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

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

YEAR SIX ANNUAL REPORT

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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 selected 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 spectroscopic 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.
available at Carnegie, that have led to the recent breakthrough in ultratough diamond\textsuperscript{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 Zr. 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.](image)

- 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 Synchrotron 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
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 Velisavljevic** (LANL) showed that the pressure of the \(\alpha-\omega\) 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.\(^4\)

- CDAC graduate student **Arianna Gleason** (Berkeley) showed that it is 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

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**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.”

**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.\(^4\)
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 SiH₄-H₂ system, postdoctoral fellow **Tim Strobel (Carnegie)** prepared the compound SiH₄(H₂)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 H₂.⁶

- Orientation-dependent SFG spectroscopy 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 °C 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 6.** Crystal structure of SiH₄(H₂)₂. Blue spheres represent the positions of the SiH₄ molecules on an fcc lattice, with the red spheres showing the rotationally averaged positions of H₂ molecules.⁶

**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.  

• 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).  

• 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. 

• 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.

• 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. 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.

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

![Figure 10. Left) Pilatus detector images of Fe$_2$O$_3$ at ambient (top) and 60 GPa (bottom). Right) Fe $K_{\beta}$ XES spectra of Fe$_2$O$_3$ at various pressures. The disappearance of the $K_{\beta}$ satellite peak, indicating a high- to low-spin transition, is cleanly resolved.](image)

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 Amorphization in Superconducting $\text{FeSe}_{0.5}\text{Te}_{0.5}$—The phenomenon of pressure-induced amorphization in the superconducting compound $\text{FeSe}_{0.5}\text{Te}_{0.5}$ has been studied to 27 GPa. Using synchrotron diffraction techniques, the Alabama group has found that the ambient pressure tetragonal phase ($P4/nmm$) 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 $\text{Fe(Se,Te)}_4$ tetrahedra under compression attributed to a kinetic hindrance to a stable phase and is likely to impact its superconducting properties under high pressures. Figure 11 shows the integrated x-ray diffraction profile (intensity versus $2\theta$) for $\text{FeSe}_{0.5}\text{Te}_{0.5}$ 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 $\text{FeSe}_{0.5}\text{Te}_{0.5}$ and a copper (Cu) pressure marker at various pressures. All spectra have been collected at the HPCAT sector using an x-ray wavelength $\lambda = 0.3875$ 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.
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$_{30}$Pd$_{70}$, but a greater Pd concentration stabilizes the ferromagnetic state, suppressing thermal Invar behavior. The composition Pd$_3$Fe does not show thermal Invar behavior. Two years ago, in CDAC-funded work, graduate student Mike Winterrose discovered pressure-induced Invar behavior in Pd$_3$Fe 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$_3$Fe 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$_3$Fe, 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$_3$Fe 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$_3$Fe was under pressure, and the Invar transition was found. Figure 13 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.

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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.  

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. 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, SiH₄(H₂)₂, that displays anomalously strong intermolecular interactions. 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 SiH₄ and eight H₂ molecules per unit cell (Fig 6). Spectroscopic measurements on this compound show the molecular H₂ 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 D₂ readily exchange with protons of SiH₄ to create H-D and Si-D stretching modes.

The unique features observed in this system suggest a range of previously inaccessible intermolecular interactions in H₂-bearing molecular systems and a potential new class of dense low-Z materials. Additionally, the combination of SiH₄ (which was previously predicted 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 Transformations 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. 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 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. 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
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$_2$O$_3$ has been measured at 32 GPa in a laser-perforated DAC using a monochromatic, micro-focused high-energy x-ray beam.\textsuperscript{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$_4$S$_3$ 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$_4$S$_3$ cages, is shown to diminish in intensity at high pressure. A kinetic effect is also observed.

\textit{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.

\textbf{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 $\beta$-tin
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 stratural properties at high pressures and temperatures. 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 $T_c \sim 1232$K and pressure $P_c \sim -12kB$).

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
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.

**Figure 18.** Pressure-volume isotherms of liquid silicon show a “van der Waals loop” below \( T_c \sim 1232 \) K. *Inset: Panchapakesan Ganesh (Carnegie).*

**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, and the first observation of the transition to the newly discovered structure. 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. 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.
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 orthoensostatite to high-pressure clinoenostatite transformation also broadly matches depths of the X discontinuity, but requires depleted and orthoensostatite-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$_2$O can displace the transition pressure of low-clinoenastatite to high-clinoenastatite by up to 2 GPa (60 km), similar to previous quench experiments on the orthoensostatite to high-clinoenostatite 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, 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
undergo $ns^1$ to $(n-1)d^1$ electronic transitions, where $n$ is the primary quantum number of the outer shell electron. 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.

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.

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.

**Figure 21.** Eutectic melting at 100 GPa in the Fe-FeS 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 FeS are marked on the bottom based on the lattice parameters $a = 8.205 \pm 0.014 \text{ Å}$ and $c = 4.122 \pm 0.011 \text{ Å}$ 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 FeS coexist. When the temperature was increased to 2600 K both phases melted simultaneously, indicative of melting close to the eutectic composition.

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 Fe₃S. 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. 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 Fe₁₀₅Te** – 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 Fe₁₀₅Te by combining synchrotron x-ray and neutron diffraction techniques. 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,
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. 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. 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 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.](image)

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-Si3N4.31-32 Previous measurements on TiO2 show that the highest-pressure phase OII is quenchable to ambient pressure at least at cryogenic temperatures. Previous experiments on high-pressure TiO2 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: $Pbcb$), 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 $\rightarrow$ CB $\rightarrow$ 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 TiO2 under both high pressure and temperature using both DAC experiments and ab-initio computations has been constructed (Fig. 24).

Zirconia (ZrO2) and hafnia (HfO2) 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 TiO2. 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 ZrO2 and HfO2 undergo the following sequence: baddeleyite $\rightarrow$ OI $\rightarrow$ OII34 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 ZrO2 and HfO2 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](image-url)
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 25. X-ray diffraction patterns for $Y_3Fe_5O_{12}$ showing transformation from the garnet structure to orthorhombic perovskite ($Y_0.75Fe_{0.25})FeO_3$ 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.

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\textsuperscript{46-50} and high hardness.\textsuperscript{51} Because of these properties, osmium is a potentially

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**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.\textsuperscript{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/mm² to 2000-3000 kg/mm² at the expense of the bulk modulus.\textsuperscript{52-53} Carbon\textsuperscript{44} and nitrogen are also predicted to enhance osmium’s mechanical properties.\textsuperscript{54} In addition, a high-temperature high-pressure EOS for Os was measured using \textit{in situ} x-ray diffraction and a multianvil apparatus\textsuperscript{19} up to 15 GPa and 1273 K. The objective of current 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 \textit{P-T} experiments on Os metal using monochromatic x-ray diffraction with \textit{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, \textit{NH}_4\textit{NO}_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 \textasciitilde6 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.\textsuperscript{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 ($P_{\text{mmn}}$), with two molecules per unit cell, from \textasciitilde0.4 GPa to 25 GPa, with an initial density of 1.726 g/cm³. The static high pressure data were used, along with knowledge of the thermodynamic parameters, to develop a

![Figure 28. Static \textit{P-V} experimental data and 3rd-order Birch-Murnaghan semi-empirical EOS fit for ammonium nitrate.](image)
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 L12 ordered Pd3Fe. This is the first study of lattice dynamics at pressures relevant to the pressure-induced Invar effect. The 57Fe 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 57Fe 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.

Rather similar behavior to L12 ordered Pd3Fe was found for disordered Pt3Fe – the results are quite similar to those published earlier this year for ordered Pd3Fe. 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 $-1.7 \text{ kJ/atom}$, 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. Such laboratory measurements are crucial for interpreting seismological observations of Earth’s interior, including the rich data provided by seismic tomography, 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.

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 gasketed diamond-anvil cell with a 4:1 methanol:ethanol pressure-transmitting medium. Results 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), 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 \( \theta \), 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. 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, 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: \( \theta = 180^\circ \)) and reflection geometries (middle two spectra: \( \theta' = 110^\circ \)), 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.

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. 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. 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. 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 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.

Elastic Moduli and Strength of Nanocrystalline Cubic BC₂N — 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 (cBN), 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-BC₂N) 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, \( K_0 = 276 \pm 20 \) GPa with a fixed pressure derivative, \( K_0' = 3.4 \) at \( \psi = 54.7^\circ \), 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-BC₂N sample could support a
maximum differential stress of \( \sim 38 \) GPa when it started to yield at \( \sim 66 \) GPa under uniaxial compression (Fig. 33). Moreover, the aggregate elastic moduli of the nanocrystalline \( c \)-BC\(_2\)N 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 \( (K_0) \) and its pressure derivative \( (K_0') \) were determined for Kel-F 800 through a Murnaghan equation-of-state (EOS) analysis (overlaid in Fig. 34b) giving \( K_0 = 7.50 \) GPa and \( K_0' = 10.0 \). For comparison, recent dilatometry results for Kel-F 800 at 33 °C are overlaid in Fig. 34b and analyzed similarly to give a \( K_0 = 2.8 \) GPa and \( K_0' = 30.0 \). The discrepancy by nearly a factor of three for separate \( K_0 \) and \( K_0' \) 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 \( K_0 \)) compared with static, dilatometric measurements and (2) disparate pressure ranges used

**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.

**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 dilatometry. 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 ($\lambda$) of muscovite mica as a function of hydrostatic pressure. Picosecond interferometry and time-domain thermoreflectance provide high precision measurements of C33 and $\lambda$, respectively, of micron-sized samples within a DAC; $\lambda$ 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 $\lambda$ 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. 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$_2$O 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.

**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-developed 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 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. 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 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. 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, 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 1200 K. 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 12.3 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.](image)

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 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 and a feature to allow for turbostratic disorder. 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.\(^8\) 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 MA\(_{2n}\)Si\(_3\)O \((M=\text{Rb, K})\) 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.](image)

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appear very similar to the defects that occur in shocked steels (Fig. 38a) with the development of twins upon $\alpha$ to $\varepsilon$ 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.

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 instrument’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 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.

Figure 40. In situ heating experiments with HIPPO: Pole figures of quartzite (a) 500$^\circ$C, (b) 625$^\circ$C, (c) 500$^\circ$C (after phase transformation). Note the perfect texture memory. Equal area projection.$^{85}$
The question of texture memory and variant selection is a hot topic in materials science and only recently, with \textit{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.\textsuperscript{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 \textbf{LANSCE} a cold-rolled sample of pure (#520-1S) uranium\textsuperscript{87} shows indeed a strong texture (Fig. 41). The texture changes somewhat during heating to 500ºC. Rapid grain growth occurs above 600ºC and in most cases it was not possible to determine a meaningful texture pattern. When the sample was just barely heated above the $\beta$-transition (677°C) the $\beta$-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 $\beta$–phase, a $\gamma$ 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 \textbf{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 \textbf{LANL} (J. Bingert and D. Brown), \textbf{APS} (Yanbin Wang) and \textbf{Berkeley}.

\textbf{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.\textsuperscript{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 $\mu$strains) than in a tectonically deformed quartz (600-1200 $\mu$strains). This figure also establishes that the observations are real by comparing deformed quartz with an ideal single crystal, where values of 400 $\mu$strains 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. 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:

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

where $P$ is 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. 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. 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 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 standard 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.](image)

**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, the Fultz group at Caltech finds 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.

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.

**Figure 46.** Iron partial phonon density of states of ErFe$_2$ as a function of temperature, showing a substantial shift towards lower energies.

**Figure 47.** Nuclear forward scattering spectra from ErFe$_2$.

**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 $\alpha \rightarrow \omega$ structural phase transition. The transformation from a ductile $\alpha$- to a brittle $\omega$-phase is observed at ~8 GPa for Ti, ~8 GPa for Zr, and ~38 GPa for Hf. The $\alpha \rightarrow \omega$ 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.

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. 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
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 $\alpha \rightarrow \omega$ 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 $\alpha \rightarrow \omega$ 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. 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.

**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 $\text{AMe}_2\text{O}_4$, 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, Fe₂TiO₄ or Fe²⁺[Fe³⁺,Ti]₂O₄ has been studied in detail using CDAC beamtime in collaboration with Professor Takamitsu Yamanaka.

Recently, novel iron arsenides AFeAsO₁₋xFₓ (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 SrFe₂As₂, and CaFe₂As₂, using X-ray emission spectroscopy and X-ray diffraction have been performed.

AFe₂As₂ and Fe₂TiO₄ 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 Fe₂TiO₄ (Fig. 49). The transition occurs much earlier than the structural transition (at 7 GPa) and in Fe²⁺ octahedral sites.

High-Pressure X-Ray Absorption Spectroscopy of Fe₂O₃ – As an archetypal transition metal oxide, hematite (Fe₂O₃) 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 Al₂O₃ structure and is an antiferromagnetic Mott insulator, with five 3d electrons in the high-spin state. Upon increasing pressure, its FeO₆ octahedron is progressively distorted, until at 40-70 GPa, the structure of hematite changes to the Rh₂O₃-II type. Along with the structural change, hematite becomes a metal with a low-spin state. Such electronic and magnetic phase transitions have been demonstrated in a number of studies: Pasternak has conducted Mossbauer spectroscopy on Fe₂O₃ at room temperature up to 82 GPa and found that the non-magnetic component in the spectrum appears from 50-55 GPa. Badro used x-ray emission spectroscopy to indicate the high spin and low spin state of Fe₂O₃ under different pressure.

The Mao group at Stanford has measured the x-ray absorption spectra of Fe₂O₃ up to 64 GPa, and for the first time, experimentally resolved the crystal field splitting of the 3d 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 1s - t₂g and 1s - e₅ excitations. Preliminary DFT calculations were also carried out to examine the electronic structure of the 3d band. More theoretical work is needed to understand the high pressure metallic state of Fe₂O₃.

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

**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 (La0.75Ca0.25MnO3) 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(Sc1/2Nb1/2)O3 (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...
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 (Pm). 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 Pm = 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 XH4 (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 SiH4 at 60 GPa.

Silane (SiH4) 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 P21/c in the pressure range of 10 and 27 GPa. The Carnegie group also provided the optical evidence for the metallization of SiH4 at pressure of 60 GPa. The electronic and lattice dynamical properties of compressed solid SiH4 in the pressure range up to 300 GPa were

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**Figure 53.** Left) The energetically favorable Cmca structure for SiH4. Right) Calculated (a) logarithmic average phonon frequency $\omega_{\text{log}}$, (b) electron-phonon coupling parameter $\lambda$, and (c) superconducting transition temperature $T_c$ of the Cmca phase of metallic SiH4 with increasing pressure.
calculated with density functional theory.\textsuperscript{101} Two energetically preferred insulating phases with $P_\text{21}/c$ and $Fd\text{d}2$ symmetries at low pressures were found, and it was demonstrated that the $\text{Cmca}$ 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 \textit{ab initio} first-principles calculations of the structural properties, GeH$_4$, within the molecular phase.\textsuperscript{102} They found that the $P_\text{21}/c$ structure evolves following a group-subgroup relation to the extended $C\text{mmm}$ structure with an insulator-metal transition at 15 GPa, followed by two metallic structures with the $P_\text{21}/m$ and $C_2/c$ 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$_2$Sr$_2$Ca$_2$Cu$_2$O$_{10+\delta}$ (Bi2223). We found that $T_c$ first increases with pressure and then decreases after passing through a maximum.\textsuperscript{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,
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) Ti42Zr24Cu15.5Ni14.5Be4 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 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).](image)

![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.](image)
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.

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).

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 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$_2$O) 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-CaF₂. 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 D₂O to avoid IR wavelengths where atmospheric water interferes. There is clearly a more prominent dangling OD at diamond interfaces than at CaF₂ interfaces. Work is underway to extend these measurements to different polarization conditions.

Aqueous Oxidation of Re Metal in Supercritical H₂O-O₂ 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 H₂O or O₂, even at extreme P-T conditions. At Carnegie, Raja Chellappa has found that that Re undergoes a series of reactions with H₂O-O₂ mixtures at pressures less than 1 GPa at room temperature, in a DAC. The reaction product (identified using Raman spectroscopy) was primarily perrhenic acid (HReO₄) which in the presence of water forms a combination of rhenium oxide hydrates: ReO₄•(H₂O)₂ and HReO₄•H₂O. The observed oxidation of Re in H₂O-O₂ 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 (ReO₄⁻) is a window to its radioactive analogue technetium (Tc) found in high level nuclear wastes.

Figure 59 shows reaction products of rhenium in H₂O-O₂ mixtures at room temperature and the Raman signatures of HReO₄ are identified in the spectra. In one of the samples, HReO₄ 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 peroxy derivative: [ReO(O₂)₂OH]₃H₂O. Extending classical metal corrosion behavior in H₂O, the electrochemical oxidation of Re is due to reduction of dissolved O₂ to form hydroxyl ions in essentially a neutral starting mixture. The formation of perrhenic acid can be represented by the following overall reaction scheme:
\[ 2 \text{Re(s)} + \frac{7}{2} \text{O}_2(g) + \text{H}_2\text{O}(l) \rightarrow 2 \text{HReO}_4(l) \quad \Delta G_f = -0.7 \text{kJ/mole.} \quad (1) \]

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

\[ E^\circ (\text{Re}/\text{ReO}_4^{--}) = -0.367 \text{V}. \]

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)

\[ 3 \text{O}_2(g) + 6 \text{H}_2\text{O}(l) + 12 \text{e}^- \rightarrow 12 \text{OH}^- \quad (\text{aq}) \quad E^\circ = +0.40 \text{V} \quad (2) \]
\[ \text{Re(s)} + 8 \text{OH}^- (\text{aq}) \rightarrow \text{ReO}_4^{--} (\text{aq}) + 4 \text{H}_2\text{O}(l) + 7 \text{e}^- \quad E^\circ = +0.58 \text{V} \quad (3) \]

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\text{2}O-O\text{2} mixtures.

**Hydrogen Interactions with Polymerica B-N-H Compounds** – Ammonia borane [NH\text{3}BH\text{3}, AB] is a prototypical Lewis acid (NH\text{3})-Lewis base (BH\text{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\text{2} in an exothermic reaction to form polyaminoborane [(NH\text{2}BH\text{3})\text{n}, PAB] at temperatures below 120 °C and decomposes further to polyiminoborane [(N\text{HBH})\text{n}, 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\text{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\text{2} interactions with AB and resulting AB-H\text{2} complexation behavior in the 6-10 GPa range.\textsuperscript{113} This has now been extended to demonstrate reactions of H\text{2} and D\text{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\text{2} and D\text{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\text{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\text{2}, and HD were obtained at 3.4 GPa. Weak, low frequency shoulders on the Q\text{1}(1) vibrations of H\text{2} and HD are also observed. On cooling to 27 °C, these low frequency peaks gain some intensity and are seen ~70 cm\textsuperscript{-1} lower than the respective Q\text{1}(1) vibrations at 4.8 GPa. Sharp peaks are seen in the 2370-2450 cm\textsuperscript{-1} range coinciding with the ν(BH\text{2}) region and are assigned as ν(NDH\text{2}) while the broad peak at ~1750 cm\textsuperscript{-1} is assigned as ν(BD\text{2}). Under high pressure D\text{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\text{2} is released with formation of a PIB-(H\text{3}, HD, D\text{2}) complex that is retained on cooling to room temperature, (b) heating cycle of AB-D\text{2} mixture.](image)
phases as seen by the formation of HD. It is possible that D2 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$_3$BH$_3$, the group of Wendy Mao at Stanford has studied NH$_3$BH$_3$ in the presence of excess H$_2$ pressure from ambient to 20.3 GPa and discovered a novel solid phase NH$_3$BH$_3$(H$_2$)$_x$, where $x \sim 1.3-2$. X-ray diffraction indicates that the new phase has a different crystal structure from pure NH$_3$BH$_3$ at the equivalent pressure.$^{114}$ This new phase forms slowly at 6.2 GPa, but the reaction rate is enhanced by crushing the NH$_3$BH$_3$ 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$_3$BH$_3$ interactions with H$_2$. In order to determine the amount of H$_2$ in NH$_3$BH$_3$-H$_2$, the pressure was measured by ruby fluorescence, and the volume for the free H$_2$ and NH$_3$BH$_3$ 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$_3$BH$_3$-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$_3$BH$_3$, 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 $v/dP$ for B-H stretching modes is $4.5 \times 10^3$ GPa, and B-H...B bridge $3.4 \times 10^3$ 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 (C₂-C₄ 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 H₂ vibron (gray line) confined in decaborane vs. free H₂ vibron (black line), taken at 3.7 GPa.](image)

**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.

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.\textsuperscript{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.

\textbf{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 Ce₃Al 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.\textsuperscript{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.\textsuperscript{119-121}).
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
Jane Kanitpanyacharoen
Lowell Miyagi

Berkeley (Wenk): Kurt D. Morgan
Jane Kanitpanyacharoen
Lowell Miyagi

Alabama (Vohra): Gopi Samudrala
Andrew Stemshorn

Illinois (Dlott): Kathryn Brown
Aaron Lozano

Arizona State (Yarger): Samrat Amin
Keri McKiernan (undergraduate)

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
Sabra 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 University, where she has continued to work in the area of high-pressure materials science. Velisavljevic 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.

**Student Publications**


**Student Presentations**


Amin, S. A., E. Soignard, M. Guthrie, Q. Mei, C. J. Benmore, and J. L. Yarger, Probing the structure of amorphous compounds at high pressure using high-energy x-rays, High Pressure Synchrotron Science Workshop (Argonne, IL, May 6-8, 2009).

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


Barkley, M. C. and R. T. Downs, The structure determination of the high-pressure analog of 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., Surface-enhanced Raman scattering at high pressure, Gordon Conference on Vibrational Spectroscopy (South Hadley, MA, August 4-8, 2008).

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).


Chen, B., G. Bartov, D. Cahill, and J. Li, Thermal conductivity of H$_2$O up to 11 GPa using time-domain thermoreflectance method in diamond anvil cell: Insights into icy planetary bodies, Geological Society of America North-Central Section, 43rd Annual Meeting (Rockford, IL, 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., Z. Mao, S. R. Shieh, Y. Meng, V. B. Prakapenka, and T. S. Duffy, Synthesis and equation of state of pervoskites in the Mg$_9$Al$_5$Si$_5$O$_{12}$-Fe$_5$Al$_5$Si$_5$O$_{12}$ system, Eos Trans. AGU Fall Meet., Suppl., 89 (2008).


Guthrie, M., E. Soignard, C. J. Benmore, S. A. Amin, and J. Yarger, X-ray diffraction from liquid water up to ~5 GPa, Joint AIRAPT-22 and HPCJ-50, International Conference on High Pressure Science and Technology (Odaiba, Tokyo, Japan, July 26-31, 2009).

Halevy, I., M. Winterrose, J. Munoz, L. Mauger, and B. Fultz, Pressure-induced electronic transition and invar behavior in Cu$_3$Au structure Pd$_3$Fe and Pd$_3$(Fe$_2$U$_{0.8}$), Actinides 2009 (Lawrence Berkeley National Laboratory, Berkeley, CA, 2009).

Halevy, I., A. T. Yue, L. Mauger, J. Munoz, J. Hu, M. Lerche, and B. Fultz, Pressure-induced invar behavior in Pd$_3$Fe and Pd$_3$(U$_{0.5}$Pd$_{0.5}$), 39èmes journées des actinides (La Grande-Mont, France, March 28-31, 2009).


Miyagi, L., In-situ laser heating and pressure change with radial diffraction, *California High Pressure Science Observatory Meeting* (University of California - Berkeley, Berkeley, CA, June 3, 2008).

Miyagi, L., Deformation of MgSiO3 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., Understanding deformation in the deep Earth through texture and anisotropy, Geophysical Laboratory Seminar (Carnegie Institution of Washington, Washington, DC, March 2, 2009).  
Miyagi, L., Understanding deformation in the deep Earth through texture and anisotropy, Princeton University (Princeton, NJ, March 9, 2009).  
Miyagi, L., Understanding deformation in the deep Earth through texture and anisotropy, University of Colorado - Boulder (Boulder, CO, March 12, 2009).  
Miyagi, L., Understanding deformation in the deep Earth through texture and anisotropy, California High Pressure Science Observatory Meeting (University of California - Berkeley, Berkeley, CA, April 21, 2009).  
Miyagi, L., Deformation and texture development in deep Earth mineral phases: Implications for deep Earth anisotropy and dynamics, University of California - Berkeley (Berkeley, CA, August 25, 2009).  
Oelker, E., High pressure investigations of vitreous BeF₂ (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 BeF₂, CDAC Winter Workshop 2009 (Argonne, IL, February 27-28, 2009).  
Seagle, C. T., Liquidus temperatures in the iron-sulfur system and melting of Fe₃S at high pressure (invited), American Geophysical Union Fall Meeting (San Fransisco, CA, December 10-14, 2008).  
Seagle, C. T., Synchrotron infrared reflectivity of iron at high pressure, American Geophysical Union Fall Meeting (San Fransisco, CA, December 10-14, 2008).  
Seagle, C. T., Far infrared reflectivity of the FeO-MgO solid solution series (invited), CDAC Winter Workshop 2009 (Argonne, IL, February 27-28, 2009).  


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


Winterrose, M. L., High pressure invar behavior and magnetism in Pd_{3}Fe (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).


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 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.

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
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 NH₃-H₂O-H₂ 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 semifinalist 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 polymers with Muhetaer Ahart, and Claire Barkett extended the work begun by Jaqueline Rivera on Fe,Al solid solutions.

2008:

Jaqueline Rivera, César Chávez Public Charter High School, Washington, DC
*Synthesis of Solid Solutions in the Fe₂O₃-Al₂O₃ System*

Manchali Madduri, Thomas Jefferson High School, Alexandria, VA
*High-Pressure Studies of H₂ in Crown Ethers*

Maura James, Convent of the Sacred Heart, Greenwich, CT
*Raman Spectroscopic Investigation of the H₂O-NH₃-H₂ System*
2009:

Claire Barkett, Good Counsel High School, Olney, MD
Low-Temperature Synthesis of Fe-Bearing Solid Solutions

Emily Sandford, Glenelg Country School, Ellicott 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.
Laura Lewis
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
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Centre National de la Recherche Scientifique, France
C. Dubourdieu
Chinese Academy of Science
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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
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H. Niu
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. Zhao
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
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H. Q. Lin
J. L. Wang
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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
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P. Cervantes
Katie M. Chynoweth
Colorado School of Mines
Carolyn A. Koh
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Z. Wu
Columbia University
C. Y. Chin
D. Walker
Cornell University
W. Bassett
Z. Wang
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B. G. Aitken
Dalhousie University, Canada
S. A. Bonev
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DePaul University
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DESY, Germany
H. P. Liermann
Drexel University
M. W. Barsoum
DTC Research Centre, UK
D. Fisher
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P. Gillet
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F. Langenhorst
Geoforschungzentrum, Potsdam
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H. J. Reichmann
F. Schilling
S. Speziale
R. Wirth
George Mason University
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I. A. Trojan
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S. Nakano
Institute for Problems of Chemical Physics, Chernogolovka Russia
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National Aerospace Laboratories,
India
A. K. Singh
National Cheng-Kung University,
Taiwan
J. Kung
National Institute for Materials Science,
Japan
T. Kikegawa
S. Nakano
S. Nimori
T. Sekine
T. Taniguchi
National Institute of Standards and Technology
B. Burton
E. Cockayne
T. Jenkins
J. Leão
S. Prosandeev
National Laboratory of Superhard Materials,
Jilin
C. Gao
National Museum of Natural History,
Smithsonian Inst.
Elizabeth Cotrell
National Research Council, Ottawa
D. J. Klug
National Synchrotron Radiation Research
Center, Taiwan
Y. Q. Cai
C. C. Chen
C. T. Chen
P. Chow
N. Hiraoka
E. P. Huang
H. Ishii
I. P. Jarringe
C. Kendziora
National University of Singapore
Y. P. Feng
Naval Research Laboratory
J. E. Butler
S. J. Charles
J. L. Feldman
New Jersey Institute of Technology
J. P. Carlo
Z. Chen
C. Cui
M. A. DeLeon
P. Gao
Y. Qin
T. Tyson
Z. Zhong
New Mexico State University
B. Kiefer
Northern Illinois University
D. E. Brown
M. R. Frank
S. J. Maglio
M. van Veenendaal
Northwestern University
K. Brister
D. Brown
C. M. Holl
Y. C. Tseng
Nuclear Research Center-Negev,
Israel
I. Halevy
Oak Ridge National Laboratory
D. Abernathy
Michelle Buchanan
O. Delaire
Oak Ridge National Laboratory, cont’d.
M. Guthrie
G. E. Ice
B. C. Larson
M. Loguillo
M. Lucas
Jamie J. Molaison
A. F. Moreira dos Santos
M. Stone
C. A. Tulk
J. Z. Tischler
Okayama University, Japan
H. Fuki
Ohio State University
K. Driver
D. M. Reaman
P. L. Rios
J. W. Wilkins
Osaka University
Y. Nakamoto
T. Okada
K. Shimizu
Pennsylvania State University
A. C. T. van Duin
Physikalisches Institut, Germany
K. J. Choi
G. Guenthrodt
Purdue University
P. C. Doerschuk
S. King
Rensselaer Polytechnic Institute
E. B. Watson
Royal Institution, London
P. McMillan
Royal Institution of Technology, Sweden
A. Delin
B. Johannson
V. Kanchana
V. G. Kucherov
G. Vaitheeswaran
Russian Academy of Sciences
A. V. Ivanov
A. A. Kaminskii
I. S. Lyubutin
S. G. Ovchinnikov
V. A. Ralchenko
Rutgers University
S. W. Cheong
Martha Greenblatt
S. B. Kim
M. V. Lobanov
C. Zhang
St. John Fisher College
Kristina M. Lantzky
Saitama University, Japan
Y. Saiga
Sam Houston State University
B. Friedman
Savannah River National Laboratory
D. Anton
Polly Berseth
Ashley C. Stowe
R. Zidan
School of Physics & Astronomy, Tel Aviv, Israel
A. Milner
M. P. Pasternak
Scripps Oceanographic Institute
I. Gan
I. Gertsman
J. E. Johnson
T. Lin
Seoul National University, Korea
S. K. Lee
Sichuan University, China
H. Dong
D. He
J. Wang
Simon Fraser University, Canada
Y. Bing
Z. G. Ye
Soliel, France
R. Fourme
South China University of Technology
Y. Pan
Southwest Jiaotong University, China
Lewei Deng
S. M. Hong
Spring-8, Japan
A. Q. R. Baron
Y. Ohishi
S. Tsutsui
Stanford University
Maria Baldini
Steacie Institute for Molecular Science, Canada
S. Patchkovskii
Stanford University
G. E. Brown
J. R. Groves
SUNY-Stony Brook
J. Chen
J. Hu
Jennifer King
B. Li
L. Li
C. D. Martin
J. B. Parise
L. Wang
D. J. Weidner
Technological Institute for Superhard and Novel Carbon Materials, Russia
V. Denisov
M. Popov
N. R. Serebryanaya
Technical University of Berlin, Germany
H. J. Eichler
H. Rhee
Technical University of Denmark
K. Stahl
Texas Christian University
R. Senter
Texas Tech University
J. Chaudhuri
D. Hou
R. Lee
V. Levitas
L. Nyakiti
J. Sandhu
J. Rasty
A. White
Tohoku University, Japan
D. X. Li
E. Ohtani
Tokyo Institute of Technology, Japan
K. Hirose
T. Kombayashi
Umeå University, Sweden
B. Sundqvist
T. Wåberg
Universidad Complutense de Madrid, Spain
J. Santamaria
M. Varela
Universidad de La Laguna, Spain
J. Lopez-Solano
A. Mujica
A. Muñoz
S. Radescu
P. Rodriguez-Hernandez
Universidad de Oviedo, Spain
Julia Contreras
Università di Roma Tre, Italy
G. Della Ventura
Università di Trento, Italy
L. Lutterotti
G. Mariotto
Università G. D’Annunzio, Italy
Gianluca Iezzi
Universidad de Valencia, Italy
C. Ferrer-Roca
N. Garro
J. Pellicer-Poers
A. Segura
Universität Bonn, Germany
Winfried Kockelmann
N. Zotov
Universitat de València, Spain
D. Errandonea
J. Ruiz-Fuertes
Universitat Jaume I, Spain
A. Beltrán
L. Gracia
Universitat Politècnica de València, Spain
F. J. Manjón
Université Catholique de Louvain, Belgium
X. Gonze
Université de Picardie, France
P. Toledano
Université des Sciences et Techniques de Lille, France
M. Roskosz
Université Lille 1, France
S. Merkel
Université Paris Nord, France
O. O. Kurakevych
V. L. Solozhenko
Université Parisé, France
P. Cartigny
University College London, UK
D. Dobson
University of Aarhus, Denmark
A. Svane
University of Alaska
T. Trainor
University of Arizona
W. B. Hubbard
D. Krishnamoorthy
A. Krishnamurthy
M. Origlieri
C. Prewitt
University of Arkansas
A. Khanna
University of Bristol, UK
H. Darwish
A. E. Mora
J. W. Steeds
University of California, Berkeley
A. A. Correa
G. Ischina
W. B. Montgomery
B. Militzer
D. Prendergast
D. Spaulding
Caterina E. Tommaseo
M. Voltoni
Z. Wu
University of California, Davis
Ilke Arslan
N. Browning
S. J. Gaudio
D. M. Krol
B. Maddox
V. Ortalan
W. E. Pickett
S. Savrasov
R. T. Scalettar
S. Sen
S. Soyer Uzun
University of California, Los Angeles
R. Kundargi
Sarah Tolbert
University of California, Riverside
H. Green, II
Larissa Dobrzheiskaya
J. Zhang
University of California, San Diego
J. J. Hamlin
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. Guilhaume
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. Lakshitanov
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
A. K. Speck

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
X. Ke
E. Kim
R. S. Kumar
M. K. Jacobsen
Kristina Lipinska-Kalita
Patricia E. Kalita
J. McClure
M. Nicol
T. Pang
Z. Quine
E. Romano
Y. Shen
W. Stanberry
Elizabeth A. Tanis
I. Tran
O. Tschauner
B. Yulga

University of Nevada-Reno
S. Chandra
W. M. Chieh
A. M. Covington
J. C. Fallas
V. K. Kamisetty

University of New Mexico
C. Agee
P. Li

University of Northern Florida
L. V. Gasparov
D. Arenas

University of Oslo, Norway
K. Bjørlykke
J. Jahren
N. H. Mondol

University of Ottawa, Canada
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

University of Pittsburgh
J. K. Johnson

University of Saskatchewan
N. Chen
J. S. Tse

University of Science and Technology of China
Y. Xie

University of Sydney, Australia
X. Liao

University of Tennessee
M. Anand
L. A. Taylor

University of Texas, Arlington
J. B. Goodenough
Y. F. Lin
S. Sharma

University of Tokyo
K. Matsubayashi
M. Takigawa
Y. Uwatoko
T. Yagi

University of Toronto
M. Fujihsaki

University of Tsukuba
A. Hushur
S. Kojima
K. Matsuishi

University of Warsaw, Poland
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
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).

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

Figure 71. CDAC visitors to Carnegie. From left: Alexander Gavriluk (Institute for High Pressure Physics), Sylvia-Monique Thomas (Northwestern University), Kai Landskron (Lehigh University), and Henry Scott (Indiana University – South Bend).
<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Activity</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Natascha Filipouitch</td>
<td>Stanford University</td>
<td>Carbon sequestration</td>
<td>November 24-28, 2008</td>
</tr>
<tr>
<td>Shibing Wang, Ling Yu Lin</td>
<td>Stanford University</td>
<td>Raman lab experiments</td>
<td>November 24-28, 2008</td>
</tr>
<tr>
<td>A. Kyono</td>
<td>University of Tsukuba</td>
<td>Work with Takamitsu Yamanaka</td>
<td>December 1-5, 2008</td>
</tr>
<tr>
<td>R. Boehler</td>
<td>Max Planck Mainz</td>
<td>Visit with Russell Hemley</td>
<td>January 7-10, 2009</td>
</tr>
<tr>
<td>Sylvia-Monique Thomas</td>
<td>Northwestern University</td>
<td>Optical absorption studies of high-pressure hydrous materials</td>
<td>January 7-30, 2009</td>
</tr>
<tr>
<td>F. Elkin</td>
<td>Institute for High Pressure Physics, Russia</td>
<td>Synchrotron x-ray diffraction, spectroscopy of correlated materials, and transport measurements in DAC</td>
<td>February 5, 2009 -</td>
</tr>
<tr>
<td>Yu Lin</td>
<td>Stanford University</td>
<td>Research with Ho-kwang Mao</td>
<td>February 23-26, 2009</td>
</tr>
<tr>
<td>C. C. Kao</td>
<td>NSLS</td>
<td>Talk on “New developments at the National Synchrotron Light Source”</td>
<td>February 25, 2009</td>
</tr>
<tr>
<td>Michelle Weinberger</td>
<td>Army Research Laboratory</td>
<td>Work on the mechanical behavior of ultrahard and ultra-incompressible materials under extreme conditions</td>
<td>March 5, 2009-</td>
</tr>
<tr>
<td>A. Kyono</td>
<td>University of Tsukuba</td>
<td>Crystallography work</td>
<td>March 13, 2009-December, 2009</td>
</tr>
<tr>
<td>E. Alp</td>
<td>Advanced Photon Source</td>
<td>High resolution inelastic x-ray scattering under pressure: Phonons, sound velocity, magnetism and local structure</td>
<td>March 24, 2009</td>
</tr>
<tr>
<td>Veronica Vaida</td>
<td>University of Colorado</td>
<td>Visit with Russell Hemley</td>
<td>April 8, 2009</td>
</tr>
<tr>
<td>C. Tulk</td>
<td>Oak Ridge National Laboratory</td>
<td>Sample Loading</td>
<td>April 8, 2009</td>
</tr>
<tr>
<td>K. Lokshin</td>
<td>University of Tennessee</td>
<td>Sample preparation for high pressure transport measurements in nickelates</td>
<td>April 27-May 1, 2009</td>
</tr>
<tr>
<td>Maaike Kroon</td>
<td>Delft University, Netherlands</td>
<td>Raman system to look some preloaded methane-hydrogen clathrate samples in DAC</td>
<td>May 11-13, 2009</td>
</tr>
<tr>
<td>A. Gavriliiuk</td>
<td>Institute for High Pressure Physics</td>
<td>Correlated electronic materials under high pressure</td>
<td>May 11-June 5, 2009</td>
</tr>
<tr>
<td>H. Scott</td>
<td>Indiana University – South Bend</td>
<td>CO2 gas loading</td>
<td>May 27-29, 2009</td>
</tr>
<tr>
<td>K. Landskron</td>
<td>Lehigh University</td>
<td>Nano-materials synthesis</td>
<td>May 27-June 21, 2009</td>
</tr>
<tr>
<td>M. Guthrie</td>
<td>HPSynC</td>
<td>Seminar on “Multiple lengthscale structural studies of disordered H-bonded matter”</td>
<td>June 6, 2009</td>
</tr>
<tr>
<td>P. Loubeyre</td>
<td>CEA, France</td>
<td>Seminar on “Calculations versus experiments in high pressure physics”</td>
<td>July 13, 2009</td>
</tr>
<tr>
<td>R. Little</td>
<td>Newcastle University, UK</td>
<td>Sample preparation of gold nitrate in DAC</td>
<td>August 4-7, 2009</td>
</tr>
</tbody>
</table>
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 BeF2*

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 FeSe1-xTe1-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 MgSiO3 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 Pd3Fe*

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**


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


Chellappa, R., Oxidation potential supercritical O$_2$-fluid H$_2$O mixtures at room temperature, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 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).


Downs, R. T., Phase transitions and crystallography at high pressure (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).


Ji, C. and Y. Ma, X-ray diffraction study of Al$_2$C$_3$ powder to 33.5 GPa, *CDAC Winter Workshop 2009* (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).


Oelker, E., High pressure investigations of vitreous BeF$_2$ (invited), *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).


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**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 Hrubiaik (Florida International), and Seth King (Purdue) listen to Mike Winterrose (Caltech) talk about his poster; Tom Duffy (Princeton) and Shiping Wang (Stanford) discuss her poster during the Poster Session.
Seagle, C. T., Far infrared reflectivity of the FeO-MgO solid solution series (invited), CDAC Winter Workshop 2009 (Argonne, IL, February 27-28, 2009).
Soignard, E., Polymorphism 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 Fe$_{x}$Se$_{y}$Te$_{1-x}$, 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).
Wenk, H. K., Deformation at ultra-high pressure (invited), CDAC Winter Workshop 2009 (Argonne, IL, February 27-28, 2009).
Winterrose, M. L., High pressure invar behavior and magnetism in Pd$_3$Fe (invited), 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 supported 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 Dortmund), 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 Bohler (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 GeO2 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 Irfune (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 University), X-ray induced dissociation of H₂O and formation of an O₂-H₂ 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.

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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.

**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.

![Figure 73. Dual undulators installed in tandem mode on beamline 16 ID at HPCAT.](image)

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 16-ID: 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...
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$_\beta$ 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$_2$O$_3$ 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 remote 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 completely 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 principle be used at any APS experimental station. Standard DAC membrane containers for forward or side diffraction, as well as inelastic scattering are currently

![Figure 74. 17-element analyzer array commissioned in June 2009 on the 16-ID-D beamline at HPCAT.](image)
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 mm³) 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

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

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 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 planned CO₂ laser heating system operational. Following interlock tests and commissioning, 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.

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

![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.](image)
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/cm². 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.

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. The methods involve the use of time-resolved (5
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 \( \text{H}_2, \text{D}_2, \text{N}_2, \text{H}_2\text{O} \) and \( \text{O}_2 \) show a broadening of intramolecular vibrations at high \( P,T \) conditions, indicating a decreasing molecular lifetime, and hence an increasing molecular dissociation. 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 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.

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 (\( \text{N}_2 \)). 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 consist 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)
- Study of Matter in Extreme Conditions Workshop (2007)
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 opportunities 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. 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 during a 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.
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 synthesis 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, announcements 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.

![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.](88)
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 liaison to the HPCAT/HPSynC groups at the APS.

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
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)
7. PLANS FOR YEAR 7 AND BEYOND

7.1 New Academic Partners

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, Fe₂O₃), 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 3d and 4f-band compounds. This work will therefore involve a significant 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 interchangeably 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.](image)

**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](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—Sectors 13 and 16
• 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:


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 conditions, 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


Gao, P., T. A. Tyson, Z. Liu, M. A. DeLeon, and C. Dubourdieu, Optical evidence of mixed-phase behavior in 
Ganesh, P., E. Cockayne, M. Ahart, R. E. Cohen, B. Burton, R. J. Hemley, Y. Ren, W. Yang, and Z. G. Ye, Origin 
Gavriluk, A. G., V. V. Struzhkin, I. S. Lyubutin, S. G. Ovchinnikov, M. Y. Hu, and P. Chow, Reversible 
Gavriluk, A. G., V. V. Struzhkin, I. S. Lyubutin, S. G. Ovchinnikov, M. Y. Hu, and P. Chow, Another 
mechanism for the insulator-metal transition observed in Mott insulators, Phys. Rev. B, 77, 155112 
(2008).
George, L., V. Drozd, A. Durygin, J. Chen, and S. K. Saxena, Bulk modulus and the thermal expansion 
coefficient of mechano-chemically synthesized Mg2FeH6 from high temperature and high pressure 
George, L., V. Drozd, S. K. Saxena, E. G. Bardaji, and M. Fichtner, Structural Phase Transitions of Mg(BH4)2 
Giefers, H. and M. Pravica, Radiation-induced decomposition of PETN and TATB under extreme conditions, J. 
Giefers, H., M. G. Pravica, W. Yang, and H. P. Liermann, Radiation-induced decomposition of explosives under 
Gleason, A. E., B. Chen, and R. Jeanloz, Grain-boundary effects in Brillouin scattering at ambient and high 
Goncharov, A. F., R. J. Hemley, and H. K. Mao, Comment on “Coherent anti-stokes Raman spectroscopy of 
highly compressed solid deuterium at 300 K: evidence for a new phase and implications for the band 
Goncharov, A. F., R. J. Hemley, and H. K. Mao, Vibron frequencies of solid H2 and D2 to 200 GPa and 
Goncharov, A. F., V. V. Struzhkin, J. A. Montoya, S. Kharlamova, R. Kundargi, J. Siebert, J. Badro, D. 
Antonageli, F. J. Ryerson, and H. K. Mao, Spin crossover in iron and thermal conductivity in the 
Earth’s lower mantle, Phys. Earth Planet. Inter., submitted.
Goncharov, A. F., P. Beck, V. V. Struzhkin, B. D. Haugen, and S. D. Jacobsen, Thermal conductivity of lower 
Goncharov, A. F., P. Beck, V. V. Struzhkin, R. J. Hemley, and J. C. Crowhurst, Laser heating diamond anvil cell 
studies of simple molecular systems at high pressures and temperatures, J. Phys. Chem. Solids, 69, 
2217-2222 (2008).
Goncharov, A. F., J. C. Crowhurst, V. V. Struzhkin, and R. J. Hemley, Triple point on the melting curve and 
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Goncharov, A. F., R. J. Hemley, and E. Gregoryanz, Comment on ”The melting line of hydrogen at high 
Goncharov, A. F., S. D. Jacobsen, V. V. Struzhkin, and P. Beck, Optical properties of minerals in the deep-earth, 
Goncharov, A. F., J. A. Montoya, N. Subramanian, V. V. Struzhkin, A. I. Kolesnikov, M. Somayazulu, and R. J. 
Hemley. Laser heating in diamond anvil cells: Developments in pulsed and continuous techniques, J. 
Goncharov, A. F., C. Sanloup, N. Goldman, J. C. Crowhurst, S. Bastea, L. E. Fried, N. Guignot, M. Mezouar, and 
Gregoryanz, E. and A. F. Goncharov, Comment on ”High-pressure melting curve of nitrogen and the liquid-
Han, W. Q., H. G. Yu, C. Zhi, J. Wang, Z. Liu, T. Sekiguchi, and Y. Bando, Isotope effect on band gap and 
Hao, J., B. Zou, P. Zhu, C. Gao, W. Li, D. Liu, K. Wang, W. Lei, and Q. Cui, In situ x-ray observation of phase 
transitions in Mg2Si under pressure, Solid State Comm., 149, 689-692 (2009).

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Lazicki, A., Y. Fei, and R. J. Hemley, High pressure differential thermal analysis measurement of the melting curve of lithium, *Solid State Comm.*, submitted.


B. CDAC Presentations


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


Amin, S., E. Soignard, M. Guthrie, Q. Mei, C. J. Benmore, and J. L. Yarger, Probing the structure of amorphous compounds at high pressure using high-energy x-rays, *High Pressure Synchrotron Science Workshop* (Argonne, IL, May 6-9, 2009).


Brown, K., Surface-enhanced Raman scattering at high pressure, *Gordon Conference on Vibrational Spectroscopy* (South Hadley, MA, August 4-8, 2008).


Ding, Y., Y. C. Tseng, E. Kaneshita, D. Haskel, M. van Veenendaal, J. Mitchell, S. V. Sinogeikin, V. Prakapenka, and H. K. Mao, Pressure-induced magnetic transition in manganite (La₀.₇₅Ca₀.₂₅Mn₃O₄),
Conference on High Pressure Science and Technology Conference on High Pressure Science and Technology (Odaiba, Tokyo, Japan, July 26-31, 2009).


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Dlott, D. D., Vibrational energy in molecules and nanostructures (invited), University of California Davis, Department of Chemistry (Davis, CA, April 15, 2008).

Dlott, D. D., Vibrational energy in molecules and nanoparticles: Applications to energetic materials (invited), Air Force Research Laboratory Nanotechnology Initiative (Fairborn, OH, May 2008).

Dlott, D. D., Vibrational energy with high time and space resolution (invited), Air Force Office of Scientific Research, Molecular Dynamics Contractor’s Meeting (Vienna, VA, May, 2008).


Dlott, D. D., Vibrational energy at interfaces (invited), Telluride Workshop on Nonlinear Optics at Surfaces and Interfaces (Telluride, CO, June 2008).


Dlott, D. D., Vibrational energy with high time and space resolution, Columbia University Department of Chemistry (New York City, NY, October, 2009).


Dlott, D. D., Vibrational spectroscopy of surfaces at high pressure, CDAC Program Review (Argonne, IL, February 26, 2009).


Dlott, D. D., Vibrational dynamics at interfaces probed by vibrational sum-frequency generation spectroscopy, ACS Colloids and Surface Chemistry Symposium (Columbia University, New York, NY, June, 2009).


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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).


Downs, R. T., Phase transitions and crystallography at high pressure (invited), *CDAC Winter Workshop* (Argonne, IL, February 27-28, 2009).


Goncharov, A., Construction of the high pressure scale at high temperature using cubic boron nitride (cBN), *Joint AIRAPT-22 and HPCJ-50, International Conference on High Pressure Science and Technology* (Odaiba, Tokyo, Japan, July 26-31, 2009).


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Hemley, R. J., New findings in materials under extreme pressures (invited), *MRL Seminar Series, California Institute of Technology* (Pasadena, CA, May 7, 2008).


Hemley, R. J., A brave new world of extreme conditions (invited), *U. S. Army Research Laboratory* (Aberdeen, MD, April 10, 2008).

Hemley, R. J., Diamond windows on extreme conditions, *NIST Sigma Xi Lecture (invited)* (Gaithersburg, MD, February 21, 2008).

Hemley, R. J., New directions in high pressure science (invited), *SUSSP 2008: High Pressure Physics, Scottish Universities Summer School in Physics No. 63* (Isle of Skye, Scotland, May 26-June 6, 2008).

Hemley, R. J., Materials under extreme conditions: From fundamental science to the pressures of the world (invited), *46th EHPRG: International Conference* (Valencia, Spain, September 7-12, 2008).

Hemley, R. J., High growth rate single crystal CVD diamond: Advances and applications (invited), *Diamond 2008* (Sitges, Spain, September 7-11, 2008).


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Hemley, R. J., Windows on a new chemistry under pressure (invited), *Kohler Lecture, University of California - Riverside* (Riverside, CA, November 5, 2008).


Hemley, R. J., Citation for Ronald E. Cohen (invited), *Goldschmidt 2009* (Davos, Switzerland, June 21-26, 2009).

Hemley, R. J., New developments and high-pressure applications of single crystal CVD diamond (invited), *Diamond and Nano Carbons Conference* (Traverse City, MI, June 8 2009).


Jacobsen, S. D., Condensed matter problems in the Earth sciences (invited), *Nortwestern University Department of Physics and Astronomy* (Chicago, IL, May 23, 2008).


Jacobsen, S. D., Effects of hydration on the elastic properties of upper mantle and transition zone minerals from atomic to geophysical scales (keynote), *Cooperative Institute for Deep Earth Research (CIDER), Planning Workshop* (Marconi Center, CA, May 19, 2009).

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Ji, C. and Y. Ma, X-ray diffraction study of Al₄C₃ powder to 33.5 GPa, *CDAC Winter Workshop 2009* (Argonne, IL, February 27-28, 2009).


Lee, K. K. M., Potassium in the deep Earth: Radioactivity under pressure (invited), *CIDER Workshop, Kavli Institute of Theoretical Physics, University of California - Santa Barbara* (Santa Barbara, CA, June 30, 2008).

Lee, K. K. M., Interface between experiment and computation (invited), *Workshop on Ab Initio Calculations in Geosciences* (Krakow, Poland, October 23, 2008).


Lerche, M., Magnetism of amorphous iron up to 35 GPa, *High Pressure Synchrotron Science Workshop* (Argonne, IL, May 6-8, 2009).

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Mao, H. K., Diamond windows on planetary interior -- minerals & rocks (Smith Lecture), *Department of Geological Sciences, University of Michigan* (Ann Arbor, MI, March 14, 2008).


Mao, H. K., Pressure: A new dimension in the physical sciences (Angstrom Lecture), *Uppsala University* (Uppsala, Sweden, May 19, 2008).


Mao, H. K., Energy frontier research in extreme environment (plenary talk), *4th Asian Conference on High Pressure Research, Seoul National University* (Seoul, Korea, October 14-17, 2008).


Mao, H. K., Pressure: A new dimension in the physical sciences (coloquium talk), *Department of Physics and Astronomy, University of California - Los Angeles* (Los Angeles, CA, January 15, 2009).


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Miyagi, L., In-situ laser heating and pressure change with radial diffraction, *California High Pressure Science Observatory Meeting* (University of California - Berkeley, Berkeley, CA, June 3, 2008).

Miyagi, L., Deformation of MgSiO3 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., Understanding deformation in the deep Earth through texture and anisotropy, *University of Colorado - Boulder* (Boulder, CO, March 12, 2009).

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Phatak, N., Synthesis and structure stability of a new compound $(\text{Cr}_{0.5}\text{V}_{0.5})_2\text{GeC}$ and $\text{M}_2\text{GeC}$ ($\text{M}=$Ti, V, Cr) at high pressure and temperature, 2008 Stewardship Science Academic Alliances Program Symposium (Washington, DC, February 26-28, 2008).


Schilling, J. S., Recent studies in superconductivity at extreme pressures (invited), 5th Conference on the Study of Matter at Extreme Conditions (SMEC2009) and the 1st International Meeting of the High Pressure Science Society of America (HiPSSA) (Miami-Western Caribbean, March 28-April 2, 2009).


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


Sinogeikin, S. V., Online optical systems (Brillouin, Raman, ruby) at HPCAT and GSECARS: Current status and new developments, High Pressure Synchrotron Science Workshop (Argonne, IL, May 6-8, 2009).


Soignard, E., Polyamorphism in SiO2 glass at high pressure, CDAC Winter Workshop 2009 (Argonne, IL, February 27-28, 2009).


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


Struzhkin, V. V., Spin crossover effects and Mott transitions in 3d metal oxides, *High Pressure Synchrotron Science Workshop* (Argonne, IL, May 6-8, 2009).


Yarger, J. L., Transitions in network and molecular glasses at high-pressure (invited), *Sixth International Conference on Synchrotron Radiation in Materials Science* (Campinas, Brazil, July, 2008).


Yarger, J. L., High pressure chemistry (invited), *Oklahoma State University Department of Chemistry Colloquium* (Stillwater, OK, September, 2008).

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).


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.

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<tr>
<th>User Name</th>
<th>Affiliations</th>
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<tr>
<td>C. Holt</td>
<td>Northwestern University</td>
<td>MgO EOS</td>
<td>October 3-5, 2008</td>
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<td>Rebecca Fisher</td>
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<td>H. Cynn</td>
<td>LLNL</td>
<td>Study of V-group elements at high (P-T)</td>
<td>October 4-7, 2008</td>
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<td>Z. Jenei</td>
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<td>W. Evans</td>
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<td>R. Kumar</td>
<td>University of Nevada – Las Vegas</td>
<td>Low temperature x-ray diffraction studies on heavy fermion compounds CeCoIn(_5) and CeIrIn(_5)</td>
<td>October 4-7, 2008</td>
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<td>S. Maglio</td>
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<td>Quantifying slab dehydration</td>
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<td>Quantifying element mass transfer of REE-monazite at subduction zone conditions using the hydrothermal DAC and in situ x-ray fluorescence</td>
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<td>P. E. Janolin</td>
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<td>N. Velisavljevic</td>
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<td>High (P-T) x-ray diffraction and electrical resistance measurements on Zr, Ti, and Sn metal</td>
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<td>Resonant x-ray emission studies on CeMIn(_5)(M=Rh,Co,Ir) and CeCu(_2)Si(_2) at high pressures</td>
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<td>J. Klepeis</td>
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<td>XES of Fe in (Fe,Mg)SiO₃ post-perovskite</td>
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<td>Z. Lin</td>
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<td>M. Laguna-Marco</td>
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<td>O. Tschauner Barbara Lavina O. Grubor-Urosevic</td>
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<td>Powder diffraction of super-conducting materials</td>
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<td>M. Pravica S. Tkachev A. Johnson Y. Z. Feng W. Pravica</td>
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<td>Studies of hydrocarbons at extreme conditions using x-ray diffraction</td>
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<td>A. Cornelius J. Baker</td>
<td>University of Nevada – Las Vegas</td>
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<td>Svetlana Kharlamova V. Struzhkin</td>
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<td>Jennifer Ciezak</td>
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<td>H. K. Mao Y. Ding</td>
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<td>NaPlasmon at high pressures</td>
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<td>M. Guthrie S. Sinogeikin E. Gregoryanz C. Guillaume</td>
<td>HPSynC HPCAT University of Edinburgh</td>
<td>High pressure structures of lithium</td>
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<td>Y. Vohra A. Stemshorn N. Cunningham</td>
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<td>Yu Lin Wendy Mao Maake Kroon S. Sinogeikin</td>
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<td>E. Kaneshita J. Chang Y. Ding Q. Zeng W. Yang</td>
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<tr>
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<td>Yu Lin</td>
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<td>O. Tschauner, S. Maglio, M. Frank</td>
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### 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.

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<td>Kin Fai Mak</td>
<td>Columbia University</td>
<td>Probing the electronic structure of graphene nanoribbons by infrared photoconductivity</td>
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<td>High pressure study of C60 nanomaterials</td>
<td>September 29-30, 2008 Oct. 1, 2008</td>
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<td>High-pressure IR Study gases storage in boron nitride nanotubes)</td>
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<td>Wendy Panero, J. Pigott, Z. Liu</td>
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<td>Solubility of two component systems at high-presures and temperatures</td>
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<td>S. Yu</td>
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<td>Investigation of H2O and some organic substance storage in the nanotubes by using high pressure</td>
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<td>Infrared spectroscopy on energetic materials at high pressure and temperature</td>
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<td>Infrared studies of cyclooctatetraene at high pressure</td>
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<td>Infrared and Raman spectroscopic studies of FeS under high pressure</td>
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<td>In situ measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR</td>
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<td>A. Goncharov</td>
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<td>Infrared spectroscopy of hot dense hydrogen (proposal # 10052)</td>
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<td>J. Smedley</td>
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<td>Characterization of impurities in diamond</td>
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<td>T. Tyson, P. Gao</td>
<td>New Jersey Institute of Technology</td>
<td>High pressure IR measurements on manganites</td>
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<td>M. Lang, F. Zhang</td>
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<td>Phase transitions in minerals induced by ion beams and high pressure: A novel approach in geosciences</td>
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<td>W. Han</td>
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<td>IR reflectivity of sodium</td>
<td>February 5-7, 2009</td>
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<td>B. Yulga, S. Tkachev</td>
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<td>Infrared spectroscopy on energetic materials at high pressure and temperature</td>
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<td>Wendy Panero</td>
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<td>Solubility of two component systems at high-pressure and temperatures</td>
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<td>K. Otsuka, G. Amulele</td>
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<td>In situ measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR</td>
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<td>M. Lang, F. Zhang</td>
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<td>M. Ma</td>
<td>Graduate University of the Chinese Academy of Sciences</td>
<td>Effect of water on properties of olivine at high pressure and high temperature</td>
<td>April 2-3, 2009</td>
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<td>T. Tyson, P. Gao</td>
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<td>G. Yang</td>
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<td>Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe</td>
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<td>M. Pravica, S. Tkachev, E. Romano</td>
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<td>Characterization of impurities in diamond</td>
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<td>Y. Lee</td>
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<td>Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application</td>
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