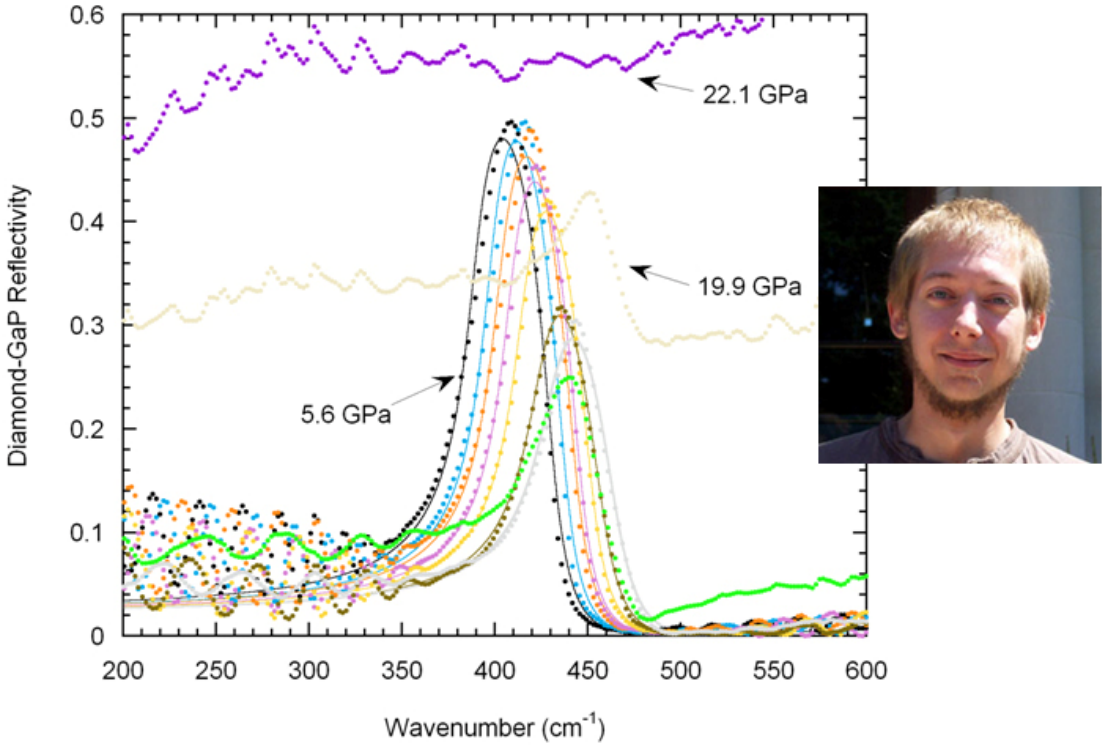


Figure 7. *Reflectivity of the Diamond-GaP interface at high pressure. The main peak in the spectrum is due to the TO phonon mode which shifts to higher wavenumber and decreases in intensity as pressure is increased. The disappearance of the phonon mode and sharp rise in the magnitude of the reflectivity are associated with the metallization of GaP at ~20 GPa. The solid lines are fits to the lower pressure data using the Lorentz oscillator model. Inset: CDAC Graduate Student **Chris Seagle (Chicago)**.*[9]

- At HPCAT, **Yogesh Vohra's** group at **Alabama-Birmingham** discovered a tetragonal to amorphous phase transition at 11.5 GPa in the superconducting compound $FeSe_{0.5}Te_{0.5}$. Disordering of $Fe(Se,Te)_4$ tetrahedra appear to accompany the phase transformation, which has a significant hysteresis.[8]

- CDAC graduate student **Chris Seagle** (**Chicago**) used the infrared beamline U2A at NSLS to study the reflectivity of semiconductors at high pressure and showed that the disappearance of the TO phonon mode in GPa at ~20 GPa is associated with band gap closure and metallization (Fig. 7).[9]

- Visiting Scientist **Pierre Toledano** (**Universite de Picardie**) has developed a group theory approach to the problem of predicting the structures of the high-pressure, low- temperature broken symmetry phases (phases II and III) of solid hydrogen. Analysis of the behavior of order parameters with pressure provides evidence for a partially ordered structure for H_2-II and an ordered structure for H_2-III, as well as a new phase, H_2-I', isostructural with H_2-III.[10]

- CDAC graduate student **Susannah Dorfman** at **Princeton** has for the first time directly compared the equations of state of metals and MgO, one of the best constrained pressure calibrants. In an experiment carried out to 226 GPa, the pressures indicated by the MgO and Pt scales differed by as much as 10% above 200 GPa. This result has provided the incentive to understand the origin of these differences, which have important implications for the accuracy of high *P-T* experiments.

Technique Development

CDAC groups continue to pioneer new directions in experimental methods, which are crucial in enabling the next level of advancement in high *P-T* science. In addition to key upgrades in the capabilities at synchrotron sources, highlights for Year 6 in the area of technique development include a number of improvements to laboratory-based techniques, such as laser heating instrumentation, spectroscopic methods for investigation of laser shocks, and gigahertz interferometry for elasticity measurements. These will be described in detail in Section 4.

- CDAC Academic Partner **Steven Jacobsen** (**Northwestern**) has developed a hybrid optical-mechanical interferometer that allows measurements of sample thicknesses to be carried out with a precision about ± 0.01 mm (Fig 8). The resulting uncertainty in the measurement of elastic constants has now been improved by an order of magnitude.

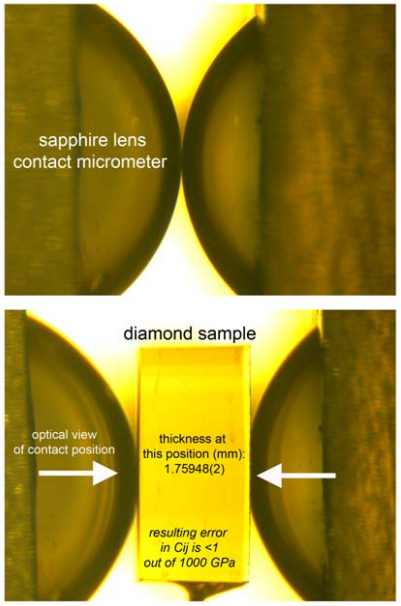


Figure 8. *Micrometer component of the length-measuring instrument, composed of two sapphire lenses, which allow optical access to view the contact position.*

- In the group of CDAC Academic Partner **Dana Dlott**, graduate student **Kathryn Brown** has developed a method for fabricating photonic substrates for diamond anvil cell (DAC) work. The substrates consist of silver-coated nanospheres that enhance the Raman spectra of adsorbate monolayers by a factor of about 10^6 through the surface-enhanced Raman scattering effect. In related work, the sum-frequency generation technique is now applied to obtaining the vibrational spectra of flash-heated adsorbates.[11] The group has also developed a method for measuring the spectroscopy of reactive materials initiated by the high-speed impact of laser-launched flyer plates. An interferometer accurately measures the velocity history of the flyer plate at velocities up to 6 km/s.

- Picosecond interferometry and time-domain thermoreflectance measurements carried out by CDAC Academic Partner **Jie Lie** and colleague **David Cahill** (**Illinois**) allow high precision measurements of the thermal conductivity of materials in the DAC. The technique has been applied to both problems of heat conduction in layered crystals as well Earth materials in the Earth's lower mantle and core.

- **Hans-Rudolf Wenk's** group at **Berkeley**, in collaboration with the HPCAT staff, designed and built a resistance furnace for use at beamline 16-BM-D. The furnace provides for stable heating to ~30 GPa and 1100 °C for radial diffraction experiments, which are crucial for the analysis of texture development at high pressure, as shown in Fig 9.

Figure 9. A *resistance furnace at beamline 16 BMD of HPCAT for high temperature diffraction studies used by* ***Lowell Miyagi (Berkeley).***

- At **HPCAT**, Beamline Scientist **Stanislav Sinogeikin** has developed a membrane control system adaptable to every variety of DAC. The membrane system gives a much finer control of pressure on the DAC than the standard method of turning screws. This improvement is particularly important in studying phase transitions, where small increments in pressure are crucial.

- At **Washington University**, CDAC graduate student **Wenli Bi** has developed photolithography techniques for preparing coils for DAC transport measurements. Deposited onto the diamond culet, the coils will allow AC susceptibility and resistivity measurements on samples as small as 50 μm at multimegabar pressures.

- Beamline Scientists **Paul Chow** and **Yuming Xiao** at **HPCAT** have commissioned a Pilatus detector for use on the x-ray spectroscopy beamline 16-ID-D. The detector provides for higher sensitivity for low-count rate experiments such as x-ray emission (Fig 10).

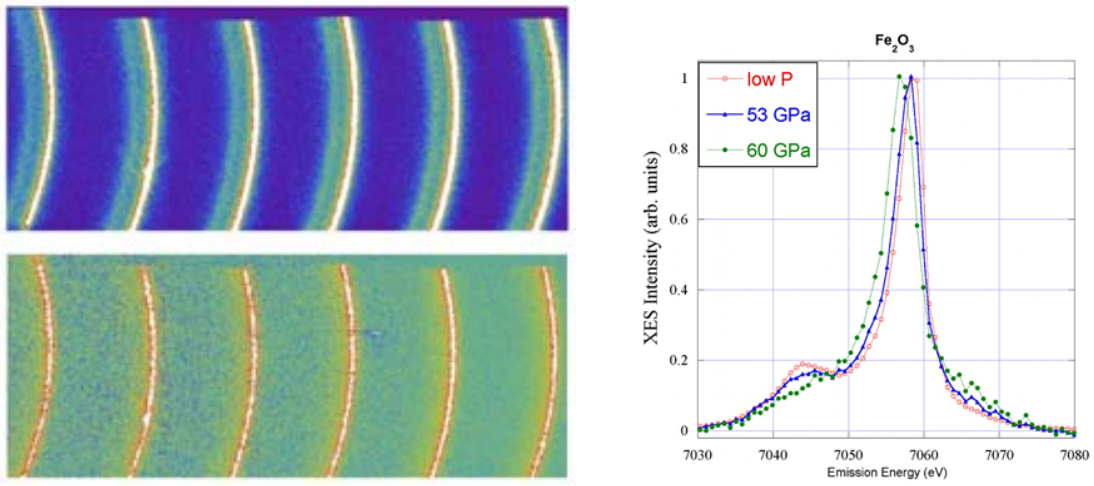


Figure 10. *Left) Pilatus detector images of Fe_2O_3 at ambient (top) and 60 GPa (bottom). Right) Fe K_β XES spectra of Fe_2O_3 at various pressures. The disappearance of the K_β satellite peak, indicating a high- to low-spin transition, is cleanly resolved.*

2. SCIENTIFIC PROGRESS

CDAC continues to make impressive scientific progress in each of our six key areas of research, even as new interests arise with breakthroughs in experimental techniques. We classify the CDAC research effort into six principal research areas, although we have become increasingly

interdisciplinary as our program has matured over the last six years, and new areas of scientific interest have emerged. This section describes scientific progress in the following general areas.

1. High *P-T* Phase Relations and Structures
2. *P-V-T* EOS Measurements
3. Phonons, Vibrational Thermodynamics and Elasticity
4. Plasticity, Yield Strength and Deformation
5. Electronic and Magnetic Structure and Dynamics
6. High *P-T* Chemistry

2.1 High *P-T* Phase Relations and Structures

Structural relationships at high pressure and temperature provide the key background information for understanding the effects of pressure on materials, and this area of research has always been at the center of CDAC research efforts. Technical advancements at HPCAT and NSLS have increased the resolution with which structural changes may be determined, and at the same time the array of materials of interest to CDAC groups continues to increase. Over the last year, interest in semi-crystalline amorphous solids as well as iron-based superconductors has been a focal point of activity in several CDAC groups. New findings in hydrogen and hydrogen-containing systems also continue to highlight work in the area of high *P-T* structural science.

Reversible Pressure-Induced Amporphization in Superconducting $FeSe_{0.5}Te_{0.5}$ – The phenomenon of pressure-induced amorphization in the superconducting compound $FeSe_{0.5}Te_{0.5}$ has been studied to 27 GPa. Using synchrotron diffraction techniques, the **Alabama** group has found that the ambient pressure tetragonal phase (*P*4/*nmm*) transforms to an amorphous phase at 11.5 GPa during compression and reverts back to the tetragonal phase during decompression at 2.8 GPa. The onset of the tetragonal to amorphous transition is detected at 11.5 (± 1.0) GPa, with disordering of $Fe(Se,Te)_4$ tetrahedra under compression attributed to a kinetic hindrance to a stable phase and is likely to impact its superconducting properties under high pressures.[8] Figure 11 shows the integrated x-ray diffraction profile (intensity versus 2θ) for $FeSe_{0.5}Te_{0.5}$ at various pressures. Figure 11a shows the tetragonal phase at ambient conditions after pressure cycling to 27.2 GPa. This x-ray spectrum is identical to that of the starting tetragonal sample. The spectrum in Fig. 11a at ambient pressure was measured outside the high pressure cell with sample contained in the metallic gasket after the high pressure experiment. All ten observed diffraction peaks in Fig. 11a can be assigned to a tetragonal phase. Figure 11b shows the onset of the transformation at 11.5 GPa where a broad peak characteristic of an amorphous phase marked by an asterisk is beginning to appear along with the tetragonal phase. The transformation to an amorphous phase is completed by 15.2 GPa and

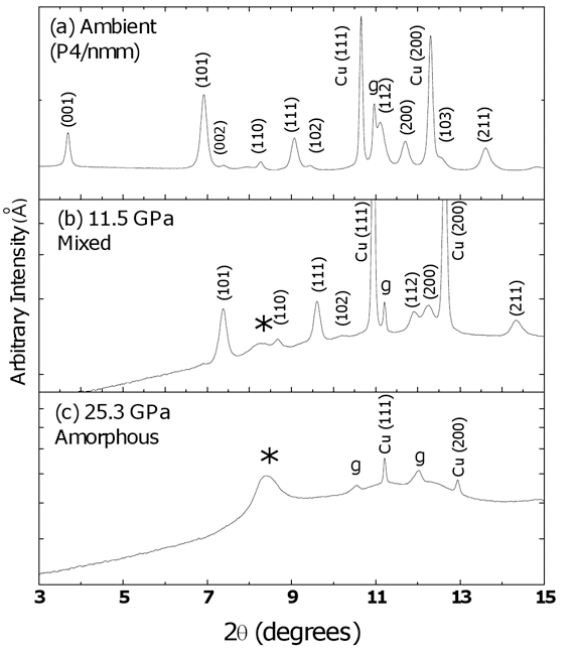


Figure 11. *Angle-dispersive x-ray diffraction patterns of $FeSe_{0.5}Te_{0.5}$ and a copper (Cu) pressure marker at various pressures. All spectra have been collected at the HPCAT sector using an x-ray wavelength λ= 0.3875 Å. a) Sample in the tetragonal phase at ambient pressure after pressure release from 27.2 GPa. b) Sample at 11.5 GPa at the onset of the transition to the amorphous phase. c) Sample in pure amorphous phase showing a broad peak denoted by an asterisk. The diffraction peaks from the Cu pressure marker are also indicated and "g" represents weak peaks from the spring steel gasket.*[8]

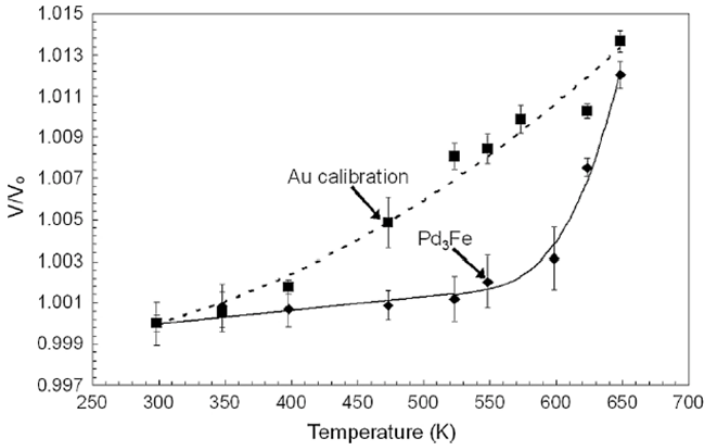


Figure 12. *Volume-temperature data for Pd_3Fe (diamonds) and Au (squares) obtained from externally heating the diamond anvil cell at an approximately constant pressure of 7 GPa. The Pd_3Fe shows practically no thermal expansion up to 573 K.*

the amorphous phase was found to be stable to the highest pressure of 27.2 GPa. The measured spectrum for the amorphous phase at 25.3 GPa is shown in Fig. 11c and is dominated by a strong peak of amorphous phase at an interplanar spacing of 2.644 Å. The tetragonal to amorphous phase transformation is reversible on decreasing pressure and a back-transformation is observed to start at 2.8 GPa, with the pure tetragonal phase recovered at ambient conditions as shown in Fig. 11a.

Pressure-Induced Invar Phenomena – Thermal Invar behavior in the Pd-Fe system is well known for compositions around $Fe_{70}Pd_{30}$, but a greater Pd concentration stabilizes the ferromagnetic state, suppressing thermal Invar behavior. The composition Pd_3Fe does not show thermal Invar behavior. Two years ago, in CDAC-funded work, graduate student **Mike Winterrose** discovered pressure-induced Invar behavior in Pd_3Fe with the ordered $L1_2$ structure. He has now completed an important phase of this work, the results of which have been published recently.[2]

In this work on Pd_3Fe under pressure, synchrotron x-ray diffraction (XRD) measurements were performed at NSLS, and nuclear forward scattering (NFS) measurements performed at HPCAT. Both NFS and XRD measurements were performed at a fixed temperature of 300 K at pressures up to 33 GPa. XRD measurements were also performed at a fixed pressure of 7 GPa at temperatures up to 650 K. The NFS spectra 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, confirming Invar behavior (Fig. 12). Density functional theory (DFT) calculations were performed on $L1_2$-ordered Pd_3Fe, and showed the ferromagnetic state to be the ground state, and that several antiferromagnetic states had comparable energies at pressures above 20 GPa.

In subsequent work, it was found that the effect of composition and the effect of pressure on the electronic band structure of ordered Pd_3Fe are very similar. Under pressure, the occupied but antibonding spin-up t_{2g} states are pushed up in energy. At the pressure of the Invar transition, these cross the Fermi level, and spin down states become occupied, changing the magnetism. The same effect is found by decreasing the Pd concentration, and very similar electronic band structure is found at ambient pressure around compositions of $Fe_{70}Pd_{30}$.

In a follow-up experiment at HPCAT, the temperature was decreased when Pd_3Fe was under pressure, and the Invar transition was found. Figure 13

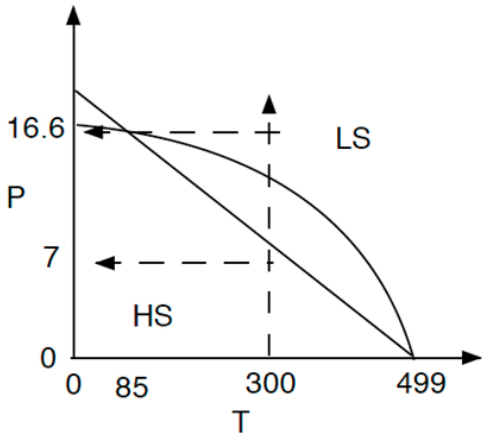


Figure 13. *Pressure-temperature phase diagram of the Invar transition in ordered Pd_3Fe. Dashed arrows are paths taken in experimental measurements. (LS denotes low-spin, HS denotes high-spin region.) A straight line boundary for the Invar transition is predicted by a simple Weiss-like mode; the curved line corresponds to experimental transition under pressure at 300 K.*

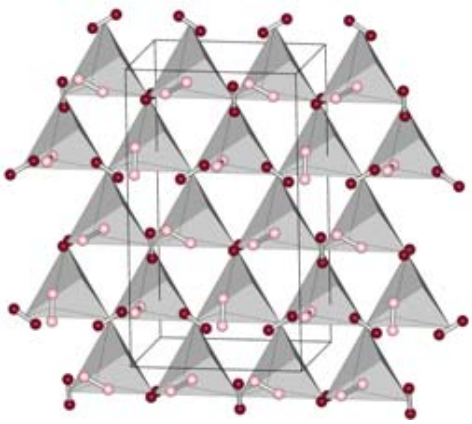


Figure 14. *The $Cmc2_1$ structure of H_2-III in the conventional unit cell.*[10]

shows an approximate phase diagram, compiled using available data of the Invar transition in temperature and pressure. A simple thermodynamic prediction with independent effects of pressure and temperature gives a straight line, but it seems that there is an increased stability of the high-spin phase when temperature and pressure are both present simultaneously.

Progress in Understanding the Behavior of Dense Solid Hydrogen – The structure of hydrogen in the dense molecular state remains challenging both experimentally and theoretically. Working with CDAC scientists at **Carnegie**, Visiting Scientist **Pierre Toledano** of the **Universite de Picardie** developed a group-theory approach and combined it with available experimental data to predict the structures of the elusive high-pressure, low-temperature broken symmetry phases of solid molecular hydrogen (phases II and III). Data from spectroscopy and diffraction experiments do not provide unambiguous structural information for these orientationally ordered phases, but do suggest that the corresponding transitions are quasi-continuous and not reconstructive. This fact allows the use of the Landau theory to predict potential structures of the high pressure phases by constraining the number of possible mechanisms available for their formation.[10]

Analysis of the behavior of order parameters with pressure suggests that H_2-II has a partially ordered structure, while H_2-III has an ordered isotranslational structure (Fig. 14). In addition, the existence of another high-pressure phase, H_2-I' isostructural with H_2-III, has been predicted. This new phase is defined by a boundary in the phase diagram that meets the boundaries of H_2-I and H_2-III at a second triple point. The results have important implications for metallization predicted at higher pressures.

Pressure-Induced Compound Formation in the Xe-H_2 System – Using a combination of x-ray diffraction and optical spectroscopy measurements, a **Carnegie** group led by **Maddury Somayazulu** has recently discovered the formation of a stable compound in the Xe-H_2 binary system. At 4.8 GPa, a unique, hydrogen-rich structure forms that can be viewed as a tripled solid hydrogen lattice modulated by layers of Xe (Fig. 5), consisting of xenon dimers and the formation of unusual bonding states. Varying the applied pressure tunes the Xe-Xe distances in the solid over a broad range from that of an expanded xenon lattice (ambient pressure-low temperature structure) to the distances observed in metallic xenon at megabar pressures. Infrared and Raman spectra indicate a weakening of the H_2 covalent bond as well as the persistence of semiconducting behavior in the compound to at least 255 GPa. High quality single crystal diffraction data collected over a large reciprocal space allows the details of the xenon electron density in this structure to be determined. A striking spread of electron density towards the interstitial hydrogen molecules is the first direct evidence in this class of compounds that points to overlap between the low-lying xenon bonding states and the energetically high-lying hydrogen antibonding states. Raman spectroscopy measurements to the highest pressure of 255 GPa (well above the metallization pressure of 133 GPa in pure Xenon) show no indications of weakening of the H-H covalent bond. Synchrotron IR spectroscopy measurements show no signatures of Drude absorption at these pressures.[4] Put together, these experimental observation indicate that metallization in electron-rich van der Waals compounds such as $Xe(H_2)_8$ does not take place readily although the compound itself is stable against dissociation at these extreme compressions.

Intermolecular Interactions in the SiH_4-H_2 System at High Pressure – The behavior of molecular hydrogen over a range of thermodynamic and chemical environments is of fundamental importance to basic condensed matter physics, astrophysics and energy applications. While the role of H_2 in most simple molecular compounds is well described by small perturbations to bulk H_2,

Carnegie researchers **Timothy Strobel**, **Madurry Somayazulu**, and **Russell Hemley** have discovered a new hydrogen-rich compound, $SiH_4(H_2)_2$, that displays anomalously strong intermolecular interactions.[6]

The new compound, which crystallizes above ~7 GPa, was characterized by synchrotron x-ray diffraction, Raman and synchrotron IR spectroscopy, and optical microscopy. Results show that the structure is face-centred cubic (fcc) with four SiH_4 and eight H_2 molecules per unit cell (Fig 6). Spectroscopic measurements on this compound show the molecular H_2 bond weakens at remarkably low pressure (Fig. 15), indicating tendency towards dissociation with increasing pressure and eventual metallization. Additional evidence for enhanced interactions in this system is provided by the observation of isotopic exchange experiments in which deuterium atoms from D_2 readily exchange with protons of SiH_4 to create H-D and Si-D stretching modes.

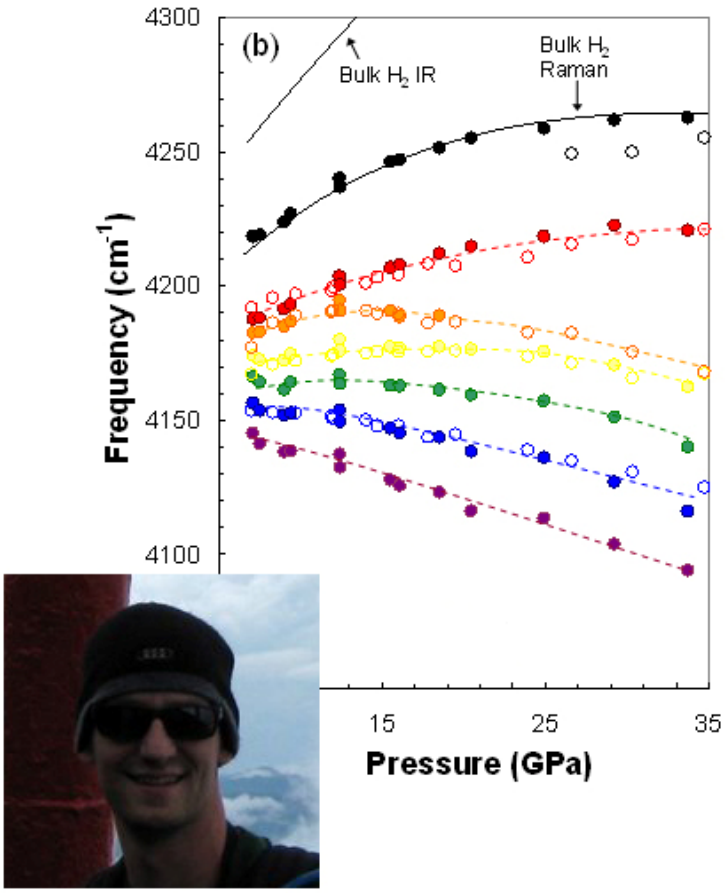


Figure 15. *Raman (filled symbols) and IR (open symbols) vibron frequencies for hydrogen in $SiH_4(H_2)_2$ with increasing pressure. Raman and IR vibron frequencies for bulk H_2 are given by solid lines; dashed lines are drawn to guide the eye. Inset:* ***Tim Strobel (Carnegie).***[6]

The unique features observed in this system suggest a range of previously inaccessible intermolecular interactions in H_2-bearing molecular systems and a potential new class of dense low-Z materials. Additionally, the combination of SiH_4 (which was previously predicted[12] and experimentally verified[13-14] to undergo an insulator to metal transition and exhibit superconductivity), with a second hydrogen-rich sublattice represents an alternative path for the pressure-induced dissociation of molecular hydrogen.

Phase Tranformations in Eu Metal at High Pressure – In the group of CDAC Academic Partner **Jim Schilling** at **Washington University**, superconductivity was recently discovered in Eu metal at pressures above 75 GPa.[15] It is important to determine whether the appearance of superconductivity is accompanied by a structural phase transition and how the Eu valence changes under pressure. The goal of the present work was to extend earlier published studies on pure Eu to 27 GPa[16] to much higher pressures in order to gain information on whether or not Eu undergoes an increase in valence from divalent to trivalent. CDAC graduate student **Wenli Bi** discovered a phase transition above 30 GPa (Fig. 16). Wenli is currently collaborating with **Ravhi Kumar** at **HiPSEC/UNLV** on an analysis of the experimental data. Further information on experimental advances that have enabled these challenging experiments is provided in Section 2.5.

Polyamorphic Systems at High Pressure and Temperature – In recent work, the **Yarger** group at **Arizona State University** has realized an urgent need to develop better DAC methods to characterize the structure and dynamics of liquids and glasses at pressure. The group is

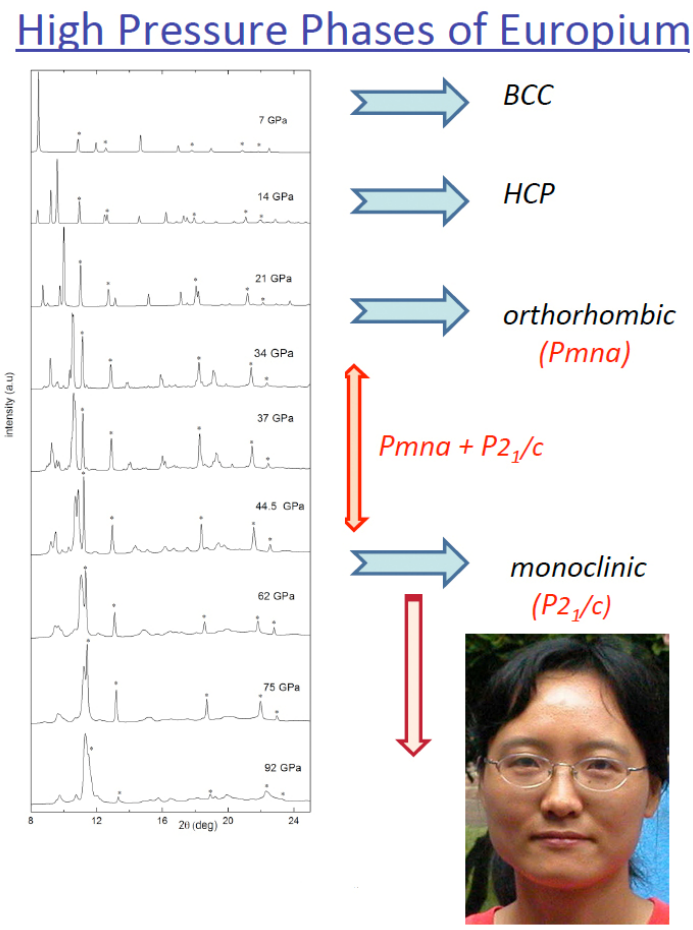


Figure 16. *Synchrotron x-ray diffraction data for Eu metal to 92 GPa, indicating phase transition above 30 GPa. Inset: CDAC graduate student* ***Wenli Bi (Washington University).***

currently developing the technology of perforated DACs for *in-situ* x-ray diffraction of liquids and glasses at high pressure and temperature. The x-ray structure factor of vitreous As_2O_3 has been measured at 32 GPa in a laser-perforated DAC using a monochromatic, micro-focused high-energy x-ray beam.[17] In the process of this work, experimental x-ray DAC instrumentation and data analysis and filtering techniques have been developed that have greatly improved the ability to characterize liquids and glasses at high pressure. Laser-perforated diamonds were used to minimize the amount of anvil material in the beam path and thereby the Compton scattering from the DAC, while maintaining a relatively high strength. **Emmanuel Soignard**, a research professor working in collaboration with the CDAC partnership has been primarily responsible for developing perforated DACs for use in x-ray diffraction of liquids and glasses at pressure. **Soignard** has also worked closely with both graduate and undergraduate students to teach them high-pressure loading and *in situ* characterization techniques.

CDAC graduate student **Samrat Amin** and undergraduate student **Keri McKiernan** have teamed up to study polyamorphism in chalcogenide glasses and liquids at high pressure, and are developing DAC NMR techniques for investigating these materials. Research has begun with a preliminary study of GeAsS glasses. A structural collapse of the As_4S_3 cages that are found in the ambient glass and liquid are believed to be the primary structural mechanism for a phase transition in this material. As shown in Fig. 17, the Raman mode at 270 cm-1, which is associated with the As_4S_3 cages, is shown to diminish in intensity at high pressure. A kinetic effect is also observed.

In-situ DAC Raman experiments were conducted under the same conditions, differing only in the time held at high pressure. The pressures chosen were 9 GPa, and 14 GPa, and the times held at high pressure were 1 and 4 hours. Through these experiments it can be seen that there is a clear correlation between time held under high pressure and the intensity of the molecular peak recovered. A major concern of this system is its glass transition temperature, resting just above room temperature at 29°C. This raises the question of whether peak recovery is strictly a function of kinetics, or whether thermodynamics play a role. To answer this question a series of experiments are planned for the future to repeat the previous pressure-time quench experiments at temperatures both considerably above and below T_g in order to more completely understand the nature of such amorphous-amorphous phase transitions.

Liquid-Liquid Transition in Supercooled Silicon – At low pressure, crystalline silicon adopts the diamond structure and is an indirect band-gap semiconductor. With increasing pressure, crystalline Si transforms from the diamond phase through a more highly-coordinated metallic ß-tin

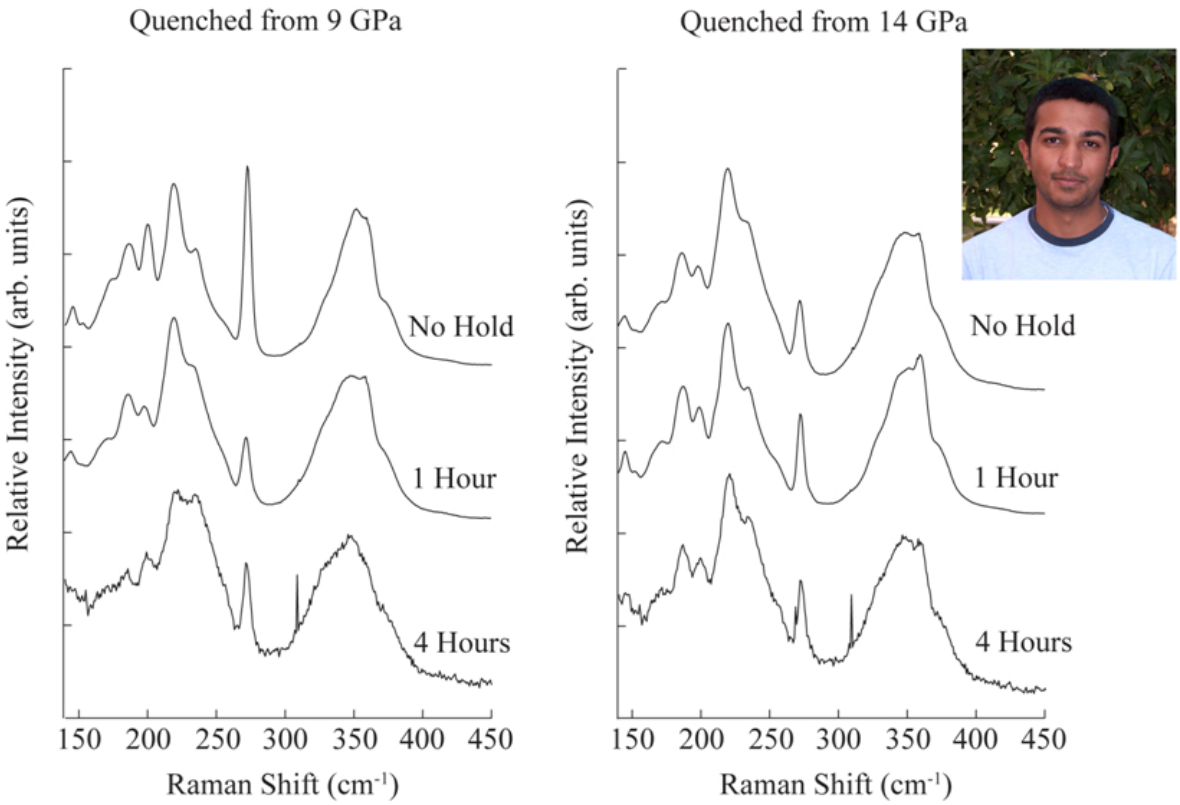


Figure 17. *Raman spectra of quenched GeAsS samples held at 9 GPa (right) and 14 GPa (left) for specified amounts of time (indicated by the label to the right of each spectrum). Inset: CDAC graduate student* ***Samrat Amin (Arizona State)****.*

phase, and then to a hexagonal phase. Such polymorphic phase transitions are usually accompanied by interesting changes in electronic properties. Similar to crystalline silicon, amorphous Si is also known to exhibit polymorphism. At equilibrium, liquid Si is metallic and is denser than its crystalline counterpart, very similar to the case with water. In spite of the widespread use of Si in industry, the nature of the transition of the dense metallic liquid to an open network semiconducting solid is poorly understood.

Panchapakesan Ganesh, a postdoctoral fellow at **Carnegie**, has explored the structures of liquid and supercooled liquid Si using first-principles molecular-dynamics simulations, which allow the most realistic predictions for strutural properties at high pressures and temperatures.[18] The method is unhindered by the intrinsic inaccuracy of phenomenological potentials, and has the ability to accurately capture the chemical nature of the atoms in the simulation. In the simulation, the thermodynamic pressure as a function of temperature was determined at different volumes. A "van der Waals loop" in a pressure-volume isotherm (at constant temperature) occurs when a region of positive slope interrupts the generally negative slope of the isotherm. This positive slope corresponds to negative isothermal compressibility, which in the real physical system would lead to a separation of the coexisting phases. The presence of the van-der Waals loop in the pressure-volume isotherm (Fig. 18) clearly shows the presence of a liquid-liquid thermodynamic phase transition in supercooled liquid Si, and indicates that the transition is first-order (critical temperature T_c ~ 1232K and pressure P_c ~ -12kB).

The work shows that the two coexisting polymorphic liquid phases are the high-density liquid (HDL), which can be considered as a metastable extension of the high-temperature equilibrium liquid (HTEL), and the low-density liquid (LDL) which is tetracoordinated and has a more open structure, like that of semiconducting solid Si. The high degree of orientational order in

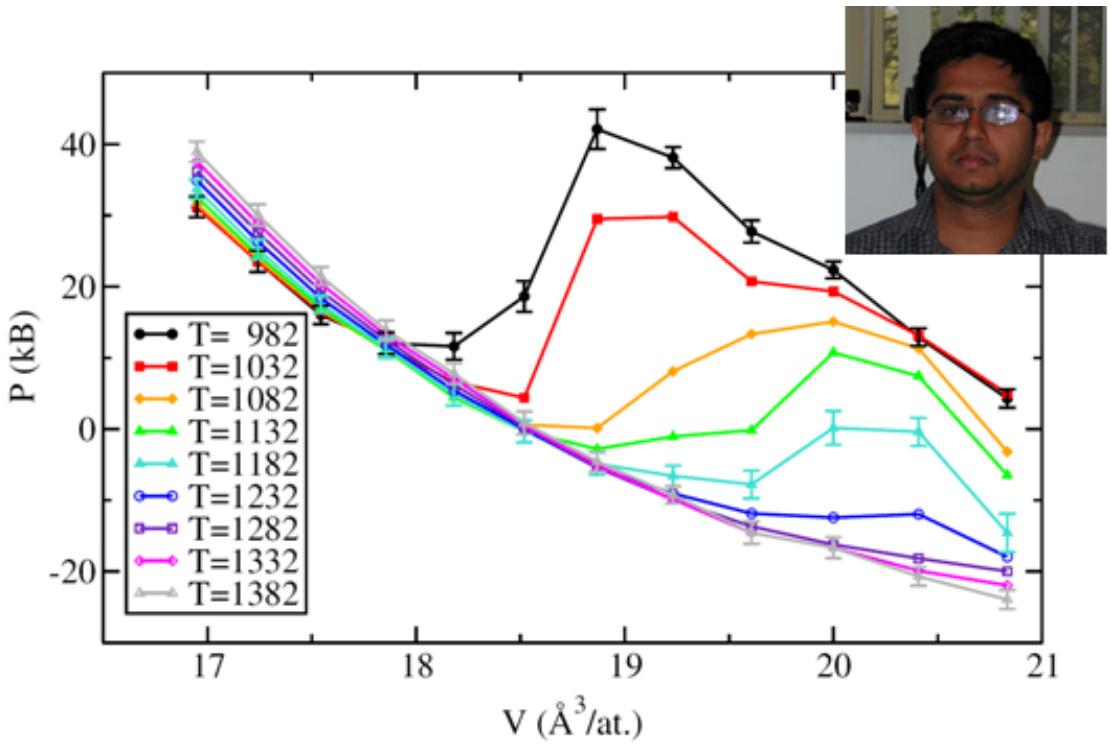


Figure 18. *Pressure-volume isotherms of liquid silicon show a "van der Waals loop" below T_c ~ 1232 K. Inset:* ***Panchapakesan Ganesh (Carnegie)****.*[18]

the open, tetrahedrally coordinated LDL Si compared to the disordered HDL Si has been proposed as the driving force behind this phase transition. The simulations also show that HDL Si is metallic, similar to liquid Si, while LDL Si has a semimetallic character, close to that of semiconducting crystalline Si.

Novel High-Pressure Phase of Elemental Boron – Because of its low mass, high strength, and response to neutron irradiation, boron has important applications in technology, including nuclear engineering and in extreme environments. In recent work on the high-pressure properties of elemental boron, it has been discovered that under compression, the B_{12} icosahedra present in the ambient pressure phase contract, leaving two boron atoms in the inter-icosahedral voids to form a B_2 dimer, leading to a denser structure.

The present work builds on the discovery of superconductivity in elemental boron in 2001 by researchers at **Carnegie**,[19] and the first observation of the transition to the newly discovered structure.[20] That study revealed superconductivity with a relatively high transition temperature for an element, but the underlying structure and mechanism have remained unexplained. The current structural and spectroscopic work provides an important step toward understanding the transition to superconductivity in boron under pressure. Samples of the material were prepared in the laboratory of **Yingwei Fei** at **Carnegie** by **Y. Ma** and at **Stony Brook University** by co-workers from **Florida International University**, **Stony Brook University** and **University of Paris XIII**. Spectroscopic (U2A) and diffraction (X17C) work was then carried out at the NSLS by groups headed by **Z. Liu** and **Y. Ma**, respectively. **Artem Oganov** (**Stony Brook University**) led the effort, along with colleagues from **ETH Zurich**, **University of Milan**, and **Jilin University**. The theorists were able to predict the crystal structure of the high pressure phase and provide a rationale for its formation at high pressure and temperature.[21] The new phase was formed at above 12 GPa and 1400 degrees Celsius using multi-anvil techniques, and is stable upon quenching to ambient conditions. Computations show that this phase should be stable between approximately 19 and 89 GPa.

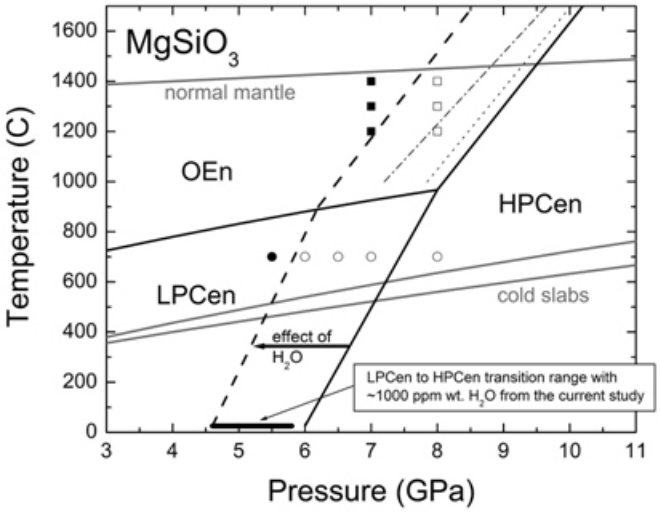


Figure 19. *Effect of hydration on the phase boundary in $MgSiO_3$ between low-pressure clinoenstatite (LPCen), orthoenstatite (Oen), and high-pressure clinoenstatite (HPCen) shown by the dashed line. The variation of transition pressure with water content may explain why the seismic velocity reflector at 270-330 km, known as the X-discontinuity, displays so much depth variability.*

Effect of water on high-pressure phase transitions in $MgSiO_3$ – The mantle X-discontinuity, usually assigned to positive seismic velocity reflectors at 270-330 km depth, has proved difficult to explain in terms of a single mineralogical phase transformation, in part because of its depth variability. The coesite to stishovite transition of SiO_2 matches deeper X-discontinuity depths, but requires 5-10% free silica in the mantle to match the observed impedance contrast. The orthoenstatite to high-pressure clinoenstatite transformation also broadly matches depths of the X discontinuity, but requires depleted and orthoenstatite-rich lithology at 300 km depth in order to match the observed seismic impedance contrast. On the basis of high pressure infrared spectroscopy carried out at the U2A beamline at **NSLS**, x-ray diffraction work done at **HPCAT**, and Raman spectroscopy, **Steven Jacobsen** at **Northwestern** shows that variation of water content in $MgSiO_3$ from 0 to ~1300 ppm weight H_2O can displace the transition pressure of low-clinoenstatite to high-clinoenstatite by up to 2 GPa (60 km), similar to previous quench experiments on the orthoenstatite to high-clinoenstatite phase transition (Fig. 19). If the mantle X-discontinuity results from pyroxene transitions in a depleted harzburgite layer, because of the strong influence of minor amounts of water on the transformation boundary, the depth of the mantle X-discontinuity could be a potentially sensitive indicator of water content in the upper mantle.

Exploring a New High Pressure Metallurgy – Two important questions that lie at the heart of metallurgy guide research in the **Panero** group at **Ohio State**, as they seek to develop metallurgy at high pressures. First, how does the electronic structure of a material evolve with pressure in the simplest metals? The second question begins to stake out the territory for a metallurgical engineering at high pressures and temperatures. How do mesoscopic structures, for example those due to cold rolling or cold forming, evolve at high pressures and high temperatures? The heavy alkali metals, K, Rb, and Cs, take on a variety of complex structures at high pressures, including incommensurate host-guest and modulated structures,[22] largely due to the complexities of the pressure dependence of the electronic structure. At low pressures, the low electronegativity of the alkalis causes these elements to dominantly bond ionically, forming oxides, halides, and silicates. The effect of pressure, however, is for these elements to

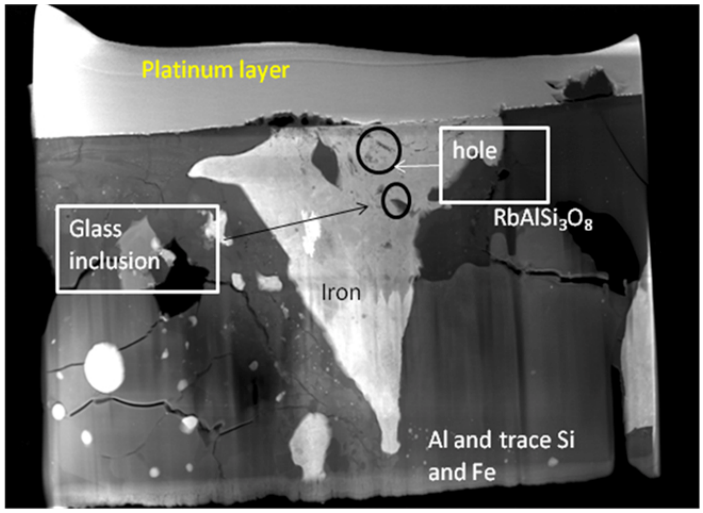


Figure 20. *Sample synthesized at 20 GPa and 2700 K, and extracted using focused-ion beam milling. Preliminary S/TEM shows Rb concentration in the iron foil below the detection limit (~1000 ppm).*

undergo ns^1 to $(n\text{-}1)d^1$ electronic transitions, where n is the primary quantum number of the outer shell electron.[23-24] This transition changes the chemical behavior of the alkali metal to a transition metal-like behavior, allowing for the formation of intermetallic alloys. The electronic transition occurs over a broad pressure range at room temperature as the energy states of the s-shell electrons overlaps with the d-shell electrons. Novel materials and structures can be formed in the in and above this pressure range through the reaction of alkali metals and transition metals.[25]

CDAC graduate student **Sabrina Huggins** performed laser-heated DAC (LHDAC) experiments on alkali feldspars mixed with iron at pressures of 10-90 GPa, heated to the melting temperature of iron. The reactivity of the iron was used as a marker for the electronic transition, as the formation of intermetallic phases, an expansion of the transition metal lattice, or the direct detection of the alkali in the metal after synthesis can be used to detect the transition. Samples were constructed with layers of high purity, natural potassium feldspar, $KAlSi_3O_8$, or high purity rubidium feldspar, $RbAlSi_3O_8$ (provided by **Guy Hovis, Lafayette College**), with iron foil between the silicate layers. The results show that there is a significant effect of the sample preparation with iron powder loaded in air showing the greatest K and Rb incorporation. When using foil samples, however, the results are indistinguishable between those samples loaded in the room environment and those never exposed to oxygen.

Room-temperature x-ray diffraction measurements are then made to determine the crystal structure of the metal and silicate phases. Initial results show that the zero-pressure volume of iron in experimental runs above the s-to-d transition pressure is expanded by 1-2% relative to pure iron. The chemistry of the iron metal needs to be analyzed directly to determine the cause of the expansion. Extraction of a foil through the sample using focused ion beam milling (FIB) allows for the S/TEM analysis of the samples. In Fig. 20, textures relating to the melting of iron in a silicate matrix are evident, as well as the inclusion of silicate sample material in the metal. However, the concentration of alkali metals is below the detection limit in the metal foil (~1000 ppm), indicating that the lattice expansion is a result of oxygen uptake instead.

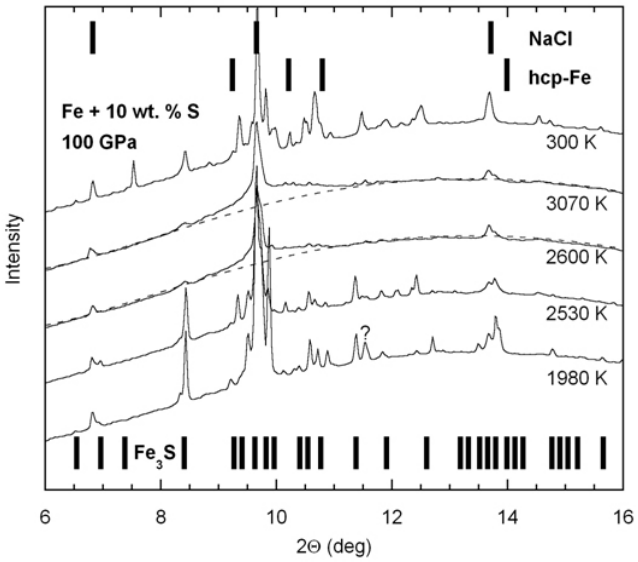


Figure 21. *Eutectic melting at 100 GPa in the Fe-Fe_3S system. Diffraction patterns are presented in order of collection from bottom to top, the temperature of each pattern is indicated to the right. Peak positions of the NaCl pressure medium and hcp iron are indicated on the top of the figure. All peak positions allowed by symmetry for Fe_3S are marked on the bottom based on the lattice parameters a = 8.205 ± 0.014 Å and c = 4.122 ± 0.011 Å determined from the 1980 K pattern; one peak (indicated by the question mark) at ~11.5° in the 1980 K pattern remains unidentified. Below 2530 K, solid hcp iron and Fe_3S coexist. When the temperature was increased to 2600 K both phases melted simultaneously, indicative of melting close to the eutectic composition.*[26]

The high-pressure structure of $RbAlSi_3O_8$ has the hollandite structure between ~12-25 GPa. The EOS of this material indicates that the hollandite structure behaves very similarly to the $KAlSi_3O_8$-hollandite, indicating that Rb is likely stored with K in the mantle, and that the hollandite structure is sufficiently flexible to accommodate many larger cations, as has been suggested as a component of SYNROC for disposal nuclear materials including cesium.

Melting Studies Using Simultaneous Diffraction and Laser Heating – An ongoing theme in the **Heinz** group at **Chicago** has been the measurement of melting temperatures for materials important for Earth's core. Technology has sufficiently advanced to the

point where it is now possible to couple double-sided laser heating with synchrotron x-ray diffraction. Figure 21 shows a series of integrated x-ray diffraction patterns of an iron plus iron sulfide mixture at 100 GPa. The bulk composition of the sample at this pressure was 10 wt% sulfur. At subsolidus temperatures at this pressure, two solid phases coexist, hcp-Fe and Fe_3S. When the sample temperature was increased to 2600 K, both solid phases were completely exhausted into the melt suggesting that the eutectic composition is very close to the initial bulk composition of the sample material. This data shows that the eutectic composition in the iron-sulfur system continues to evolve towards iron with increasing pressure, consistent with lower pressure data.[26] This is important because if Earth's core is predominantly iron with sulfur, one would expect the composition to fall on the iron rich side of the eutectic composition at core pressures, but this is unlikely to be the case because at least 14 wt. % sulfur would be required in the core, but the eutectic composition is less that 10 wt. % sulfur and decreasing at 100 GPa.

Pressure-Induced Lattice Collapse in $Fe_{1.05}Te$ – Exploring superconductors with high critical temperatures has long been an important topic in condensed matter physics. Currently the Fe-based compounds are being examined as potential candidates in achieving higher critical temperatures compared to cuprate superconductors. It has been found that pressure plays a significant role in tuning superconductivity in these compounds. Among them, binary compounds such as FeSe are of interest because they are safe systems due to the absence of toxic arsenic. Structural studies are the first step toward understanding the observed physical properties.

The **Carnegie** group performed the first experimental investigations of the high-pressure structure of $Fe_{1.05}Te$ by combining synchrotron x-ray and neutron diffraction techniques.[27] This work has provided direct evidence for pressure-induced lattice collapse at 4 GPa at which a 'transition' from the tetragonal to the collapsed tetragonal phase also takes place. An Fe spin state change is proposed to account for the lattice collapse. Further studies at higher pressures are currently underway.

Understanding Hydrogen Environments in Minerals – The purpose of CDAC research in the group of **Bob Downs** at **Arizona** is to understand how Nature stores hydrogen in solids. One of the challenges facing society is alternative energy sources. The federal government has identified hydrogen fuel as a potentially clean and cheap solution. Practical aspects of hydrogen storage in materials are hindered by the simple problem of how to store hydrogen safely and in sufficient concentration for practical applications. The work seeks to identify the ways that nature stores hydrogen in minerals, and then explore the response of these systems to concentrating the hydrogen though compression and increasing density. The study of hydrogen environments in minerals provides a vast catalogue of structural types from which examples may be drawn.

Behoite, $Be(OH)_2$, is isostructural with cristobalite, but silica does not undergo room-temperature reversible transformations between cristobalite, tridymite, quartz, coesite or stishovite that leave the crystal intact, as behoite appears to do. Thus, it appears that the phase transitions in behoite offer a chance to examine the effect of hydrogen as a "lubricant" in its phase transitions (Fig 22).

CDAC graduate student **Madison Barkley** has collected diffraction data on single crystals of both materials at the **GSECARS** sector of the APS, for $Be(OH)_2$ at 0.34, 7.31,

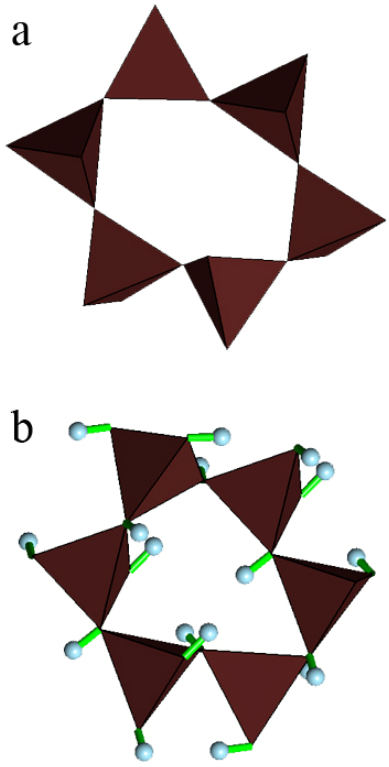


Figure 22. *a) Polyhedral image of the six-membered ring of silicate tetrahedra in cristobalite. b) Equivalent ring of $Be(OH)_4$ tetrahedra in behoite.*

9.64, and 8.43 GPa, with methanol-ethanol as the pressure medium, and at 12.83, 19.25, and 25.08 GPa with He gas as the pressure medium. Preliminary data suggest a phase transition to an orthorhombic structure. Data were also collected for a single crystal of cristobalite at five pressures from 0.7 to 5.3 GPa with methanol-ethanol, and then to 18.1 GPa with He gas. Preliminary results surprisingly point to two separate transitions in the cristobalite structure, at approximately 3 and 2 GPa, suggesting that previous structural results for high-pressure experiments on cristobalite are in error. Current work is aimed now at resolving these discrepancies correlating the behavior of these two isostructural materials.

2.2 *P-V-T* EOS Measurements

Stewardship science relies heavily on accurate *P-V-T* EOS data in order to provide for accurate predictions of the behavior of materials over a wide range of conditions. DAC methods such as x-ray and neutron diffraction and sound velocity measurements provide data that can be combined with that obtained in dynamic compression studies to more fully understand material properties at conditions relevant to stewardship science applications. Metals, simple and complex crystalline solids, superhard materials and polymers, liquids and glasses highlight the wide range of materials under investigation in CDAC research groups.

Static Compression to Multimegabar Pressures – The study of materials under static loading to pressures greater than 1 Mbar is hampered by the difficulty in achieving and characterizing a quasi-hydrostatic sample environment. Use of helium as a pressure transmitting medium is known to provide very good quasi-hydrostatic conditions to pressures up to about 1 Mbar but its use at higher pressures has not been explored. Furthermore, pressure calibration is a fundamental and critical problem in DAC experiments at ultrahigh pressures. Pressure uncertainties are introduced by uncertainties in the equations of state of pressure calibrants, discrepancies between different pressure scales, and non-hydrostatic stress conditions in the DAC. At pressures up to ~1 Mbar, Dewaele et al.[28] and others have attempted to resolve these differences by co-compressing metals commonly used as pressure calibrants in a He medium, the most hydrostatic pressure medium available. However, no previous experiment has directly compared the equations of state of metals and MgO, one of the most popular and best constrained pressure calibrants, to Mbar pressures in He. In the experiments of CDAC graduate student **Susannah Dorfman** at **Princeton**, a mixture of Pt and MgO powders was loaded in a DAC with 50 um beveled culets.[29] Helium or neon was loaded as a pressure transmitting medium using the high-pressure loading system at GSECARS of the Advanced Photon Source. X-ray diffraction experiments were performed to a maximum pressure of 226 GPa, as measured using the EOS of MgO. Above 200 GPa, the pressures indicated by MgO and Pt scales differed by as much as 10%. Differential stress in the platinum sample was estimated by lattice strain theory[30] and diffraction peak width analysis to range from 1-4 GPa, or a maximum of ~2% of the mean pressure (Fig. 23). Ongoing work is continuing to explore the differences in stress states obtained using various pressure media, different loading conditions, and the effects of laser annealing.

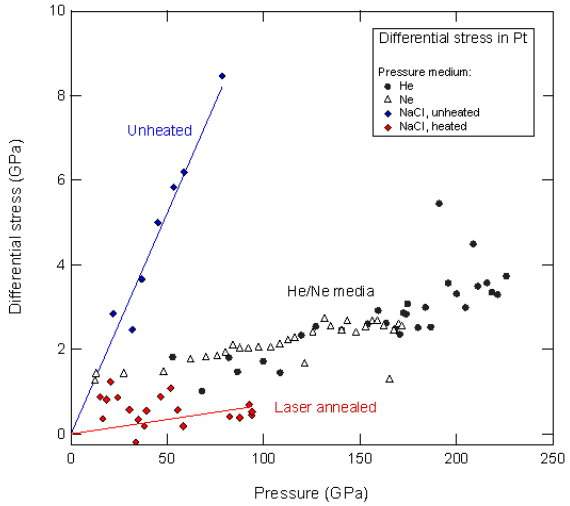


Figure 23. *Comparison of differential stress in a platinum sample for various pressure media (Ne, He, NaCl) that has (NaCl) or has not (Ne, He, NaCl) been laser annealed. Rare gas media or laser annealing reduce differential stresses to ~1-2% of the total pressure.[30]*

Structures and Phase Transitions in Transition Metal Oxides – The nature of bonding in titanium dioxide TiO_2 is of interest as it is a superhard material with many industrial

applications. During the last several years, **Yahya Al-Khatatbeh** in the group of **Kanani Lee** at **New Mexico State University** has been investigating the structural properties of some key oxides. It is expected that the yield strength of materials increases with increasing pressure either within a single phase or across volume-reducing phase transitions. Thus, the possibility of quenching high-pressure phases and maintaining them at ambient pressure can generate novel superhard materials with increased mechanical strength as well as other properties. This strategy to synthesize novel superhard materials by quenching high-pressure phases to ambient pressures has been successfully applied to other materials such as c-Si_3N_4.[31-32] Previous measurements on TiO_2 show that the highest-pressure phase OII is quenchable to ambient pressure at least at cryogenic temperatures. Previous experiments on high-pressure TiO_2 polymorphs show that this compound can adopt several different structures: rutile (RT, tetragonal, space group: $P4_2/mnm$), anatase (AN, tetragonal, space group: $I4_1/amd$), brookite (BR, orthorhombic, space group: *Pbca*), columbite (CB, orthorhombic, space group: *Pbcn*), baddeleyite (MI, monoclinic, space group: $P2_1/c$), orthorhombic I (OI, orthorhombic, space group: *Pbca*), fluorite (FL, cubic, space group: *Fm3m*), and cotunnite (OII, orthorhombic, space group: *Pnma*). The low-pressure phase transition sequence in all studies at room temperature is: RT or AN or BR → CB → MI. On the other hand, the high-pressure phases (OI, FL, and OII) were only observed after heating at high pressures.[33] A clear phase diagram for TiO_2 under both high pressure and temperature using both DAC experiments and ab-initio computations has been constructed (Fig. 24).

Zirconia (ZrO_2) and hafnia (HfO_2) are well-known components of modern ceramic materials, which lead to important industrial applications because of their superior mechanical properties.[34-35] Both oxides also follow structural behavior similar to that of TiO_2. Previous experimental and theoretical studies predict different structural phase transition sequences under high pressure and/or temperature. The most recent first-principles computations predict that ZrO_2 and HfO_2 undergo the following sequence: baddeleyite → OI → OII[34] in good agreement with previous measurements.[36] The cotunnite phase of both oxides is dense with a high bulk modulus, that approaches that of diamond. Previous work on ZrO_2 and HfO_2 shows several possibilities of the

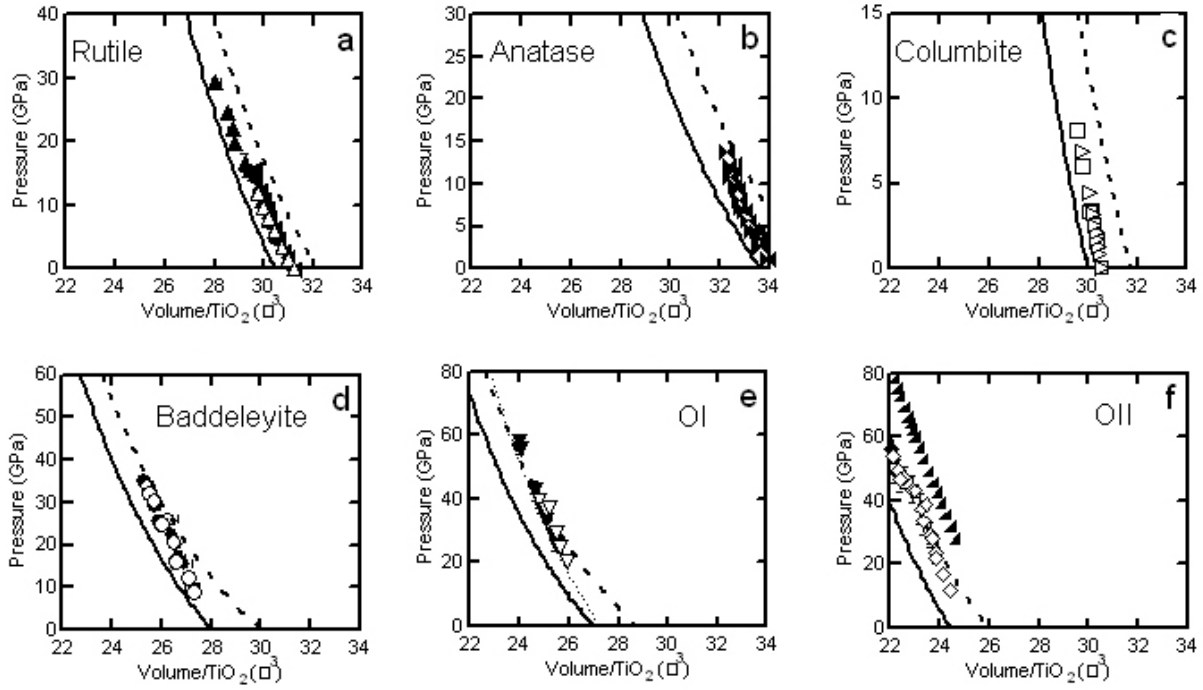


Figure 24. *Series of plots showing the agreement between computed equations of state from LDA (solid lines) or GGA (dashed lines) and compiled experimental results. Open symbols, compression; filled symbols, decompression.*[33]

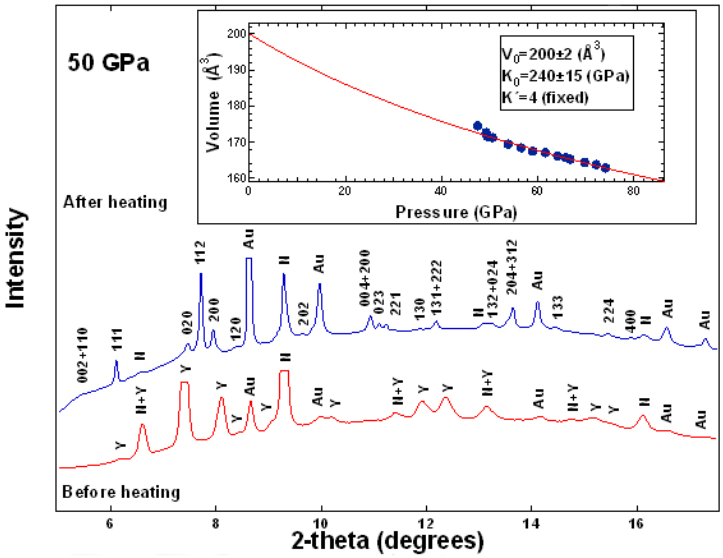


Figure 25. *X-ray diffraction patterns for $Y_3Fe_5O_{12}$ showing transformation from the garnet structure to orthorhombic perovskite $(Y_{0.75}Fe_{0.25})FeO_3$ after laser heating to ~1600 K near 50 GPa. Inset shows preliminary equation of state data yielding a bulk modulus of ~240 GPa for the high-pressure phase. Perovskite peaks are labeled with hkl value. Y – YIG, N – NaCl insulating medium, Au – gold pressure standard.*

transition sequence as well as different phases in each sequence under high pressure and temperature, where tetragonal and cubic phases are also expected.[35-37]

Phase Transition and EOS of $Y_3Fe_5O_{12}$ at High Pressures – The garnet structure type is of fundamental importance in materials science. High-pressure investigations of oxide garnets composed of transition and rare earth elements have revealed a range of interesting phenomena including pressure-induced amorphization, phase transitions, magnetic collapse, and potential transformation to superhard solids.[38-41]

Yttrium iron garnet, $Y_3Fe_5O_{12}$ (YIG) has been widely studied due to its extensive technical applications.[42-43] At high pressure, YIG was observed to become suddenly amorphous upon 300 K compression to 55 GPa accompanied by magnetic collapse and a spin transition.[41] At low *P* and *T* (0-4 GPa, 1600 K), there are conflicting reports of different phase transitions that have never been resolved,[44-45], and no high-temperature experiments have previously been performed at significantly elevated pressures. To address this issue, the **Princeton** group of CDAC Academic Partner **Tom Duffy** performed an extensive synchrotron x-ray diffraction experiment on YIG in the DAC at the GSECARS sector of the Advanced Photon Source. During room temperature compression, the results reproduce previous findings of amorphization near 50 GPa. Upon heating above 1600 K at this pressure, a phase transition from the cubic garnet structure to a new structure whose peaks match an orthorhombic $GdFeO_3$-type perovskite phase was observed, as illustrated in Fig. 25. This provides a new example of a garnet – orthorhombic perovskite transition similar to that observed in the $(Mg,Fe)(Si,Al)O_3$ system. Volume compression data were obtained by further compression (and heating) of YIG up to 74 GPa yielding a preliminary EOS. The transformation of YIG to a single-phase orthorhombic perovskite at high pressures implies that Fe^{3+} cations are distributed into both the A and B sites and there is A-site disorder in the high-pressure polymorph.

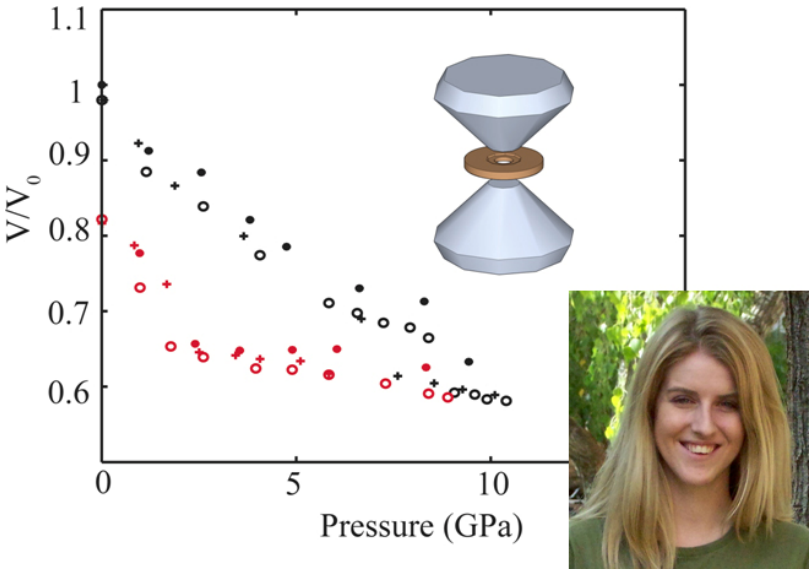


Figure 26. *Measured DAC EOS for amorphous red phosphorus. The three sets of symbols represent separate runs. The compression data is in black and the decompression data is in red. Inset: CDAC graduate student* ***Erin Oelker (Arizona State)****.*

Equations of State for Liquids and Amorphous Solids – During the past year, the **Yarger** group at **Arizona State University** has focused on the high-pressure behavior of chalcogenide and pnictide glasses and liquids. The group works to find new polyamorphic systems, quench new high-density glasses and further develop *in-situ* EOS measurements for the DAC. An example for the DAC EOS measurement made on the red to black phase transition in amorphous elemental phosphorus is shown in Fig. 26. The technique relies on capturing images of a polished flat glass in a DAC as a function of pressure. The development of EOS measurements at high-pressure is critical to understanding the thermodynamics of glasses and liquids as well as being a requirement for proper scaling of x-ray and neutron diffraction data for pair distribution function (PDF) analysis.

Amorphous red phosphorus (a-rP) is a semiconducting material, which undergoes an insulator-metal transition at high pressure. Furthermore, liquid phosphorus is the only known material to undergo an equilibrium first-order liquid-liquid phase transition. This can be directly observed in *P-V* measurements and is seen at ~7-8 GPa in red amorphous phosphorus at room temperature. The observed transition is not polyamorphic; rather it is a quasi-first order transition from red amorphous phosphorus to crystalline black phosphorus. The black phosphorus phase is then recovered upon decompression. CDAC graduate student **Erin Oelker** has done extensive Raman, Brillouin and x-ray diffraction measurements as a function of pressure to better characterize this amorphous to crystalline transition, and is currently developing a structural model for red amorphous phosphorus, with the preliminary findings to be published in the near future.

High P-T EOS of Osmium – Osmium, a third row transition metal in the iron group, has an hexagonal close-packed structure and is characterized by its high density, extremely low compressibility[46-50] and high hardness.[51] Because of these properties, osmium is a potentially

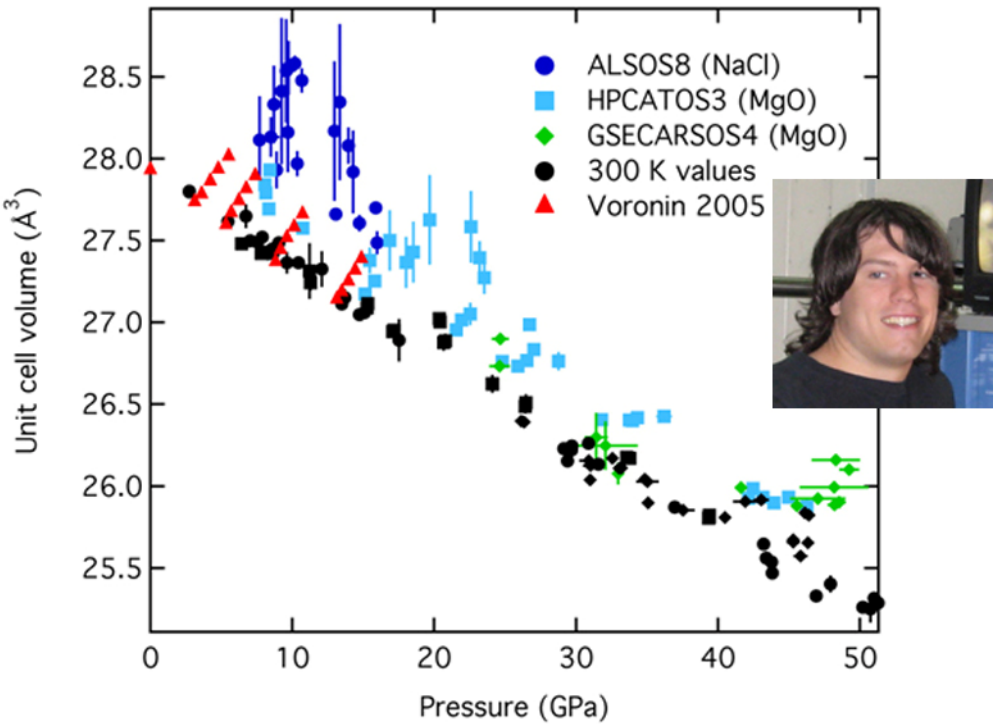


Figure 27. *Complete dataset on osmium. Blue circles are high temperature data from the ALS. Blue squares are data from HPCAT, and green diamonds are from GSECARS. Black markers are room temperature data from each of the above datasets. Data from Ref.* [49] *is represented by red triangles, in which volumes were measured along isotherms of 300 K, 523 K, 773 K, 1023 K, and 1273 K. Inset: CDAC graduate student* ***Matt Armentrout (UCLA)****.*

important matrix material for the synthesis of ultra-hard materials. For example, addition of boron raises osmium's Vicker's hardness from 400 kg/mm^2 to 2000-3000 kg/mm^2 at the expense of the bulk modulus.[52-53] Carbon[44] and nitrogen are also predicted to enhance osmium's mechanical properties.[54] In addition, a high-temperature high-pressure EOS for Os was measured using *in situ* x-ray diffraction and a multianvil apparatus[49] up to 15 GPa and 1273 K. The objective of currrent work in the **Kavner** group at **UCLA** is to extend the measurement the EOS of osmium to pressures of 50 GPa and temperatures up to 2000 K. The ultimate goal is to provide a baseline measurement for the osmium metal endmember, which can be used to compare with future measurements of the thermal behavior of osmium-based ultra-hard materials.

Several sets of high *P-T* experiments on Os metal using monochromatic x-ray diffraction with *in situ* double-sided laser heating in the DAC were performed by CDAC graduate student **Matt Armentrout** at three different beamlines: at 12.2.2. at the Advanced Light Source (ALS), at 13-ID-D at GSECARS and 16-ID-D at HPCAT. This redundancy allows this study to function as a check on the agreement between data collected at multiple beamlines and with different pressure standards. Pressures were determined by fitting the measured lattice parameters of NaCl B1 or B2 or MgO to their high pressure, high temperature equations of state using an isothermal third order Birch-Murnaghan EOS in conjunction with a Mie-Gruneisen-Debye model of thermal pressure. Volumes as a function of pressure at room temperature and elevated temperatures are shown in Fig. 27.

Equations of State for High Explosives – A key part of the research program of CDAC Laboratory Partner **Dana Dattlebaum** at **LANL** is determining the equations of state of explosive materials. Historically, however, static high pressure EOS data on high explosives (HE) has been difficult to determine, in particular due to the low scattering intensity and radiation damage caused by the x-ray beam. However, advances in synchrotron radiation intensity now allow for structural determination of low-Z materials. In addition, by using a monochromatic x-ray beam, such as 16-ID-B at HPCAT, it is possible to select input energies that significantly reduce or eliminate radiation damage.

In the past year the **LANL** group has investigated the high pressure properties of ammonium nitrate (AN, NH_4NO_3), which is perhaps the most widely used mining explosive in the world. In explosive applications, the ammonium nitrate prills are prepared so that they readily absorb ~6 wt% fuel oil, forming an ammonium nitrate-fuel oil composite (ANFO). ANFO is known to be a non-ideal explosive with measured detonation velocities near 4 km/s.[55] While there have been numerous studies of the detonation properties of ANFO, there are limited reports of the EOS and initiation properties of pure AN. The present work involves using both static high pressure x-ray diffraction measurements and gas gun-driven plate impact (shock compression) experiments to determine valuable EOS information.

AN is known to exist in at least 6 phases in addition to the melt as a function of temperature and pressure. Analysis of the ADXD patterns at room temperature (298K) and elevated pressures reveal that the high pressure crystal structure(s) could be indexed as Phase IV, an orthorhombic phase (*P*mmn), with two molecules per unit cell, from ~ 0.4 GPa to 25 GPa, with an initial density of 1.726 g/cm^3. The static high pressure data were used, along with knowledge of the thermodynamic parameters, to develop a

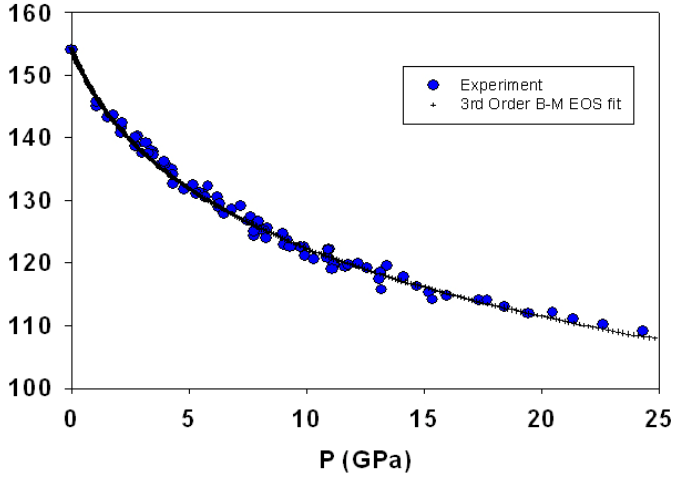


Figure 28. *Static P-V experimental data and 3rd-order Birch-Murnaghan semi-empirical EOS fit for ammonium nitrate.*

thermodynamically-consistent EOS for neat AN at a variety of initial densities, which was further compared to the available shock Hugoniot data. The isothermal bulk modulus and its pressure derivative were determined from a 3rd-order Birch Murnaghan semi-empirical EOS fit to the room temperature isotherm derived from the x-ray diffraction experiments at 16-ID-B, shown in Fig. 28. Additional work is underway to completely analyze higher temperature isotherms, and determine the source of the scatter in the data near 6-8 GPa.

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

The vibrational properties of materials provide access to key thermodynamic information that is used to both predict material behavior at extreme conditions and constrain theoretical models. Synchrotron x-ray diffraction, x-ray spectroscopy and infrared spectroscopy are supplemented by laboratory Brillouin scattering techniques to investigate a wide variety of physical properties of alloys and semiconductors, crystalline solids, polymers and molecular materials.

Understanding Invar Behavior at the Microscopic Level – CDAC graduate student **Mike Winterrose** in the **Fultz** group at **Caltech** has used a variety of experimental methods, combined with theory, to unravel the Invar behavior of iron-containing alloys. A key technique in this work has been nuclear resonance spectroscopy at HPCAT. Following up on the experiments described in Section 2.1, the Fultz group is currently completing a manuscript on the phonon partial density of states (PDOS) of Fe at high pressures in $L1_2$ ordered Pd_3Fe. This is the first study of lattice dynamics at pressures relevant to the pressure-induced Invar effect. The ^{57}Fe PDOS was measured using nuclear resonant inelastic x-ray scattering (NRIXS), and calculated for four magnetic states (ferromagnetic, antiferromagnetic, low-spin, and nonmagnetic) with density functional theory (DFT). At lower pressures, NRIXS revealed stiffening of the ^{57}Fe PDOS with increasing pressure, but an anomalous softening occurs around 12 GPa. Comparison with the constrained volume DFT calculations showed that the softening could result from the pressure-induced magnetic transition from the high-moment (HM) to low-moment (LM) states (Fig. 29). Further, the *ab initio* calculations showed second-neighbor Fe-Fe interactions to be as important as first-neighbor Fe-Pd interactions for controlling the phonon dynamics through the HM to LM transition, and the phonon modes most affected were those that involve distortions of the Fe sublattice. Extraction of the individual interatomic force constants from the NRIXS data using an inversion-iteration process is underway.

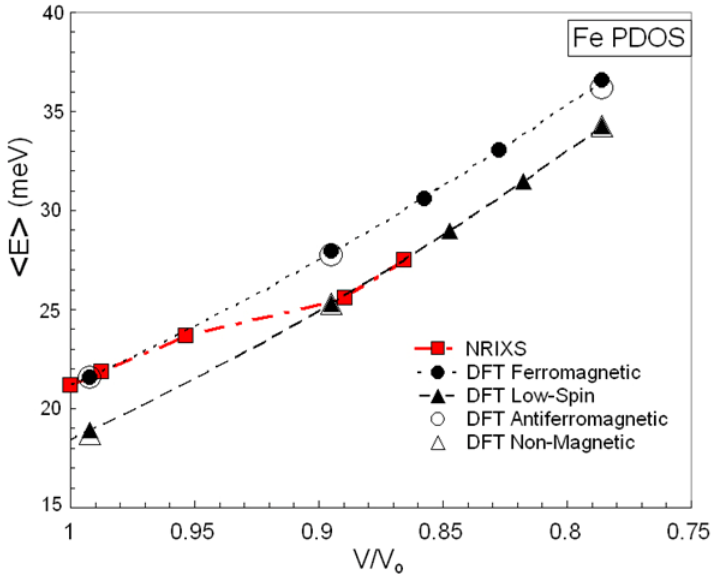


Figure 29. *Measured and calculated average vibrational frequencies as a function of reduced volume for the Fe partial phonon density of states in ordered Pd_3Fe. The dashed lines are trend lines for the ferromagnetic and low-spin data, drawn as guides to the eye.*

Rather similar behavior to $L1_2$ ordered Pd_3Fe was found for disordered Pt_3Fe – the results are quite similar to those published earlier this year for ordered Pd_3Fe. Nevertheless, the transition region is somewhat different.

Invar behavior has proved useful for understanding the effects of pressure on the stability of materials at the level of the electrons. In Invar materials, the various electron states respond very differently to pressure, causing significant effects at relatively low pressures.

Vibrational Entropy of Vacancies in Fe-Al – The alloy FeAl can be prepared with vacancy concentrations as high as 4%, making it possible to observe effects of vacancies on the phonon entropy in this material. The phonon density of states (DOS) and phonon entropy of B2 FeAl were determined as functions of the Fe site vacancy concentration using several scattering techniques (including nuclear resonant inelastic x-ray scattering at HPCAT) and first-principles calculations. On the average, the temperature and pressure trends of phonon frequencies were consistent with the quasiharmonic model, where the phonon energy levels depend linearly on the change in volume. The decrease in specific volume associated with the introduction of vacancies caused a stiffening of the DOS that was generally consistent with the experimentally determined Grüneisen parameter. Nevertheless, there were features associated with vacancies in the DOS that are not well explained by the quasiharmonic model, especially in the gap between the acoustic and optic branches. First-principles calculations indicated that these gap modes are primarily associated with vibrations of Al atoms in the first-nearest-neighbor shell of the vacancy, with some vibration amplitude also involving the second nearest neighbor Fe atoms. At the vacancy concentrations of this study, the phonon entropy of vacancy formation was found to be approximately −1.7 k_B/atom, about half as large and of opposite sign as the configurational entropy of vacancy formation. This work has been written for publication, and is in review with *Physical Review B*.

Elastic Properties from Powder Samples – Recent work by CDAC graduate student **Arianna Gleason** in the **Jeanloz** group at **Berkeley** has been focused on Brillouin spectroscopy, which is a well-established technique for determining the acoustic-wave velocities of single crystals under pressure.[56] Such laboratory measurements are crucial for interpreting seismological observations of Earth's interior, including the rich data provided by seismic tomography,[57] yet they are limited by phase transitions, shear stresses and heating, all of which compromise the integrity of single-crystal samples. More generally, it may be impossible to maintain a given sample material in single-crystal form, which motivates establishing methods for obtaining elastic moduli from powders.

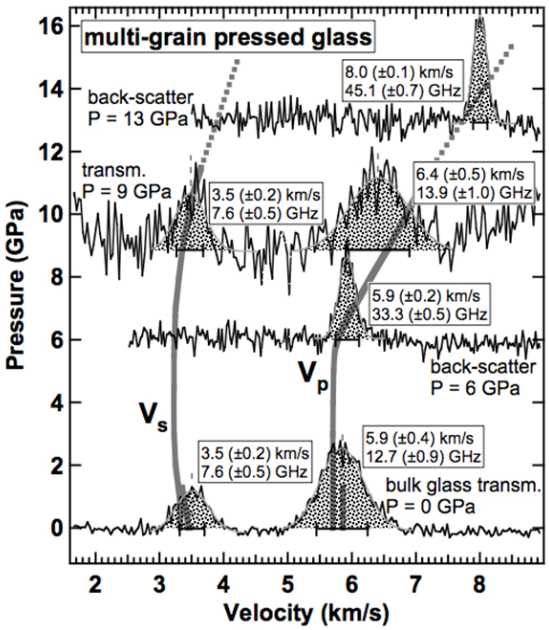


Figure 30. *Brillouin spectra (black traces) of bulk glass at zero pressure (bottom: transmission geometry), and of pressed glass powder (upper three traces) at 6, 9 and 13 GPa (transmission and back-scatter geometries, with only the compressional mode visible in back-scattering). The traces are shifted so as to match the baseline for each spectrum with the pressure scale (left). Thick solid grey curves show compressional (V_P) and shear (V_S) wave velocities for float glass as a function of pressure, based the ultrasonic measurements to 1.3 GPa of Li et al.*[62,63]

Brillouin spectra were collected at room temperature and pressure from both bulk and powder (10 μm average grain size) forms of Erie Electroverre soda-lime glass. Spectra were also collected from multi-grain samples at high pressure, using a gasketted diamond-anvil cell with a 4:1 methanol:ethanol pressure-transmitting medium.

Results[58] support the model of multiple-elastic scattering dominating the Brillouin spectra of powder (including polycrystalline) samples, and provide new experimental strategies for mitigating the scattering effects. Specifically, the experiments show that powder (or polycrystal) spectra become indistinguishable from Brillouin spectra of bulk (single-crystal) specimens when immersed in a medium matching the index of refraction of the sample. Sintering offers another means of reducing multiple-scattering in the Brillouin spectra of multi-grain samples (*e.g.*, Ref [59-60]), and this can be

accomplished through quasi-hydrostatic compression, even at room temperature, as illustrated in Fig. 30 (see also Ref [61]).

The high-pressure powder spectra are characterized by symmetric peaks, as is the case for the bulk sample or the powders immersed in an index-matching medium at zero pressure (Fig. 31). The spectra are qualitatively different from those affected by multiple-elastic scattering in this regard, and yield results in quantitative agreement with independent measurements of room-temperature acoustic-wave velocities as a function of pressure. As with the zero-pressure spectra, the peaks are observed at different frequency shifts, depending on scattering angle θ, yet the resulting acoustic-wave velocities are entirely consistent with each other (Fig. 31).

Measurements have also been completed on polycrystalline argon, measured at pressures up to 30 GPa in 180° and 70° scattering geometries, providing the first experimental determination of the refractive index and polarizability of pressurized solid argon. The experimental results provide a direct examination of the assumption of constant polarizability in previous calculations of the high pressure properties of solid argon.[64] Elasticity information is derived from Brillouin scattering data, independent of a high-pressure x-ray diffraction (XRD) data series. Fitting with the Birch-Murnaghan EOS, the bulk modulus and pressure derivative are 13.1 (± 1.0) GPa and 3.4 (± 0.3) at 2 GPa. The EOS obtained from this study agrees well with the results of independent XRD studies,[65] documenting that high-pressure Brillouin scattering methods can be suitable for characterizing the elasticity of polycrystalline materials.

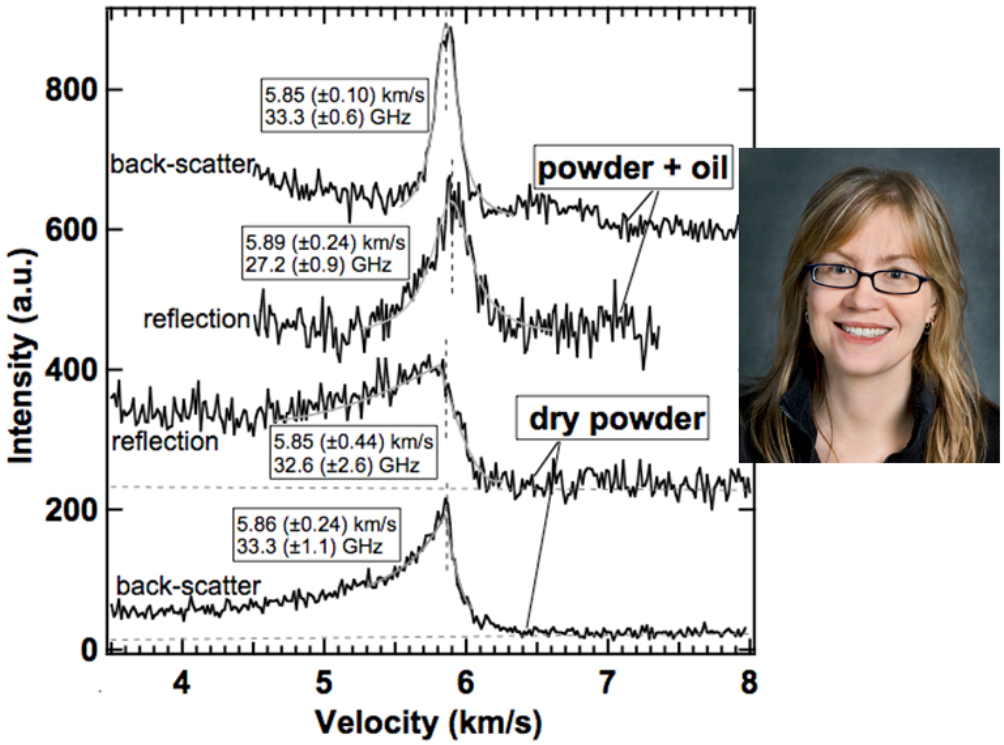


Figure 31. *Brillouin spectra (black traces) of soda-lime glass powder at ambient conditions (P = 0 GPa, T = 290 K) in back-scatter (top and bottom spectra: θ = 180°) and reflection geometries (middle two spectra: θ = 110°), plotted as a function of velocity rather than frequency shift in order to document alignment of the acoustic peaks. The bottom two traces are from dry powder and the top two traces from powder in an index-matching oil. Inset: CDAC graduate student* ***Arianna Gleason (Berkeley)****.*

Infrared Reflectivity Studies on Semiconductors – In the last year the **Heinz** group at **Chicago** has been studying infrared active phonons of semiconductors at the **U2A** beamline of the **NSLS**. In particular, GaP was studied because of its technological relevance. The data provide the

pressure dependence of the frequencies of the transverse optic (TO) and longitudinal optic (LO) phonon modes, which can be used to constrain the optic and thermal Grüneisen parameters, as well as elastic and dielectric properties as a function of pressure.

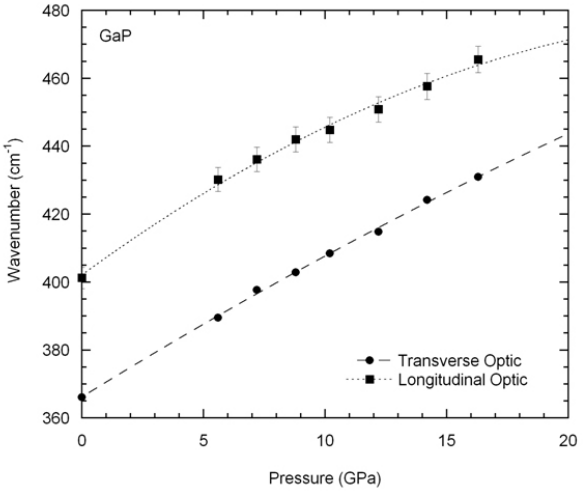


Figure 32. *Transverse and longitudinal optic mode frequencies of GaP as a function of pressure. The 1 bar data is from Ref. [72]. Errors are smaller than the symbols for the TO mode data.*

Synchrotron FTIR reflectivity measurements were carried out by CDAC graduate student **Chris Seagle** using DAC techniques and with a liquid helium cooled bolometer. The ratio of the intensity of light reflected off of the sample-diamond interface multiplied by the reflectivity of diamond gives the diamond-sample reflectivity.[66] In the far IR, (~100-700 cm^{-1}), GaP possesses a phonon mode which can interact with the oscillating electric field of the synchrotron beam.[67] This interaction causes a peak in the reflectivity spectrum which may be used to calculate the dielectric and averaged vibrational properties of the material. An example of the reflectivity spectra obtained is presented in Fig. 7. The main feature in these spectra arise from the TO phonon mode, which decreases in intensity with increasing pressure, finally disappearing from the spectrum at ~20 GPa where a phase transition in GaP occurs.[68] The reflectivity data below 20 GPa was treated with a classical dispersion analysis. The long wavelength dielectric constant was known previously from index of refraction measurements at high pressure[69] and thus was fixed to its independently measured value as a function of pressure in the fitting of the data. Figure 32 shows the pressure dependence of the TO and LO modes for this material derived from the reflectivity data. These mode frequencies may be used to constrain the optic and thermal Grüneisen parameters which are important properties in the in the theory of thermoelasticity.[70-71]

Elastic Moduli and Stregth of Nanocrystalline Cubic BC_2N – A continuing theme in the work of **Tom Duffy's** group at **Princeton** is the investigation of potential superhard materials. Cubic B-C-N phases are reported to have hardness values greater than that of cubic boron nitride (*c*BN), along with better chemical stability and the ability to withstand oxidation at a higher temperature than diamond. This significantly adds to the attractiveness of cubic B-C-N phases as superhard materials for potential industrial applications. In work carried out in collaboration with **Yusheng Zhao** at **LANL**, the stress behavior of nanocrystalline cubic boron carbon nitride (*c*-BC_2N) was investigated using radial and axial x-ray diffraction in the DAC under nonhydrostatic compression up to ~100 GPa. The radial x-ray diffraction data yields a bulk modulus, K_0=276±20 GPa with a fixed pressure derivative, K_0'=3.4 at ψ =54.7°, which corresponds to the hydrostatic compression curve. A comparative study of the observed compression curves from radial and axial diffraction shows that the ruby fluorescence pressure scale may reflect the maximum stress under nonhydrostatic compression. It was found that the nanostructured *c*-BC_2N sample could support a

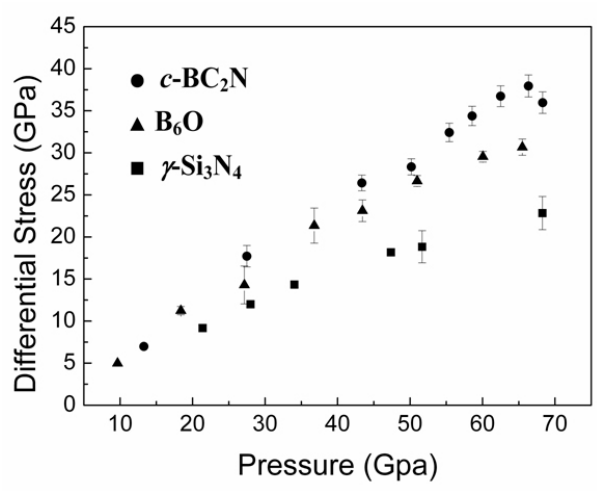


Figure 33. *A comparison of differential stress supported by c-BC_2N, γ-Si_3N_4 and B_6O under uniaxial compression in DACs.*

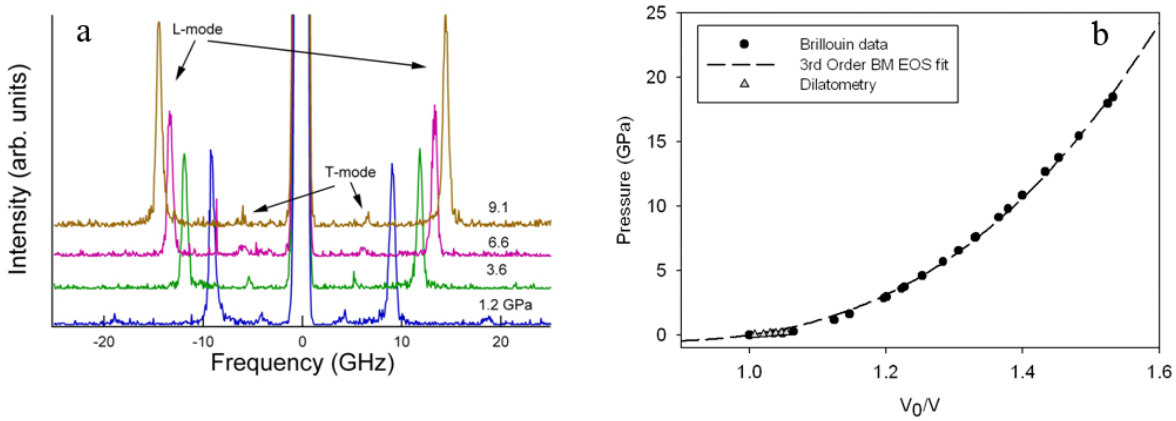


Figure 34. a) *Brillouin spectra recorded as a function of pressure for Kel-F 800.* b) *Room temperature isotherm for Kel-F 800 in the pressure-volume plane. The solid symbols (•) are derived from the Brillouin measurements. Overlaid in the plot are data from low pressure bulk dilatometry measurements to 0.2 GPa, and the third-order Birch-Murnaghan EOS fit to the Brillouin data.*

maximum differential stress of ~38 GPa when it started to yield at ~ 66 GPa under uniaxial compression (Fig. 33). Moreover, the aggregate elastic moduli of the nanocrystalline *c*-BC_2N have been determined from the radial x-ray diffraction data at high pressures.

EOS of Polymers by Brillouin Scattering – Polymeric materials are routinely subjected to extreme environments either in use or during manufacturing, but the predominantly amorphous character of many polymeric materials presents an unique challenge for establishing their isothermal compressibility to pressures beyond those achieved in dilatometry. Through combination with DAC techniques, Brillouin scattering is now firmly established as a means to broaden the phase diagrams of polymers into new *P-T* regimes. At Carnegie, **Muhetaer Ahart** is collaborating with **Dana Dattelbaum** at **LANL** in the development of Brillouin scattering techniques for the study of polymeric materials at high pressure.

Typical Brillouin spectra at selected pressures are shown for Kel-F 800 in Fig. 34a. The spectra were collected at room temperature which is coincidentally near the glass transition temperature for Kel-F 800. T_g is strongly pressure dependent, shifting monotonically higher with pressure.

The isothermal bulk modulus (K_o) and its pressure derivative (K_o') were determined for Kel-F 800 through a Murnaghan equation-of-state (EOS) analysis (overlaid in Fig. 34b) giving K_o = 7.50 GPa and K_o' = 10.0. For comparison, recent dilatometry results for Kel-F 800 at 33 °C are overlaid in Fig. 34b and analyzed similarly to give a K_o = 2.8 GPa and K_o' = 30.0. The discrepancy by nearly a factor of three for separate K_o and K_o' determinations is perhaps a consequence of two factors: (1) the sound speeds are measured at GHz frequencies and thus the polymer response may be stiffer (larger K_o) compared with static, dilatometric measurements and (2) disparate pressure ranges used

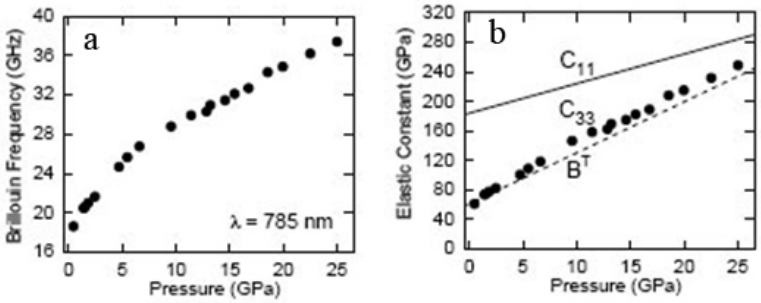


Figure 35. *a) Example data for the ratio V_{in}/V_{out} as a function of delay time and fits (solid lines) to the heat flow model of Ref.[73]; data and fits are labeled by the pressure. b) Example data for the oscillations in V_{in} as a function of delay time that are used to measure the Brillouin frequency of muscovite.*

in the EOS analysis, *i.e.* 18.5 GPa for the Brillouin measurements and 0.2 GPa in the dilatometry analysis.

To illustrate this latter point, the isotherm determined from Brillouin scattering was reanalyzed over a limited pressure range to 5.5 GPa. The resulting fit from this second analysis yielded K_o = 2.8 GPa and K_o' = 30.6, which are significantly more consistent with those determined from dilatometery. Above this limited pressure range, the parameters represent those determined initially over the entire pressure range. This is suggestive of a phase transition above ~ 5 GPa; however, in general EOS analyses, particularly for polymers that are known to display non-linear compression behavior at low pressure, must be compared with caution.

Pressure Tuning of Thermal Conductivity in a Layered Crystal – In the group of **Jie Li** (**Illinois**), the physics of heat conduction in layered, anisotropic crystals is probed by measurements of the cross-plane elastic constant C33 and thermal conductivity (λ) of muscovite mica as a function of hydrostatic pressure. Picosecond interferometry and time-domain thermoreflectance provide high precision measurements of C33 and λ, respectively, of micron-sized samples within a DAC; λ changes from the anomalously low value of 0.46 W m^{-1} K^{-1} at ambient pressure to a value more typical of oxide crystals with large unit cells, 6.6 W m^{-1} K^{-1}, at P = 24 GPa. Most of the pressure dependence of λ can be accounted for by the pressure dependence of the sound velocities and elastic anisotropy, as illustrated in Fig. 35.

Thermal Conductivity Modeling of Dense Hydrogen Fluids – Callisto, the second largest moon of Jupiter, poses a challenge to our understanding of icy bodies in the solar system. The existence of a subsurface ocean in Callisto is difficult to reconcile with its largely undifferentiated interior. The dichotomy between Callisto and its brother moon Ganymede has also remained a mystery in planetary sciences.[74] The **Li** group at **Illinois** now reports experimental data showing that ice VII, stable at pressures above ~ 3 GPa, is at least twice as conductive as that of its lower-pressure polymorph ice VI. Highly conductive ice VII in Callisto's undifferentiated core quickly brings its internal heat to shallower depths where the melting temperature of H_2O is the lowest, thus forming a subsurface ocean while keeping the deeper region in the subsolidus state (Fig. 36). A small difference in ice to rock ratio, through combined effects on the rates of radiogenic heating and convective cooling, may be sufficient to explain Ganymede and Callisto's divergent paths of evolution.

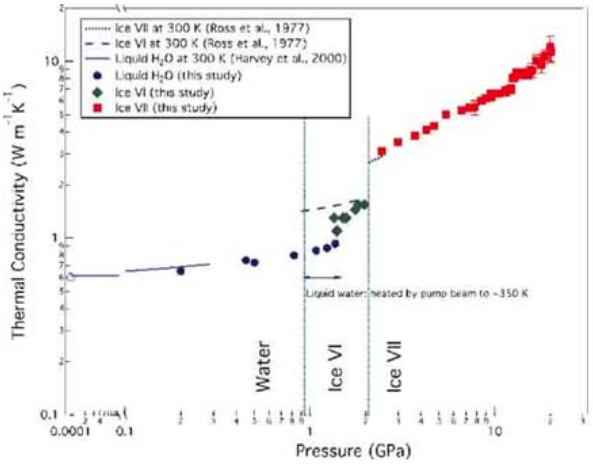


Figure 36. *Thermal conductivity of H_2O up to 22 GPa. At 300 K, liquid water transforms to ice VI at 0.93(3) GPa and ice VI transforms to ice VII at 2.08(5) GPa. The blue curves represent existing data on liquid H_2O, ice VI and VII up to 2.4 GPa.*

2.4 Plasticity, Yield Strength, and Deformation

High strain rates are included in the group of extreme conditions, along with extremes of pressure and temperature, that are of importance to stewardship science applications. CDAC groups have applied newly-devloped experimental techniques to the analysis of strain-induced texture development in both metals and crystalline solids, and continue to pioneer new methods in both neutron and x-ray diffraction. The results of these investigations give valuable insight into possible mechanisms for phase transformations in a wide variety of materials.

Deformation Measurements at High Pressure – Radial diffraction in conjunction with the DAC is a useful technique used by the group of **Rudy Wenk** at **Berkeley** to study the

development of lattice strains and lattice preferred orientation, *in-situ* at pressures relevant to the deep Earth. These experiments provide useful rheological information on high-pressure mineral phases that can be used to constrain deformation mechanisms in the deep Earth and interpret observed seismic anisotropies. However, earlier work using the DAC in radial diffraction were all performed at ambient temperature. It is questionable whether room temperature studies are appropriate for extrapolation to behavior in planetary interiors where materials are deforming at both high pressure and temperature. In order to address this limitation the **Wenk** group, led by CDAC graduate student **Lowell Miyagi,** has developed a laser heating system[75] and a novel combination of *in-situ* laser heating with a remote pressure increase utilizing a gas membrane driven panoramic DAC. This device has been used to study bcc (α), fcc (γ) and hcp (ε) iron at a range of pressures and temperatures up to 30 GPa and 1900 K.[76] This device, developed first for ALS beamline 12.2.2. is easily transportable and has also been used at HPCAT sector 16-BM-D.

In parallel with their efforts efforts to develop an *in-situ* laser heating system for radial diffraction, the **Wenk** group has also been working to develop a system for resistive heating and radial diffraction in collaboration with staff at HPCAT. This new technique combines radial diffraction geometry with external heating using a graphite heater and membrane pressure control. The current coverage in pressure and temperature is ~30 GPa and 1100 °C. Although the temperature range is more limited than that provided by laser heating, this technique has the advantage over laser heating of more uniform temperatures in the sample.

This method was applied to collect *in situ* texture measurements on the high-pressure and temperature phases of iron.[77] In the experiment, a (100) and (111) texture in bcc-Fe was observed, which made it possible to track the evolution of the texture with increasing temperature and during the bcc to fcc phase transition. Finally, the plastic deformation in the fcc phase between 5 and 15 GPa at 850 °C, which generates a (110) texture, was observed (Fig. 37). This is consistent with observations made using *in-situ* laser heating,[76] validating this technique.

Recently the group has also used this technique to systematically vary pressure and temperature conditions to explore changes in deformation mechanisms for MgO. They have now deformed MgO up to 40 GPa at 900 K and 25 GPa at 1050 K, and 65 GPa at 1200K. At 1200 K they observe a change in texture type. It appears that this is due to activation of {111} slip which is typical of NaCl type structures at high temperature versus {110} slip at low temperature.

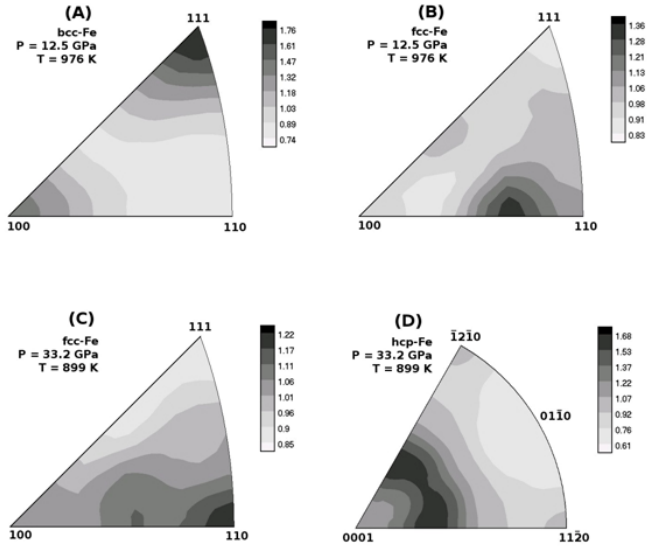


Figure 37. *High pressure-temperature DAC experiments with a resistance furnace. Inverse pole figure of the compression direction for bcc- and fcc-iron at 12.5 GPa and 976 K (A,B) and FCC- and HCP-iron at 33.2 GPa and 899 K (C,D). Equal area projection. Linear pole density scale in m.r.d.*

Clearly a large amount of the credit for the success with radial DAC experiments goes to MAUD, the Rietveld code Materials Analysis Using Diffraction developed by **Luca Lutterotti**, first at Berkeley[78] and since then upgraded and expanded in close coordination. It was first introduced to use the Rietveld method for neutron diffraction but has now been expanded for a full 2D image analysis. With this method it is possible not only to analyze textures, but also stress, phase proportions, crystallographic data and microstructural data as well. Among some features are a new approach for monoclinic crystal symmetry[79] and a feature to allow for turbostratic disorder.[80] A website that is constantly

updated provides detailed instructions for both neutron and synchrotron x-ray analysis with test examples. This helps beginners to get started with this very complex system (http://www.ing.unitn.it/~maud/tutorial.html).

Deformation in Hexagonal Metals – For some time there has been interest in texture development in hexagonal metals due to important applications as light structural materials (Ti) and applications in the reactor industry (Zr, Hf). The **Wenk** group has initiated an investigation of the high pressure properties of osmium based on a recent report that suggests strong anisotropy at high pressure.[81] Indeed, Os, compressed in a radial DAC and supposed to be very strong, shows immediate texture development already at 1 GPa, and strengthening to 54 GPa (Fig. 1). This is very different from Zn with a gradual texture development and a practically random texture at 10 GPa (Fig. 1). These pilot experiments are very intriguing and the group plans to systematically investigate hexagonal metals at high pressure to document differences and interpret patterns in terms of slip systems and mechanical twinning. CDAC graduate student **Jane Kanitpanyacharoen** is taking a leading role lead in this project.

Microstructure Evolution at High Pressures – Experiments of the type carried out in the **Panero** group at **Ohio State** (see **Section 2.1**) require using iron foil or powder and examination in the TEM. One concern in the experiments is whether or not the Rb and K in the alkali feldspars $MAlSi_3O$ (M=Rb, K) reside in grain boundaries and defects present at high temperature or grain boundaries formed upon decompression, or if the measured Rb and K content represent true dissolution. This has led an independent yet linked line of inquiry concerning the high-pressure, high-temperature microstructure evolution of metals.

The development and healing of such defects have first-order control on the creep mechanism in the deformation and material transport in high-pressure, high-temperature metals. Initial experimental samples are composed of a 10 μm thick, $Fe_{64}Ni_{36}$ alloy foil, cleaned of oxidation under high vacuum (10^{-10} torr) with an electron beam. Without exposing the sample to air, a uniform layer (300-500 nm) of Ni or Fe is sputtered onto the surface of the substrate. The samples are loaded into a LHDAC in an Ar pressure medium. After compression and heating, foils are extracted from the diamond cell for *ex-situ* analysis. Using FIB milling, a ~100-200 nm thick slice is extracted through the center of the hotspot and removed and thinned to electron transparency.

Panero and her students have analyzed the microstructure of these samples with respect to dislocation densities as a function of pressure and temperature. Initial results show that the effect of 50 GPa hydrostatic pressure noticeably increases the defect density. The defects in these alloys

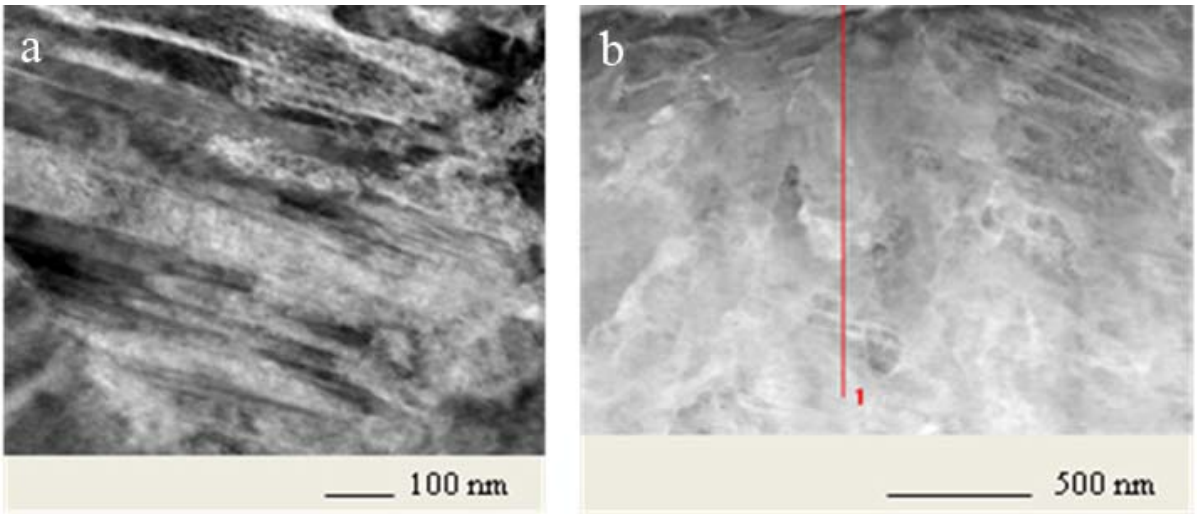


Figure 38. *TEM micrographs of iron-nickel alloys hydrostatically compressed to 60 GPa at room temperature (a) and heated to ~2900 K for 50 sec (b) showing a significant healing of defects through heating. Note the different length scales.*

appear very similar to the defects that occur in shocked steels (Fig. 38a) with the development of twins upon α to ε phase transitions. We observe that locations of twinning occur in regions of a high defect density in the foil as rolled, leading to regions of shear localization in the room temperature samples, which can explain the observations of non-homogeneous distribution of defects upon shock loading. Laser heating to 95% of the melting temperature, however, significantly anneals defects on timescales of <1 minute (Fig 38b). We have observed significant mixing between the pure deposited layer and the alloy substrate indicating transport times 2-5 orders of magnitude in excess of those expected by lattice diffusion. We therefore infer that material transport is occurring along grain boundaries and through defects.

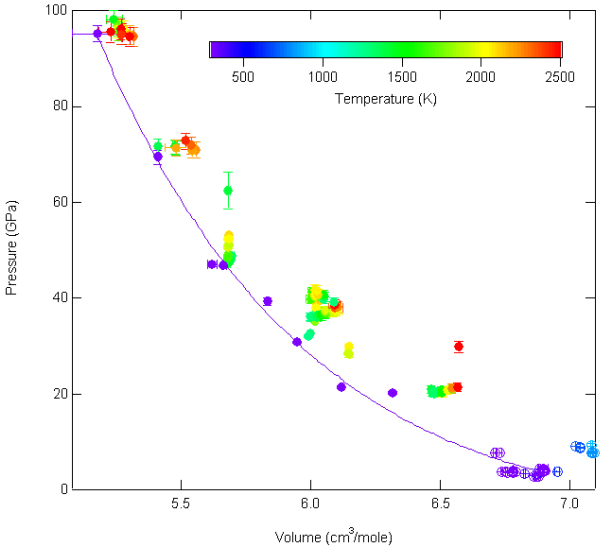


Figure 39. *P-V data for fcc $Fe_{64}Ni_{36}$ alloy. Open symbols are data at 298-1023 K in the hydrothermal diamond anvil cell (data from NSLS X17C), and closed symbols are data at 298-3000 K in the laser-heated diamond anvil cell.*

The $Fe_{64}Ni_{36}$ alloy is an Invar material exhibiting very low thermal expansion at ambient pressure and temperatures. At high pressures, the alloy was found to not undergo any phase transitions to 100 GPa and 3000 K, yet exhibiting no such Invar behavior. As a model material for the Earth's core, $Fe_{64}Ni_{36}$ provides a definitive constraint on the stabilization of the fcc structure with increasing nickel content. Such high-pressure, high-temperature results (Fig. 39) illustrate the very high quality of measurements attainable from *in-situ* measurements at facilities such as HPCAT.

Uncovering the Role of Phase Transformations in Texture Changes – The **Wenk** group has been regular users at the HIPPO TOF neutron diffractometer at **LANSCE**, where they use the intstrument's unique features to measure *in situ* texture changes during phase transformations. The research on zirconium[82] and titanium[83] documented regular variant selection during the hcp-bcc-hcp transformation based on a Burgers relationship. Similarly, variant selection occurs in iron during the bcc-fcc transformation.[84] A most amazing "texture memory" is observed in the trigonal-hexagonal-trigonal transformation in quartz, where a crystal remembers exactly the orientation it came from, as shown in Fig. 40.[85] In the quartz study this memory effect was attributed to stresses imposed by neighboring grains.

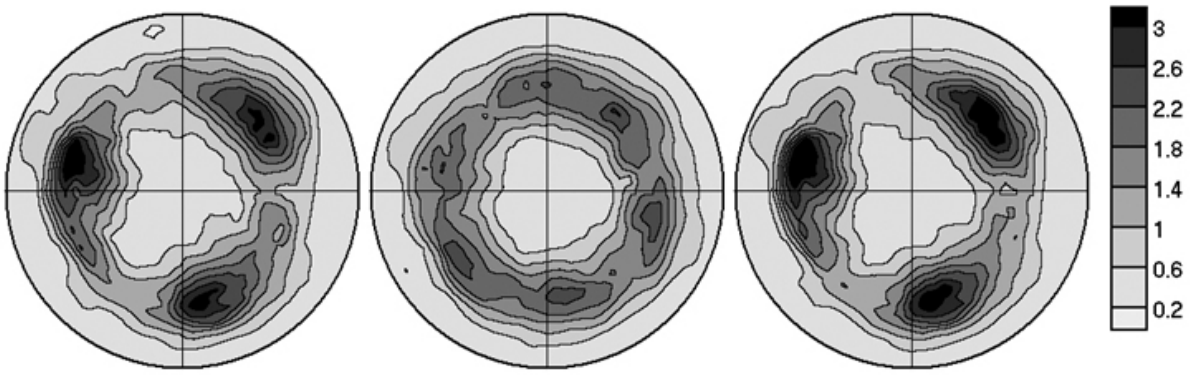


Figure 40. *In situ heating experiments with HIPPO: Pole figures of quartzite (a) 500°C, (b) 625°C, (c) 500°C (after phase transformation). Note the perfect texture memory. Equal area projection.*[85]

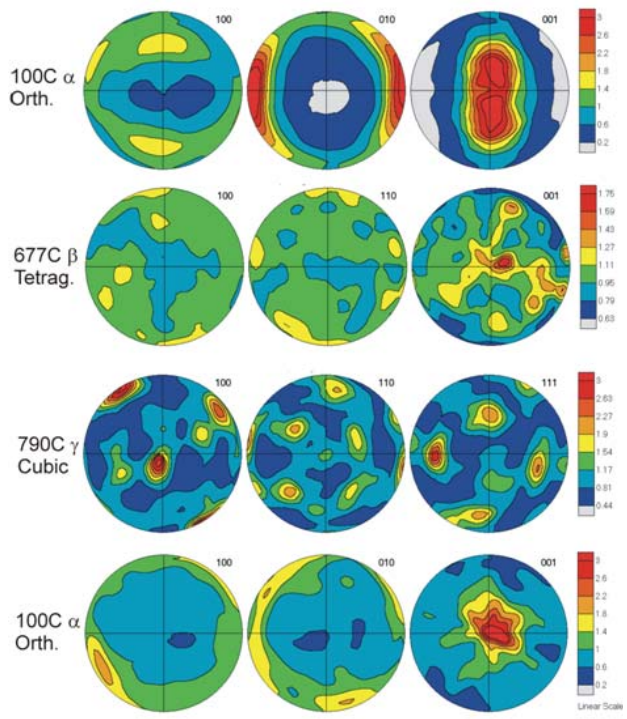


Figure 41. *Texture changes in pure uranium measured at the HIPPO diffractometer at LANSCE.*[87]

The question of texture memory and variant selection is a hot topic in materials science and only recently, with *in situ* high pressure-high temperature experiments, is there sufficient data to document the changes. Phase transformations occur in many low symmetry minerals and it is critical to understand the significance of applied stress during a phase transformation. For this reason the Wenk group has begun investigating uranium, a low-symmetry system. In uranium there are two phase transformations: orthorhombic up to 660ºC, tetragonal, from 668ºC to 766ºC and bcc above 766ºC.[86] The fundamental question at issue in this work is: Does an orthorhombic crystal remember its orientation after transforming to a cubic structure?

In a first round of experiments with neutron diffraction at **LANSCE** a cold-rolled sample of pure (#520-1S) uranium[87] shows indeed a strong texture (Fig. 41). The texture changes somewhat during heating to 500°C. Rapid grain growth occurs above 600°C and in most cases it was not possible to determine a meaningful texture pattern. When the sample was just barely heated above the ß -transition (677°C) the ß-texture could be refined with a weak pattern and c-axes predominantly parallel to the orthorhombic c-axis. If the sample is cycled rapidly through the ß –phase, a g cube texture can be identified (790°C).

Current work includes investigating U-0.7Ti, where small precipitates prevent grain growth. In December 2009 the group has beam time to carry out some experiments with the D-DIA apparatus at the **APS**, changing temperature and pressure, to induce phase transformations under stress analogous to what CDAC graduate student **Lowell Miyagi** found for postperovskite, but this alloy is extremely brittle and strong. High pressure experiments are relevant to make the material ductile and at the same time apply stress. There is very little work on anisotropy of uranium during phase transformations. Uranium is not only a fascinating system because of the low crystal symmetries, but it also shows shape memory properties (U-Nb). This is a collaborative project between researchers at **LANL (J. Bingert and D. Brown)**, **APS (Yanbin Wang)** and **Berkeley**.

Residual Stress in Deformed Crystals – Residual elastic strain in deformed crystals can be measured quantitatively in thin sections with a new high spatial resolution Laue microdiffraction technique with white synchrotron x-rays (beamline 12.2.2 at ALS). The measurements, with a resolution of one micron, allow a quantitative determination of the deviatoric strain tensor as a function of position within the crystal investigated. The method was first applied to a moderately deformed quartz crystal (undulatory extinction) and equivalent strain values of 800-1200 microstrains were documented.[88] The measured equivalent strain translates into an equivalent stress in the order of ~ 50 MPa. We have followed up investigating shock-deformed quartz with deformation lamellae (Fig. 42a). In these crystals high shear stresses exist along lamellar boundaries (Fig. 42b). Histograms illustrate that equivalent stresses in shock-deformed quartz are much higher (1000-4000 μstrains) than in a tectonically deformed quartz (600-1200 μstrains). This figure also establishes that the observations are real by comparing deformed quartz with an ideal single crystal, where values of 400 μstrains correspond to the current resolution of the method. Prospects for

pursuing this method to map residual stresses, with the potential of applying them as paleopiezometer, are encouraging.

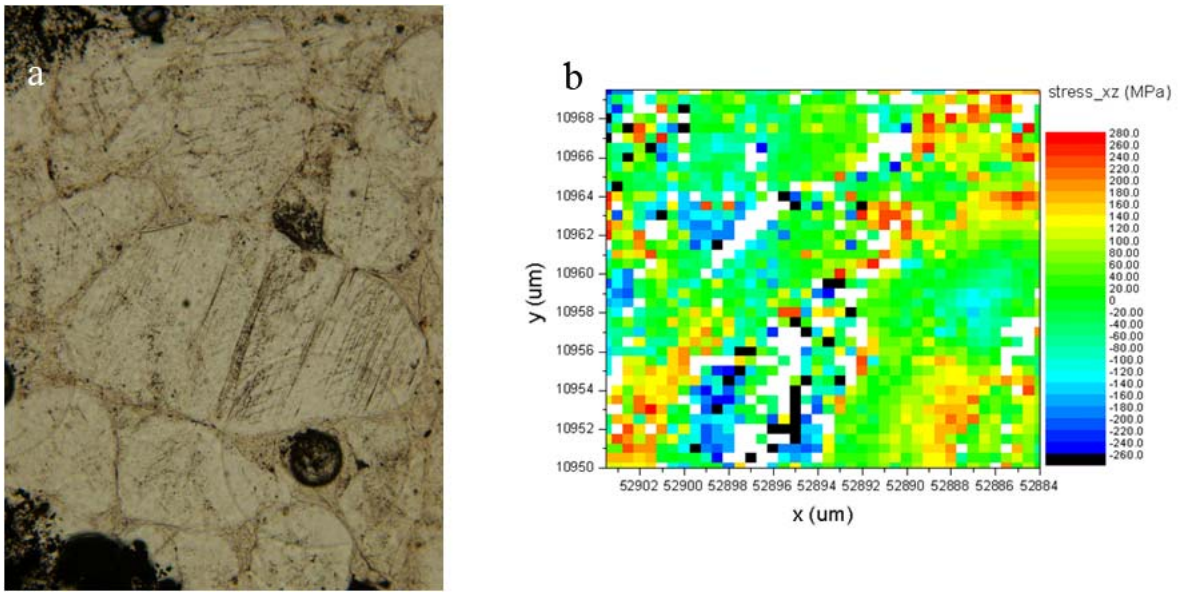


Figure 42. *Stress mapping in Vredfort quartzite with deformation lamellae. a) Petrographic thin section. b) Shear stress map across some lamellae. In the bands there is low stress but high stress is concentrated along the boundaries*

2.5 Electronic and Magnetic Structure and Dynamics

The behavior of new materials, such as the recently-discovered iron based superconductors, along with well-studied materials such as transition metal oxides, alloys, and rare earth metals, provide valuable new information on their electronic and magnetic properties when investigated at high pressures and the extremes of temperature. Breakthroughs in experimental techniques and the refinement of classical methods, including those available at synchrotron sources, are enabling physical property measurements of unprecedented accuracy and resolution and are leading to new insights concerning the physics that govern transport properties at high pressures.

Amorphization and Superconductivity in Layered Fe-Based Materials – High pressure superconductivity in the iron based superconductor $FeSe_{0.5}Te_{0.5}$ has been studied up to 15 GPa and 10 K by the **Alabama** group, using an eight probe designer diamond anvil in a DAC device. Four probe electrical resistance measurements show the onset of superconductivity (T_c) at 14 K at ambient pressure with T_c increasing with increasing pressure to 19 K at a

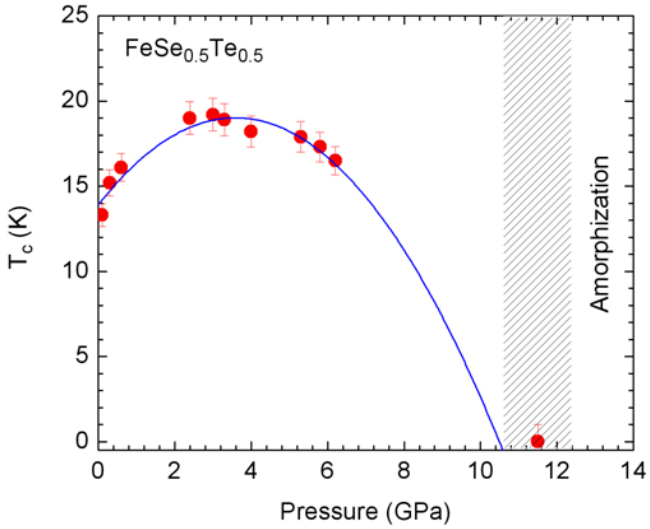


Figure 43. *Measured superconducting transition temperature for $FeSe_{0.5}Te_{0.5}$ as a function of pressure to 14 GPa. The solid curve is a quadratic fit to the data and is described in the text. The amorphization pressure range of 11.5 ± 1.0 GPa at room temperature is also indicated.*

pressure of 3.6 GPa. At higher pressures beyond 3.6 GPa, T_c decreases and extrapolation suggests non-superconducting behavior above 10 GPa. This loss of superconductivity coincides with the pressure induced amorphization of $Fe(SeTe)_4$ tetrahedra reported at 11 GPa in x-ray diffraction studies at ambient temperature.[8] The variation of T_c measured in these experiments is plotted as a function of pressure in Fig. 43. There is no evidence in the data for superconductivity at 11.5 GPa. The measured T_c variation can be fit by the following quadratic equation over the entire pressure range:

$$T_c \text{ (in Kelvin)} = -0.40\,P^2 + 2.86\,P + 13.97, \text{ P in GPa.}$$

The measured value of dT_c/dP at ambient pressure is 2.86 GPa/K. This is lower than the value of dT_c/dP of 4.87 K/GPa reported earlier in measurements confined to lower pressures between 1-2 GPa. The maximum T_c from the fit is at 3.6 GPa and has a value of 19.1 K. The measured extrapolation of the parabolic fit to the T_c data predicts that material will be non-superconducting above a pressure of 10 GPa.[89] This prediction coincides with the observations in our x-ray diffraction studies that the $FeSe_{0.5}Te_{0.5}$ sample becomes amorphous under high pressures above 11.5 ± 1.0 GPa at ambient temperature (see p. 10). The range of amorphization pressures is shown in Fig. 43. It should be added that amorphization pressure indicated in Fig. 43 is an approximation and does not include the temperature dependence of this phase boundary.

Low temperature x-ray diffraction studies have been combined with electrical resistance measurements on single crystals of the iron based layered superconductor FeSe to a temperature of 10 K and a pressure of 44 GPa. The low temperature, high pressure x-ray diffraction studies were performed at HPCAT, 16-BM-D, and superconductivity at high pressure was studied using designer diamond anvils. At ambient temperature, FeSe shows a phase transformation from a PbO-type tetragonal phase to a NiAs-type hexagonal phase at 10 ± 2 GPa. On cooling, a structural distortion from the PbO-type tetragonal phase to an orthorhombic *Cmma* phase is observed below 100 K. At low temperature (10 K), compression of the orthorhombic *Cmma* phase results in a gradual transformation to an amorphous phase above 15 GPa. The transformation to the amorphous phase is completed by 40 GPa at 10 K. A loss of superconductivity is observed in the amorphous phase and a dramatic change in the temperature behavior of electrical resistance indicates the formation of a semiconducting state at high pressures and low temperatures.[90] The formation of an amorphous phase is attributed to a kinetic hindrance to the growth of a hexagonal NiAs-structured phase under high pressures and low temperatures. The superconducting properties of single crystal specimens of FeSe have also been investigated using an eight-probe designer diamond anvil. Four-probe electrical resistivity measurements were performed on an FeSe single crystal to 10 K and 20 GPa. The onset of superconductivity was detected by a sudden decrease in electrical resistivity at low temperatures. The reported pressures the are an average of ruby pressure values measured during the superconducting transition measurements. Figure 44 shows the four probe electrical resistance measurement on FeSe at a pressure of 9.5 GPa where the onset of superconductivity is observed (T_c=36 K). In the amorphous

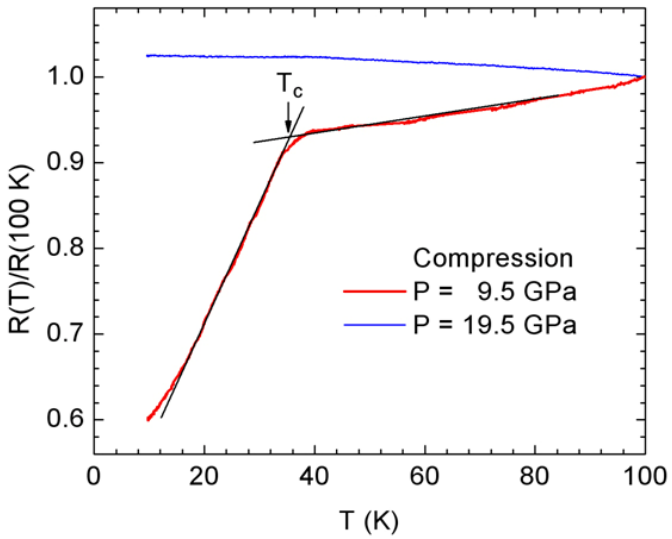


Figure 44. *The normalized four-probe electrical resistance measurements on FeSe samples using designer diamond anvils. The sample is superconducting at a pressure of 9.5 GPa with a superconducting transition temperature T_c of 36 K. At higher pressure of 19.5 GPa, no superconductivity is detected and sample resistance is observed to increase with decreasing temperature characteristic of a semiconducting material.*

phase, no superconducting transition is detected at a pressure of 19.5 GPa. Instead, in the amorphous phase, electrical resistance is observed to increase with a decrease in temperature and is characteristic of a semiconducting material.

Magnetic Properties of Rare Earth Metals at High Pressure – In **Jim Schilling's** group at **Washington University**, CDAC graduate student **Wenli Bi** has been developing experimental techniques for demanding measurements of magnetic properties at high pressure. For multimegabar experiments, where sample dimensions are below 50 microns, the standared method for fixing Pt electrical leads into a DAC sample is now unsatisfactory. Photolithography techniques are now used to fashion the coil systems needed for transport measurements in the DAC. Using specialized AutoCAD techniques, patterns for photolithographic masks have been created. Figure 45 shows such a mask containing approximately 480 individual lithographic patterns, two of which are shown to the right in detail, one for ac susceptibility and the other for four-point resistivity measurements. In the former only the 10-turn secondary coil spiral is shown; on top of it comes an insulating layer and then a straight lead to the center of the spiral. Electron beam lithography is available at Washington University's **Center for Materials Innovation** and will be used to sharply reduce the winding dimensions, thus allowing even secondary coils with 100 - 1000 turns.

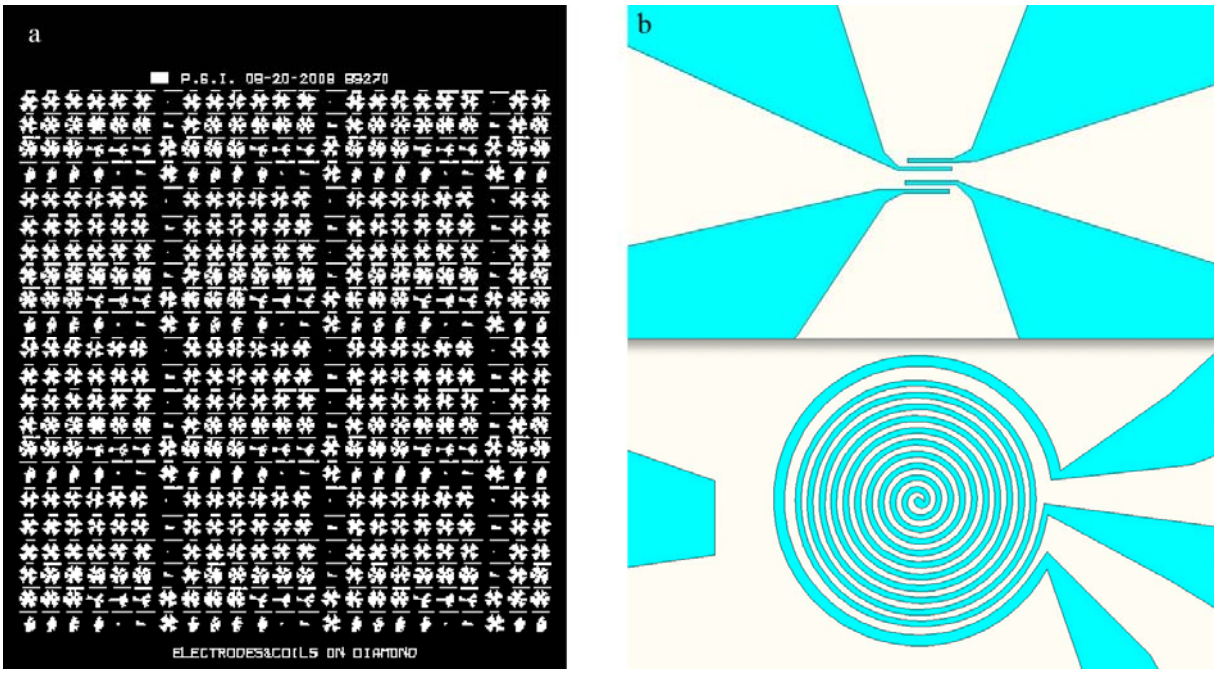


Figure 45. *a) Detail of coil patterns for AC susceptibility measurements (top) and four-point resistivity measurements (bottom). b) Photolithographic mask.*

Rare Earth-Iron Laves Phases at High Pressure and Temperature – The cubic rare-earth-iron Laves phases (C15 structure) have been studied extensively because of their unique magnetic and magneto-mechanical properties, particularly giant magnetostriction. A famous example is the pseudo-binary compound $Tb_{0.3}Dy_{0.7}Fe_2$ (Terfenol-D), which shows giant magnetostriction with a high Curie temperature that saturates at moderate magnetic fields. When there is a strong coupling between shape and magnetism, magnetic effects on phonons are expected, but effects of magnetism on phonons have received little attention. The intricate interaction between the iron 3d electrons and the lanthanide 4f electrons should be affected significantly by pressure.

Using data from the literature,[91-93] the **Fultz** group at **Caltech** finds find that the Grueneisen parameter for many C15 compounds is around 4, which is unusually large. In recent NRIXS measurements of $ErFe_2$ (Fig. 46), a similarly anomalous Grueneisen parameter is found. While the temperature range of these measurements is modest (300 K), the softening is substantial.

It is tempting to attribute this behavior to magnetic and magnetoelastic properties, but other explanations are possible.

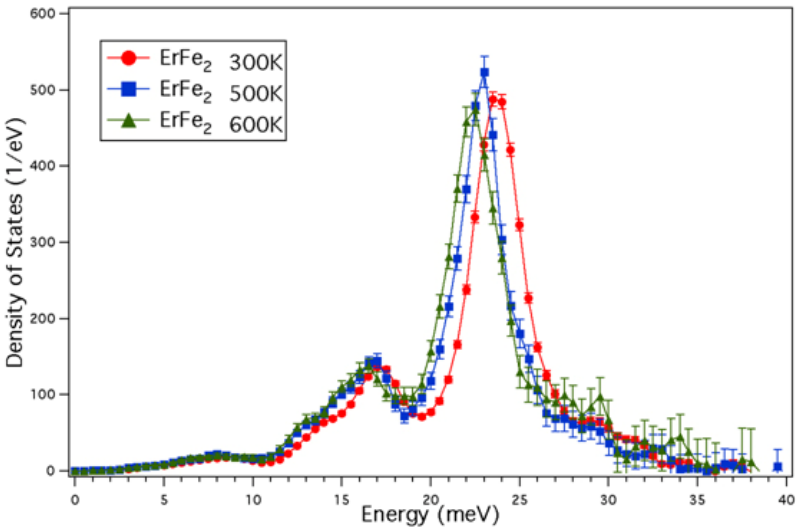


Figure 46. *Iron partial phonon density of states of $ErFe_2$ as a function of temperature, showing a substantial shift towards lower energies.*

As a preliminary to measuring phonons under pressure, nuclear forward scattering under pressure in $ErFe_2$ was measured to detect changes in magnetism. These results in Fig. 47 are fresh, and not fully analyzed. Nevertheless, they do show a change in the magnetic beat pattern below 5 GPa, and a transition to a paramagnetic phase between 5 and 10 GPa. Curiously, it seems that some of the magnetic beat pattern returns between 14.7 and 19 GPa, but this would be surprising. Evidently pressure does induce a change in the spin polarization, and likely the magnetic structure, that ought to be evident in the phonons as measured by nuclear resonant inelastic x-ray scattering. These measurements will be carried out at HPCAT 16-ID-D in the near future.

Structural and Electronic Properties of Group IV Metals – Research on group IV metals (titanium, zirconium, and hafnium) has been one focus of CDAC Laboratory Partners **Nenad Velisavljevic** and **Neal Chesnut** at **LANL** during the past year. An important aspect of this work is understanding and detecting the onset of a high pressure α → ω structural phase transition. The transformation from a ductile α- to a brittle ω-phase is observed at ~8 GPa for Ti, ~8 GPa for Zr, and 38 GPa for Hf. The α → ω phase boundary decreases to lower pressures at high temperatures, and can severely limit the use of group IV metals in industrial applications. A large part of the available static high pressure data on group IV metals has been obtained by the energy dispersive x-ray diffraction (EDXD) technique. Problems in detecting structural phase transitions using EDXD arise from preferred crystal orientation, grain growth, transition kinetics, and other effects encountered at high static pressures. Furthermore, detection of the onset of structural phase transition using angle dispersive (ADXD) or EDXD methods may be hindered by the ability to measure and resolve the diffracted beam intensity of the initially strong parent phase versus the weak daughter phase.

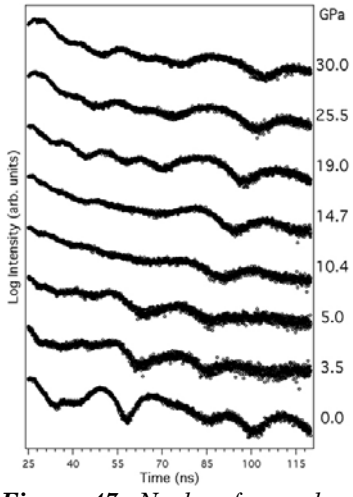


Figure 47. *Nuclear forward scattering spectra from $ErFe_2$.*

In order to overcome some of the issues associated with detection of structural phase transitions, the LANL group has performed simultaneous electrical resistance/x-ray diffraction experiments. Designer diamond anvils mounted in a gas membrane driven DAC were used to record changes in electrical resistance as a function of applied pressure, while ADXD data were taken at each pressure point, at beamline 16-BM-D at HPCAT. Comparison of the electrical resistance and ADXD data allows a correlation of the changes in electrical resistance with the evolution of a structural phase transition.[3] Furthermore, since designer anvils were mounted in a gas membrane DAC, pressure can be adjusted while performing *in situ* electrical resistance and x-ray measurements. In one of the experiments, a Ti sample was loaded in a pre-indented spring steel gasket. During the initial pressure increase a decrease in electrical resistance for Ti, followed by a

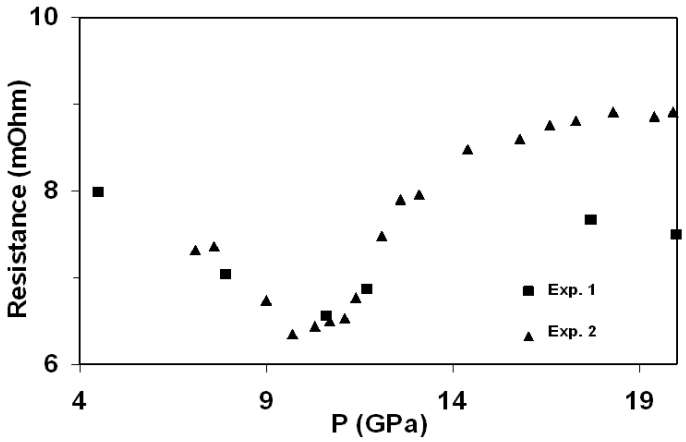


Figure 48. *The α → ω structural phase transition in Ti, detected using electrical resistance. The change in electrical behavior is caused by the phase transition.*

sharp increase above 10 GPa was observed (Fig. 48). The measurements show a sharp increase in electrical resistance during a pressure increase from 8.9 to 9.5 GPa, while ADXD measurements taken over the same time interval confirm that the change in electrical resistance is caused by the α → ω structural phase transition.

By performing *in situ* electrical resistance and x-ray diffraction measurements, it is possible to pinpoint with much higher accuracy the onset of the α → ω structural phase transition in Ti. In addition to collecting phase boundary data, the measurements provide valuable information on kinetic effects on structural phase transitions, which can also be used in conjunction with dynamic compression experiments.

Thermal Conductivity of Simple Oxides – The key to understanding Earth's evolution, including how our atmosphere gained oxygen and how volcanoes and earthquakes form, is to look deep into the Earth's lower mantle. At Carnegie, **Alexander Goncharov**, former **Carnegie** Summer Scholar **Ben Haugen** (**University of Colorado**) and CDAC partner **Steven Jacobsen** (**Northwestern**), recently investigated the high pressure thermal conductivity of iron-containing periclase and silicate perovskite, and discovered that the concentration of ferric iron plays a key role in moving radiative heat in the mantle, which in turn influences material movement throughout the deep Earth.[94] The group also discovered that ferrous iron has much less effect than expected — two to five times lower than previous models suggested. These results now call into question current models of mantle dynamics. Up to 130 GPa for silicate perovskite and up to 59 GPa for ferropericlase, the data show that heat absorption is governed by the concentration of ferric iron. Changes in absorption related to spin-state transition were also observed, but the effects are smaller than previously believed.

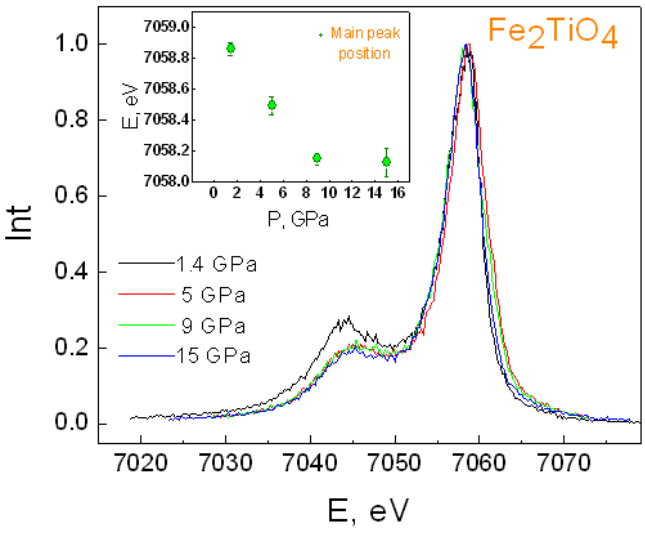


Figure 49. *X-ray emission spectra of Fe K_β collected from a single crystal of Fe_2TiO_4 at high pressures and room temperature. The spectra were normalized to unity and shifted in energy to compensate for the pressure induced shift of the line maximum based on the main fluorescence peak (K_β) at 7058 eV. The presence of the satellite peak (K_β`) at 1.4 GPa is characteristic of the high-spin state of iron whereas the reduction of the satellite peak at 5, 9 and 15 GPa indicates the occurrence of the intermediate or low-spin state of ferrous iron in Fe_2TiO_4.*

Spin Transitions in Transition Metal Oxides – A longstanding interest at **Carnegie** is the behavior of transition metal oxides at high pressure. **Viktor Struzhkin** has recently focused on spin transitions that take place in spinel-type oxides AMe_2O_4, which are abundant in the crust of the Earth. Oxide spinels with transition elements or mixed-charge cations have been intensively studied before: their magnetic, electronic, or

elastic properties, phase transitions and structures under ambient and extreme conditions have been scrutinized because of their importance in understanding magnetic and electronic conditions in the Earth's crust and mantle. The end member of the titanomagnetite family, Fe_2TiO_4 or $Fe^{2+}[Fe^{3+},Ti]_2O_4$ has been studied in detail using CDAC beamtime in collaboration with Professor **Takamitsu Yamanaka**.

Recently, novel iron arsenides $AFeAsO_{1-x}F_x$ (A=La, Ce, Sm, Pr, Nd, Sr, Ba, etc.) have been found as a second important class of high-T_c superconductors. Research activity is focused on identifying the mechanism responsible for superconductivity in these materials. To reveal the evolution of superconductivity and magnetism, and to investigate the interplay between these two collective phenomena high-pressure, low temperature studies of the $SrFe_2As_2$, and $CaFe_2As_2$, using X-ray emission spectroscopy and X-ray diffraction have been performed.

AFe_2As_2 and Fe_2TiO_4 have been investigated in the pressure ranges from 0.5 up to 4.4 GPa, and 1.4 to 15 GPa, respectively, at room temperatures. A high- to low-spin transition was found at between 0 and 3 GPa in Fe_2TiO_4 (Fig. 49). The transition occurs much earlier than the structural transition (at 7 GPa) and in Fe^{2+} octahedral sites.

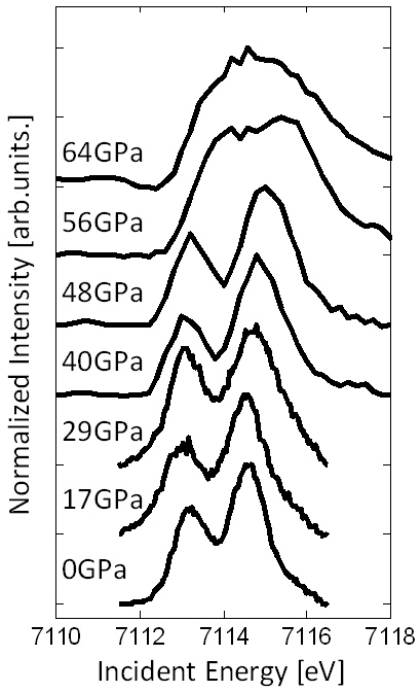


***Figure 50**. Fe K pre-edge of Fe_2O_3 at high pressure. 0, 17 and 29 GPa data were taken at BL12XU, SPring-8, while 40, 48, 56 and 64 GPa data at 16-ID-D of HPCAT.*

High-Pressure X-Ray Absorption Spectroscopy of Fe_2O_3 – As an archetypal transition metal oxide, hematite (Fe_2O_3) undergoes a series of electronic transitions and structural changes under high pressure, which have significance for condensed matter physics. At ambient conditions, hematite adopts the Al_2O_3 structure and is an antiferromagnetic Mott insulator, with five 3d electrons in the high-spin state. Upon increasing pressure, its FeO_6 octahedron is progressively distorted, until at 40-70 GPa, the structure of hematite changes to the Rh_2O_3-II type.[95] Along with the structural change, hematite becomes a metal[96] with a low-spin state.[97] Such electronic and magnetic phase transitions have been demonstrated in a number of studies: Pasternak[96] has conducted Mossbauer spectroscopy on Fe_2O_3 at room temperature up to 82 GPa and found that the non-magnetic component in the spectrum appears from 50-55 GPa. Badro[97] used x-ray emission spectroscopy K_{β}' feature to indicate the high spin and low spin state of Fe_2O_3 under different pressure.

The **Mao** group at **Stanford** has measured the x-ray absorption spectra of Fe_2O_3 up to 64 GPa, and for the first time, experimentally resolved the crystal field splitting of the 3*d* levels as a function of pressure (Fig. 50). The crystal field splitting energy increases from 1.4 eV at ambient conditions to 1.9 eV at 48 GPa, just below the pressure at which the series of structural and electronic transitions occur. The pre-edge features change dramatically after these phase transitions, indicating a complicated contribution from the 1*s* - t_{2g} and 1*s*- e_g excitations.[98] Preliminary DFT calculations were also carried out to examine the electronic structure of the 3*d* band. More theoretical work is needed to understand the high pressure metallic state of Fe_2O_3.

Bigger, Better Diamond Single Crystals – Impurities and defects in diamond can be purged by annealing, but this can also turn diamond to graphite. In order to prevent graphitization, diamond treatments generally have required pressures up to 6 GPa during annealing, which is costly and limits the size and quantities of diamond treated. **Yufei Meng** and colleagues at **Carnegie** have annealed CVD diamond at temperatures up to 2000° C using a microwave plasma at pressures below atmospheric pressure. The crystals, which are originally yellow-brown if produced at very high

growth rates, turn colorless or light pink under this treatment process. Despite the absence of stabilizing pressure graphitization takes place. Using photoluminescence and absorption spectroscopy, it has been possible to identify the specific crystal defects that give rise to specific color changes. In particular, the rosy pink color is produced by nitrogen vacancy (NV) centers, in which nitrogen atoms take the place of carbon atoms in the diamond crystal lattice.[99]

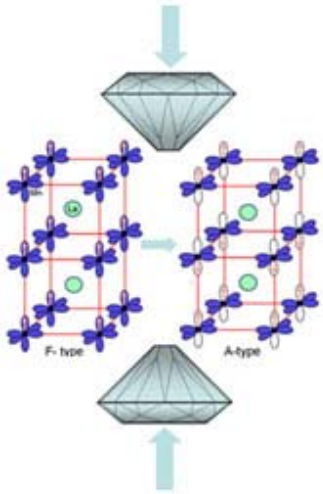


Figure 51. *Magnetic structures for* $La_{0.75}Ca_{0.25}MnO_3$. *Left, F-type ferromagnetic structure. Right, A-type antiferromagnetic structure.*

Enhanced Magnetic Effects at High Pressure – Understanding and ultimately controlling the intricate coupling between electrical conductivity and magnetism in colossal magnetoresistance (CMR) manganites remains a challenge, due to the coupling between lattice, charge, spin, and orbital degrees of freedom. Scientists from **Carnegie** and **APS**, led by **Yang Ding (HPSynC)** report new progress in using high pressure techniques to unravel its subtleties, with recent work showing that the CMR manganite ($La_{0.75}Ca_{0.25}MnO_3$) is subject to a magnetic transition coupled with a Jahn-Teller distortion at approximately 23 GPa.

In this work, x-ray magnetic circular dichroism (XMCD) and angular-dispersive diffraction techniques at the APS were combined to study the effect of pressure on the magnetic and electronic properties of the material.[100] XMCD is a newly-developed technique that uses high-brilliance, circularly polarized x-rays to probe the magnetic state of materials under pressure in the DAC. The results show that the predominant effect of applied external pressure is an increase in the strength of the superexchange interaction relative to the double exchange interaction. As a result, the system tends to increase the number of through-bond antiferromagnetic interactions by decreasing the dimension of the ferromagnetic region from three to two. This leads to an anisotropic redistribution of the 3d-e_g electrons in the Mn atoms. The resultant non-uniform electron density couples to the lattice *via* the Jahn-Teller effect causing a strained distortion of the crystal structure even under a uniform hydrostatic pressure. Ultimately, manganite transforms from an F-type ferromagnet to an A-type antiferromagnet at 23 GPa (Fig. 51).

Pressure Effects on the Properties of Relaxor Ferroelectrics – The application of pressure can tune the physical properties of relaxors and introduce new phenomena. **Muhetaer Ahart** and **Ronald Cohen** at **Carnegie** have been studying the pressure and temperature dependencies of the dielectric properties of disordered $Pb(Sc_{1/2}Nb_{1/2})O_3$ (PSN) and have extended its *P-T* phase diagram using Brillouin scattering techniques. Results of these and similar studies suggest that PSN presents a typical example of pressure-induced ferroelectric–to-relaxor crossover in lead-based perovskite materials. Motivated by the strong interest in developing a better understanding of the relaxation properties of highly disordered ferroelectrics, high pressure Brillouin scattering methods have been used to investigate the behavior of single crystal PSN from ambient to 12 GPa. Figure 52 shows the pressure dependence of linewidth and frequency of the Brillouin shifts of the L-mode of PSN. These spectra clearly exhibit elastic

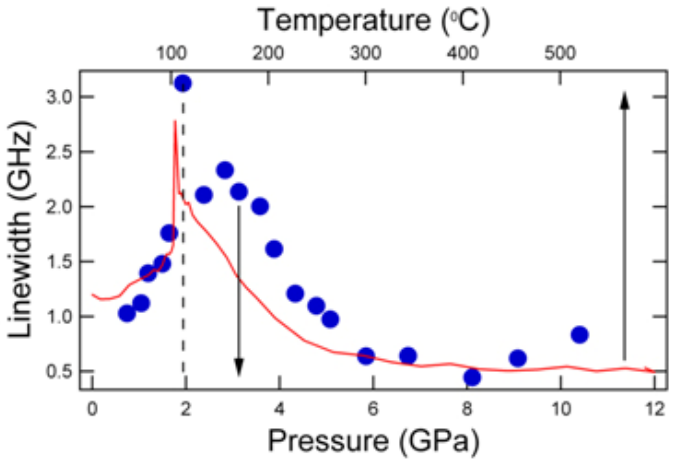


Figure 52. *Pressure dependence of the L-mode frequency of PSN (solid circles). For comparison, the temperature dependence of the L-mode frequency is also plotted (solid line).*

anomalies near the transition pressure (2 GPa).

The high pressure work on relaxor ferroelectrics demonstrates that the pressure may have more profound effects. By analogy to the temperature effects, it is possible to define a pressure point where polar nanoregions (PNRs) appear upon decompression (P_m). However, the diffuse scattering and dielectric measurements indicate that relaxor behavior only exists between 1 and 4 GPa in PSN samples at room temperature, suggesting $P_m = 4$ GPa. A significant softening of the acoustic mode upon decompression, similar to that appearing with temperature in other relaxors, was also observed. Because pressure suppresses the magnitude of dipole moments and the correlations of PNRs, at sufficiently high pressure, the correlation of PNRs do not become large enough to permeate the whole sample and precipitate a ferroelectric transition. Instead, the PNRs exhibit a dynamic "slowing down" of their fluctuations leading to the observed relaxor behavior. Thus, relaxor materials have a macro-averaged structure (host matrix) and a local structure represented by PNRs. PNRs tend to couple with acoustic modes via electrostrictive forces and cause the softening of the acoustic mode as seen in the measurements.

Metallization and Superconductivity in Group IVA Hydrides – Hydrogen constitutes more than 90% of all atoms in the visible universe and most are at extreme conditions. It has been proposed that compressed hydrogen might cross over into a metallic state and eventually become a superconductor with a high transition temperature. Although metallic hydrogen in the solid form has not yet been achieved, Group IVa hydrides XH_4 (X=C, Si, Ge, and Sn) are being examined as potential pathways toward achieving metallic hydrogen at modest pressures. This idea is based on the fact that hydrogen atoms probably have undertaken "chemical precompression" by the Group IVa atoms within the unit cell. Therefore, the chemical pressure environments in Group IVa hydrides may greatly reduce the physical pressure necessary for metallizing hydrogen. The idea has been proved to be particularly true in the experimental findings of metallization and superconductivity in solid SiH_4 at 60 GPa.

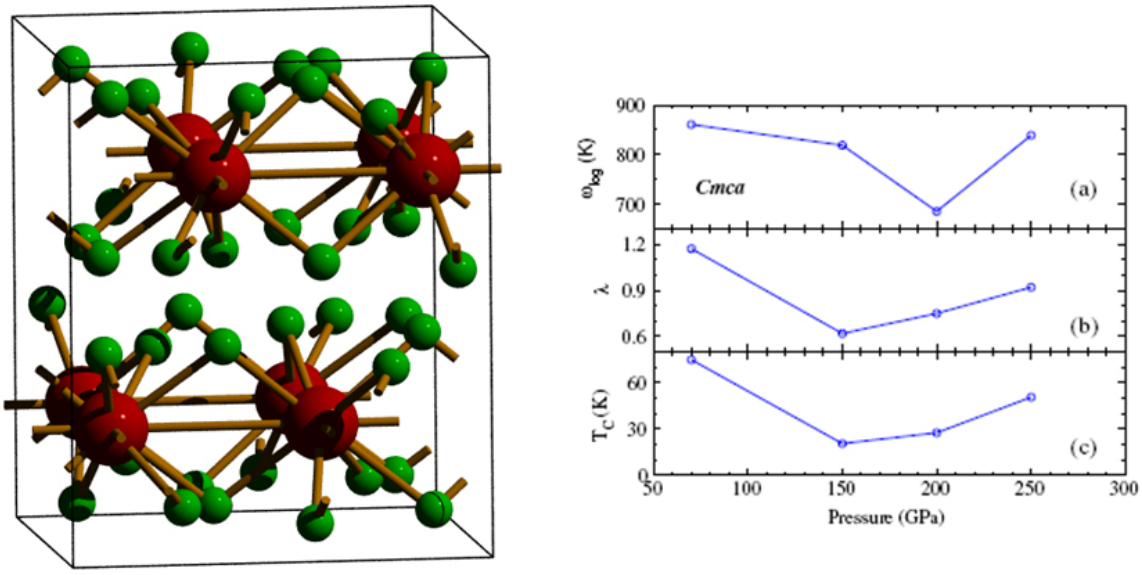


Figure 53. *Left) The energetically favorable Cmca structure for SiH_4. Right) Calculated (a) logarithmic average phonon frequency ω_{log}, (b) electron-phonon coupling parameter λ, and (c) superconducting transition temperature T_c of the Cmca phase of metallic SiH_4 with increasing pressure.*

Silane (SiH_4) has been the subject of several recent high-pressure studies. Experiments performed by **Xiao-Jia Chen** at **Carnegie** had determined the first high-pressure crystal structure with the symmetry of space group $P2_1/c$ in the pressure range of 10 and 27 GPa. The Carnegie group also provided the optical evidence for the metallization of SiH_4 at pressure of 60 GPa. The electronic and lattice dynamical properties of compressed solid SiH_4 in the pressure range up to 300 GPa were

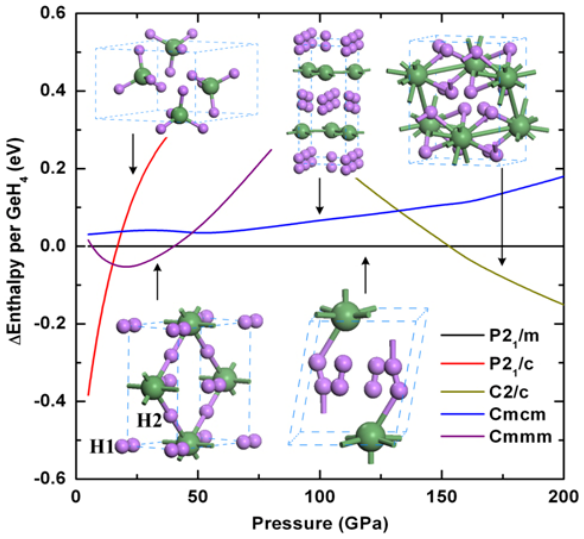


Figure 54. *The enthalpy versus pressure for five competitive structures of solid GeH_4 and the decomposition ($Ge+2H_2$) enthalpies for various possible structural combinations of Ge and H_2. Inset: the structures of the competitive solid GeH_4. The green and purple spheres represent Ge and H atoms, respectively. Enthalpy of $P2_1/m$ is taken as reference.*

calculated with density functional theory.[101] Two energetically preferred insulating phases with $P2_1/c$ and $Fdd2$ symmetries at low pressures were found, and it was demonstrated that the *Cmca* structure having a layered network is the most likely candidate for the metallic phase of SiH_4 over a wide pressure range above 60 GPa (Fig. 53) The superconducting transition temperature in this layered metallic phase was predicted to be in the range of 20–75 K.

Germane (GeH_4) is another promising candidate. Experimentally, structural determination of hydrogen-containing materials is difficult, due to the very low hydrogen scattering cross section in most diffraction methods. Thus, structural predictions are of great importance. **Chen** and co-workers performed *ab initio* first-principles calculations of the structural properties, GeH_4, within the molecular phase.[102] They found that the $P2_1/c$ structure evolves following a group-subgroup relation to the extended *Cmmm* structure with an insulator-metal transition at 15 GPa, followed by two metallic structures with the $P2_1/m$ and $C2/c$ symmetry at high pressures at least up to 200 GPa (Fig. 54). The metallization pressure for solid GeH_4 is considerably lower than that for SiH_4, pointing to a potential route to achieving metallic hydrogen. The prediction of superconductivity at 40 K suggests that this material is also a potential candidate for high-temperature superconductivity.

Effects of Pressure-Induced Competition in Electronic Order – Finding ways to achieve higher transition temperatures in superconductors remains a great challenge. Copper-oxide high-temperature superconductors (HTSCs) remain the superconducting materials having highest T_c both at ambient conditions and under pressure. The superconducting phase is one of several competing types of electronic order including antiferromagnetism and charge density waves. An emerging trend documented in heavy fermion compounds and organic conductors is that the maximum T_c for superconductivity occurs under external conditions that cause the critical temperature for a competing order to go to zero. Recently, such competition has been found in multilayer HTSCs which possess two crystallographically inequivalent CuO_2 planes in the unit cell. However, whether one can suppress the competing electronic state in order to enhance T_c in HTSCs remains unsettled.

Xiao-Jia Chen (**Carnegie**) and co-workers report the experimental finding that pressure-driven phase competition leads to a novel two-step enhancement of T_c in optimally doped $Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$ (Bi2223). We found that T_c first increases with pressure and then decreases after passing through a maximum.[103] Remarkably, T_c increases again with increasing pressure above a critical pressure around 24 GPa and considerably surpasses the first maximum. The presence of this critical pressure is a manifestation of the crossover from the competing order to superconductivity in the inner CuO_2 plane. It is suggested that the latter T_c increase occurs as a result of competition between pairing and phase ordering in different CuO_2 planes. These observations have important implications for engineering superconductors with much higher T_c at ambient conditions.

2.6 High *P-T* Chemistry

Investigations addressing the compositional basis of materials properties continue to be an important part of the CDAC research effort. CDAC groups are uncovering novel phenomena and reactivity in a broad range of systems such as small molecules, hydrogen-containing mixtures,

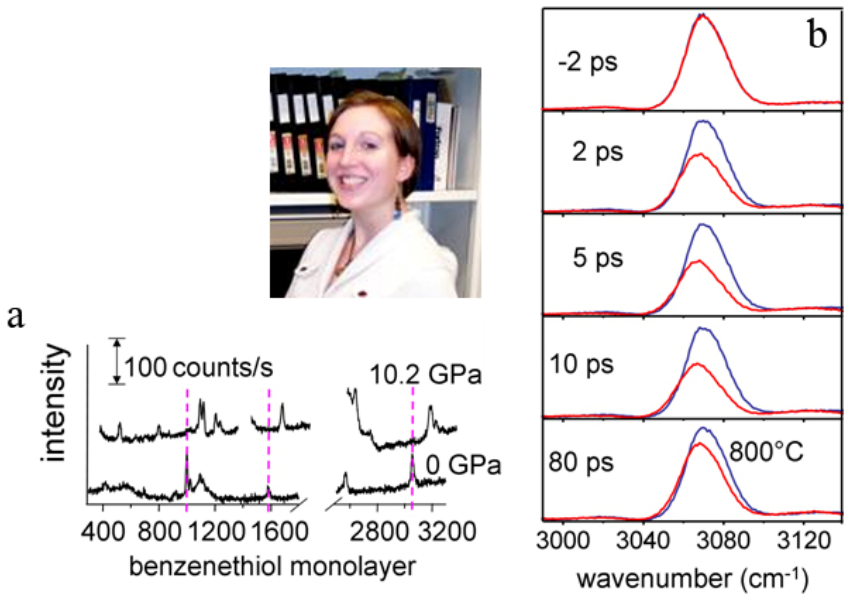


Figure 55. *a) Raman spectrum of benzenethiol monolayer on photonic substrate in the DAC at 10.2 GPa. b) Benzenethiol CH-stretch at 800°C studied by flash-heating. Inset: CDAC graduate student* ***Kathryn Brown (Illinois)****.*

organic molecules on surfaces, and complex systems of geochemical interest including the diamond anvil cell itself. Both laboratory and synchrotron-based techniques are central to this aspect of the CDAC program, which benefits significantly from advances in these methods.

Special Properties of Bulk Metallic Glasses – In the **Alabama** group, high pressure x-ray diffraction studies have been carried out on the two group IV transition metal-based bulk metallic glasses (BMG) $Zr_{57}Cu_{15.4}Ni_{12.6}Al_{10}Nb_5$ and $Ti_{42}Zr_{24}Cu_{15.5}Ni_{14.5}Be_4$ to a pressure of 30 GPa at ambient temperature. Image plate x-ray diffraction studies under high pressure were carried out at HPCAT 16-BM-D. Two BMG diffraction peaks can be followed to the highest pressure using an internal copper pressure standard. The amorphous phase is observed to be stable to a static pressure of 30 GPa suggesting that the phase change observed in dynamical pressure experiments is related to an increase in temperature.[104]

Spectroscopy of Monolayers Under Extreme Conditions – Current research in the group of **Dana Dlott** at **Illinois** is aimed at extending the study of molecular materials under extreme conditions of high temperature, high pressure and dynamic high pressure to molecular monolayers. Monolayers at high pressure provide new insights into the molecular dynamics of lubrication and adhesion, and monolayer spectroscopy of shock compression provides the ultimate in time and space resolution of the shock wave-molecule interaction.

CDAC graduate student **Kathryn Brown** has now developed and constructed a DAC Raman apparatus, and has fabricated photonic substrates that fit into a DAC, consisting of polymer nanospheres coated with Ag that enhance the Raman spectra of adsorbate monolayers by about one million *via* the surface-enhanced Raman scattering (SERS) effect. Using Ar as the pressure medium, spectra of benzenethiol and other monolayers up to 10 GPa, have been measured, as shown in Fig. 55. In related work, a new method has been developed for obtaining vibrational spectra

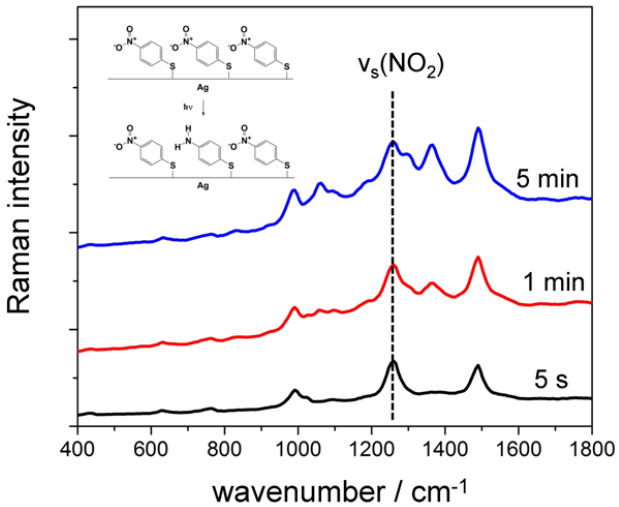


Figure 56. *Raman spectrum of nitrobenzene thiol monolayer. After 5s irradiation with a 532 nm laser, the nitro spectrum is clearly seen. After a minute or two some of the nitro groups are photoreduced to amine groups as depicted in the reaction scheme. This reaction and others can be studied in the DAC.*

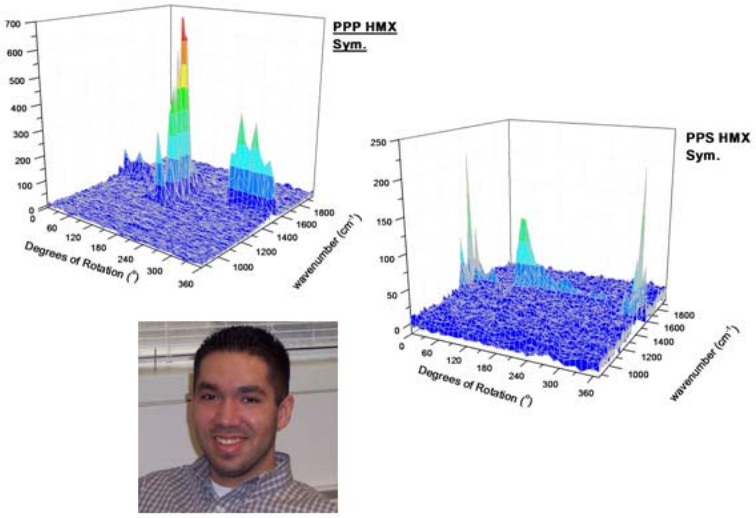


Figure 57. *SFG spectra of HMX (001 plane) showing symmetric stretch transitions of surface nitro groups in two polarization conditions, ppp and pps (SFG, vis, IR) as the crystal is rotated. Spectra such as these should determine the orientation of surface nitro groups. Inset: CDAC graduate student* ***Aaron Lozano*** *(**Illinois**).*

of adsorbates that have been flash-heated up to about 800 °C using nonlinear coherent sum-frequency vibrational spectroscopy (SFG). The spectra are obtained in a few picoseconds after the energy levels have thermalized, but before the adsorbate layer can decompose.[11, 105] A spectrum of benzenethiol at 800 °C is also shown in Fig. 55. The capability now exists to obtain spectra of molecular monolayers under conditions of high T and P, which we can compare to dynamic shock compression measurements using the technique developed by former CDAC graduate student **James Patterson**.

Figure 56 shows the Raman spectrum of a nitrobenzenethiol monolayer. The SERS substrate amplifies the laser's (a mW laser focused to 20 μm giving a few kW/cm^2) electric field by about 30 and the intensity by about 1000. Under this intense irradiation, in air, the nitro groups are photoreduced to amino groups. The laser intensity was adjusted to make this happen in a few minutes. It is therefore now possible to do real-time photochemistry on monolayers. Extension of this technique to high pressures is currently under development.

Surface Chemistry and Spectroscopy – Also in the **Dlott** group at **Illinois**, CDAC graduate student **Aaron Lozano** is studying the structure of nitro groups on the surface of HMX and RDX single crystals, as described in Fig. 57, by measuring the SFG spectra of nitro symmetric and asymmetric stretching transitions on single-crystal surfaces as a function of polarization and crystal orientation. In SFG there are two input beams and one output beam and eight polarization conditions. With postdoctoral fellow **Prabuddha Mukerjee**, the group has calculated how the nitro stretching spectra should depend on polarization and orientation.[7] This was done for nitro groups having the same structure on the surface as in the bulk. These experiments can therefore discriminate whether this is the case or not, and if not, it appears possible to extract the actual surface structure. A specialized goniometer has been fabricated that makes it possible to obtain SFG spectra as crystals are rotated about their surface normal. Some example spectra are shown in Fig. 57. The the rather complicated alignment of the SFG system varies slightly as the goniometer is rotated, but the apparatus is undergoing improvements to solve some of the

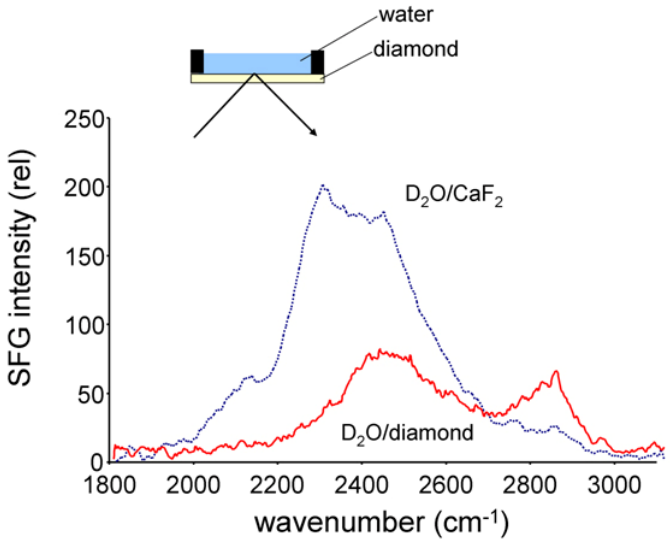


Figure 58. *SFG spectra of water (D_2O) at CaF_2 and diamond interfaces. The sharper peak at 2900 cm^{-1} is indicative of non-hydrogen bonded interfacial OD groups.*

alignment issues. Some orientation-dependent spectra are shown in Fig. 57.

Chris Berg, an undergraduate in the **Dlott** group, has been assisting with SFG work, and has made the first measurements of water at the diamond-water interface, using a CVD diamond window. There have been extensive studies of air-water interfaces, which show a peak at higher frequency not seen in bulk water, that has been associated with free non-hydrogen bonded OH at the interface. There have been studies of other interfaces such as water-quartz and water-CaF_2. As an initial guess, the water-diamond interface might be similar to water-oil, since diamond surfaces are usually highly hydrophobic. The first spectra are shown in Fig. 58. It is convenient to use D_2O to avoid IR wavelengths where atmospheric water interferes. There is clearly a more prominent dangling OD at diamond interfaces than at CaF_2 interfaces. Work is underway to extend these measurements to different polarization conditions.

Aqueous Oxidation of Re Metal in Supercritical H_2O-O_2 Mixtures – Rhenium (Re) is commonly used as gasket material in DAC experiments due to favorable materials properties such as high yield strength and plasticity, even at extreme pressures. Although Re is known to interact with aqueous geochemical samples, no such reactivity has been reported with H_2O or O_2, even at extreme *P-T* conditions. At **Carnegie**, **Raja Chellappa** has found that that Re undergoes a series of reactions with H_2O-O_2 mixtures at pressures less than 1 GPa at room temperature, in a DAC.[106] The reaction product (identified using Raman spectroscopy) was primarily perrhenic acid ($HReO_4$) which in the presence of water forms a combination of rhenium oxide hydrates; $Re_2O_7 \cdot (H_2O)_2$ and $HReO_4 \cdot H_2O$. The observed oxidation of Re in H_2O-O_2 mixtures in this study has wide implications from a fundamental point of view as well as an applications perspective. For example, Re is widely used in various space and nuclear related applications and its corrosion in the moderate pressure-temperature conditions of this study is of relevance. Also, the chemistry of perrhenate ion (ReO_4^-) is a window to its radioactive analogue technetium (Tc) found in high level nuclear wastes.[107-112]

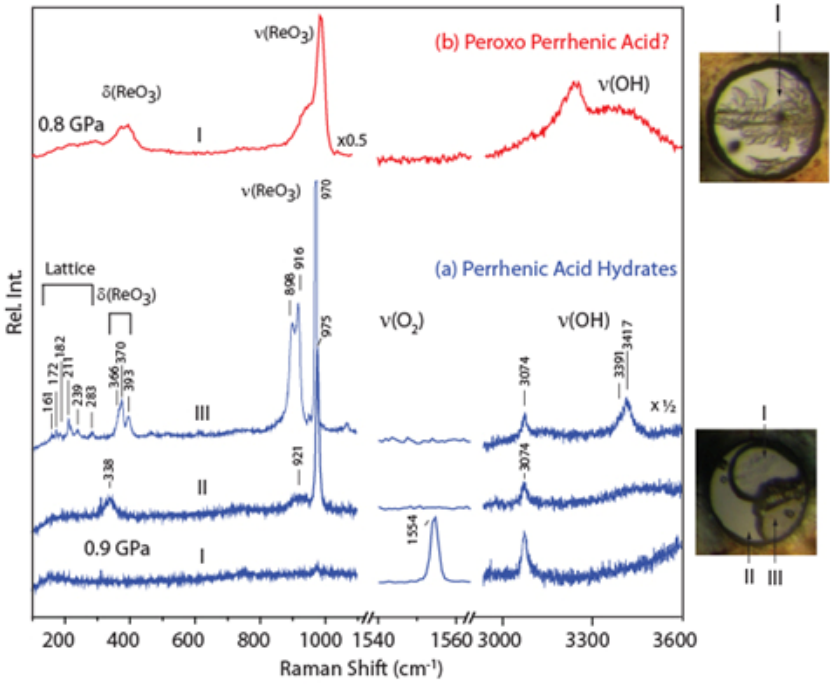


Figure 59. *Raman spectra and photomicrographs showing the reaction products from H_2O-O_2 mixtures in a rhenium gasket; (a) formation of perrhenic acid and its hydrates (0.9 GPa) after 12 days, (b) dendritic crystal growth in $HReO_4$-rich region with ν(OH) modes similar to ice VI (unstable on exposure to laser and likely to be an oxygen rich peroxo-$HReO_4$ compound).*

Figure 59 shows reaction products of rhenium in H_2O-O_2 mixtures at room temperature and the Raman signatures of $HReO_4$ are identified in the spectra. In one of the samples, $HReO_4$ crystallized into a mixture of perrhenic acid hydrates, and while the reaction product of another sample showed unusual instability on exposure to laser radiation. It is suspected that this may be an oxygen-rich peroxo derivative: $[ReO(O_2)_2OH].H_2O$. Extending classical metal corrosion behavior in H_2O, the electrochemical oxidation of Re is due to reduction of dissolved O_2 to form hydroxyl ions in essentially a neutral starting mixture. The formation of perrhenic acid can be represented by the following overall reaction scheme:

$$2\ Re(s) + 7/2\ O_2(g) + H_2O(l) \longrightarrow 2\ HReO_4(l) \quad \Delta G^o_f = -0.7\ kJ/mole. \qquad (1)$$

Based on the standard Gibbs energy of formation, the half-cell potential is

$$E^o\ (Re/ReO_4^-) = -0.367\ V.$$

The redox couple occurring on the walls of the gasket consists of a cathodic half-cell reaction (2) and an anodic half cell reaction (3)

$$3\ O_2(g) + 6\ H_2O(l) + 12\ e^- \longrightarrow 12\ OH^-(aq) \qquad E^o = +0.40\ V \qquad (2)$$

$$Re(s) + 8\ OH^-(aq) \longrightarrow ReO_4^-(aq) + 4\ H_2O(l) + 7\ e^- \qquad E^o = +0.58\ V \qquad (3)$$

The observed corrosion of rhenium with aqueous samples with high oxygen content suggests that caution should be exercised in the use of Re gaskets in containing oxidative aqueous samples (relevant for hydrothermal studies). The suggested reaction mechanisms and the calculated variations in chemical potential of dissolved oxygen explain the oxidative nature of supercritical H_2O-O_2 mixtures.

Hydrogen Interactions with Polymerica B-N-H Compounds – Ammonia borane [NH_3BH_3, AB] is a prototypical Lewis acid (NH_3)-Lewis base (BH_3) adduct that is a stable molecular crystal at ambient temperature and pressure. It is an attractive candidate for on-board hydrogen storage due to its high theoretical gravimetric and volumetric hydrogen densities with 19.6 wt. % H and 0.145 kg /L. Upon heating, AB releases H_2 in an exothermic reaction to form polyaminoborane [$(NH_2BH_2)_x$, PAB] at temperatures below 120 °C and decomposes further to polyiminoborane [$(NHBH)_x$, PIB] above 120 °C. A major challenge to its potential for practical application is the inability of reversing hydrogen release, i.e., addition of H_2 to PAB and/or PIB. A deeper understanding of hydrogen interactions with AB, PAB, PIB in a broad *P-T* range will provide guidance to designing hydrogen storage materials derived from B-N-H ternary system. At **Carnegie**, **Raja Chellappa** has recently reported on pressure-induced H_2 interactions with AB and resulting AB-H_2 complexation behavior in the 6-10 GPa range.[113] This has now been extended to demonstrate reactions of H_2 and D_2 with PAB and PIB in the 2-4 GPa pressure range and temperatures up to 220 °C, *in situ* in a DAC. Isotopic scrambling of H_2 and D_2, when thermodynamics prevent reversible reactions, is proposed to occur by a mechanism involving 'polymeric' frustrated Lewis pairs (FLPs).

In Fig. 60, the Raman spectra of a AB-D_2 mixture pressurized to 2.2 GPa and subject to a heating cycle is shown. Prior to decomposition at 2.3 GPa (165 °C), an H-D exchange process was observed by the formation of HD. With further heating to 216 °C, a mixture of PAB, H_2, and HD were obtained at 3.4 GPa. Weak, low frequency shoulders on the $Q_1(1)$ vibrons of H_2 and HD are also observed. On cooling to 27 °C, these low frequency peaks gain some intensity and are seen ~70 cm^{-1} lower than the respective $Q_1(1)$ vibrons at 4.8 GPa. Sharp peaks are seen in the 2370-2450 cm^{-1} range coinciding with the $\nu(BH_2)$ region and are assigned as $\nu(ND_2)$ while the broad peak at ~1750 cm^{-1} is assigned as $\nu(BD_2)$. Under high pressure D_2, an H/D exchange process occurs with PAB, PIB and mixed

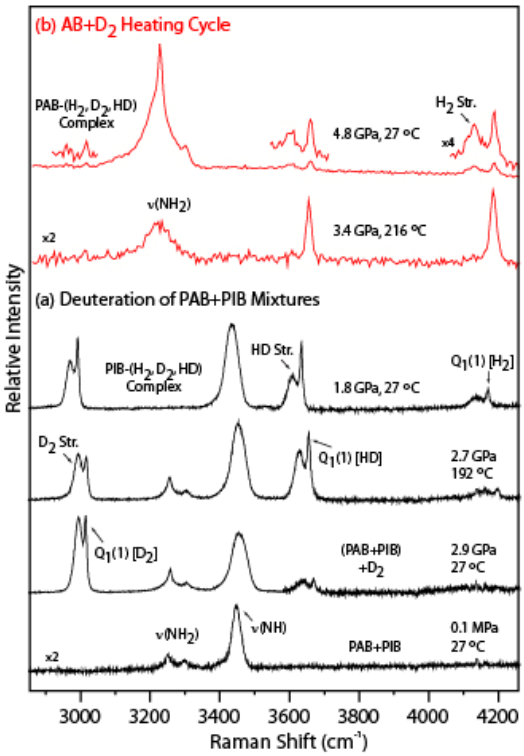


Figure 60. *Raman spectra showing (a) deuteration of PAB-PIB mixture showing H-D exchange and complexation at 2.9 GPa. On heating, further H_2 is released with formation of a PIB-(H_2, HD, D_2) complex that is retained on cooling to room temperature, (b) heating cycle of AB-D_2 mixture.*

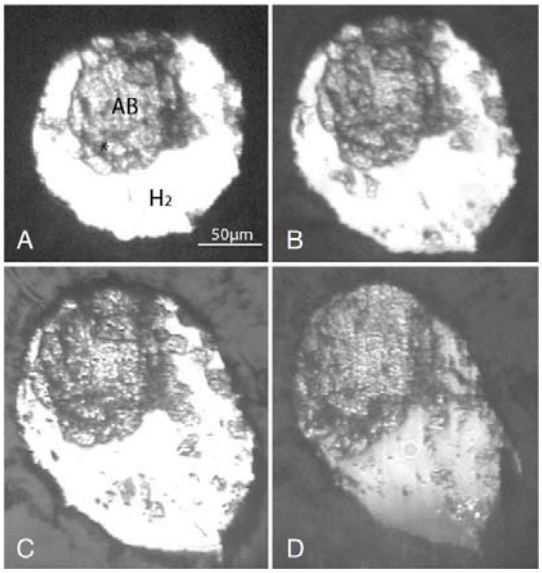


Figure 61. *Photomicrographs of ammonia-borane and H_2 in a Be–Cu 150 micron gasket hole as the reaction took place. A) Sample at 8.0 GPa without reaction occurring. B) Sample after increasing pressure to 10.1 GPa, the highest pressure reached in this sample. The previously circular gasket hole has started to deform and become oval. C) Sample experienced a rapid pressure drop to 8.2 GPa. D) AB sample kept growing at the expense of H_2 and the gasket shrank as the DAC was held at 8.6 GPa.*

phases as seen by the formation of HD. It is possible that D_2 interacts with the partially filled p-orbital of unsaturated boron in PIB resulting in H-D exchange with H bonded to boron.

The *P-T* stability of PAB-H_2, and PIB-H_2 complexes (as well as their D_2 and HD analogues) up to 8.7 GPa and 220 °C is notable. The kinetics of PAB, PIB complexation with H_2 are considerably faster (seen on compression between 2-4 GPa) compared to AB-H_2 complexes. It is of interest to determine if the complexation observed here can be accomplished by tuning *P-T* to more practical conditions. In fact, pressure-quenching suggests that these complexes are stable on recovery to ambient conditions.

Behavior of the NH_3-BH_3-H_2 System at High Pressure – Inspired by the high H_2 content in NH_3BH_3, the group of **Wendy Mao** at **Stanford** has studied NH_3BH_3 in the presence of excess H_2 pressure from ambient to 20.3 GPa and discovered a novel solid phase $NH_3BH_3(H_2)_x$, where x ~ 1.3 – 2. X-ray diffraction indicates that the new phase has a different crystal structure from pure NH_3BH_3 at the equivalent pressure.[114] This new phase forms slowly at 6.2 GPa, but the reaction rate is enhanced by crushing the NH_3BH_3 sample to increase its contact area with H_2. The formation of the new phase was accompanied by the appearance of two new H_2 vibrons from the absorbed H_2, and the changes in the N-H and B-H stretching modes resulting from the NH_3BH_3 interactions with H_2. In order to determine the amount of H_2 in NH_3BH_3-H_2, the pressure was measured by ruby fluorescence, and the volume for the free H_2 and NH_3BH_3 regions before and after the reaction was determined by optical microscopy and interferometry, H_2 vibron intensity by Raman spectroscopy, and optical density by absorption spectroscopy. Based on two measurements, an estimated 8 - 12 wt% molecular H_2 can be stored in the new NH_3BH_3-H_2 compound (Fig. 61). This represents a significant amount of H_2 storage which when added to the amount of H_2 chemically stored in NH_3BH_3, and demonstrates that this new phase a very promising material for additional study.

Boranes and Their Interactions with H_2 Under Extreme Conditions – Decaborane ($B_{10}H_{14}$) and its interaction with additional molecular hydrogen up to 11 GPa at room temperature has been studied using Raman spectroscopy.[115] The observed frequency dependence with pressure (dv/dP) and mode Grüneisen parameters varied for different spectral groups. The average dln ν/dP for B-H stretching modes is 4.5 /10^3 GPa, and B-H…B bridge 3.4 /10^3 GPa. For B-B skeletal stretching modes at 200-1100 cm^{-1}, the dv/dP covers a wide range from 2.8 /10^3 GPa to 7.3 /10^3 GPa, due to the wide spectral spreading of the modes. The dv/dP remains constant at approximately 2.1 cm^{-1}/GPa for all the skeletal modes. It can be seen that the B-H bonds are the most sensitive to pressure and show the most changes in Raman shift. The B-H...B bonds show intermediate changes on Raman shifts with pressure. The B-B backbone stretching modes are the least sensitive to pressure. We also identify a possible transition at approximately 3 GPa, represented by several new features from Raman spectroscopy. In addition, we found that decaborane could store additional molecular hydrogen with the application of pressure. Specifically, at 4.5 GPa it can hold 1 wt% of hydrogen (Fig. 62).

Hydrocarbon Condensation Reactions under Pressure – The extent to which there are contributions from hydrocarbon compounds synthesized beneath Earth's surface under elevated pressures and temperatures from abiogenic precursor molecules remains an open question. It has been proposed that hydrocarbon compounds generated in the upper mantle could transport through deep faults to shallower depths in the Earth's crust. One of the main obstacles for further understanding of the role of this mechanism has been the lack of reliable and reproducible experimental results confirming the possibility of the spontaneous synthesis of complex hydrocarbon systems under the conditions of the upper mantle. At **Carnegie**, **Alexander Goncharov** and co-workers used Raman spectroscopy in laser heated DACs to monitor the chemical reactivity of methane and ethane under the conditions of the upper mantle, including oxygen fugacity. It was found that methane above 2 GPa and 1000-1500 K partially reacts and forms saturated hydrocarbons (C_2-C_4 alkanes), molecular hydrogen and graphite. Formation of methane in similar experiments on ethane suggests the reversibility of hydrocarbon formation. These results support proposals of abiogenic pathways for the formation of hydrocarbons in the Earth's upper mantle.[116]

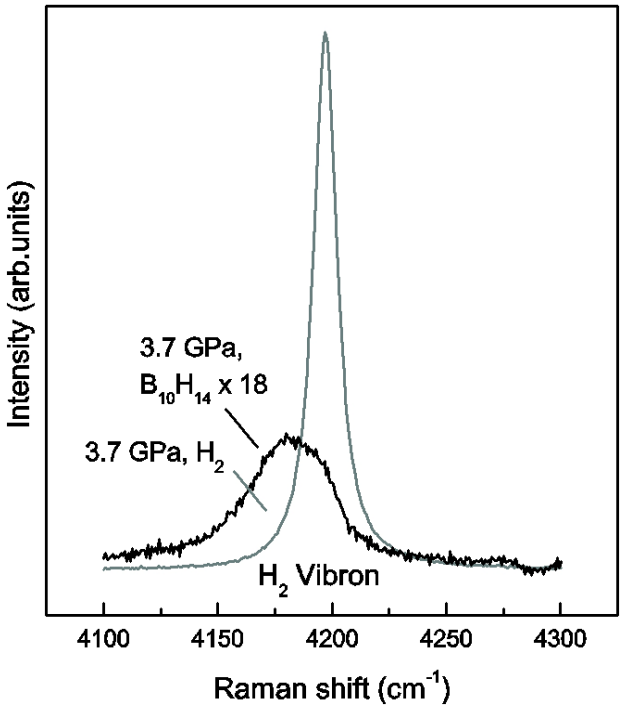


Figure 62. *The Raman spectra of the H_2 vibron (gray line) confined in decaborane vs. free H_2 vibron (black line), taken at 3.7 GPa.*

Recalibrating the Time Scale of Planet Formation – Researchers from **Caltech** and **UNLV**, with the support of scientists from **Carnegie**, have demonstrated a new way to create in the laboratory a mineral that only exists in meteorites and deep below the Earth's crust. The discovery indicates that the formation of planets and certain minerals in the early solar system may have involved collisions between much smaller bodies than previously thought.

Figure 63. *Tenham H6, a meteorite that contains wadsleyite (light colored areas), a high pressure polymorph of $(Mg,Fe)_2SiO_4$.*

In work carried out in part at **NSLS-U2A** and at **HPCAT**, the group, led by former **Carnegie** postdoctoral fellow **Oliver Tschauner** (**UNLV**), reports evidence for small quantities of the mineral wadsleyite formed upon shock compression of thin layers of magnesium oxide and fused quartz. Wadsleyite is widely believed to be the most abundant mineral in the Earth between 410 and 520 km depth. The conditions under which wadsleyite forms are known from static high pressure experiments, but it had never before been recovered from a laboratory-scale shock wave experiment, which has a much shorter time scale. However, wadsleyite has been found in some meteorites that consist of debris that formed upon natural shock events during collisions of proto-planetary bodies in the early solar system, as shown in Fig. 63. Based on the size of the wadsleyite grains recovered from the experiment,

it can be inferred that the wadsleyite in the meteorites from the early solar system could be generated by collisions between bodies one to five meters in diameter, or a thousand times smaller than calculated by earlier models.[117] Therefore high-velocity, destructive collisions among objects in the early solar system may have developed at an early stage of its evolution. Infrared spectroscopy, carried out at **NSLS-U2A** and x-ray diffraction, carried out at **HPCAT**, were used to do the initial characterization of the shocked sample. Using backscattered electron diffraction techniques, the size of the wadsleyite grains could then be determined to be several micrometers in diameter. Thus, growth rates of the wadsleyite grains during shock were in the range of several meters per second. Usually crystal growth occurs on rates many orders of magnitude slower.

Can Pressure Modify the Rules for Alloy Formation? – In the search for new alloys, metallurgists are guided by the empirical Hume-Rothery rules, which state that two elements can form an alloy only if they are similar in atomic size and electronegativity. With atomic radii of 1.83 Å, and 1.43 Å, respectively, cerium and aluminum would appear to be incompatible with respect to the formation of an alloy, particularly since the electronegativity of cerium is much lower than that of aluminum.

Both cerium and aluminum do, however, form many useful alloys with other metals, and can even form chemical compounds together, as well disordered mixtures (bulk metallic glasses), but a cerium-aluminum alloy would appear to be impossible. **Qiaoshi Zeng** (**HPSynC**) and co-workers from **Carnegie**, **HPCAT**, **Stanford University**, **PNC-CAT** (APS), **Uppsala University**, and the **Stanford Linear Accelerator Center** prepared a Ce-Al alloy at high pressure by transforming crystalline and metallic glass Ce_3Al into similar substitutive alloys. Using DAC techniques at HPCAT, transitions to the alloy phase were observed by x-ray diffraction to occur at 15 GPa for the crystal and 25 GPa for the glass. Once formed, the alloys persisted when the pressure was released. It is suspected that the Kondo volume collapse of cerium at high pressure causes its 4f electrons to delocalize, reducing the required difference in size and electronegativity between the two types of atoms.[118] Pressure-induced delocalization may therefore be a promising route for making novel alloys with unusual electronic and magnetic properties. The properties of the new alloy are currently under investigation, with one key finding being that after quenching, the delocalized electrons become localized again, suggesting that the alloy may retain some of the magnetic properties of cerium. Rare earth elements such as cerium are components of the strongest known magnets, and the new alloy could therefore have novel electronic and mechanical properties.

3. EDUCATION, TRAINING, AND OUTREACH

3.1 CDAC Graduate Students and Post-doctoral Fellows

The education, training and outreach mission of CDAC continues to focus on the support of graduate student preparation in the areas of high pressure research important to stewardship science. CDAC graduate students continue to work on a wide variety of problems in experimental high pressure research relevant to stewardship science, with projects in the fields of materials science, physics, chemistry as well as high-pressure mineral physics and geophysics. In addition, the integration of computational theory with experimental work in a number of CDAC groups has created an environment in which graduate students working in the area of high *P-T* materials research are acquainted with not only advanced experimental techniques and results, but also with state-of-the-art computational methods (*e.g.*, Refs.[119-121]).

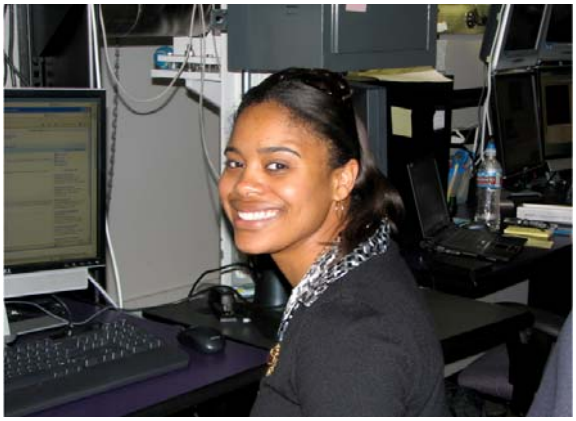


Figure 64. *CDAC graduate student* ***Madison Barkley (University of Arizona)***

In Year 6 of the CDAC program, 17 academic partners supported a total of 26 graduate students.

Princeton (Duffy):	**Susannah Dorfman**
	Zhu Mao
Caltech (Fultz):	**Lisa Mauger**
	Jorge Munoz
	Michael Winterrose
Chicago (Heinz):	**Chris Seagle**
Berkeley (Wenk):	**Jane Kanitpanyacharoen**
	Lowell Miyagi
Alabama (Vohra):	**Gopi Samudrala**
	Andrew Stemshorn
Illinois (Dlott):	**Kathryn Brown**
	Aaron Lozano
Arizona State (Yarger):	**Samrat Amin**
	Keri McKiernan (undergraduate)
	Erin Oelker
New Mexico State/Yale (Lee):	**Yahya Al-Khatatbeh**
Florida International (Saxena):	**Lyci George**
UCLA (Kavner):	**Matt Armentrout**
Northwestern (Jacobsen):	**Yun-yuan Chang**
Illinois (Li):	**Bin Chen**
Berkeley (Jeanloz):	**Arianna Gleason**
Ohio State (Panero);	**Daniel Reaman**
	Sabrina Whitaker
Arizona (Downs)	**Madison Barkley**
Washington Univ. (Schilling):	**Wenli Bi**
Stanford (Mao)	**Yu Lin**
	Shibing Wang

Eighteen graduate students have now received their Ph.D. degrees with CDAC support. Four of them, **James Patterson, (Illinois**, 2004), **Wendy Mao** (**Chicago**, 2005), **Nenad Velisavljevic** (**Alabama-Birmingham**, 2006), and **Raja Chellappa** (**Nevada-Reno**, 2004) have continued working in the area of stewardship science. **Patterson** pursued a postdoctoral appointment at the **Institute of Shock Physics, Washington State University**. **Mao** was an Oppenheimer Fellow at **LANL** working in the **LANSCE** division and has gone on to a faculty position at **Stanford Universtity**, where she has continued to work in the area of high-pressure materials science. **Velisavjlevic** is at **Los Alamos National Laboratory** working in the group of CDAC Laboratory Partners **Neal Chesnut** and **Yusheng Zhao**. **Chellappa** is now a CDAC postdoctoral fellow at **Carnegie**, working on both stewardship science and energy storage projects. **Matt Lucas** has gone on to a postdoctoral research position at the Spallation Neutron Source at **Oak Ridge**, and **Jeff Montgomery**, who worked on a Master's degree at **New Mexico State** with CDAC Academic Partner **Kanani Lee**, has now joined the group of **Yogesh Vohra** at **Alabama** to pursue doctoral studies.

Figure 65. Lowell Miyagi *received his Ph.D from* ***Berkeley*** *in 2009.*

The full list of graduate students who have received the PhD degree with CDAC support is as follows:

James Patterson (Illinois, 2004)
Raja Chellappa (Nevada-Reno, 2004)
Wendy Mao (Chicago, 2005)
Jenny Pehl (Berkeley, 2005)
Sergio Speziale (Princeton, 2005)
Tabitha Swan-Wood (Caltech, 2005)
Alexander Papandrew (Caltech, 2006)
Nenad Velisavjevic (Alabama-Birmingham, 2006)
Emre Selvi (Texas Tech, 2007)
Joanna Dodd (Caltech, 2007)
Matthew Lucas (Caltech, 2008)
Resul Aksoy (Texas Tech, 2008)
Mike Winterrose (Caltech, 2009)
Lowell Miyagi (Berkeley, 2009)
Chris Seagle (Chicago, 2009)
Bin Chen (Illinois, 2009)
Sabrina Whitaker (Ohio State, 2009)
Zhu Mao (Princeton, 2009)

Publications and presentations involving CDAC-supported students and postdoctoral fellows in Year 6 are listed below.

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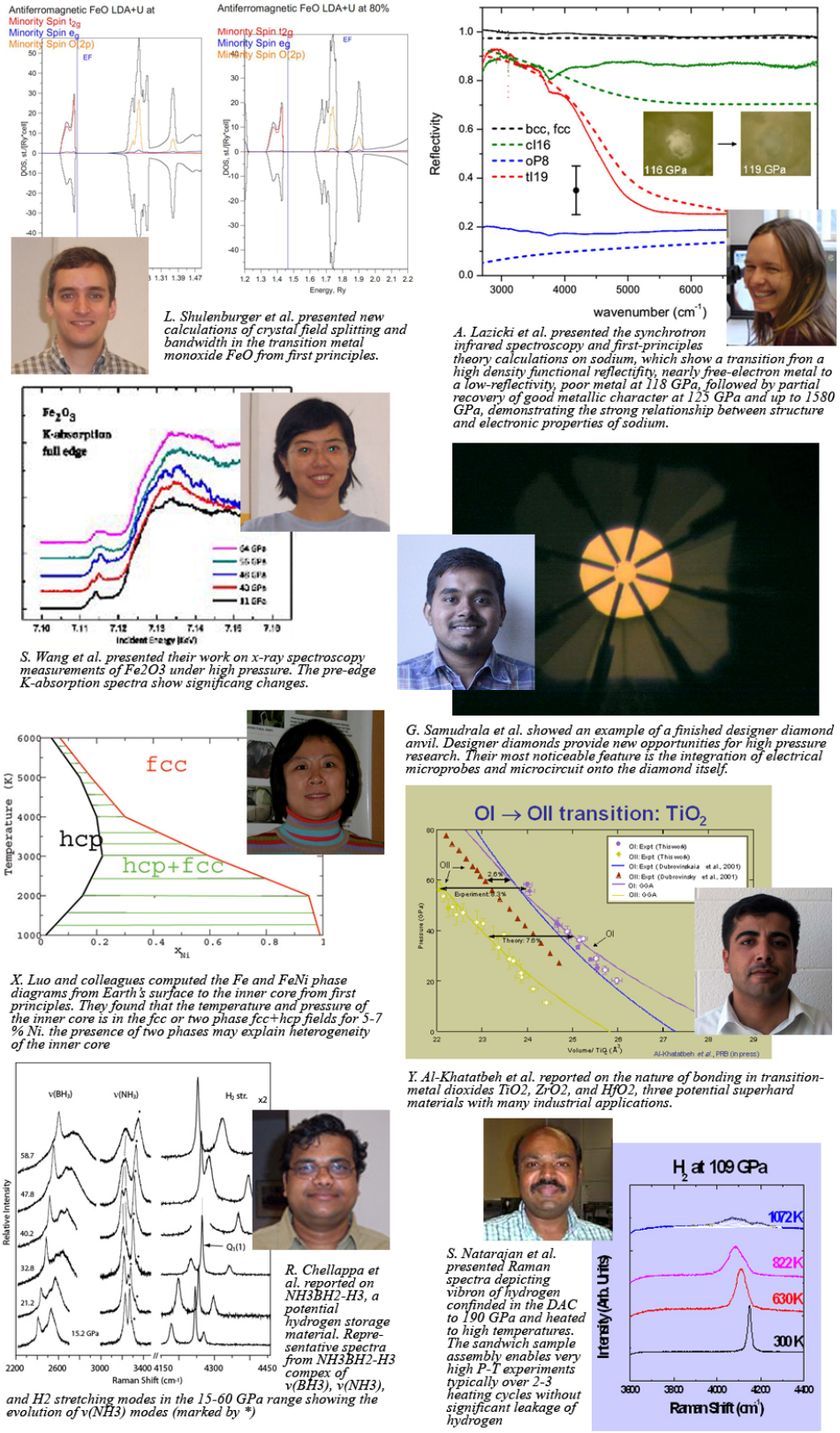

Figure 66. *CDAC Academic and Laboratory Partners, postdoctoral fellows, and graduate students were well represented at the March 2009 meeting of the American Physical Society held in Pittsburgh, PA.*

3.2 Undergraduate Student Scholars

A number of university undergraduate students participating in the highly successful Carnegie Summer Intern Program (Fig. 67) have worked on projects directly related to CDAC goals during the past year. This NSF-funded program, which is run by CDAC coordinator **Stephen Gramsch**, seeks to identify students at smaller institutions who may not have the opportunity for front-line research during the academic year, or students without a significant research background. At **Carnegie**, such students experience a rigorous an introduction to scientific research, and within the structure of CDAC, are learning about the important problems in the field of high-pressure research. During the summers of 2008-2009, the following students participated in this program with the **Carnegie** high pressure group.

Figure 67. *2009 Carnegie Summer Scholars*

Figure 68. *2009 Summer Scholar* ***Neil Foley (Carleton College)*** *examines a meteorite during a trip to the Smithsonian's Natural History Museum.*

2008:

Violeta Castro, Bucknell University
The Partitioning Behavior of Sulfur and Oxygen between Metal and Silicate
Caitlin Farnsworth, University of California-Davis
Structure and Symmetry of Oxygen at 350 GPa
Rohan Kundargi, University of California-Los Angeles
In-situ Thermal Diffusivity Measurements of $MgSiO_3$ Perovskite at Lower Mantle Pressures

2009:

Neil Foley, Carleton College
Fractionation of Sulfur Isotopes in the Formation of Mars
Zhili Liang, Lehigh University
Crystallization of Periodic Mesoporous Organosilicas
Alexander Savello, Emory University
Measurement of the Thermal Conductivity of $(MgFe)SiO_3$ Perovskite at High P and T
Angela Schad, University of Notre Dame
High Pressure Raman Studies of Ferroelectric Perovskites

Figure 69. *2009 Summer Scholars* ***Zhili Liang (Lehigh University)****,* ***Angela Schad (University of Notre Dame)****, and* ***Alexander Savello (Emory University)*** *present their work at the Carnegie Institution of Washington Summer Scholars Research Symposium.*

3.3 DC Area High School Outreach

Every year at **Carnegie**, several local high school students are hosted and offered guidance in their science fair projects and in other areas of research (Fig. 70). In 2008, **Jaqueline Rivera** worked on chemical synthesis methods for the preparation of Fe- and Al-containing solid solutions with **Stephen Gramsch**. **Maura James** investigated the NH_3-H_2O-H_2 system at high pressure and temperature with **Gramsch** and CDAC Research Scientist **Maddury Somayazulu**, and submitted her work to the Intel Science Talent Search and Siemens Competition for Math, Science, and Technology. **Manchali Madduri** was a semifinalst in the 2008 Siemens competition for Math, Science, and Technology, placing her among the top 300 entrants throughout the country. She investigated hydrogen complexation in crown ethers. Ms. Rivera is now studying biochemistry at the **Catholic University of America** in Washington, DC; Ms. James is now a student at the **University of Chicago**, and Ms. Madduri has enrolled at **Stanford University**. In 2009, **Emily Sandford** studied the Brillouin spectroscopy of prolymers with **Muhetaer Ahart**, and **Claire Barkett** extended the work begun by **Jaqueline Rivera** on Fe,Al solid solutions

Figure 70*. 2009 High School Summer Scholars. Left:* ***Emily Sandford (Gleneleg Country School)****. Right:* ***Claire Barkett (Good Counsel High School)****.*

2008:

Jaqueline Rivera, César Chávez Public Charter High School, Washington, DC
Synthesis of Solid Solutions in the Fe_2O_3-Al_2O_3 System
Manchali Madduri, Thomas Jefferson High School, Alexandria, VA
High-Pressure Studies of H_2 in Crown Ethers
Maura James, Convent of the Sacred Heart, Greenwich, CT
Raman Spectroscopic Investigation of the H_2O-NH_3-H_2 System

2009:

Claire Barkett, Good Counsel High School, Olney, MD
Low-Temperature Synthesis of Fe-Bearing Solid Solutions
Emily Sandford, Glenelg Country School, Ellicot City, MD
High-Pressure Brillouin Spectroscopy of Polymers

CDAC Coordinator **Stephen Gramsch** continues to teach a laboratory-intensive Advanced Placement Chemistry course for senior-level students at **Cesar Chavez Public Charter High School** in Washington, DC.

3.4 CDAC Collaborators

As discussed above, CDAC also has established active collaborations with high-pressure groups throughout the country and around the world. These collaborations play an important role fulfilling the mission of the center, specifically by training new students and researchers in high-pressure materials science and exposing them to problems of importance to the NNSA Labs. Some other collaborations are just starting and still others that are in the preliminary planning stages, but in all cases the infrastructure made possible by CDAC has given leverage to work on a number of exciting new research directions. The CDAC collaborators to date include faculty and students from the following institutions:

Aarhus University, Denmark
A.N. Christensen
Abdus Salam International Center for Theoretical Physics, Italy
M. S. Lee
S. Scandolo
Academia Sinica, Taiwan
F. C. Hsu
Y. L. Huang
M. K. Wu
K. W. Yeh
Academy of Sciences of Moldova
E. V. Rusu
V. Vu. Uraski
Albert Ludwig University, Germany
J. Majzlan
Argonne National Laboratory
A. Atalas
C. J. Benmore
J. A. Cowan
G. W. Crabtree
D. Haskel
E. Kaneshita
J. C. Lang
P. L. Lee
B. M. Leu
J. Mitchell
Y. Ren
A. H. Said
S. D. Shastri
H. Sinn
W. Sturhahn
N. M. Souza-Neto
Y. C. Tseng
J. Urquidi
Argonne National Laboratory, cont'd.
M. van Veenendaal
R. Yang
J. Zhao
Arizona State University
K. Leinenweber
A. K. McNamara
T. G. Sharp
J. Yarger
Auburn University
J. Dong
T. Tzeng
Bayerisches Geoinstitut, Bayreuth
Tiziana Boffa Ballaran
R. Caracas
L. S. Dubrovinsky
A. El Goresy
D. J. Frost
Anastasia P. Kantor
I. Y. Kantor
Catherine A. McCammon
Beijing Institute of Spacecraft Environment Engineering, China
Z. Gong
Beijing University of Technology, China
X. D. Han
Bhabha Atomic Research Centre, India
S. N. Achary
A. K. Tyagi
Brookhaven National Laboratory
Y. Cai
G. L. Carr
O. Gang
W. Q. Han
J. Hanson
C. C. Kao

Brookhaven National Laboratory, cont'd.
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M. M. Maye
Lisa Miller
W. Wen
D. Yi
Bulgarian Academy of Sciences
I. K. Bonev
I. Mitov
Daniela Paneva
Rossitsa D. Vassileva
California Institute of Technology
C. Ahn
T. Ahrens
P. D. Asimow
C. Brown
J. C. Castillo
O. Delaire
W. A. Goddard, III
Jennifer M. Jackson
N. Konstandova
J. Keith
S. Kung
C. Ma
J. Purewal
H. Su
Carleton College
Frances R. Reid
Carnegie Mellon University
M. Widon
Case Western Reserve University
J. Van Orman
CEA Marcoule, France
C. Poinssot
Centre National de la Recherche Scientifique, France
C. Dubourdieu
Chinese Academy of Science
L. G. Bai
G. F. Chen
L. C. Chen
M. Chen
C. Dong
X. L. Dong
T. D. Hu
S. Jiang
C. Q. Jin
X. D. Li
Y. Li
Y. C. Li
Z. Li
J. Lia
J. Liu
L. Liu
Q. Q. Liu
Y. W. Long
Y. X. Lv
W. Lu
X. Ma

Chinese Academy of Science, cont'd.
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Q. Shan
B. G. Shen
J. R. Sun
L. L. Sun
W. Sun
L. Tang
C. Tu
F. W. Wang
N. L. Wang
X. C. Wang
J. Wen
W. Ziao
L. X. Yang
W. Yi
S. J. You
R. C. Yu
X. Yu
X. H. Yu
Y. Yu
C. Zhang
D. Zhang
H. Zhang
H. W. Zhang
S. J. Zhang
Y. Zhang
T. Y. Zhao
Z. X. Zhao
Chinese University of Hong Kong
Y. Li
H. Q. Lin
J. L. Wang
City University of Hong Kong
C. Zhang
R. Q. Zhang
CLCR Rutherford Appleton University
M. Guttman
W. G. Marshall
Cleveland State University
J. Vitali
Colby College
Elizabeth Littlefield
Colorado College
T. D. Atkinson
P. Cervantes
Katie M. Chynoweth
Colorado School of Mines
Carolyn A. Koh
E. D. Sloan
Z. Wu
Columbia University
C. Y. Chin
D. Walker
Cornell University
W. Bassett
Z. Wang
Corning, Inc
B. G. Aitken

Dalhousie University, Canada
S. A. Bonev
Delaware State University
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Democritos National Simulation Center, Trieste
A. F. Young
DePaul University
G. B. Gonzalez
DESY, Germany
H. P. Liermann
Drexel University
M. W. Barsoum
DTC Research Centre, UK
D. Fisher
Duke University
P. M. Wu
East China Normal University, China
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P. Beck
P. Gillet
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J. Rasty
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University of Aarhus, Denmark
A. Svane
University of Alaska
T. Trainor
University of Arizona
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A. Krishnamurthy
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A. Khanna
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J. Zhang

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University of California, Santa Cruz
Q. Williams
University of Cambridge, UK
R. Needs
P. Lopez Rios
M. Towler
University of Chicago
X. Hong
A. Kuznetsov
J. J. Pluth
V. B. Prakapenka
M. L. Rivers
W. Schildkamp
S. R. Sutton
W. Zhang
University of Chile (Chile)
E. Menendez-Proupin
University of Colorado
B. D. Haugen
J. R. Smyth
H. Spetzler
University of Connecticut
P. D. Mannheim
University of Edinburgh
C. L. Bull
Olga Degtyareva
E. Gregoryanz
C. Guillhaume
H. Hamidov
K. Komatsu
I. Loa
J. Loveday
L. F. Lundegaard
Miriam Marques
H. E. Maynard
R. J. Nelmes
G. Stinton
University of Exeter, UK
K. Evans
Jennifer J. Williams
University of Florence, Italy
F. Gorelli
University of Florida
D. P. Norton
University Firenze, Italy
R. Bini
M. Ceppatelli
D. Chelazzi
M. Santoro
V. Schettino
University of Georgia
Z. W. Pan
University of Guelph
D. T. Jiang
University of Hawaii
X. Hong
F. Li
M. H. Manghnani
S. Marriappan
L. Ming
X. Qin
S. Sharma
P. V. Zinin
University of Hyogo, Japan
Y. Akahama
H. Kawamura
University of Illinois
J. D. Bass
B. Chen
L. Gao
H. Hellwig
W. Huang
J. Kim
A. S. Lagutchev
D. L. Lakshtanov
C. C. Lundstrom
Y. Pang
J. P. Perrillat
Carmen Sanches-Valle
J. Wang
H. Yavas
University of Kaiserlautern, Germany
H. J. Jodl
J. Kreutz
University of Kentucky
G. Cao
University of Kiel, Germany
H. Katzke
University of Leeds, UK
G. E. Lloyd
University of Leige, Belgium
M. Ausloos
J. F. Fagnard
P. Vanderbemden
University of Louisville
G. A. Lager
University of Manitoba, Canada
F. Hawthorne
University of Maryland
A. J. Campbell
B. Liang
W. F. McDonough
N. Miller
University of Michigan
U. Becker
R. C. Ewing
M. Lang
V. Pointeau
L. C. Shuller
F. X. Zhang

University of Minnesota
S. Demouchy
University of Missouri, Columbia
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University of Missouri, Kansas City
B. Chen
E. P. Gogol
M. B. Kruger
J. Murowchick
University of Nebraska at Omaha
J. Liu
W. N. Mei
University of Nevada-Las Vegas
S. Bajar
C. Chen
A. L. Cornelius
M. Daniel
H. Giefers
C. L. Gobin
T. Hartmann
D. Hartnet
O. A. Hemmers
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M. Nicol
T. Pang
Z. Quine
E. Romano
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A. M. Covington
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C. Agee
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J. Jahren
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S. Desgreniers
R. R. Flacau
J. S. Smith
University of Oxford, UK
A. Boothroyd
D. Prabhakaran
University of Paris VI
J. Badro
G. Calas
G. Fiquet
Chrystele Sanloup
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University of Tokyo
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M. Takigawa
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W. Grochala
M. Pekala
University of Warwick, UK
D. L. Carroll
Zoe A. D. Lethbridge
M. L. Newton
J. Vorberger
R. I. Walton
University of Washington
J. M. Brown
University of Western Ontario, Canada
C. Murli
S. R. Shieh
Y. Song
S. Xie
University of Wyoming
S. Sampath
University Ulm, Germany
U. Kaiser
Z. L. Zhang

Uppsala University, Sweden
R. Ahuja
S. Arapan
A. Blomqvist
W. Luo
Ural State Technical University, Russia
S. V. Streltsov
Verkin Institute, Kharkov
Y. A. Freiman
A. Grechnev
M. A. Strzhemechny
S. M. Tret'yak
Vernadsky Institute, Moscow
Delia Tchkhetia
M. A. Nazarov
Virginia Polytechnic Institute
R. J. Angel
B. E. Hanson
Nancy L. Ross
J. Zhao
Waseda University, Tokyo
Y. Ohki
Washington State University
W. Bi
M. Debassi
T. Matsuoka
K. Perkins
S. J. Turneaure
K. Zimmerman
Washington University, St. Louis
J. Y. Chen
S. Deemyad
J. J. Hamlin
M. Kim
K. M. Pitman
Brigitte Wopenka
C. S. Yoo
Wayne State University
J. D. Cook
T. Stremler
Wilbur Wright College
W. Pravica
Woods Hole Oceanographic Institution
N. Shimizu
Zhejiang Normal University, China
Y. Z. Feng
F. M. Wu
Zhejiang University, China
W. Chen
C. M. Feng
M. Y. Ge
Y. He
J. Z. Hong
J. Z. Jiang
E. Z. Liu
N. H. Shu
H. Wang
Q. S. Zeng

3.5 Visitors to CDAC

As part of CDAC's outreach program, **Carnegie** receives many visiting scientists each year. These scientists utilize the **Carnegie** laboratory facilities to prepare and perform experiments that would be impossible to do at their home institutions. Scientists from around the country and the world have visited **Carnegie** to take advantage of this program (Fig. 71).

Figure 71. *CDAC visitors to* ***Carnegie****. From left:* ***Alexander Gavriliuk (Institute for High Pressure Physics)****,* ***Sylvia-Monique Thomas (Northwestern University)****,* ***Kai Landskron (Lehigh University)****, and* ***Henry Scott (Indiana University – South Bend)****.*

Visitors	Affiliation	Project	Date
K. Driver	Ohio State University	Research with Ronald Cohen	October 6-20, 2008
P. Toledano	Universite de Picardie	Theory of high-pressure phases in molecular systems	November 17-December 19, 2008

Natascha Filipouitch	Stanford University	Carbon sequestration	November 24-28, 2008
Shibing Wang Ling Yu Lin	Stanford University	Raman lab experiments	November 24-28, 2008
A. Kyono	University of Tsukuba	Work with Takamitsu Yamanaka	December 1-5. 2008
R. Boehler	Max Planck Mainz	Visit with Russell Hemley	January 7-10, 2009
Sylvia-Monique Thomas	Northwestern University	Optical absorption studies of high-pressure hydrous materials	January 7-30, 2009
F. Elkin	Institute for High Pressure Physics, Russia	Synchrotron x-ray diffraction, spectroscopy of correlated materials, and transport measurements in DAC	February 5, 2009 -
Yu Lin	Stanford University	Research with Ho-kwang Mao	February 23-26, 2009
C. C. Kao	NSLS	Talk on "New developments at the National Synchrotron Light Source"	February 25, 2009
Michelle Weinberger	Army Research Laboratory	Work on the mechanical behavior of ultrahard and ultra-incompressible materials under extreme conditions	March 5, 2009-
A. Kyono	University of Tsukuba	Crystallography work	March 13, 2009- December, 2009
E. Alp	Advanced Photon Source	High resolution inelastic x-ray scattering under pressure: Phonons, sound velocity, magnetism and local structure	March 24, 2009
Veronica Vaida	University of Colorado	Visit with Russell Hemley	April 8, 2009
C. Tulk	Oak Ridge National Laboratory	Sample Loading	April 8, 2009
Alexandra Navrotsky	University of California – Davis	Talk on "Carbon, Sulfur, and Nitrogen in the Deep Earth and Other Planets: Some Unconventional Materials and their Thermodynamics"	April 23, 2009
K. Lokshin	University of Tennessee	Sample preparation for high pressure transport measurements in nickelates	April 27-May 1, 2009
Maaike Kroon	Delft University, Netherlands	Raman system to look some preloaded methane-hydrogen clathrate samples in DAC	May 11-13, 2009
A. Gavriliuk	Institute for High Pressure Physics	Correlated electronic materials under high pressure	May 11-June 5, 2009
H. Scott	Indiana University – South Bend	CO_2 gas loading	May 27-29, 2009
K. Landskron	Lehigh University	Nano-materials synthesis	May 27-June 21, 2009
M. Guthrie	HPSynC	Seminar on "Multiple lengthscale structural studies of disordered H-bonded matter"	June 6, 2009
P. Loubeyre	CEA, France	Seminar on "Calculations versus experiments in high pressure physics"	July 13, 2009
R. Little	Newcastle University, UK	Sample preparation of gold nitrate in DAC	August 4-7, 2009

3.6 2009 CDAC Winter Workshop

As outlined in Section 2.1, CDAC hosted the first Winter Workshop in February 2009 (Figs. 3 and 72). The event offered the opportunity for CDAC graduate students to hear tutorials in fundamental aspects of high-pressure materials science from CDAC academic partners, to interact with NNSA Laboratory Partners and hear presentations on their research activities at the respective laboratories, and to give presentations on their own dissertation research. The list of presentations is provided below. In addition, the Winter Workshop included a poster session and banquet where guests were entertained by the musical stylings of Gene Ice of Oak Ridge National Laboratory.

Lecturers supported by CDAC funds (staff, partners, postdoctoral fellows, or students) are designated by an asterisk (*).

Friday, February 27th:

Dana Dlott* (University of Illinois), *Laser-driven shock waves and molecular spectroscopy*
Kathryn Brown* (University of Illinois), *High pressure Raman spectroscopy of molecular monolayers of organic thiols on a nanotextured metal surface*
Chris Seagle* (University of Chicago), *Far infrared reflectivity of the FeO-MgO solid solution series*
Erin Oelker* (Arizona State University), *High pressure investigations of vitreous BeF_2*
Rip Collins (LLNL), *Exotic behavior in ultra-condensed matter: A few observations and questions*
Robert Downs* (University of Arizona), *Phase transitions and crystallography at high pressure*
Matt Armentrout* (UCLA), *High pressure and temperature equation of state of osmium*
Sara Whitaker* (Ohio State University), *High-pressure electronic transitions: Might Rb and K be compatible with iron at high pressure?*
Andrew Stemshorn* (University of Alabama-Birmingham), *Pressure induced amorphization in superconducting $FeSe_xTe_{1-x}$ compounds*
Neal Chesnut (LANL), *Los Alamos National Laboratory: Science & Research*

Saturday, February 28th:

Tom Duffy* (Princeton), *Elastic properties of solids at high pressures and temperatures*
Hans-Rudolf Wenk* (UC-Berkeley), *Deformation at ultra-high pressure*
Surendra Saxena* (Florida International University), *Thermodynamic view of Earth's interior*
Yogesh Vohra* (University of Alabama – Birmingham), *Physical property measurements at high pressure using designer diamond anvils*
Lowell Miyagi* (UC-Berkeley), *Deformation of $MgSiO_3$ perovskite at high pressure using DACs and in-situ radial diffraction*
Susannah Dorfman* (Princeton), *Static compression to multimegabar pressure under quasi-hydrostatic conditions: Platinum and magnesium oxide to 226 GPa in a helium medium*
Michael Winterrose* (Caltech), *High pressure invar behavior and magnetism in Pd_3Fe*
Marcus Knudson (SNL), *Shock wave compression and ultra-high pressure Hugoniot experiments on the Sandia Z Machine*

Posters Presented at the 2009 CDAC Winter Workshop

Al-Khatatbeh, Y., K. K. M. Lee, and B. Kiefer, Large volume change across OI --> OII phase transition in transition-metal dioxides TiO_2, ZrO_2, and HfO_2 as determined by experiment and theory, *CDAC Winter Workshop, 2009* (Argonne, IL, February 27-28, 2009).

Armentrout, M., High pressure and temperature equation of state of osmium (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Armentrout, M. and A. Kavner, The high pressure and temperature equation of state of osmium metal, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Barkley, M. C. and R. T. Downs, The determination and categorization of hydrogen environments in hydrous minerals, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Barkley, M. C., R. T. Downs, and H. Yang, The high-pressure behavior of the framework mineral behoite, $Be(OH)_2$: Insight into the effect of H as a lubricant in silica, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Bi, W., J. S. Schilling, and Y. Meng, The creation, evolution, and destruction of magnetism in rare-Earth systems at ultrahigh pressures, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Brown, K., High pressure Raman spectroscopy of molecular monolayers of organic thiols on a nanotextured metal surface (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Brown, K., Y. Fang, and D. D. Dlott, High pressure Raman spectroscopy of molecular monolayers of organic thiols on a nanotextured metal surface, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Chang, Y. Y. and S. D. Jacobsen, A gigahertz-ultrasonic interferometer for material elasticity studies at high pressures, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Chellappa, R., Oxidation potential supercritical O_2-fluid H_2O mixtures at room temperature, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Chen, B., D. Cahill, G. Bartov, and J. Li, Thermal conductivity of H_2O up to 11 GPa using time-domain thermo-reflectance method in diamond anvil cell: Insights into icy planetary bodies, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Dlott, D. D., Laser-driven shock waves and molecular spectroscopy (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Dlott, D. D., Vibrational spectroscopy of surfaces at high pressure, *CDAC Program Review* (Argonne, IL, February 26, 2009).
Dorfman, S., Static compression to multimegabar pressures under quasi-hydrostatic conditions: platinum and magnesium oxide to 226 GPa in a helium medium (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Dorfman, S., V. Prakapenka, and T. Duffy, Static compression to multimegabar pressures under quasi-hydrostatic conditions: platinum and magnesium oxide to 226 GPa in a helium medium, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Downs, R. T., Phase transitions and crystallography at high pressure (invited), *CDAC Winter Workshop* (Argonne, IL, February 27-28, 2009).
Duffy, T. S., Single-crystal elastic properties of materials (invited), *CDAC Program Review* (Argonne, IL, February 26, 2009).
Fischer, R. A., S. D. Jacobsen, C. M. Holl, K. A. Adams, E. S. Martin, C. R. Bina, J. F. Lin, V. Prakapenka, A. Kubo, and P. Dera, Compression of single-crystal magnesium oxide to 118 GPa and a ruby pressure gauge for helium pressure media, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Fultz, B., M. Winterrose, L. Mauger, and J. Munoz, Pressure-induced invar effect in Pd_3Fe (invited), *CDAC Program Review* (Argonne, IL, February 26, 2009).
Gao, L., B. Chen, E. E. Alp, W. Sturhahn, Y. Wang, and J. Li, Density and sound velocities of Fe_3C: implications for the Earth's inner core, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
George, L., V. Drozd, and S. K. Saxena, An overview of hydride research at CeSMEC, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Hrubiak, R., A. Durygin, and S. K. Saxena, Direct measurement of high-temperature thermal conductivity of materials using heat transfer analysis of temperature gradient of laser spot heated surfaces, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Hu, D., Y. Ma, J. Chaudhuri, and H. Yang, Compression of a crystalline ZnO nanotube: An experimental exploration of the B4 to B1 transition mechanism, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Ji, C. and Y. Ma, X-ray diffraction study of Al_4C_3 powder to 33.5 GPa, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Kanitpanyacharoen, W., L. Miyagi, H. P. Liermann, S. Merkel, M. Kunz, J. V. Nasiatka, M., J. Knight, and H. K. Wenk, In-situ deformation experiments at ultra-high pressure and temperature, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Lin, Y., W. L. Mao, V. Drozd, J. Chen, L. L. Daemen, and J. Shu, Ammonia borane at high pressure, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Lozano, A., P. Mukjeree, and D. D. Dlott, Investigating high explosive surfaces using nonlinear coherent vibrational spectroscopy, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).
Mao, Z., S. Dorfman, S. Shieh, Y. Meng, and T. Duffy, High-pressure phase of $Gd_3Ga_5O_{12}$: A New Superhard Solid?, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Figure 72. *CDAC Winter Workshop. Clockwise from top left:* ***Rip Collins (LLNL)*** *presents a talk on "Exotic behavior in ultra-condensed matter;"* ***Neal Chesnut (LANL)*** *gives a talk about some of the scientific and research being done at Los Alamos; CDAC graduate student* ***Lowell Miyagi (Berkeley)*** *presents his talk on the experimental determination of the high pressure deformation properties of perovskite and post-perovskite;* ***James Schilling (Washington University – St. Louis)****,* ***Rostislav Hrubiak (Florida International)****, and* ***Seth King (Purdue)*** *listen to* ***Mike Winterrose (Caltech)*** *talk about his poster;* ***Tom Duffy (Princeton)*** *and* ***Shibing Wang (Stanford)*** *discuss her poster during the Poster Session.*

Mauger, L., J. A. Munoz, M. L. Winterrose, I. Halevy, B. Fultz, and J. Hu, High pressure x-ray diffraction at elevated temperatures: An external resistive heater for DAC experiments, *CDAC Winter Workshop* (Argonne, IL, February 27-28, 2009).

Miyagi, L., Deformation of $MgSiO_3$ perovskite at high pressure using diamond anvil cells and in-situ radial diffraction (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Miyagi, L., W. Kanitpanyacharoen, M. Kunz, Y. Meng, M. Voltolini, and H. K. Wenk, Deformation of $MgSiO_3$ perovskite at high pressure using diamond anvil cells and in-situ radial diffraction, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-29, 2009).

Oelker, E., High pressure investigations of vitreous BeF_2 (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Oelker, E., E. Soignard, S. Amin, A. Chizmeshya, C. Benmore, and J. L. Yarger, High pressure investigations in vitreous BeF_2, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Samudrala, G. K., Y. K. Vohra, S. T. Weir, D. D. Jackson, and S. Falabella, Development of designer diamond anvils for high-pressure and high-temperature diamond anvil cell experiments, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Schilling, J. S., The creation, evolution, and destruction of magnetism in rare-earth systems at ultrahigh pressures (invited), *CDAC Program Review* (Argonne, IL, February 26, 2009).

Seagle, C. T., Far infrared reflectivity of the FeO-MgO solid solution series (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Seagle, C. T., W. Zhang, D. L. Heinz, and Z. Liu, Infrared dielectric and vibrational properties of rocksalt-type oxides at high pressure, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Soignard, E., Polyamorphism in SiO_2 glass at high pressure, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Stemshorn, A., P. M. Wu, and Y. K. Vohra, Reversible pressure induced amorphization and T_c in superconducting compounds $FeSe_xTe_{1-x}$, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Strobel, T., Raman studies of hydrogen bearing clathrates, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Vohra, Y. K., Physical property measurements at high pressure using designer diamond anvils (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Wang, S., W. L. Mao, Y. Cai, N. Hiraoka, H. Ishii, Y. Ding, Y. Xiao, P. Chow, H. K. Mao, J. Shu, and C. C. Kao, Fe K pre-edge of Fe_2O_3 (hematite) at high pressure, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Wenk, H. K., Deformation at ultra-high pressure (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Whitaker, S., D. M. Reaman, J. E. Kabbes, J. S. Piggott, G. L. Hovis, A. J. Campbell, E. Cottrell, and W. R. Panero, High-pressure electronic transitions: might Rb and K be compatible with iron at high pressure?, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Winterrose, M. L., High pressure invar behavior and magnetism in Pd_3Fe (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Winterrose, M. L., I. Halevy, J. A. Munoz, L. Mauger, M. S. Lucas, B. Fultz, M. Lerche, and J. Hu, High-pressure stabilization of antiferromagnetism and competing magnetic states in the Pd-Fe system, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

Zhang, W., C. T. Seagle, H. Zhou, and D. L. Heinz, Size effect of molecular dynamics simulation of $MgSiO_3$ perovskite, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).

3.7 High Pressure Synchrotron Science Workshop

The High Pressure Synchrotron Science workshop was held at the Advanced Photon Source on May 6-8, 2009. CDAC provided support for graduate students from Academic Partner groups and other high-pressure research groups throughout the country to attend the workshop. The emphasis of the workshop was on forefront science using synchrotron radiation and the technological advances that are needed to meet scientific grand challenges in the field. A list of presentations made at the workshop is provided below.

Lectures – Talks were given by scientists from institutions around the world. Lecturers suppored by CDAC funds (staff, partners, postdoctoral fellows, or students) are designated by an asterisk (*).

Wednesday, May 6th:

Scientific Session I: *Fundamental matter under extreme conditions*
(Chair: **Ho-kwang Mao**,* Carnegie)

Eugene Gregoryanz (University of Edinburgh), *"Simple" systems at high pressure*
Chris Benmore (Argonne), *Polyamorphism: Implications for glass science*
Alexander Goncharov* (Carnegie), *Melting of simple molecular solids at high pressures*

Scientific Session II: *Extreme biology: X-ray techniques and the study of proteins under pressure*
(Chair: **Keith Brister**, Northwestern University)

Roland Winter (Technical University Dortmond), *Exploring the configurational and free energy landscape of biomolecules under extreme conditions: From model biomembranes to proteins*
Chae-Un Kim (Cornell University), *Pressure study on water inside protein crystals*

Roger Fortune (Synchrotron Soleil), *Recent developments in high pressure macromolecular crystallography*

Scientific Session III: Physics *and chemistry of earth and planetary interiors*
(Chair: **Vitali Prakapenka**, University of Chicago)

Leonid Dubrovinsky (Geoinstitut Bayreuth), *Iron partitioning between ferropericlase and silicate perovskite: is Earth lower mantle spin transition zone chemically distinct?*
Reinhard Boehler (Max Planck Institute for Chemistry), *Melting by x-ray diffraction and x-ray absorption with a portable laser heating system*
Thomas Duffy* (Princeton University), *Chemical complexity in Earth's deep mantle*

Technical Session I: *Future high-pressure science using nano-beams*
(Chair: **Zonghou Cai**, Argonne National Laboratory)

Lin Wang* (HPSynC), *Application of nano/submicron-focused x-ray probes for ultrahigh-pressure studies*
Wenge Yang* (HPCAT), *Nanoscale diffraction and imaging techniques for high pressure science*
Wenjun Liu (Argonne), *Polychromatic and monochromatic x-ray scanning micro/nano-diffraction probe for high-pressure research*

Thursday, May 7th:

Scientific Session IV: *Dynamic compression: Frontiers in real time*
(Chair: **Guoyin Shen***, HPCAT)

William Evans (LLNL), *The dynamic diamond anvil cell (dDAC): A novel device for studying the dynamic properties of materials at high pressure*
Gilbert Collins (LLNL), *Exotic behavior of materials at ultra-high densities*

Scientific Session V: *Magnetism in dense matter*
(Chair: **Daniel Haskel**, Argonne National Laboratory)

Viktor Struzhkin* (Carnegie), *Spin crossover effects and Mott transitions in 3d metal oxides*
Narcizo Souza-Neto (Argonne), *Spin-dependent electronic structure under high pressure: The case of EuX (X=O, S, Se, Te) magnetic semiconductors*
Wolfgang Sturhahn (Argonne), *High pressure magnetism studied with nuclear resonant spectroscopy*

Scientific Session VI: *High pressure phenomena in liquids and glasses*
(Chair: **Chris Benmore**, Argonne)

Robert Mayanovic (Missouri State University), *High P-T x-ray spectroscopic studies of oxides, glasses, and inorganic metal complexes in aqueous fluids*
Qiang Mei* (HPSynC), *Structural investigation of vitreous GeO_2 under high pressure*
Aleksandr Chumakov (European Synchrotron Radiation Facility), *Putting pressure on glass to understand its anomalies*

Technical Session II: *Transformative instrumentation for the next decade of high pressure research*
(Chair: **George Strajer**, Argonne)

Jianwei Miao (University of California – Los Angeles), *X-ray diffraction microscopy and its applications in materials science and nanoscience*
Yogesh Vohra* (University of Alabama – Birmingham), *Designer diamond anvils for high pressure research at synchrotron x-ray sources – Recent developments and applications in iron based superconducting materials)*

Sakura Pascarelli (European Synchrotron Radiation Facility), *Energy dispersive x-ray absorption spectroscopy applied to studies at extreme conditions*

Friday, May 8th:

Scientific Session VII: *3D imaging at high pressure*
(Chair: **Francesco de Carlo**, Argonne)

Mark Rivers (University of Chicago), *X-ray microtomography at high pressure*
Ian McNulty (Argonne), *Opportunities for nanoscale imaging at high pressure by coherent x-ray diffraction*
X. Xiao (Argonne), *Measuring mass density with tomography*

Scientific Session VIII: *Novel materials and properties at high pressure*
(Chair: **Innokenty Kantor**, University of Chicago)

Tetsuo Irifune (Ehime University), *Synthesis of nano-polycrystalline diamond at high pressure and some physical properties*
Natalia Dubrovinskaia (University of Heidelberg), *Structure-property relationship in superhard materials of the B-C-N system*
Michael Lerche* (HPSynC)*, Magnetism of amorphous iron up to 35 GPa*

Scientific Session XI: *Frontiers in inelastic spectroscopy*
(Chair: **Ercan Alp**, Argonne)

Ingo Loa (University of Edinburgh), *Dynamics in elemental metals with incommensurate crystal structures*
Wendy Mao* (Stanford Universtiy), *X-ray induced dissociation of H_2O and formation of an O_2-H_2 compound at high pressure*
Krzysztof Parlinski (Nuclear Physics Institute, Poland), *Ab initio phonon calculations*

Technical Session III: *Online optical spectroscopy*
(Chair: **Mark Rivers**, University of Chicago)

Alexander Goncharov* (Carnegie), *Online optical spectroscopy and laser heating in the DAC: recent developments and future prospective*
Stanislav Sinogeikin (HPCAT), *Online optical systems (Brillouin, Raman, Ruby) at HPCAT and GSECARS: Current status and new developments*
Vitali Prakapenka (University of Chicago), *Various aspects of on-line laser heating and optical spectroscopy at extreme conditions*

3.8 Carnegie CDAC Group Meetings

The members of CDAC located at **Carnegie** meet several times a month to discuss their research and a brief talk is given by one of the members or by a guest speaker. In addition, members of the group will share recently published papers with their colleagues.

Speaker	Affiliation	Topic	Date
L.Shulenberger	Carnegie	A theoretical exploration of the structure of iron bearing post-perovskite	February 6, 2009
X. J. Chen	Carnegie	Methane at megabar pressures	February 6, 2009
X. J Chen	Carnegie	Pressure-induced metallization in germane: Band closure or molecular dissociation	February 13, 2009
R. Chellappa	Carnegie	Pressure-induced interactions in NH_3BH_3-H_2 system	February 13, 2009

H. Yang	Carnegie	Barite-bearing UHP eclogite from the main borehole core of the Chinese continental scientific drilling	February 20, 2009
C. C. Kao	NSLS	New developments at the National Synchrotron Light Source	February 20, 2009
Anat Shahar	Carnegiev	Experimental high *P-T* isotope geochemistry - Sulfides on Mars	February 26, 2009
V. Struzhkin	Carnegie	Spins in the lower mantle	March 6, 2009
P. Ganesh	Carnegie	First-principles study of diffuse scattering in $Pb(Sc_{1/2}Nb_{1/2})O_3$	March 11, 2009
L. Shulenberger	Carnegie	High pressure phase transitions in FeO from density functional theory, quantum Monte Carlo and dynamical mean field theory	March 11, 2009
Rose Xuan Luo	Carnegie	First-principles calculation of iron and iron-nickel phase diagram	March 11, 2009
A. Sharma	Carnegie	Abiogenic hydrocarbon pathways at high pressure & temperature	March 13, 2009
Svetlana Kharlamova	Carnegie	Spin transition of Fe^{2+} in Fe_2TiO_4	March 20, 2009
S. Yamashita	Carnegie	*In-situ* spectroscopic observation of silicate melts and NOH fluids under reduced conditions	April 3, 2009
Q. Liang	Carnegie	Recent developments in CVD diamond	April 9, 2009
T. Strobel	Carnegie	Hybrid clathrate materials for hydrogen storage	April 17, 2009
F. El'kin	Carnegie	The strain gauge technique at high pressures and temperatures	April 30, 2009
J. Janik	Carnegie	Diamond electronics	May 15, 2009
S. Natarajan	Carnegie	Automation of laser heating experiments	May 22, 2009
H. Scott	Indiana University – South Bend	Simple hydrocarbon synthesis in planetary interiors	May 29, 2009
D. Foustoukos	Carnegie	Theoretical geochemistry at the extremes: Fe speciation at supercritical water conditions	June 5, 2009
F. McCubbin	Carnegie	Detection of structurally bound water in lunar apatite	June 12, 2009
M. Guthrie	HPSynC	Multiple lengthscale structural studies of disordered H-bonded matter: Applications for energy research	June 19, 2009
T. Yamanaka	Carnegie	Crystallography Short Course: Part I	July 3, 2009
P. Griffin	Carnegie	Developments in high pressure microbiology	July 10, 2009

T. Yamanaka	Carnegie	Crystallography Short Course: Part II	July 16, 2009
T. Yamanaka	Carnegie	Crystallography Short Course: Part III	July 17, 2009
Emily Sandford	Gleneleg Country School	Determining the EOS of polymer 5cs using Brillouin scattering	August 28, 2009

4. TECHNOLOGY DEVELOPMENT

4.1 Technical Improvements at HPCAT

The HPCAT sector at the APS remains the centerpiece of the CDAC program. Not only does CDAC directly support the facility at the level of 30% of the operating costs on a yearly basis, the majority of fundamental scientific advances made within CDAC are a direct result of the cutting-edge capabilities available on the sector's four beamlines. In this section, we outline some of the improvements made at HPCAT during Year 6.

Figure 73. *Dual undulators installed in tandem mode on beamline 16 ID at HPCAT.*

A Second Undulator on the Insertion Device Beamline – Clearly the most significant advancement in experimental capabilities within CDAC took place on the insertion device beamline during 2009, as with APS support, a second U33 undulator was installed at 16-ID. In the first phase of operations, this second undulator is installed in tandem mode (Fig. 73). The clear benefits of dual undulator operation include (1) eliminating the energy dependence between 16-ID-B and 16-ID-D, thus increasing user beam time by 50%, (2) energy scanning capability will be allowed for the spectroscopy station 16-ID-D, and (3) increasing the brightness of each branch by a factor of two. In order to limit the heat load before the upgrade of high heat load optics, however, the minimum gap of each undulator is currently set at 13.5 mm.

In the second phase of the installation, APS will, with recent ARRA funding, reconfigure the 16-ID undulator from the tandem mode to two canted undulators and will rebuild the front end (with the consideration of an extended straight section) by May 2011. The two branches, 16-ID-B and 16-ID-C-D-E, will then be completely independent and can be optimized to the full extent. The canted-undulator system will allow independent control of undulator parameters for concurrent operation of the two 16-ID branches, thus providing optimal operation in both branches as two independent beamlines and increasing the usable ID beam time. This will bring an additional factor of two to three gain in brightness on each beamline.

Beamline ID-D: X-Ray Spectroscopy – HPCAT beamline scientists **Paul Chow** and **Yuming Xiao** have commissioned a 17-element analyzer array for the study of electronic excitations and x-ray Raman spectroscopy. It was economically designed and fabricated by HPCAT staff and

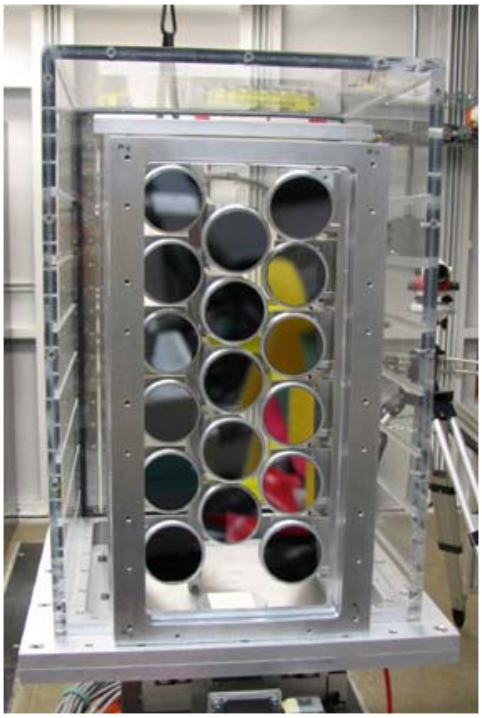

Figure 74. *17-element analyzer array commissioned in June 2009 on the 16-ID-D beamline at HPCAT.*

has been in use since June 2009. The compact analyzer array consists of 17 bent Silicon [111] wafers, individually aligned on a 1-meter Rowland circle. (Fig. 74) The overall energy resolution of this backscattering spectrometer when used with the diamond [111] monochromator is 1 eV. The array is housed in a helium-filled chamber which is coupled to the flight path to decrease absorption.

A short working distance (SWD) spectrometer for Fe K_β XES has been designed, built, installed and tested. The spectrometer has seven Ge [620] crystals which are 25 mm long, ~15 mm wide and 2 mm thick. For the desired energy resolution (~1eV) and the available detector area, the effective collection angle of the optic will be roughly equivalent to 4.5 'usual' spherical bent analyzers of 10 cm diameter at 1m working distance, representing a much improved performance. During commissioning in run 2009-2, this new spectrometer was used to measure x-ray emission spectra of Fe_2O_3 under ambient, 53 and 60GPa, and a clear high- to low-spin transition is observed. The collection time for ambient and 53GPa spectra is 10 minutes, and for the 60 GPa spectrum, the collecting time is 20 minutes.

Beamline ID-B: Microfocused X-Ray Diffraction – The ID-B beamline at HPCAT must accommodate a wide variety of DAC experiments, and therefore must remain extremely versatile even as it is upgraded continuously. One of the key improvements to the ID-B station made by beamline scientist **Stas Sinogeikin** in Year 6 has been the implementation of two romote pressure control devices, a gearbox and a gas-driven membrane apparatus.

The gearbox is designed for fast data collection and will provide a dramatic increase in productivity with standard symmetric and other compatible DACs (Fig. 75). The gear mechanism provides high (20-400 times) force amplification, and when driven by a stepper motor it offers a mechanical pressure adjustment with an "infinitely" small screw rotation / pressure increment. The new gearbox offers ompletely remote operation from outside the experimental station with the possibility of automatic sequencing and data collection. Finally, different models of the gearbox can be used at room and elevated temperatures, as well as with a cryostat. In a recent test run, the B1-B2 transition in a single crystal of NaCl was resolved to about 0.25 GPa.

The new universal remote control membrane system (Fig. 76) can be used with any variety of DAC in experiments with a cryostat or with resistive heating. A controller has been designed to accommodate any commercial or custom membrane system and can in prinicple be used at any APS experimental station. Standard DAC membrane containers for forward or side diffraction, as well as inelastic scattering are currently

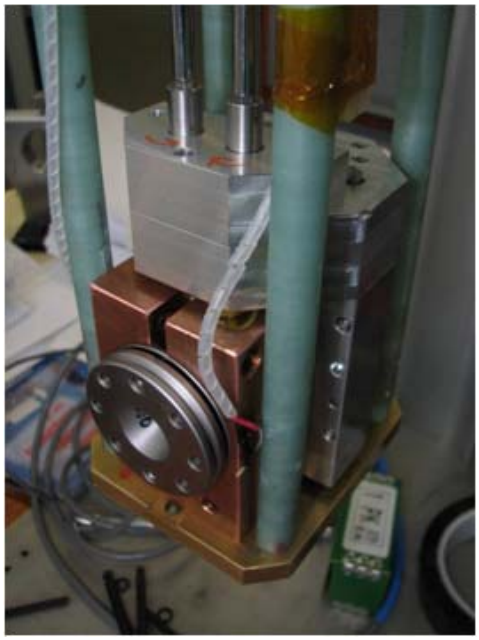

Figure 75. *Symmetric DAC in gearbox assembly.*

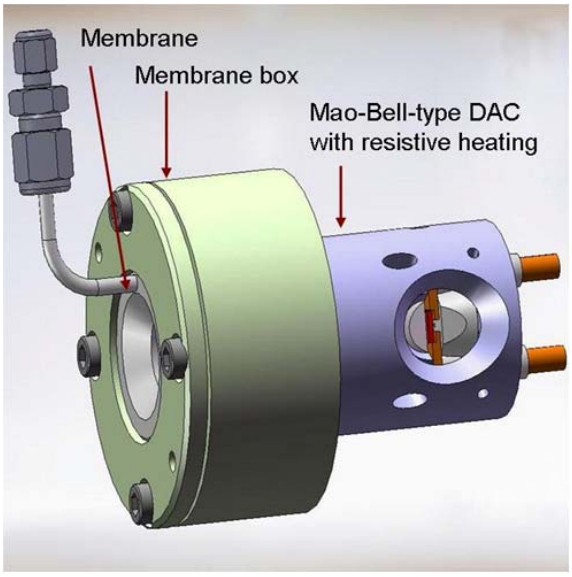

Figure 76. *Threaded membrane container for the standard symmetric DAC.*

available at HPCAT, and customized adapter boxes can be easily made on-site to accommodate specialized DACs.

To improve efficiency during simultaneous laser heating/x-ray diffraction experiments, beamline scientists **Yue Meng** and **Arun Bommanavar** have developed a data logging procedure to automatically record temperature measurement (both sides of the cell for double-sided heating) and x-ray diffraction data files names. The new procedure correlates the temperature measurements with the respective diffraction patterns automatically.

A neutral density filter system to allow temperature measurement at much higher temperatures has also been installed. Improvements for the near future include a new IR fiber laser to replace the currently used photonics YLF laser and a new CCD detector and spectrograph with improved capability for temperature measurement at lower temperatures than provided by the current apparatus.

Beamline 16-BM-D: High-Resolution Powder Diffraction – During Year 5, the HPCAT staff demonstrated the capability of scanning angle powder diffraction with a monochromatic beam on bending magnet beamline 16-BM-D. Preliminary results in Year 6 indicate that a factor of 5~8 better angular resolution is now achievable. This can provide a great advantage to check small peak splitting or distortions on the powder pattern. The routine powder diffraction apparatus can be set up (2D area detector) at one side (say 2theta from 0-30 degrees), and the point detector set up at the other side (2theta from -2->-30 degrees). When several angular regions need the high resolution scans determined by regular powder diffraction, one can use the scanning point detector technique to probe only small regions with much higher angular resolution.

Beamline 16-BM-B: PE-Cell Development – **This** new project started in early 2009 through a collaboration with GSECARS and Ehime University. The Paris-Edinburgh pressure cell can hold a large sample volume (~1-3 mm^3) while it can compress up to 15 GPa and heat up to 2000 K (depending on heater dimensions). The suitability of the setup at the 16-BM-B experimental hutch (Fig. 77) was tested through 2009-1 and 2009-2 run periods. The test was successful and the preliminary results showed that S(Q) with the maximum Q up to ~20 $(angstrom)^{-1}$ could be obtained. Safe operational procedures for pressure and temperature controls, and the related control

Figure 77. *In-situ heating experimental setup. A custom-made precision collimator is applied to obtain a high signal to background ratio, which is one of the key challenges, especially for low-Z and non-crystalline materials. We expect this PEC setup at 16-BM-B will bring more opportunities to study materials properties and phase transitions in amorphous and liquid materials and oxide/silicate minerals under high pressure and temperature, which will be complementary to DAC measurements.*

software are currently under development. In the 2009-3 cycle, the first tests for for ultrasonic and radiography measurements will take place, which provide additional capabilities to study material properties combined with the diffraction probe.

4.2 Technical Improvements at NSLS-U2A

High and Low Temperature Capabilities – Progress continues on making the planed CO_2 laser heating system operational. Following interlock tests and comissioning, the U2A beamline will be able to provide laser heating for DAC experiments to 1000 K. In addition, a new cryostat with a compact design for a standard symmetric DACs has been purchased and will be delivered in December 2009.

Expanded Facilities – There is increasing interest from the high-pressure community in conducting experiments that require very high spatial resolution, such as IR mapping below the diffraction limit of 5 μm. An exciting opportunity has arisen to create a side station on the beamline as a result of new space that has been created next to the U2 port, where a vacuum pipe for beam delivery was installed in 2006 for the gas-gun shock wave experiments. The distance from the synchrotron source to the IR system would then be only about 3 meters, which will remove the problem of beam divergence and image distortion. Funding from COMPRES, UNLV and CDAC has allowed the purchase of the necessary instrumentation, which will be installed and operational in the January-April 2010 run period.

4.3 Infrastructure Development at Carnegie and Academic Nodes

Development of a Hybrid Optical-Mechanical Interferometer – Research in the group of CDAC Academic Partner **Steven Jacobsen** at **Northwestern** focuses on elastic properties of materials using a unique high-frequency (GHz) ultrasonic method. GHz-ultrasonic interferometry is being used to carry out CDAC-supported work on the nature of superhard materials. Single-crystal elastic properties measurements of natural and synthetic forms of diamond and other superhard materials probe physical properties at the atomic scale related to interatomic bonding. Using ultrasound with near-optical wavelengths at 1-2 GHz, the technique makes possible sound velocity measurements of materials that are not easily studied with other techniques such as Brillouin scattering or resonance ultrasound, either because samples are opaque, or not available in sub-millimeter sizes.

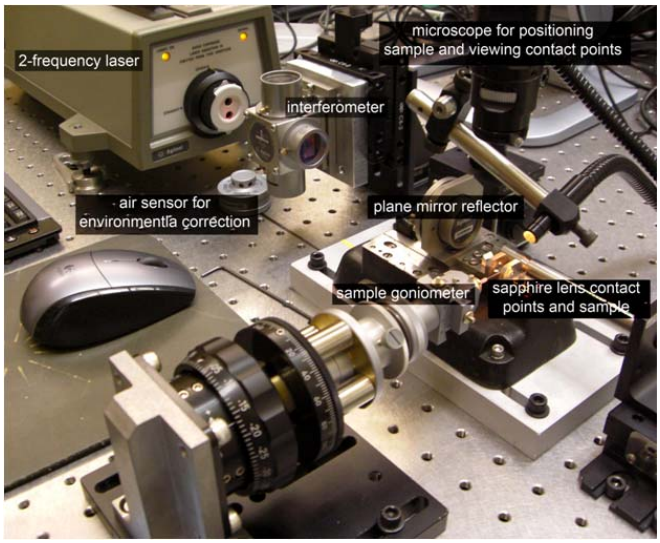

Figure 78. *Newly developed sample-length measuring interferometer to support GHz-ultrasonic measurements of material elasticity. The instrument has reduced experimental uncertainty of elastic constants from GHz-ultrasonics by about one order of magnitude.*

Although relative changes in travel time on compression or heating are measured with a standard deviation of about 0.02 nanoseconds out of 20-200 ns (depending on sample thickness), the absolute accuracy of ultrasonic measurements of elastic properties at standard conditions, required to anchor high *P-T* measurements, has been limited by our ability to measure sample thickness mechanically at STP, usually carried out with a simple micrometer and ±1 μm precision, at best. **Jacobsen's** group has developed a new sample length measuring device, which improves the ability to measure zero-pressure lengths with high accuracy and a precision of about ±0.01 μm. The resulting uncertainty in elastic constants measurements has been improved by one order of magnitude. For example, the group has determined the C_{11} and C_{44} elastic

constants of natural type-IA diamond to be 1076.2(6) GPa and 575.8(4) GPa, respectively. These values are in excellent agreement with classic, low-frequency ultrasonic measurements, but have better than one order of magnitude improvement in uncertainty. These new tools will allow evaluation of the elastic properties of challenging materials with unprecedented accuracy and precision. The group plans to explore, for example, variations in elastic properties of superhard materials with varying defect concentrations and structures.

The length-measuring instrument, pictured in Fig. 78, includes a commercial, double-pass optical heterodyne interferometer coupled with a high-precision linear stage. The stage holds a contact micrometer, which consists of a pair of sapphire lenses (Fig. 8). Because the contact points are also lenses, we can view through the sapphire and record exactly the point of contact, allowing accurate maps of thickness variations across samples, and pinpoint the location of ultrasonic measurements to be combined with the length measurements. It is possible to achieve $\lambda/4$ fundamental optical resolution with $\lambda/128$ (about 5 nm) system resolution through software-based interpolation. By adding real-time corrections for air temperature, humidity, and pressure applied to the laser wavelength, one can achieve high accuracy with standard deviations of about 0.01 micrometers in the thickness measurements.

Laser-Launched Flyer Plates – **Kathryn Brown** is working with postdoctoral fellow **Hiroki Fujiwara** on laser-launched flyers to study the spectroscopy of reactive materials such as nano-Al + Teflon initiated by high-speed impact. The concept of these measurements is shown in Fig. 79. A laser produces a uniform top-hat beam profile with fluence (8 ns) up to 20 J/cm^2. Flyer plate substrates have been fabricated, and a high speed 8 GHz displacement interferometer has been constructed to monitor the velocity history of the flyers. An 8 GHz interferometer can accurately track velocities up to 6 km/s. Prior to the implementation of the interferometer, the velocity of a 2 μm thick Al flyer at 4 km/s was measured using a fast photomultiplier to observe the flash of light generated when the flyer hits a window. The Al Hugoniot gives the shock pressure as 118 GPa for a 4 km/s impact.

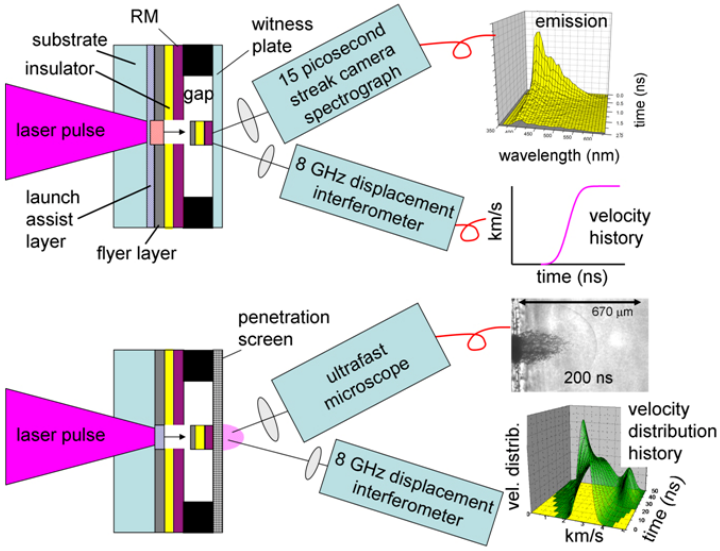

Figure 79. *Concept for laser-driven miniflyer studies of reactive material (RM) dynamics. Top) A miniflyer impacts the RM against a transparent witness plate at velocities of 0.1 - 5 km/s. A 25 ps streak camera spectrograph detects the emission burst. A displacement interferometer (DISAR) monitors the flyer velocity history. Bottom) The RM impacts a screen causing it to fragment. The fragments are monitored using ultrafast microscopy. The DISAR measures the time dependent velocity distribution.*

Development of Laser Heating Techniques – The laser heated diamond anvil cell (LHDAC) techniques represent a fast developing tool for the study of materials under extreme conditions of high pressures and temperatures. With these methods, investigations are now possible at pressures and temperatures approaching the center of the Earth. These experimental studies have a profound impact on fields that include Earth science, planetary science, and new materials chemistry. However, further developments are needed to increase the pressure range available, temperature measurements range and accuracy, ability to overcome chemical reactivity, and provide more uniform temperature conditions. At **Carnegie**, **Alexander Goncharov** and his group have made significant advances in the development of continuous and pulsed laser heating techniques and finite element calculations for DAC experiments.[122] The methods involve the use of time-resolved (5

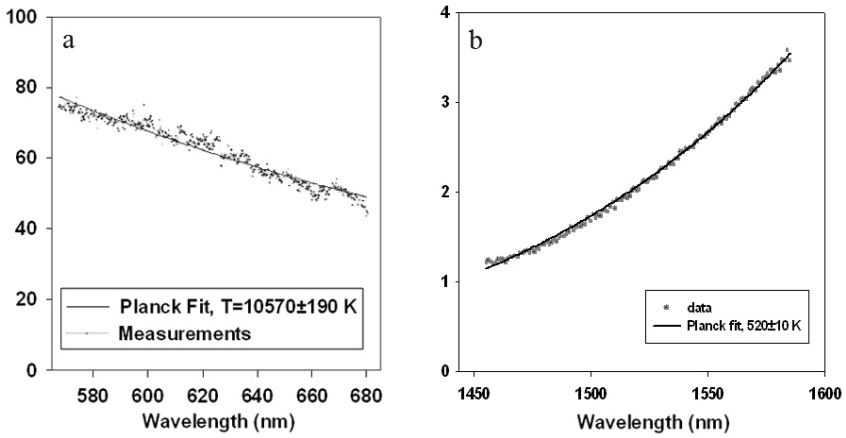

Figure 80. *a) Example of the incandescent spectrum measured in the DAC at 124 GPa with 10 ns temporal resolution. The uncertainty in temperature determination is given at one sigma level. b) Example of the incandescent spectrum measured in a laser heated DAC using a InGaAs nitrogen cooled array detector. The uncertainty in temperature determination is given at one sigma level.*

ns gated), incandescent light temperature measurements to determine the time dependence of heat fluxes, while near IR incandescent light temperature measurements (Fig. 80) allow temperature measurements to as low as 500 K. Further optimization of timing in pulsed laser heating together with sample engineering will provide additional improvements in data collection in very high *P-T* experiments.

The laser heating techniques described above have been applied to a variety of molecular solids at high pressure. Sample preparation procedures for these simple molecular materials (diatomic molecules and water) under high pressure in the DAC have now been optimized, and experiments are now carried out using both continuous and pulsed laser heating methods. Experiments were carried out using Raman spectroscopy, and the time evolution of the temperature of the metallic coupler that is used to absorb laser radiation and heat the sample was analyzed as well. Raman measurements of H_2, D_2, N_2, H_2O and O_2 show a broadening of intramolecular vibrations at high *P-T* conditions, indicating a decreasing molecular lifetime, and hence an increasing molecular dissociation.[123] In diatomic molecules the intramolecular bonding can be further probed by observations of sidebands corresponding to vibrational transitions from excited states; the energies of these sidebands imply intramolecular potentials that become increasingly less anharmonic as pressure is increased. It has also been shown that the pulsed heating technique combined with instantaneous radiative temperature measurement provides a useful tool for studies of thermochemical properties and phase transformation boundaries.

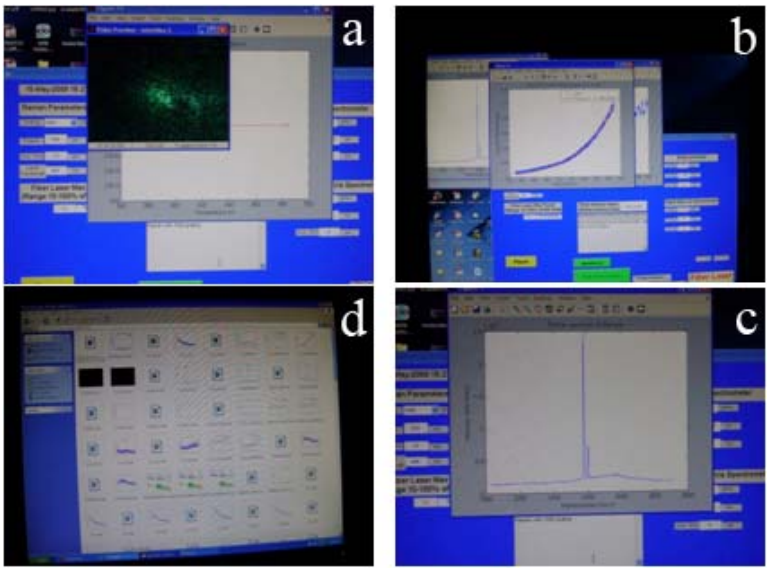

Figure 81. *Screen shots from a typical automated LHDAC-Raman experiment. a) Recording of speckle movie while fiber laser power is being raised to detect changes associated with melting or reactions. b) On-the-fly Planck function fit to estimate sample temperature from thermal radiation spectrum. c) High P/T Raman spectrum of the sample (N_2). d) A thumbnail view of the large number of data files in different formats that must be automatically archived during the experiment automatically.*

Automation of Laser Heating-Raman Spectroscopy Experiments – A typical simultaneous double sided laser heating and Raman spectroscopy

experiment at GL's LHDAC-Raman facility involves electromechanical operation of several flipping devices, shutters, polarizers, control and data acquisition from multiple spectrometers for temperature and Raman spectra measurements, control of a heating IR fiber laser and recording of speckle movies and other images. Further, data files have to be stored in the individual controlling computers. These operations have to be done at each step when laser power is raised to heat up the sample. Attempts to do this manually at each experimental step lead to more than 80-85% of precious experiment time spent on the data handling. With reactive and diffusive samples (*e.g.* hydrogen at extreme conditions), it was realized that attempts to minimize this excess time using an automation program can be beneficial.

At **Carnegie**, **Natarajan Subramanian** performed a thorough analysis of the various components and their functions, and created an algorithm to achieve complete automation of the LHDAC-Raman experiments, which constist of 11 distinct steps. Implementation of the algorithm has been done at two levels. At the backend level, several scripts written on three individual "slave" computers establish interfacing with the set of devices to which they are connected. Both serial and parallel interface protocols are used to communicate with the devices. At the next level, a Graphics Users Interface (GUI, see Fig. 81) program running on a "master" computer is employed to control and communicate with the slave computers using the TCP/IP protocol on a LAN. This GUI program is the frontend level, where the user can decide the experimental parameters (choice of spectrometers; gratings, grating positions, spectra acquisition times, fiber laser power and a master directory name for archiving all data). The master computer program is also used to enable remote ON/OFF of viewing lamps, acquire video and snap shots, perform on-the-fly spectrum analysis (optimizing Raman signals; Planck fit to estimate sample temperature). Options for emergency laser-off, user variable laser power step size, choice of heating or cooling cycle and semi-automatic operation have been implemented.

The modular nature of the object oriented program offers easy implementation of other physical property measurements that may be thought of in the future. The successful automation of the LHDAC-Raman system has turned out to be one of the key factors that have allowed several key high P/T experiments on hydrogen in the recent months.

5. INTERACTIONS WITH NNSA/DP LABORATORIES

5.1 Overview

One of the primary goals of CDAC from the start of the program in 2003 has been to facilitate interactions between NNSA Laboratory Scientists and the CDAC Academic Partners. To that end we have provided beam time at the synchrotron beamlines that we manage, and to the CDAC-supported laboratory facilities at Carnegie. In addition, our Academic Partners have made their specialized laboratory facilities available to NNSA Laboratory Partners. By virtue of their participation in CDAC as Laboratory Partners, NNSA Lab scientists may also attend the regularly scheduled HPCAT meetings at the APS. The NNSA plays a significant role in HPCAT operations and attendance at HPCAT meetings gives our Laboratory Partners the opportunity to provide input to the HPCAT operational plan. CDAC continues to organize, provide support to and participate in other venues that afford Laboratory Partners an opportunity for interaction with Academic Partner groups. These have included:

- *CDAC Summer School* (2005)
- *SSAAP Symposia* in Albuquerque (2004) and Las Vegas (2005) and Washington, DC (2007 and 2008)
- *Synergy of 21st Century High-Pressure Science and Technology Workshop* (2006)
- *Study of Matter in Extreme Conditions Workshop* (2007)

- *High Pressure Synchrotron Science Workshop* (2009)
- *CDAC Winter Workshop* (2009)

These events have all been highly successful vehicles for introducing Laboratory Partners to the work taking place in Academic Partner groups, and also for introducing CDAC graduate students to the opportunites available in the NNSA Labs. During the 2005 CDAC Summer School and in the 2009 Winter Workshop, described more fully in Section 3.3, Laboratory Partners from each of the NNSA Labs provided lectures in which they introduced CDAC graduate students to their research programs. The opening reception, poster session and banquet all provided opportunities for one-on-one interaction between Laboratory Partners and the CDAC academic community. The following aspects of the CDAC program also provide opportunities for interaction and collaboration.

5.2 Beam time for Experiments at HPCAT

Each year, groups from **LLNL** and **LANL** may obtain beam time provided by CDAC to carry out experimental work at one of the sectors at HPCAT. To date, each of the four sectors has been utilized by Laboratory Partners for their research, and over the past several years, approximately 25% of the available time on the diffraction beam lines ID-B and BM-D at HPCAT has been used by National Lab scientists for NNSA program-related work. Although the H-Division of LLNL retains a share of beam time by virtue of membership, CDAC has made available beam time to H-Division and to other research groups at LLNL. CDAC plans to continue our commitment to Laboratory Partner groups in the pursuit of program goals.

CDAC beam time at HPCAT is allocated based on the membership shares of each of the contributing members. Currently, CDAC contributes 30% of the annual operating expenses of HPCAT and is therefore entitled to 30% of the beam time available on each of the four beamlines.

Figure 82. *Screen shot of the CDAC website, http://cdac.gl.ciw.edu*

The present membership of HPCAT is as follows. **Carnegie** (25%), CDAC (30%), **LLNL** H-Division (20%), and **University of Nevada-Las Vegas** (25%). For CDAC, this amounts to approximately 40 eight-hour shifts on each of the four beamlines duringa run period, with three run periods supported during a calendar year. On a consistent basis, about 20% of available CDAC time on station ID-B (microdiffraction with laser heating capabilities) and 30% of time on station BM-D (microdiffraction with cryostat capabilities) has been made available to NNSA Laboratory Partners. During Year 6, all CDAC users who requested beam time were able to receive it, whether through the General User Proposal system, or through the

CDAC discretionary share. A detail of those who obtained beam time at HPCAT and the experiments they performed is given in Appendix II.

5.3 Other Interactions

- ***Carnegie High-Pressure facilities.*** Throughout the first six years of our program we have interacted and collaborated on a continuing basis with the high-pressure groups from **LLNL** and **LANL**, from hosting individuals and groups for specialized experimental procedures and sample preparation to arranging loans of specialized high-pressure cells for experiments at **HPCAT** and **NSLS**. In Year 6, 31 different people visited **Carnegie** for work at CDAC facilities. In addition, the CVD diamond group at Carnegie continues to collaborate actively with the **SNL** group to support dynamic compression experiments through the synthisis of diamond plates used for impedance matching.

- ***Academic Partner Participation at NIF.*** Through the work of Steering Committee member Rip Collins, Academic Partner Raymond Jeanloz and CDAC Director Russell Hemley, CDAC has been active in the potential use of NIF for Academic Partner Research. In anticipation of academic use of NIF, several CDAC academic groups are developing shock compression programs that will compliment ongoing static compression activities. We expect that five to seven CDAC groups will be interested in applying for time at NIF as their programs reach the appropriate stage.

- ***CDAC Website.*** The CDAC website, located at *http://cdac.gl.ciw.edu*, serves as a primary source of information to the CDAC community and the public (Fig. 82). The site, which is updated weekly, provides news and information from CDAC groups, announcmeents of meetings of interest to the CDAC community, and serves as a general portal to high pressure research activities, not only within CDAC, but in the US and worldwide. The site also provides publication records and abstracts for the CDAC community, which are updated continuously. Research highlights detailing information on new papers or research breakthroughs that have been supported by CDAC are also featured.

6. MANAGEMENT AND OVERSIGHT

No fundamental changes have taken place in CDAC management and oversight from Year 4 through Year 6, with essentially all committees and personnel remaining in place. A brief review of the organizational structure of the Center is provided below (Fig. 83), along with listings of key personnel, including postdoctoral fellows. Our Steering and Advisory committees are composed of leading scientists in academia and the National Labs familiar with the high pressure research community.

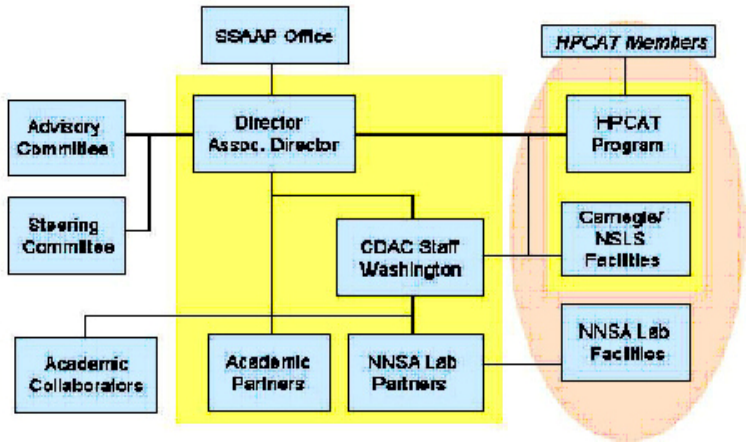

Figure 83. *CDAC organizational chart. The yellow area designates the principal components of CDAC. The oval area encompasses the three different groups of experimental facilities associated with CDAC.*

6.1 CDAC Organization and Staff

CDAC is managed at Carnegie by a core staff comprised of the Director, Associate Director, Coordinator, Administrative Assistant and two Laboratory Managers. Day-to-day operations of the Center are handled by the Director, Coordinator and Assistant, while CDAC laboratory facilities at Carnegie are supervised by the Laboratory Managers. The Associate Director serves as a liason to the HPCAT/HPSynC groups at the APS.

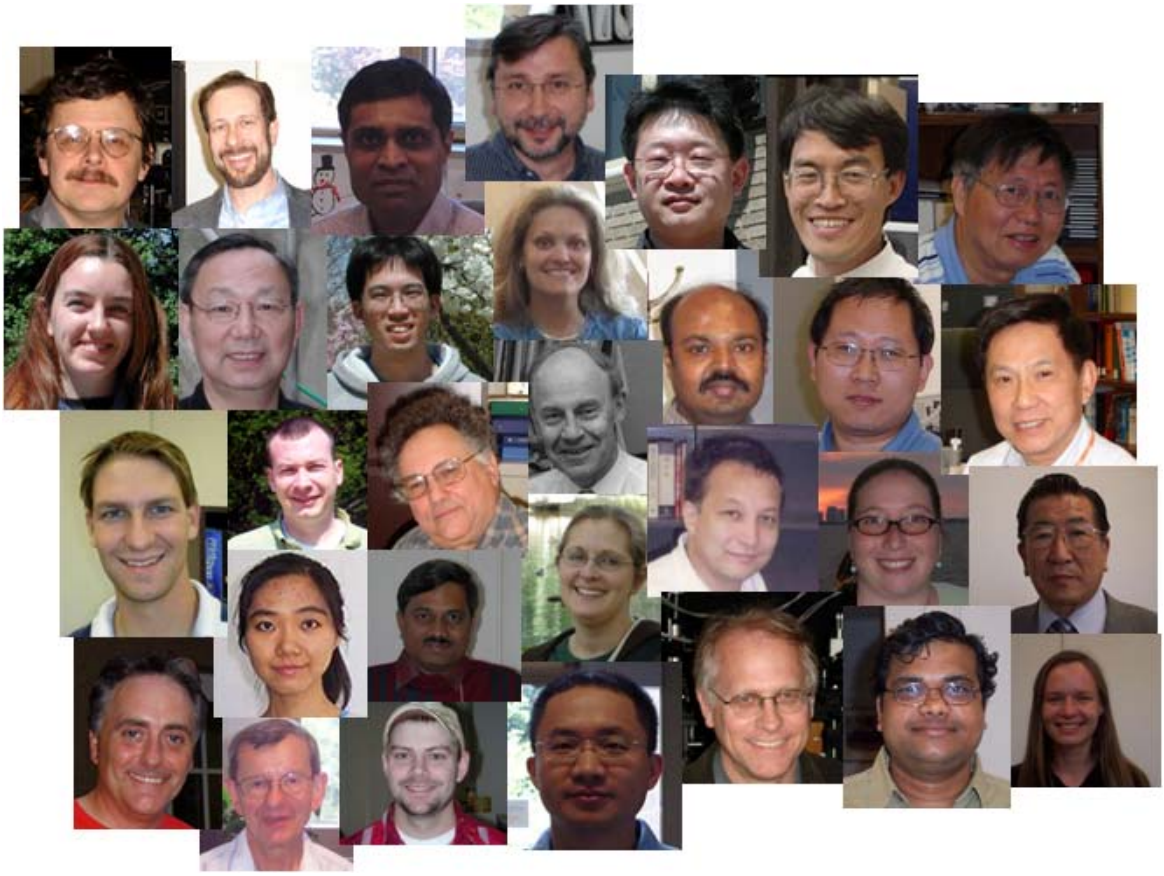

Figure 84. *CDAC affiliated personnel at* ***Carnegie***

Russell Hemley, Director, and **Ho-kwang Mao**, Associate Director are Staff Scientists at **Carnegie.** Other members of the Scientific Staff at **Carnegie** that are involved directly with CDAC are:

- **Ronald Cohen** Computational Theory
- **Yingwei Fei** Geochemistry, Petrology and Materials Science
- **Joe Feldman** Senior Visiting Fellow
- **Alexander Goncharov** Optical Spectroscopy
- **Dudley Herschbach** Senior Visiting Fellow
- **Viktor Struzhkin** Electronic, Magnetic, and Structural Properties
- **Takamitsu Yamanaka** Senior Visiting Fellow

CDAC staff at **Carnegie** directly supported by the CDAC grant and **Carnegie** Institution matching funds (*i.e.*, indirect cost return) are:

- **Stephen Gramsch** CDAC Coordinator/Research Scientist
- **Morgan Phillips** Administrative Assistant
- **Maddury Somayazulu** Lab Manager/Research Scientist

- **Chang-sheng Zha** Lab Manager/Research Scientist

Research Scientists at **Carnegie** working on CDAC-related projects include:

- **Muhetaer Ahart** (Brillouin Spectroscopy)
- **Xiao-Jia Chen** (Low-Z materials, neutron diffraction)
- **Szczesny Krasnicki** (CVD diamond)
- **Qi Liang** (CVD diamond)
- **Jinfu Shu** (Sample preparation and powder diffraction)
- **Chih-shiue Yan** (CVD diamond)

A number of predoctoral and postdoctoral fellows at **Carnegie** supported by the Institution, other grants, or outside fellowships worked on CDAC tasks during Year 6. Their contributions also include training CDAC students, undergraduate summer scholars, and visitors in high-pressure experimental techniques:

- **Raja Chellappa** (former CDAC student from **University of Nevada – Reno**)
- **Jennifer Ciezak**
- **Douglas Allen Dalton**
- **Patrick Griffin** (now a graduate student at **Johns Hopkins University**)
- **Svetlana Kharlamova**
- **Joseph Lai**
- **Amy Lazicki** (now at **CEA**, France)
- **Yufei Meng**
- **Subramanian Natarajan**
- **Tim Srobel**
- **Ravindran Thoguluva** (now at **Indira Ghandi Center for Atomic Research**)
- **Michelle Weinberger**

6.2 CDAC Oversight

CDAC Steering and Advisory Committees have been organized to provide guidance to the CDAC research program. The Steering Committee members informally advise CDAC management on near-term operational issues and act as points of contact with their respective Directorates and Divisions. Steering Committee members also evaluate yearly proposals for graduate student support from the Academic Partners. The CDAC Steering Committee consists of

- **Neal Chesnut** (UWGa)
- **Gilbert W. (Rip) Collins** (LLNL)
- **Dana Dattelbaum** (LANL)
- **Daniel Dolan** (SNL)
- **Jon H. Eggert** (LLNL)
- **Daniel Farber** (LLNL)
- **David Funk** (LANL)
- **Marcus Knudson** (SNL)
- **Choong-shik Yoo** (WSU)
- **Yusheng Zhao** (LANL)

The Advisory Committee assists with long-term strategic planning, advises CDAC management on the scientific program, and provides points of contact between CDAC and the NNSA Labs, other SSAA Centers, and the broader academic community. Current members of the CDAC Advisory Committee are

- **Neil W. Ashcroft** (Cornell)
- **Robert Cauble** (LLNL)
- **Yogendra M. Gupta** (WSU)
- **Alan J. Hurd** (LANL)

- **Chi-chang Kao** (Brookhaven)
- **Christian Mailhiot** (LLNL)
- **Tom Melhorn** (SNL)

Members of both CDAC oversight committees are invited to attend regular HPCAT meetings and are invited to attend all CDAC functions. Committee members are updated regularly on progress in the scientific program, innovations in technique development, and plans for outreach. Each of the members of the two CDAC committees has renewed their commitment to serving into Year 7.

7. PLANS FOR YEAR 7 AND BEYOND

7.1 New Academic Partners

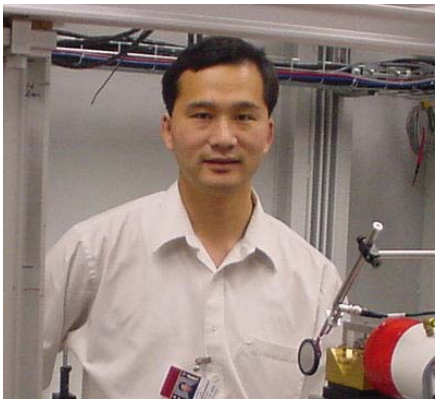

***Figure 85**. New CDAC partner **Jung-Fu Lin (University of Texas at Austin)**.*

In May 2007 the renewal proposal for CDAC was submitted, and the five-year renewal was granted in November 2007. This allowed Year 6 of the CDAC program to begin on March 1, 2008. Fully one-third of CDAC funding now goes directly to the support of graduate students in Academic Partner groups. In addition to the Academic Partners and their graduate students mentioned in Sections 2 and 3, **Jung-Fu Lin** (Fig. 85), from the **University of Texas at Austin** has joined CDAC as an Academic Partner. Professor Lin's work will focus on the electronic structures and associated changes in physical properties of the transition metal oxides under extreme pressure-temperature conditions using an array of recently developed synchrotron-based techniques. These include inelastic x-ray scattering spectroscopies (IXS), including resonant and non-resonant inelastic x-ray spectroscopy with energy resolution ranging from 1 meV (*i.e.*, high-resolution IXS) to 1 eV (*i.e.*, x-ray emission spectroscopy and x-ray Raman), x-ray absorption spectroscopy, synchrotron Mössbauer spectroscopy (SMS), and nuclear resonant inelastic x-ray scattering (NRIXS). Materials of interest will be compounds with the rocksalt-type and corundum-type structures, such as iron oxides (*i.e.*, FeO, Fe_2O_3), manganese oxides, nickel oxides, and cobalt oxides, and ultimately the *f*-band metals such as Gd, Dy, and Pr. A number of pressure-induced electronic phenomena occur in the transition metal oxides, including the Mott transition, high-spin to low-spin transitions, valence transformations, Verwey transition, and the quenching of the orbital term. These electronic phenomena may induce or be a consequence of structural transformations, a question that is extremely subtle but of central importance in high pressure research. The complexity of transition metal oxide systems occurs in cases in which several physical interactions—spin, charge, lattice, and/or orbital—are simultaneously active. With recent advances in the IXS instrumentation, it is now possible to study in detail the coupling between charge, lattice, orbital, and spin degrees of freedom of the 3*d* and 4*f*-band compounds. This work will therefore involve a signficant amount of synchrotron technique development.

7.2 HPCAT Upgrade

In October 2009, the HPCAT sector at the Advanced Photon Source reaches an important milestone--10 years of operation and innovation in service to the high pressure research community. The renewal proposal for HPCAT to partially fund operations for the next five years has been submitted and approved for 35% of the total operating budget.

The key component of the renewal proposal is the plans for the HPCAT upgrade, which anticipated a planned upgrade of the undulator by the APS. As discussed in Section 4.1, the second

undulator has been added on the insertion device beamline 16-ID in the summer of 2009. Additional plans are outlined below.

7.2.1 High Brilliance: Undulator Source Upgrade by APS

Considerations for advancing frontier capabilities start from the brightest possible x-ray source. The original insertion device at HPCAT was a standard APS type-A, which was designed conservatively in early 1990s and has a 2.5-m length, 33-mm magnet period (U33). New undulator technology advances, such as double or triple length, shorter period, higher magnetic field, etc. can each double or triple the source brightness at specific energies, resulting in 10- 30 times higher brightness when combined. Some of the newer design features have been installed and tested successfully in the newly constructed APS beamlines. APS is planning the overall upgrade of the entire ring. Due to the importance of HP science and the urgency of the upgrade, APS is giving HPCAT an early start; *i.e.*, we were the first "old beamline" to receive the second "Undulator A" in a three-phase undulator upgrade plan which will eventually increase the 16-ID brightness by 10-30 times. APS will take responsibility for the cost of upgrading the undulator source and front-end components on the storage ring side of the shield wall. In accordance with the APS renewal plan in the next decade, we have discussed this with the APS management and developed a three phase approach for the enhancement of 16-ID undulator operation, among which Phase 1 of the project has already started as of February 2009.

Phase 1 – Addition of a second undulator in May 2009. With APS support, a second U33 undulator was installed at 16-ID in tandem mode. The clear benefits of the Phase-1 dual undulator operation include (1) eliminating the energy dependence between 16-ID-B and 16-ID-D, thus increasing the user beam time by 50%, (2) energy scanning capability will be allowed for the spectroscopy station 16-ID-D, and (3) increasing the brightness of each branch by a factor of 2. In order to limit the heat load before the upgrade of high heat load optics, however, the minimum gap of each undulator is currently set at 13.5 mm.

Phase 2 – Installation of canted undulators (August 2009 – May 2011). With very recent ARRA funding, APS is committed to reconfigure the 16-ID undulator from the tandem mode to two canted undulators and rebuild the front end (with the consideration of an extended straight section) by May 2011. The two branches, 16-ID-B and 16-ID-C-D-E, will then be completely independent and can be optimized to the full extent. The canted-undulator system will allow independent control of undulator parameters for concurrent operation of the two 16-ID branches, thus providing optimal operation in both branches like two independent beamlines and increasing the usable ID beam time. This will bring an additional gain of a factor of 2-3 to each branch..

Phase 3 – Preparation and implementaion for an extended straight section with multiple undulators in canted mode (June 2011-May 2014). Extending the straight section is one of the important considerations in the APS renewal plan. A feasibility study shows that a straight section for insertion devices can be as long as 12.5 meters at APS. Compared to the current available space of 5 m, this length increase together with new undulator technology will increase the brilliance of the undulator source by more than an order of magnitude. APS will conduct research to clarify technical issues on (1) a 12.5 m straight section at 16-ID, (2) four (2+2) canted undulators, including operating interchangeablely all undulators in tandem, and (3) heat load optics for higher current (200 mA) operation proposed for the future upgrade. A higher operation current will proportionally increase the x-ray brilliance. The choice of undulator period length and power management issues have been discussed with the APS undulator group.

In the APS long-range renewal plan, 16-ID will be extended to a 12.5 m long straight section, potentially with four interchangeable canted undulators. The total improvement by a factor of 10-30 (comparing to the present status) will put HPCAT in a leading competitive position. The versatile undulator operation options will maximize the brilliance from the undulators for flux-demanding experiments such as IXS, time resolved experiments, and high resolution XRD coupled with sub-micron beams.

7.2.2 High Heat Load and High Efficiency Beamline Optics

High Heat Load Optics – The upgrade of the x-ray optics components that receive the brighter undulator source are HPCAT's responsibility. The upgrade optics will accommodate the maximum heat load for the fully upgraded APS source in 2014, and at the same time benefit the present operation immediately. All high heat load optics components are installed in 16-ID-A. Two canted beams from the undulators will first go through the primary slits, and then will encounter the double crystal monochromator (DCM), branching double crystal monochromator (BDCM), thermal apertures, and thermal beam stops as shown in Fig. 85. We propose to upgrade all these heat load components in order to meet the expected brighter undulator source.

HPCAT will design the optimized x-ray optics for canted undulators with sufficient allowance for the maximum power. All components will be able to withstand the heat load of enhanced undulator operation at 200 mA which doubles the present 100 mA. With the future APS upgrade project starting in 2014, HPCAT will be prepared for the further increase in brilliance. The first priority at HPCAT is to upgrade the high heat load x-ray optics in the FOE in order to accept the greatly increased power (and heat load) corresponding to the three phases of APS undulator upgrade.

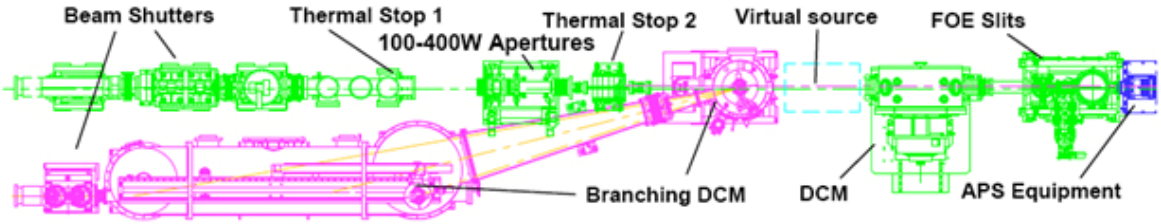

Figure 85. *Planned major beamline optics in the 16-ID-A hutch. The component in blue is the APS equipment. Components in green are for the outboard canted branch to 16-ID-C-D-E; while those in purple for the inboard branch delivered to 16-ID-B. Some components (e.g., FOE slits) are designed to operate for both branches.*

Canted Beamlines – The canted undulators will free the two 16-ID lines for totally independent operation, and will increase the available 16-ID beamtime by more than 50%. More significantly the independent control will allow optimization of the 16-ID-B x-ray diffraction and 16-ID-D x-ray spectroscopy optics, resulting in a total of more than ten times improvement in efficiency and effective beam time. The current HPCAT beamline layout is well suited for the planned layout. Only the optics components in the first optics enclosure need to be modified. The change to the rest of the beamline will be minor, thus having minimum impact on HPCAT operation.

Supplementary Material – To read the entire HPCAT renewal proposal, which contains a detailed overview of the science enabled by the facility, please see:
http://cdac.gl.ciw.edu/images/stories/HPCATSupplement2009.pdf

7.3 New Initiatives

7.3.1 HPSynC Science and Outreach

The mission of the High Pressure Synergenic Center (HPSynC) at the APS is to advance the state of the art in high pressure science and technology at APS beamlines that can be adapted and optimized for high pressure work in their current configurations. In this way, the particular strengths of many different beamlines can be utilized for specific studies. In Year 6, HPSynC has received some operational funding from CDAC, and has initiated the following collaborations with APS beamlines, headed by HPSynC staff scientists **Yang Ding** and **Michael Lerche**:

- Submicron Laue diffraction (single crystal)—Sector 34-ID-D
- Submicron diffraction imaging (single crystal)—Sector 2-ID-D
- High pressure x-ray magnetic circular dichroism—Sector 4-ID-D
- Resonant magnetic x-ray scattering—Sector 6-ID
- Spin-selective emission XANES—Sectors13 and16
- X-ray inelastic scattering on liquids—Sector 4-ID

A number of new experimental methods pioneered by HPSynC and research projects facilitated by HPSynC staff have resulted in significant new scientific directions that would not have been possible without HPSynC involvement. These include the following publications:

Ding, Y., D. Haskel, Y. C. Tseng, E. Kaneshita, M. van Veenendaal, J. Mitchell, S. V. Sinogeikin, V. Prakapenka, and H. K. Mao, Pressure-induced magnetic transition in manganite ($La_{0.75}Ca_{0.25}MnO_3$), *Phys. Rev. Lett.*, **102**, 237201 (2009).

Gao, L., B. Chen, M. Lerche, E. E. Alp, W. Sturhahn, J. Zhao, H. Yavas, and J. Li, Sound velocities of compressed Fe_3C from simultaneous synchrotron x-ray diffraction and nuclear resonant scattering measurements, *J. Synchrotron Rad.,* in press.

Jackson, J., W. Sturhahn, O. Tschauner, M. Lerche, and Y. Fei, Behavior of iron in $(Mg,Fe)SiO_3$ post-perovskite assemblages at Mbar pressures, *Geophys. Res. Lett.*, **36**, L10301 (2009).

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Shim, S. H., A. Bengtson, D. Morgan, W. Sturhahn, K. Catalli, J. Zhao, M. Lerche, A. Kubo, and V. B. Prakapenka, Electronic and magnetic structures of the postperovskite-type Fe_2O_3 - Implications for planetary magnetic records and deep interior transitions, *Proc. Nat. Acad. Sci.*, **106**, 5508-5512 (2009).

Wang, L., Y. Pan, Y. Ding, W. Yang, W. L. Mao, S. V. Sinogeikin, Y. Meng, G. Shen, and H. K. Mao, High-pressure induced phase transitions of Y_2O_3 and Y_2O_3:Eu^{3+}, *Appl. Phys. Lett.*, **94**, 061921 (2009).

Winterrose, M. L., M. S. Lucas, A. F. Yue, I. Halevy, L. Mauger, J.A. Muñoz, Jingzhu Hu, M. Lerche, and B. Fultz, Pressure-Induced Invar Behavior in Pd_3Fe, *Phys. Rev. Lett.*, **102**, 237202 (2009).

Zeng, Q. S., Y. Ding, W. L. Mao, W. Luo, A. Blomqvist, R. Ahuja, W. Yang, J. Shu, S. V. Sinogeikin, Y. Meng, D. L. Brewe, J. Z. Jiang, and H. K. Mao, Substitutional alloy of Ce and Al, *Proc. Nat. Acad. Sci.*, **106**, 2515 (2009).

7.3.2 New Facilities and Projects

CDAC personnel are closely involved with several major new DOE/NNSA facilities that are in the planning stages or are being made available to the user community. CDAC participation in these programs represent progress toward a key goal, which is the combination of static and dynamic compression techniques to access transient, high-energy states of matter that are inaccessible by the individual methods applied separately. At NIF, CDAC is helping to coordinate academic use of the facility through Academic Partner **Raymond Jeanloz** (**Berkeley**) and Laboratory Partner **Rip Collins** (**LLNL**). In addition, CDAC groups are beginning to carry out experiments at other laser facilities (*e.g.,* Omega) in anticipation of experiments at NIF in the near future.

Two new facilities that are progressing through the planning process are **DC-CAT**, to be built as a Collaborative Acces Team facility at the Advanced Photon Source, and the **MaRIE** (Matter-Radiation Interactions in Extremes) facility to be constructed at LANL. CDAC participated in facilitating the pilot experiments at HP-CAT and NSLS (described in more detail in our Year 4 and Year 5 annual reports), which established the feasibility of characterizing shock compression events with synchrotron radiation. These experiments have now laid the groundwork for DC-CAT, which will be a new sector at the Advanced Photon Source dedicated to shock compression science. The potential for shock compression measurements on precompressed samples will continue to be a major goal of CDAC as we move forward. CDAC Director **Russell Hemley** actively participates on the advisory panel for the MaRIE facility, which will provide experimental capabilities to address an additional dimension to the science of extreme consitions, that is extremes of radiation in combination with high pressure-high temperature methods. Both of these facilities will enhance the science of matter at extreme conditions for stewardship science applications, and CDAC will foster

collaborations between these unique experimental facilities and the CDAC academic community in the spirit of the SSAA partnership.

CDAC is also participating in a new effort at **Sandia**, where **Jean-Paul Davis** and **Marcus Knudson** have initiated a project to investigate multimegabar isentropic compression of metals using the Sandia's Z machine. CDAC Director **Russell Hemley** and CDAC Coordinator **Stephen Gramsch** are collaborating with the Sandia team on the project, which will open new avenues of collaboration between the high pressure static compression and dynamic compression communities.

APPENDIX I: CDAC Publications and Presentations for Year 6

We list publications and presentations for 2008-2009, including all work supported fully or in part by CDAC. This list therefore includes work carried out at HPCAT by all of its members and users during this period.

A. CDAC Publications

Aberg, D., B. Sadigh, J. C. Crowhurst, and A. F. Goncharov, Thermodynamic ground states of platinum metal nitrides, *Phys. Rev. Lett.,* **100**, 095501 (2008).

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Ahart, M., A. Hushur, Y. Bing, Z. G. Ye, R. J. Hemley, and S. Kojima, Critical slowing down of relaxation dynamics near the Curie temperature in the relaxor $Pb(Sc_{0.5}Nb_{0.5})O_3$, *Appl. Phys. Lett.,* **94**, 142906 (2009).

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Yarger, J. L., Polyamorphism and liquid-liquid transitions (invited), *University of California - Irvine* (Irvine, CA, September, 2008).

Yarger, J. L., Energetic materials at high pressure (invited), *Arizona Institute for Renewable Energy (AIRE) Workshop* (Tempe, AZ, November, 2008).

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Yarger, J. L., Liquids and glasses at high pressure (invited), *Annual Meeting of the International Commission on Glass (ICG) and the American Ceramic Society's Glass and Optical Minerals Division (GOMD) Conference, PACRIM 8* (Vancouver, Canada, June, 2009).

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APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for Year 6

A. HPCAT (APS)

A large part of our annual budget was dedicated to the completion of construction and commissioning of the HPCAT facility. In addition to the 30% membership obtained by CDAC in HPCAT, the support generated by SSAAP funding made possible significant scientific productivity of this state-of-the-art high-pressure facility.

User Name	Affiliations	Project	Dates
C. Holt Rebecca Fisher	Northwestern University	MgO EOS	October 3- 5, 2008
H. Cynn Z. Jenei W. Evans	LLNL	Study of V-group elements at high *P-T*	October 4-7, 2008
R. Kumar S. Veeramalai S. Sinogeikin	University of Nevada – Las Vegas HPCAT	Low temperature x-ray diffraction studies on heavy fermion compounds $CeCoIn_5$ and $CeIrIn_5$	October 4-7, 2008
S. Maglio M. Frank	University of Nevada – Las Vegas Northern Illinois University	Quantifying slab dehydration	October 5-7, 2008
A. Simon S. Maglio	University of Nevada – Las Vegas	Quantifying element mass transfer of REE-monazite at subduction zone conditions using the hydrothermal DAC and *in situ* x-ray fluorescence	October 5-7, 2008
Yue Meng	HPCAT	High-pressure phase transitions in Eu	October 8-10, 2008
A. Simon S. Maglio	University of Nevada – Las Vegas	Quantifying slab dehydration and element mobility during subduction	October 8-11, 2008
O. Tschauner	University of Nevada – Las Vegas	Single crystal diffraction	October 8-15, 2008
S. Maglio A. Simon O. Tschauner M. Frank	University of Nevada – Las Vegas Northern Illinois University	Quantifying slab dehydration and element mobility during subduction	October 10-14, 2008
O. Tschauner	University of Nevada – Las Vegas	Powder diffraction with 2d and 1d detector	October 11-14, 2008
Q. Zeng	HPSynC	Direct probing the 4f electronic structure of high pressure induced polyamorphism transition in CeAl binary metallic glass by RIXS	October 11-16, 2008
C. S. Zha	Carnegie	High-pressure diffraction of Ni and W at megabar pressures	October 15-16, 2008
P. E. Janolin	Carnegie	Ferroelectric nanopowders	October 15-17, 2008
N. Velisavljevic A. Stemshorn	LANL University of Alabama – Birmingham	High *P-T* x-ray diffraction and electrical resistance measurements on Zr, Ti, and Sn metal	October 16-17, 2008
R. Kumar	University of Nevada – Las Vegas	Resonant x-ray emission studies on $CeMIn_5$(M=Rh,Co,Ir) and $CeCu_2Si_2$ at high pressures	October 16-19, 2008
H. P. Liermann	HPCAT	Single crystal diffraction	October 16-20, 2008

M. Pravica S. Tkachev W. Pravica	University of Nevada – Las Vegas Wilbur Wright College	Damage studies of hard materials	October 17-20, 2008
W. Evans M. Lipp B. Baer	LLNL	X-ray diffraction studies at high pressure/Powder diffraction, DAC, resistive heating, high-temperature: EOS of simple materials/DOE interest	October 17-20, 2008
H. P. Liermann	HPCAT	Single crystal development	October 22-24, 2008
H. Cynn Krystle Catalli S. H. Shim	LLNL Massachusetts Institute of Technolgoy	X-ray emission spectroscopy of Fe-bearing silicates $MgFeSiO_3$	October 22-26, 2008
H. Cynn	LLNL	Grain boundary mapping	October 22-27, 2008
D. Ikuta	HPCAT	Single crystal development	October 24-25, 2008
M. Somayazulu	Carnegie	*P-V-T* EOS studies of boron carbide	October 24-25, 2008
Olga Shebanova	HPCAT	EXAFS study on Cs-Pt in DAC	October 25-26, 2008
Amy Lazicki	Carnegie	Single crystal diffraction	October 25-26, 2008
Q. Meng G. Shen	HPCAT	Anomalous absorption study in DAC	October 26-27, 2008
V. Struzhkin Svetlana Kharlamova	Carnegie	X-ray emission spectroscopy of superconductors	October 26-November 6, 2008
J. Klepeis B. Baer Chantel Aracne	LLNL	Sn, V, and Si in DAC under high *P-T*	October 27-31, 2008
Amy Lazicki	Carnegie	Single crystal diffraction	October 29-November 2, 2008
Michelle Weinberger	Carnegie	Hydrogen storage materials in DAC	October 31-November 1, 2008
M. Pravica W. Pravica	University of Nevada – Las Vegas Wilbur Wright College	Carbon- and nitrogen-containing compounds	November 1-3, 2008
H. K. Mao J. Shu Wendy Mao	Carnegie Stanford University	High *P-T* phase transitions and EOS of ferromagnesian oxides and silicates at the Earth's core conditions	November 1-3, 2008
W. Yang	HPCAT	Powder diffraction of micron and nano-crystalline materials ($BaFe_2As_2$, Ni powder)	November 5-6, 2008
H. P. Liermann S. Merkel	HPCAT Universite de Lille	Side diffraction in DAC	November 5-8, 2008
Yue Meng Wenli Bi	HPCAT Washington University – St. Louis	XRD study of Eu to Mbar pressures	November 6-7, 2008
H. P. Liermann P. Dera	HPCAT GSECARS	Single crystal diffraction of marokite and stishovite to high pressure	November 7-8, 2008
W. Evans S. Weir	LLNL	EOS of simple metals	November 8-11, 2008

H. K. Mao Y. Ding Wendy Mao	Carnegie Stanford University	XES of Fe in $(Fe,Mg)SiO_3$ post-perovskite	November 8-11, 2008
Z. Lin	LANL	Powder diffraction	November 9-11, 2008
H. Cynn	LLNL	Grain boundary mapping	November 11-17, 2008
G. N. Chesnut	LANL	Powder diffraction	November 13-14, 2008
L. Wang	HPSynC	Powder diffraction	November 13-15, 2008
Amy Lazicki	Carnegie	$NbSe_2$ EOS	November 15-17, 2008
M. Somayazulu Yue Meng	Carnegie HPCAT	*P-V-T* EOS studies of boron carbide	November 16-17, 2008
W. Yang	HPCAT	Anomalous scattering of amorphous material	November 17-21, 2008
Shibing Wang	Stanford University	X-ray emission spectroscopy of hemanite (Fe_2O_3) above 40 GPa	November 17-24, 2008
H. Cynn. J. Klepeis	LLNL	Simple metal (Be, BeCu, Si, Ta, TaW) melting at high pressure using laser heating	November 18-22, 2008
S. Saxena V. Drozd A. Durygin	Florida International University	Hydride studies in high *P-T*	November 19-21, 2008
M. Laguna-Marco	University of Zaragoza	$BaIrO_3$ compounds induced by Sr doping	November 21-22, 2008
Q. Mei	HPCAT	Anomalous absorption study in DAC	November 22-24, 2008
Dana Dattlebaum N. Velisavljevic	LANL	High pressure behavior of explosive molecules toward understanding hot spot related sensitization	November 22-24, 2008
W. Yang	HPCAT	Laue absorption spectroscopy	November 23-26, 2008
Melike Abliz	HPSynC	Powder diffraction of heavy fermion materials	November 24-25, 2008
M. Lerche	HPSynC	Powder diffraction of light materials	November 25-26, 2008
O. Tschauner Barbara Lavina O. Grubor-Urosevic	University of Nevada – Las Vegas	High pressure single crystal diffraction	November 25-29, 2008
H. Liu	Harbin Institute of Technology	Powder diffraction of super-conducting materials	November 28-December 2, 2008
M. Pravica S. Tkachev A. Johnson Y. Z. Feng W. Pravica	University of Nevada – Las Vegas Wilbur Wright College	Studies of hydrocarbons at extreme conditions using x-ray diffraction	November 29-December 1, 2008
A. Cornelius J. Baker	University of Nevada – Las Vegas	High pressure diffraction studies on $AuAl_2$ and $AuIn_2$	December 1, 2008
W. Yang	HPCAT	ESAFS scan development	December 3-5, 2008
L. Wang Q. Zeng H. K. Mao	HPSynC Carnegie	High pressure phase transitions of Y_2O_3 nanocrystal and $Ce_{55}Al_{45}$	December 3-5, 2008

Olga Shebanova	HPCAT	ESAFS study on Cs-Pt in DAC	December 5-6, 2008
Svetlana Kharlamova V. Struzhkin	Carnegie	Low temperature x-ray diffraction of Fe pnictides	December 5-6, 2008
Jennifer Ciezak	Carnegie/ARL	Single crystal diffraction	December 5-16, 2008
Lyci George V. Drozd Yue Meng	Florida International University HPCAT	High *P-T* characterization and phase diagrams of some selected hydrides	December 6-7, 2008
Q. Zeng	HPSynC	Amorphous study in DAC	December 6-8, 2008
H. K. Mao Y. Ding	Carnegie HPSynC	NaPlasmon at high pressures	December 6-11, 2008
M. Guthrie S. Sinogeikin E. Gregoryanz C. Guillaume	HPSynC HPCAT University of Edinburgh	High pressure structures of lithium	December 7-12, 2008
Q. Yang	HPCAT	Amorphous study in DAC	December 8-9, 2008
L. Wang	HPSynC	Nano-size sample diffraction in DAC	December 10-11, 2008
Y. Vohra A. Stemshorn N. Cunningham	University of Alabama – Birmingham	Nanocrystals and amorphous in BMG	December 11-16, 2008
Yu Lin Wendy Mao Maake Kroon S. Sinogeikin	Stanford University HPCAT	X-ray diffraction of hydrogen-rich molecular compounds at high pressures and low temperatures	December 12-13, 2008
E. Kaneshita J. Chang Y. Ding Q. Zeng W. Yang	ANL Carnegie HPCAT	Study of pressure-induced phase transitions between diagonal and vertical stripe states in $La_{2-x}Sr_xNiO_4$	December 13-16, 2008
Maria Baldini G. Amulele	Stanford University	Bonding changes in amorphous and crystal boron at high pressures	December 11-15, 2008
S. Gramsch	Carnegie	B6O ambient x-ray Rama	December 15-18, 2008
M. Aihaiti	Carnegie	Powder diffraction	December 17-18, 2008
C. S. Yoo A. Sengupta	Washington State University	X-ray crystallography in DAC	December 17-21, 2008
M. Pravica	University of Nevada – Las Vegas	X-ray damage of crystals	December 18-20, 2008
W. Evans H. Cynn M. Lipp	LLNL	f-metal behavior at high temperatures and high pressures using an external heating/DOE interest	December 18-20, 2008
M. Aihaiti	Carnegie	Phase transition in relaxor $PbSc_{1/2}Nb_{2/3}O_3$	December 21-22, 2008
Barbara Lavina B. Yulga O. Grubor-Urosevic	University of Nevada – Las Vegas	Single crystal diffraction at high pressure on carbonates	January 29-February 1, 2009
H. Cynn B. Lipp	LLNL	Oxygen under high *P-T*	January 30-February 3, 2009

H. K. Mao Amy Lazicki Y. Ding	Carnegie HPSynC	SKB compression on electron gas in sodium and H_2O conversion	January 31-February 8, 2009
H. Liu L. Wang J. Zhao Z. Yu W. Yang X. Xiao P. Lee	Harbin Institute of Technology HPCAT ANL	3DXRD studies for powder Fe and Ti phase transition under pressure	February 2-3, 2009
D. Ikuta	HPCAT	Thin-section study	February 1-2, 2009
M. Somayazulu T. Strobel	Carnegie	Single crystal Xe-H_2	February 2-3, 2009
Barbara Lavina	University of Nevada – Las Vegas	Single crystal NiSe	February 5-7, 2009
H. Liu L. Wang J. Zhao Z. Yu	Harbin Institute of Technology	3 dimensional XRD studies of powder Fe and Ti phase transition under pressure	February 6-7, 2009
M. Somayazulu	Carnegie	Single crystal Xe-H_2	February 7-8, 2009
H. K. Mao J. Shu Wendy Mao	Carnegie Stanford University	Synthesis of post-perovskite phase of $(Mg_{0.6},Fe_{0.4})Si0_3$ at high P/T for single crystal studies at sector 34	February 7-9, 2009
D. Ikuta	HPCAT	Thin-section study	February 8-9, 2009
Y. Ren Z. Nie	APS-XOR	Martinsite phase transition	February 11-13, 2009
S. Maglio	University of Nevada – Las Vegas	Yttrium fluorescence quantifying trace element mass transfer of monazite at subduction zone conditions	February 11-14, 2009
H. Cynn J. Klepeis B. Baer	LLNL	Simple metal (Be, BeCu, Si, Ta, TaW, V) melting at high pressure using laser heating	February 11-14, 2009
H. Cynn	LLNL	Grain boundary mapping	February 12-16, 2009
L. Wang	HPSynC	Nano phase transition	February 13-15,2009
Melike Abliz	HPSynC	$ZrTe_3$ phase transition	February 15-16, 2009
M. Somayazulu Jennifer Ciezak D. Dandekar	Carnegie Army Research Laboratory	*P-V-T* EOS of B_4C; strength and elasticity studies in B_4C and AL-O-N (nitride)	February 15-16, 2009
I. Troyan T. Palsyuk	Max Planck Institute	Structural study of borane at megabar pressures	February 16-17, 2009
W. Yang	HPCAT	Amorphous scattering	February 16-19. 2009
M. Lipp	LLNL	XES of f-metals at high pressure	February 16-21, 2009
L. Miyagi Waruntorn Kanitpanycharoen	University of California – Berkeley	Rheology in the lowermost mantle: *In-situ* investigation of the deformation behavior of $MgGeO_3$ at lowermost mantle pressures	February 18-21, 2009
Olga Shebanova	HPCAT	EXAFS	February 19-20, 2008

M. Pravica B. Yulga Y. Zhang	University of Nevada – Las Vegas	Low temperature radiation damage	February 19-22, 2009
A. Durigyn	Florida International University	High *P-T* ADX study of hydrides	February 20-23, 2009
L. Wang Y. Song Z. Dong	HPSynC University of Western Ontario	High pressure induced phase transitions in nanosized Y_2O_3; High-pressure XRD study of nanowire SnO_2 (different morphology)	February 21-23, 2009
V. Struzhkin Svetlana Kharlamova	Carnegie	A combined x-ray emission and diffraction study of compounds at high pressure and high temperature conditions	February 21-27, 2009
W. Yang	HPCAT	X-ray radiation	February 22-27, 2009
C. S. Yoo J. Y. Chen M. Kim	Washington State University	Novel extended nitrides at high pressures and temperatures (N_2/D_2, H_2O_2, XeF_2)	February 25-27, 2009
J. Klepeis	LLNL	Strength measurements	February 25-March 2, 2009
Johanna Nylen K. Leinenweber	Arizona State University	Phase transition under *P-T*	February 27-March 1, 2009
Amy Lazicki J. Montoya A. Goncharov	Carnegie	Transition metal nitrides (Re, ReW alloy in N_2). Au in N_2 at high *P-T*, and pure N_2 at high pressure	February 27-March 1, 2009
M. Lerche	HPSynC	Spin state in amorphous iron	February 27-March 3, 2009
H. K. Mao Li Zhang	Carnegie	*PT* phase diagram of $(Mg,Fe)SiO_3$ (En80 En60) <100 GPa, around 2500 K for phase diagram and synthesizing single crystal for studies at sector 34	March 1-3, 2009
L. Wang	HPSynC	Nano phase transition	March 2-3, 2009
M. Pravica	University of Nevada – Las Vegas	X-ray emission study of Ga-containing compounds	March 4-5, 2009
Sabrina Whitaker J. Pigott H. Scott	Ohio State University Indiana University – South Bend	K incorporation into Fe and Rb at high *P-T* (iron w/K felsbar, Rb w/K felsbar); Phase transition in $Fe_{0.63}Ni_{0.35}$/Ni at high *P-T*	March 4-7, 2009
Barbara Lavina	University of Nevada – Las Vegas	Single crystal ADX	March 4-9, 2009
W. Evans	LLNL	XES of f-metals cerium at high pressure	March 5-9, 2009
M. Lang F. Zhang	University of Michigan	High pressure phase transition in $ScPO_4$ and graphite	March 7-8, 2009
L. Wang	HPSynC	High pressure induced phase transitions in Y_2O_3 with different grain sizes	March 8-9, 2009
M.Guthrie	HPSynC	Amorphous Scattering	March 9-10, 2009
W. Yang	HPCAT	Amorphous Scattering	March 11-12, 2009
S. Maglio	University of Nevada – Las Vegas	Fluorescence quantifying trace element mass transfer of monazite at subduction zone conditions	March 11-14, 2009
M. Lipp	LLNL	High temperature melting	March 11-14, 2009
Barbara Lavina	University of Nevada – Las Vegas	Single crystal in DAC	March 13-15, 2009

R. Kumar G. Tam	University of Nevada – Las Vegas	High pressure x-ray diffraction studies on silicides and borides	March 14-16, 2009
A. Simon	University of Nevada – Las Vegas	High temperature in DAC	March 14-19, 2009
L. Wang	HPSynC	Nano phase transition	March 15-16, 2009
P. Zinin T. Acosta	University of Hawai'i	Search, synthesis, and characterization of new diamond-like phases in the B-C system under high pressures and high temperatures	March 19-21, 2009
Y. Vohra	University of Alabama – Birmingham	Low-temperature diffraction	March 19-23, 2009
W. Yang	HPCAT	X-ray absorption spectroscopy	March 19-23, 2009
H. K. Mao Wendy Mao	Carnegie Stanford University	XES of Fe in $(Mg,Fe)SiO_3$ post-perovskite	March 20-23, 2009
H. K. Mao J. Shu Wendy Mao	Carnegie Stanford University	$(Mg,Fe)SiO_3$ post-perovskite at high *P-T*	March 21-23, 2009
Amy Lazicki	Carnegie	Li melting in DAC	March 25-28, 2009
Y. Wang	LANL	Strength of nano-polycrystaline diamond	March 26-27, 2009
G. N. Chesnut	LANL	Powder diffraction	March 26-30, 2009
Elizabeth Tanis	University of Nevada – Las Vegas	NRIXS on FeDy compounds	March 27-28, 2009
H. Cynn B. Baer S. Weir	LLNL	f-medal behavior at high temperatures and high pressures using an external heating	March 27-30, 2009
M. Lipp	LLNL	Ce melting in DAC	March 28-April 2, 2009
Jennifer Jackson June Wicks Caitlin Murphy	Caltech	NRFS and NRIS on compressed samples	March 29-April 3, 2009
T. Strobel	Carnegie	Diffraction study of novel phase transitions in H_2+H_2O clathrates	March 30-April 3, 2009
V. Struzhkin	Carnegie	Powder diffraction	April 1-3, 2009
S. H. Shim Krystle Catalli B. Grocholski	Massachusetts Institute of Technology	Oxidation state of Fe in perovskite and post-perovskite under reducing conditions	April 2-5, 2009
H. Cynn A. Schwartz	LLNL	Pu phase transition low temperature	April 3-6, 2009
L. Wang	HPSynC	High pressure studies of the transitions of charge density wave of $SmTe_3$ single crystals	April 4-5, 2009
Yu Lin Maaike Kroon	Stanford University	X-ray diffraction of hydrogen-rich molecular compounds at low temperatures and high pressures	April 5-7, 2009
Svetlana Kharlamova F. Elkin	Carnegie	Insulator-metal transition in the spin-crossover regime	April 5-10, 2009
Y. Ren	APS-XOR	Superconductor at low temperature/high pressure	April 6-9, 2009
Y. Chang S. Jacobsen C. Holl	Northwestern University	EOS of ferric-iron bearing phase D	April 8-9, 2009

O. Tschauner S. Maglio M. Frank	University of Nevada – Las Vegas Northern Illinois University	Singly crystal and powder diffraction studies with hydrothermal and other diamond cells	April 9-12, 2009
G. N. Chesnut	LANL	High-*T* powder diffraction	April 9-13, 2009
R. Kumar	University of Nevada – Las Vegas	Nuclear resonant inelastic x-ray scattering experiments on FeSe and FeTe under high pressures	April 10-12, 2009
Lyci George V. Drozd S. Garimella Yue Meng	Florida International University HPCAT	High *P-T* characterization and phase diagrams of some selected hydrides	April 12-13, 2009
Lisa Mauger O. Delaire A. Moreira Dos Santos D. Abernathy	Caltech Oak Ridge	NFS measurements of ^{57}Fe partial phonon DOS and magnetism in $FeSi_{(1-x)}Ge_{(x)}$	April 12-18, 2009
W. Yang	HPCAT	EXAFS development	April 13-16, 2009
Y. Ding	HPSynC	Powder diffraction at low temperature	April 17-20, 2009
W. Evans H. Cynn B. Baer	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	April 17-20, 2009
Shibing Wang Y. Ding	Stanford University HPSynC	NRIXS and NFS on Fe_2O_3 (hematite)	April 18-22, 2009
Patricia Kalita	University of Nevada – Las Vegas	Powder diffraction of heavy metals	April 20-21, 2009
Dana Dattlebaum G. N. Chesnut N. Velisavljevic	LANL	High *P-T* behavior of explosives	April 20-22, 2009
W. Yang	HPCAT	Amorphous scattering	April 21-22, 2009
J. H. Klepeis	LLNL	Strength measurements	May 29-June 1, 2009
J. Piggot D. Reaman Wendy Panero	Ohio State University	High *P-T* EOS of rubidium hollandite	May 30-June 1, 2009
Elizabeth Tanis S. Tkachev B. Yulga	University of Nevada – Las Vegas	NRIXS on FeDy compound	May 29-June 2, 2009
M. Pravica	University of Nevada – Las Vegas	EDXD	May 30-June 4, 2009
H. Scott T. Kinney M. Frank Elizabeth Aarestad	Indiana University – South Bend Northern Illinois University	CO_2 sequestration in Earth's lower crust and mantle	June 1-2, 2009
S. Sinogeikin	HPCAT	Cryostat development	June 1-2, 2009
Barbara Lavina	University of Nevada – Las Vegas	Single crystal diffraction	June 3-4, 2009

G. Amulele Y. Al Khatatbeh	Yale University New Mexico State University	Determining the high-pressure behavior of transition metal oxides HfO_2, nano-TiO_2	June 3-5, 2009
O. Delaire J. Munoz	Oak Ridge	Measurements of ^{57}Fe partial phonon DOS at high pressure in epsilon-FeSi doped with Fe	
M. Pravica	University of Nevada – Las Vegas	Powder diffraction	June 4-6, 2009
O. Tschauner	University of Nevada – Las Vegas	White beam Laue	June 4-7, 2009
D. Shakhvorosto C. Murli	University of Western Ontario	Pressure-induced phase transition in germanium antimony alloy, glycine lithium sulphate	June 5-7, 2009
Barbara Lavina	University of Nevada – Las Vegas	Powder diffraction	June 6-8, 2009
M. Winterrose Lisa Mauger J. Munoz K. Kim H. Tan	California Institute of Technology	Low-temperature pressure-induced magnetic transitions and invar behavior in L1_2 alloys	June 6-14, 2009
M. Somayazulu	Carnegie	Single crystal x-ray diffraction studies on Xe-He solids	June 7-9, 2009
Amy Lazicki	Carnegie	White beam Laue	June 7-11, 2009
Q. Mei G. Shen	HPCAT	Amorphous heating	June 8-9, 2009
W. Yang	HPCAT	E-scan development	June 10-11, 2009
Caitlin A. Murphy Y. Liu K. Mo D. Hou C. J. Ruschman B. D. Bertram E.Cakmak P. Y. Hsieh Kelley A. Distel J. Li M. A. Kraus Illana G. Goldberg Y. L. Fang	California Institute of Technology University of Illinois at UC Texas Tech University Georgia Institute of Technology University of Tennessee – Knoxville University of Maryland – College Park Ohio State University Rutgers University University of Missouri – Columbia Georgetown University Rice University	Neutron X-ray School: XRD of structural phase transition of ZnO at high pressures	June 10-12, 2009
Olga Shebanova	HPCAT	EXAFS development	June 11-12, 2009
Barbara Lavina	University of Nevada – Las Vegas	High pressure study of Ca and Na	June 12-13, 209
M. Lipp Chantel Aracne	LLNL	Ce heating and melting	June 12-15, 2009
H. K. Mao J. Shu Yue Meng	Carnegie HPCAT	Rheology in the lowermost mantle: *In-situ* investigation of the deformation	June 13-15, 2009

L. Wang Y. Ding Yue Meng	HPSynC HPCAT	High pressure study of Terbium and FeSe	June 13-15, 2009
Y. Xiao	HPCAT	Nuclear forward scattering on FeSe	June 14-16, 2009
Susannah Dorfman T. Duffy G. Finkelstein	Princeton University	Phase transitions in molybdenum to 3000 K and 100 GPa	June 15-16, 2009
V. Arturas	Stanford University	BaFeAs low temperature phase transition	June 15-18, 2009
Y. Xiao	HPCAT	Nuclear forward scattering on FeSe	June 17-18, 2009
M. Jacobson	University of Nevada – Las Vegas	In_2Te_3 phase transition	June 18-20, 2009
R. Lacomba	Universidad de Valencia	High-pressure stability and compressibility of APO_4 (A=La, Nd, Eu, Gd, Er, and Y) orthophosphates	June 18-20, 2009
Y. Xiao P. Chow J. Seidler	HPCAT University of Washington	Mini-emission spectrometer	June 18-22, 2009
M. Lipp	LLNL	Ce heating and melting	June 18-22, 2009
D. Ikuta	HPCAT	Single crystal diffraction	June 20-22, 2009
H. K. Mao J. Shu Yue Meng Wendy Mao	Carnegie HPCAT Stanford University	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	June 20-22, 2009
X. J. Chen	Carnegie	Exploring metallic structure of solid silane (SiH_4)	June 20-22, 2009
W. Yang	HPCAT	E-scan development	June 24-26, 2009
P. Chow Y. Xiao	HPCAT	Mini-emission FeKbeta	June 24-27, 2009
Amy Lazicki	Carnegie	White beam Laue	June 24-28, 2009
G. Tsoy A. Stemshorn S. Raeman	University of Alabama – Birmingham	Low-temperature resistance measurement	June 26-July 1, 2009
R. Lacomba	Universidad de Valencia	High-pressure stability and compressibility of APO_4 (A=La, Nd, Eu, Gd, Er, and Y) orthophosphates	June 28-29, 2009
Wenge Yang	HPCAT	Laue diffraction development	June 28-July 2, 2009
H. Cynn J. H. Klepeis B. Baer	LLNL	Simple metal melting at high PT (Si, Ta, TaW, V) for phase diagram and synthesizing single crystal for studies at sector 34	June 29-July 2, 2009
S. Sinogeikin	HPCAT	Cryostat development	July 6-7, 2009
H. K. Mao J. Shu Y. Meng	Carnegie HPCAT	Fe-Mg partitioning and ultrahigh pressure in perovskite and post-perovskite	July 6-8, 2009
H. K. Mao Maria Baldini Yu Lin Wendy Mao Y. Xiao	Carnegie Stanford University HPCAT	Bonding changes in amorphous and crystal boron at high pressure	July 7-10, 2009

W. Evans	LLNL	EDXD	July 7-11, 2009
J. Mitchell H. Zheng	ANL	YCBO low-temperature transition	July 8-11, 2009
O. Tschauner	University of Nevada – Las Vegas	Structural studies at high pressure, silicates, Dy, La, Pr, FeS_2	July 9-13, 2009
O. Tschauner Barbara Lavina S. Tkachev	University of Nevada – Las Vegas	Single crystal diffraction on PETN, TATB, Dy, La, Pr	July 9-13, 2009
D. Ikuta	HPCAT	Single crystal diffraction	July 12-13, 2009
S. Sinogeikin	HPCAT	Cryostat development project	July 13-14, 2009
G. N. Chesnut	LANL	Powder diffraction	July 13-18, 2009
A. Sengupta M. Dunuwille M. Kim	Washington State University	Novel extended nitrides at high pressures and temperatures	July 15-17, 2009
M. Lipp Z. Jenei	LLNL	X-ray Raman spectroscopy of boron compounds in a DAC	July 15-19, 2009
A. Yamada T. Inoue T. Yu Y. Wang C. Park Q. Mei	Ehime University GSECARS HPCAT	PE-cell melt	July 15-31, 2009
R. Kumar S. Sinogeikin	University of Nevada – Las Vegas HPCAT	Low temperature x-ray diffraction studies on FeSe, FeTe, and $CeCu_2Si_2$ compounds	July 17-21, 2009
M. Aihaiti	Carnegie	Powder diffraction	July 18-20, 2009
H. K. Mao	Carnegie	Bonding changes in amorphous and crystal boron at high pressure	July 19-24, 2009
Yun-yuan Chen S. Jacobsen C. Holl	Northwestern University	Comparative compressibility of hydroxyl-wadsleyite	July 22-23, 2003
L. Wang	HPSynC	Powder diffraction	July 22-24, 2009
Dana Dattlebaum N. Velisavljevic G. N. Chesnut	LANL	High pressure-high temperature behavior of explosives	July 23-24, 2009
M. Lang M. Toulemonde Beatrice Shuster Christina Trautmann	University of Michigan CNRS GSI Darmstadt	Phase transitions induced by simultaneous exposure to relativistic ion beams and high pressure	July 24-26, 2009
Patricia Kalita J. Baker	University of Nevada – Las Vegas	Powder diffraction	July 24-26, 2009
S. Gramsch	Carnegie	X-ray Raman spectrum of B_6O	July 24-28, 2009
J. Jeffries A. Schwartz Kerri Blobaum	LLNL	Low-temperature powder diffraction	July 26-28, 2009
Svetlana Kharlamova V. Struzhkin S. Sinogeikin	Carnegie HPCAT	X-ray diffraction study of the novel superconductors at high pressure and low temperature	July 26-30, 2009

Olga Shebanova	HPCAT	EXAFS development	July 29-30, 2009
R. Kumar S. K. Rangasamy Veeramali	University of Nevada – Las Vegas	X-ray Raman experiments on BC_3N, ammonia borane and B_4C under pressures	July 29-August 1, 2009
D. Ikuta	HPCAT	Single crystal diffraction	July 30-August 1, 2009
S. Tkachev S. Wilde Y. Liu E. Don Romano J. Hernandez	University of Nevada – Las Vegas	X-ray powder diffraction studies of various materials under high pressure	July 30-August 1, 2009
G. Shen Q. Mei C. Park	HPCAT	PE-cell melt	July 31-August 3, 2009
Melike Abliz	HPSynC	Powder diffraction	August 1-2, 2009
R. Chellappa	Carnegie	Structural studies on B-N-H complexes	August 1-3, 2009
S. Tkachev M. Pravica	University of Nevada – Las Vegas	High-pressure x-ray Raman study of nitrogen-containing compounds	August 1-4, 2009
H. Liu	Harbin Institute of Technology	Powder diffraction	August 2-4, 2009
Patricia Kalita Kristina Lipinska-Kalita	University of Nevada – Las Vegas	High-presure x-ray diffraction of zirconium hydride and hafnium hydride	August 3-4, 2007
Q. Mei C. Park	HPCAT	PE-cell development	August 3-7, 2009
Patricia Kalita Krystina Lipinska-Kalita	University of Nevada – Las Vegas	High-pressure x-ray diffraction of a nanocrystalline composite material	August 5-7, 2009
H. P. Liermann S. Merkel L. Miyagi	DESY Universite de Lille University of California – Berkeley	High-temperature powder diffraction	August 5-8, 2009
Z. Jenei	LLNL	Nitrogen-edge x-ray Raman nitrogen compounds	August 5-9, 2009
T. Strobel	Carnegie	Diffraction studies of a pressure induced compound of silane and hydrogen	August 7-8, 2009
G. Shen Q. Mei C. Park T. Yu	HPCAT GSECARS	PE-cell melt	August 7-16, 2009
H. K. Mao J. Shu Y. Meng	Carnegie HPCAT	Fe-Mg partitioning and ultrahigh pressure in perovskite and post-perovskite	August 8-10, 2009
Kanani Lee J. Panzik J. O'Rourke	Yale University	Powder diffraction	August 8-10, 2009
S. Sinogeikin	HPCAT	Cryostat development project	August 10-11, 2009
W. Yang	HPCAT	Amorphous diffraction	August 10-14, 2009
H. Jiang H. Raines Y. Xiao	University of California – Los Angeles HPCAT	Three-dimensional high-resolution imaging of iron under high pressure using x-ray diffraction microscopy	August 10-19, 2009

H. Liu	Harbin Institute of Technology	High-pressure 3D study of Fe	August 12-14, 2009
M. Guthrie	HPSynC	Light element diffraction	August 14-15, 2009
H. Cynn J. H. Klepeis B. Baer Chantel Aracne	LLNL	f-metal behavior temperatures and high pressures	August 14-17, 2009
J. H. Klepeis	LLNL	Strength measurements	August 15-18, 2009
M. Pravica B. Yulga	University of Nevada – Las Vegas	PE-cell test	August 16-18, 2009
C. Guillaume M. Guthrie S. Sinogeikin	University of Edinburgh HPSynC HPCAT	High-pressure structures of lithium at low temperatures	August 17-19, 2009
T. Yu	GSECARS	PE-cell melt	August 18-19, 2009

B. U2A Infrared Beamline (NSLS)

Beamline U2A is managed by **Carnegie** and provides useful materials characterization capabilities not available at other beamlines. The principal source of support for this beamline is the National Science Foundation, through the EAR COMPRES consortium. CDAC has a 20% membership in the facility by virtue of **Carnegie** management. CDAC provided partial salary support for Beamline scientist **Zhenxian Liu** as well as beamline upgrades and supplies.

User Name	**Affiliations**	**Project**	**Dates**
Kin Fai Mak	Columbia University	Probing the electronic structure of graphene nanoribbons by infrared photoconductivity	September 25-26, 2008
B. Liu S. Yu	Jilin University	High pressure study of C_{60} nanomaterilas	September 29-30, 2008 Oct. 1, 2008
Amy Lazicki	Carnegie	IR reflectivity of sodium	October 2-3, 2008
W. Han	Brookhaven	High-pressure IR Study gases storage in boron nitride nanotubes)	October 9-11, 2008
Wendy Panero J. Pigott Z. Liu	Ohio State University Carnegie	Solubility of two component systems at high-pressures and temperatures	October 15-18, 2008
S. Yu Z. Liu	Jilin University Carnegie	Investigation of H_2O and some organic substance storage in the nanotubes by using high pressure	October 24-November 5, 2008
B.Yulga S. Tkachev	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high pressure and temperature	November 6-7, 2008
M. Pravica S. Tkachev E. Romano	University of Nevada – Las Vegas	Infrared studies of cyclooctatetraene at high pressure	November 8-9, 2008
T. Zhou Z. Qin	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	November 10-14, 2008
S. Yu Z. Liu	Jilin University Carnegie	Investigation of H_2O and some organic substance storage in the nanotubes by using high pressure	November 16-18, 2008

K. Otsuka	Yale University	In situ measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR	November 19-22, 2008
A. Goncharov	Carnegie	Infrared spectroscopy of hot dense hydrogen (proposal # 10052)	November 24, 2008
J. Smedley	Brookhaven	Characterization of impurities in diamond	December 1, 2008
T. Tyson P. Gao	New Jersey Institute of Technology	High pressure IR measurements on manganites	December 4-7, 2008
M. Lang F. Zhang	University of Michigan	Phase transitions in minerals induced by ion beams and high pressure: A novel approach in geosciences	January 26, 2009
W. Han	Brookhaven	High-pressure IR study gases storage in boron nitride nanotubes	January 27, 2009
X. J. Chen	Carnegie	High-pressure optical spectroscopy of hydrogen-based electron materials	January 29-February 2, 2009
Amy Lazicki	Carnegie	IR reflectivity of sodium	February 5-7, 2009
B.Yulga S. Tkachev	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high pressure and temperature	February 11-14, 2009
Wendy Panero	Ohio State University	Solubility of two component systems at high-pressures and temperatures	February 16-19, 2009
W. Han	Brookhaven	High-pressure IR Study gases storage in boron nitride nanotubes	February 20, 2009
A. Goncharov	Carnegie	Infrared spectroscopy of hot dense hydrogen	February 24-26, 2009
T. Strobel	Carnegie	Infrared spectroscopy of novel a H_2+SiH_4 compound	March 6-8, 2009
K. Otsuka G. Amulele	Yale University	*In situ* measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR	March 9-13, 2009
W. Han	Brookhaven	High-pressure IR Study gases storage in boron nitride nanotubes	March 18-20, 2009
M. Lang F. Zhang	University of Michigan	Phase transitions in minerals induced by ion beams and high pressure: A novel approach in geosciences	March 24-31, 2009
M. Ma	Graduate University of the Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature	April 2-3, 2009
T. Tyson P. Gao	New Jersey Institute of Technology	High pressure IR measurements on manganites	April 6-10, 2009
G. Yang	Brookhaven	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe	May 26-28, 2009
T. Tyson P. Gao B. Gao	New Jersey Institute of Technology	High pressure IR measurements on manganites	May 28-31, 2009
T. Strobel	Carnegie	Infrared spectroscopy of novel a H_2+SiH_4 compound	June 4-7, 2009
M. Pravica S. Tkachev E. Romano	University of Nevada – Las Vegas	Infrared studies of cyclooctatetraene at high pressure	June 10-11, 2009
W. Han	Brookhaven	High-pressure IR Study gases storage in boron nitride nanotubes	June 12, 2009
S. Garimella	Florida International University	High-pressure studies on group VI metal hexacarbonyls	June 23-25, 2009

M. Lang F. Zhang	University of Michigan	Phase transitions in minerals induced by ion beams and high pressure: A novel approach in geosciences	June 28-30, 2009
J. Smedley	Brookhaven	Characterization of impurities in diamond	July 1, 2009
Michelle Weinberger Jennifer Cizark	Army Research Laboratory/Carnegie	Elastic-plastic transformation of ultrahard materials	July 14-15, 2009
Y. Lee D. Seoung Y. Lee	Yonsei University Korea	High pressure powder diffraction studies of zeolites	July 17-20, 2009
Y. Wang	State University of New York – Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application	July 22, 2009
W. Han	Brookhaven	High-pressure IR study gases storage in boron nitride nanotubes	July 23-24, 2009
H. Liu	National Taiwan Normal University	Infrared studies of strongly correlated systems at high pressure	August 17-22, 2009
K. Otsuka G. Amulele	Yale University	*In situ* measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR	August 24-26, 2009
X. Chen	Carnegie	High-pressure optical spectroscopy of hydrogen-based electron materials	August 27-30, 2009

References

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