CDAC

CARNEGIE/DOE ALLIANCE CENTER

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

Year Five Annual Report

November 2008

Russell J. Hemley, *Director*
Ho-kwang Mao, *Associate Director*
Stephen A. Gramsch, *Coordinator*

NNSA
CARNEGIE INSTITUTION FOR SCIENCE

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

YEAR FOUR ANNUAL REPORT

1. OVERVIEW

1.1 The Mission and Scope of CDAC

Fundamental science is essential for national security. Recognizing this need, the Carnegie-Department of Energy Alliance Center (CDAC) was created to address critical needs in high *P-T* materials science in support of stewardship science campaigns in the Department of Energy/National Nuclear Security Administration (NNSA). Formed in 2003 under the Stewardship Science Academic Alliances (SSAA) program, CDAC comprises a scientifically and technically broad group of Academic and Laboratory Partners along with a growing network of collaborators, engaged in fundamental high *P-T* materials science. In this role, CDAC continues to advance and perfect high *P-T* techniques, develop and manage unique facilities, perform key measurements on important materials in newly-accessible *P-T* regimes, and integrate and coordinate static and dynamic compression studies together with theory, modeling and simulation for NNSA science. During our first five years, research groups within CDAC have addressed a wide variety of problems relevant to the NNSA, including key *d*- and *f*-electron elements and alloys, low-*Z* molecular compounds, energetic materials and detonation products, dense hydrogen, metal oxides and hydrides, and bulk materials as well as composites and interfaces. Information on material behavior in crystalline, liquid, and amorphous phases, phase transitions, equations of state (EOS), phonon dynamics, elasticity and plasticity, electronic and magnetic structures, and chemical reactions likewise are all necessary to increase the broad base of data on material properties under extreme conditions, as are accurate descriptions of matter in transient, ultra-high density states. Addressing these key issues in high *P-T* materials science requires the training of students for positions in academia and the National Labs, as well as access to state-of-the-art facilities that are not readily accessible to research groups in the NNSA Labs or universities.

Figure 1. *The Research Building (top) and Greeenwalt Building (lower) on* ***Carnegie's*** *Broad Branch Road Campus in Washington, DC.*

High *P-T* materials science, technology and student training have all benefitted tremendously from CDAC. Now at the close of our initial five-year period, CDAC continues to support the NNSA mission in stewardship science. The Center is managed at **Carnegie** (Fig. 1) by **Russell Hemley** (Director), **Ho-kwang Mao** (Associate Director), **Stephen Gramsch** (Coordinator) and **Morgan Phillips** (Administrative Assistant). CDAC now consists of 11 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)***, **Surrendra Saxena** ***(Florida International University)***, **Yanzhang Ma** ***(Texas Tech University)***, **Dhanesh Chandra** ***(University of Nevada – Reno)***, and **Jeffrey Yarger** ***(Arizona State University).***

Scientists from high-pressure research groups at all of the National Labs (CDAC Laboratory Partners) can obtain beam directly from the CDAC discretionary share, and in so doing obtain technical training and exposure to the high *P-T* technique development taking place at **HPCAT**, the dedicated high-pressure synchrotron x-ray facility at the **Advanced Photon Source (APS)**, of which CDAC is a member. Laboratory scientists are also able to take advantage of facilities at **Carnegie** and the **National Synchrotron Light Source, Brookhaven National Laboratory (NSLS)**. In addition, a number of groups within CDAC interact regularly with staff from **LANSCE (Los Alamos National Laboratory)** to develop high *P-T* neutron scattering and data analysis technques. The list of CDAC collaborators from academic and research institutions worldwide has now reached 560, representing 215 institutions.

CDAC continues to enable the next generation of high *P-T* methods. A primary focus of CDAC continues to be the HPCAT facility, a state-of-the-art sector developed for forefront research in chemistry, physics and materials science at extreme conditions. Managed by **Ho-kwang Mao** (Director) and **Guoyin Shen** (Project Manager), HPCAT provides a setting dedicated to the technical development of important spectroscopic and diffraction methods. All four beamlines at HPCAT have been accepting general users through the General User Proposal (GUP) program at the APS, even as new techniques are commissioned at each beamline. To date, more than 400 different users (*i.e.,* from National Labs and academia) have conducted experiments at the facility. The HPSynC initiative, begun in Year 4, represents a formal mechanism for coordinating high pressure research activities throughout the APS as well as for introducing new researchers in the field to the many high *P-T* techniques available at the APS. HPSynC has already facilitated an impressive number of collaborations both within and outside of the APS. Other facilities playing a key role in the CDAC effort include the high-pressure neutron facilities at LANSCE, the synchrotron infrared spectroscopy laboratory at the NSLS, and specialized high-pressure facilities at Carnegie, where developments continue in the area of high *P-T* spectroscopy and x-ray crystallography, new cell designs for a variety of experimental measurements, and advances in CVD diamond growth. Experimental work in high-pressure geoscience and planetary science is increasingly carried out with a materials science perspective and at advanced, national user facilities and therefore provides an excellent background for understanding problems in stewardship science and for future work in the NNSA/DP Labs. Interactions with theoretical groups in academia and the National Labs add significantly to the experimental work carried out within CDAC.

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 and the unprecedented accuracy needed for code validation. In just the last two years, CDAC facilities at NSLS and HPCAT have played a key role in enabling the first synchrotron x-ray measurements of dynamic compression events, complementing developments within the NNSA/DP Labs such as those at NIF and Z_R. CDAC continues to enable participation on the part of the academic community in all of these areas, which are presenting exiting new opportunities for NNSA/DP. With the potential of these and other facilities on the horizon, CDAC continues to promote the integration of static and dynamic experiments for stewardship science needs.

CDAC graduate student ***Susannah Dorfman (Princeton).***

This report covers activities from the CDAC Academic Partners, Laboratory Partners, and University Collaborators from July 2007 through July 2008. Research carried out by National Lab partners, but done outside of the CDAC facilities, is not included.

1.2 Highlights from Year 5

Outreach and Training

CDAC focuses heavily on the training and outreach aspects of its mission, both in terms of graduate student education and helping to grow the high pressure research community. Highlights for Year 5 in this critically important effort include:

- Supporting the Ph.D. thesis work of 18 graduate students at CDAC partner universities and **Carnegie**. Thus far, 15 graduate students from Academic Partner institutions have received the Ph.D. degree with CDAC support.

- Hosting undergraduate and high school interns at **Carnegie**. This past year, three undergraduate students and three high school students worked on CDAC-related research projects in our laboratories with guidance from the research staff.

Figure 2. *Carnegie Institution Headquarters Building, location of the 2008 SSAA Symposium.*

- Supporting the growth and operation of the HPCAT sector. In part, through the 30% partnership CDAC retains in HPCAT, the number of users carrying out original research and working on technique development at the facility has grown to over 400.

- Hosting the 4th Annual SSAA Symposium, held at the Carnegie Institution Headquarters Building in Washington, DC (Fig. 2) on February 26-28, 2008. Over 70 CDAC participants attended this symposium.

- Supporting the Workshop on Understanding Condensed Matter Dynamics at the Microscopic Level, held at the Advanced Photon Source on June 23-24, 2008.

Scientific Breakthroughs

During the five years since May 2003, when CDAC began formal operations, over 610 papers based on the research of Academic Partners and their graduate students, Laboratory Partners and collaborators have been published with support from the grant. This total also includes papers describing Carnegie research supported by the CDAC grant and research carried out at HPCAT and CDAC facilities at NSLS. (This does not include the large amount of research performed by high-pressure groups within the National Labs not done at CDAC-supported facilities). These papers represent a significant amount of student and post-doctoral training, and many describe important technique development as well. An increasing number of the papers in this list represent work carried out in collaboration with NNSA/DP Lab scientists. The number of articles appearing in high-impact journals continues to grow: to date 38 papers have appeared in *Physical Review Letters*, 11 in *Science*, 22 in *Nature* magazines, and 29 in the *Proceedings of the National Academy of Sciences.*

- *Invar effects induced by pressure in Pd_3Fe:* A combination of x-ray diffraction, nuclear forward scattering and *ab-initio* computational methods has allowed the **Caltech** group to work out the origin of Invar effects under pressure in the palladium-iron alloy Pd_3Fe.[1, 2]

- *Elasticity across a ferroelastic phase transition in MgF_2:* The complete elastic tensor of the model compound MgF_2 has been determined at high pressure by the **Princeton** group, in an effort to more fully understand the nature of ferroelastic transitions.

- *Nanocrystals in bulk metallic glasses:* During the synthesis of bulk metallic glass materials, the **Alabama** group isolated a pure nanocrystalline Zr_2Ni phase stable to 74 GPa.[3]

- *Texture development in Zr and U:* At the HIPPO diffractometer at **LANSCE**, Academic Partner **Hans-Rudolf Wenk's** group has carried out texture measurements of zirconium and uranium during phase transformations that take place under processing conditions.[4]

- *Novelty in the noble metal nitrides:* In a collaborative effort, groups at **Carnegie** and **LLNL** used theoretical methods[5] to evaluate the stability of different possible crystal structures of PtN_2 in an effort to provide a guide to high *P-T* synthetic strategies.

- *Origin of morphotropic phase boundaries in ferroelectrics:* A team from **Carnegie** showed that pressure can be used to drive phase transitions through morphotropic phase boundaries in a pure compound, without the need for complex microstructures or compositions, to obtain a colossal piezoelectric response.[6]

- *Elasticity of (Mg,Fe)O through the spin transition of iron:* A collaboration between **Carnegie**, **LLNL**, **University of Washington**, and **Northwestern** has identified unusual electronic properties of (Mg,Fe)O that make sound propgate slowly, suggesting that the material at high pressure is softer than previously thought.[7]

Tanja Cuk

- *Loss of magnetism in magnetite under pressure:* A team from **HPSynC**, the **Russian Academy of Sciences**, and **Krasnoyarsk State University** shows that the magnetic strength of magnetite declines drastically under pressure.

- *Superconductors get a boost from pressure:* A team lead by **Tanja Cuk** (then a graduate student at **Stanford**), including scientists from **Carnegie**, showed that in addition to chemical doping, applied pressure can raise the transition temperature of high T_c cuprates.[8]

- *Superconductivity in compressed silane:* In collaboration based at **Carnegie**, the superconducting properties of the hydrogen-rich molecular compound silane (SiH_4)[9] have been predicted from first principles. This theoretical study confirms their experimental findings of pressure-induced metallization in SiH_4.[10]

- *Intermolecular bonding in solid O_2:* Researchers from **Carnegie**, **HPCAT**, **University of Chicago**, **University of Saskatchewan**, and **NSLS** found that under pressure, individual oxygen molecules interact through their outermost, highest energy molecular orbitals.[11]

- *Surprising stability of molecular nitrogen at high pressure and temperature:* **Carnegie** and **LLNL** scienctists have obtained Raman spectra up to 120 GPa and 2500 K for both solid and fluid nitrogen in an effort to clarify the behavior of this system at high *P-T*.[12]

- *Anomalous high-pressure behavior of selenium:* A team from **Harbin Institute of Technology**, **ANL**, **Harvard**, and **Carnegie** has discovered an unexpected volume expansion associated with pressure-induced crystallization of amorphous selenium.[13]

Technique Development

Advances in high *P-T* materials science rely on the development of enabling techniques across the spectrum of experimental methods. During Year 5, CDAC has made progress in a number of key areas, particularly in the area of experimental facilities. Examples include the following:

- *Real-time synchrotron measurements of shock compression events:* Following up on feasibility studies carried out with CDAC support, a group from the Institute for Shock Physics at **WSU** led by CDAC advisory committee member **Yogendra Gupta** performed the first synchrotron x-ray diffraction measurements during shock compression on a variety of materials at **HPCAT.**

*CDAC student **Aaron Lozano (Illinois**).*

- *SFG measurements of surfaces and interfaces of high explosives:* A third-generation apparatus for vibrational sum-frequency generation (SFG) measurements developed in Year 4 at **Illinois** is now used routinely for studies of the surface spectroscopy of energetic materials.[14]

- *Single crystal white-beam diffraction:* A **Carnegie** group has refined the white-beam techniques developed in Year 4 at HPCAT station BM-B for structural refinements from high-pressure single crystal diffraction data.

- *Infrared reflectivity measurements of infrared-active phonons:* The **Chicago** group, working at NSLS-U2A, developed an infrared reflectivity method to evaluate the pressure dependence of the dielectric constants of simple oxides.[15]

- *Isotopically enriched C-13 diamond layers:* The **Alabama** group continues work on the fabrication of a pressure sensor employing C-13 enriched layers prepared by CVD on diamond anvil substrates.

- *Texture development in Fe at high P-T:* The **Berkeley** group has developed an apparatus for radial diffraction at high *P-T* with laser heating and used it to uncover unexpected effects in texture development mechanisms.[16]

- *Diamond cell techniques for amorphous solids:* The **Arizona State** group is working on special diamond anvil cells (DACs) employing perforated diamonds that give dramatically improved diffraction data in studies of glass formation from high *P-T* liquids.[17]

- *High P-T Pressure Calibration:* Work at **Carnegie** and **LLNL** combining x-ray diffraction, Raman spectroscopy and Brilloiuin scattering has established cubic boron nitride (c-BN) as a robust and accurate pressure calibrant for laser heated DACs.[18, 19]

2. SCIENTIFIC PROGRESS

We classify the ongoing research work of the CDAC program into six principal areas of interest, although the interdisciplinary nature of high *P-T* materials science allows much of our work to be characterized by two or more of these six divisions. At the close of Year 5, we continue to progress beyond the milestones outlined in our original work plans and explore new directions in each of our principal research areas. The following six sections outline the Year 5 progress in each of these key fields.

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 investigations on materials at extreme *P-T* conditions continue to progress at an impressive rate, and are made possible by technical advances at HPCAT. Studies of phase relations and structures at high pressure and temperature have been a cornerstone of the CDAC program from the beginning and encompass a broad range of materials from molecular materials to metals to minerals with intriguing properties. In the area of technique development, improvements in laser heating and resistive heating,[20] *in situ* high *P-T* Raman measurements with laser heating,[21] and refinement techniques continue to be the focus of the HPCAT team. As we come to the close of Year 5, studies of nanomaterials and glasses under pressure have begun to take on a prominent role within a number of CDAC research groups.

Melting of Hydrogen at High Pressure and Temperature – Hydrogen has long been predicted to become a metal at ultrahigh pressures, and experimental efforts have been ongoing to discover this novel form of hydrogen under static high pressures for the past few decades.[22] Most of the experiments in the past have concentrated on the pressure-induced behavior of hydrogen at room temperatures or lower. In the recent years, a few experiments on hydrogen employing either laser-heating or resistive heating techniques in conjunction with *in situ* spectroscopic measurements have been reported.[23, 24] Apart from enabling determination of the melting curve of hydrogen as a function of pressure, such experiments seek to explore the as-yet unknown phase diagram of hydrogen and deuterium at extremely high pressures and temperatures in a search for novel phases, including the molecular and monoatomic metallic phases.

Modest progress has been made at **Carnegie** in confining hot and dense hydrogen while not compromising on the ability to make spectroscopic measurements. This has been accomplished partly by "locking-up" the hydrogen in a microscopic cavity (8 mm diameter) made in an IR absorbing coupler, which in turn is sandwiched in an inert, IR and visible light transmitting buffer insulation layer between the tips of the two diamond anvils. With this configuration, **Subramanian Natarajan** has performed *in situ* Raman spectroscopy measurements on hydrogen while simultaneously laser heating at pressures close to a megabar and temperatures up to about 1100 K (Fig. 3). As part of the work on identifying the buffer materials, detailed pressure induced fluorescence (PIF) experiments were carried out on the candidate materials up to ~50 GPa. This is necessitated by the fact that PIF is a major factor in high-pressure high-temperature experiments on hydrogen that lead to significant reduction of signal-to-noise ratio.

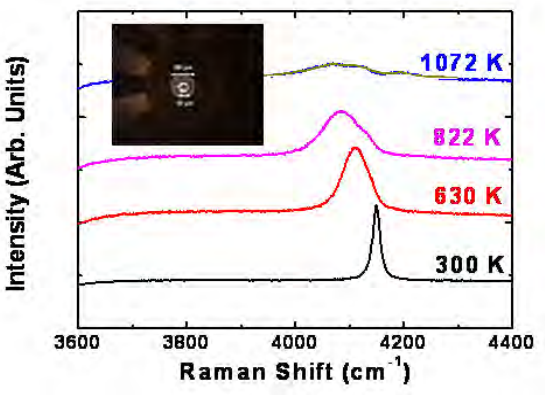


Figure 3. *Softening and broadening of the Raman vibron of hydrogen at 109 GPa contained in the composite coupler-buffer assembly at various temperatures. Hydrogen can be confined for several minutes at this pressure up to ~1500 K. Inset: view of the sample chamber.*

Molecular Oxygen at High Pressure – Molecular oxygen (O_2) changes its form dramatically with compression, transforming to a solid with spectacular colors, and eventually becoming metallic and superconducting at sufficiently high pressures. The underlying mechanism for these remarkable phenomena has been a source of debate for decades, in particular the origin of the recently discovered molecular cluster $(O_2)_4$ in the dense solid, red phase. **Yue Meng** (**HPCAT**), and researchers from **Carnegie**, **Argonne National Laboratory**, **University of Saskatchewan**, and **NSLS** found that under pressure the individual molecules interact through their outermost, highest energy molecular orbitals. This pairing interaction brings four oxygen molecules together to form discrete $(O_2)_4$ clusters at a pressure of about 10 GPa. With increasing pressure, the effective

radial extent of the molecular orbitals on individual molecules increases, promoting the interaction of unpaired electrons on adjacent molecules (Figs. 4a and b).

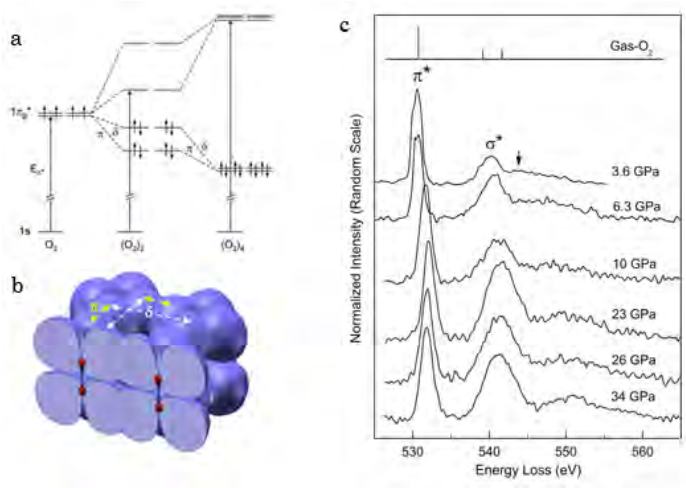


Figure 4. *a) Molecular orbital diagram showing the stabilization of the unusual $(O_2)_4$ cluster from the interactions of eight degenerate π^* orbitals of four O_2 molecules. b) Topology of π^* orbital interactions in the $(O_2)_4$ cluster, illustrating the two different interactions in which each π^* orbital participates as the cluster is formed from four O_2 molecules. The energy levels of an idealized $(O_2)_2$ dimer in a) illustrate the effect of the two interactions. C) Representative IXS K-edge spectra of condensed oxygen phases at high pressure, plotted as normalized scattering intensity (normalized to incident beam intensity) versus energy loss. The peaks labeled π^* and σ^* correspond to the 1s-$1\pi_g^*$ and 1s-$3\sigma_u^*$ transitions, respectively.*

Using newly developed high pressure inelastic x-ray scattering techniques, is has been possible to track the behavior of the relevant molecular orbitals on the oxygen molecules with compression. The fact that the energy of the scattered x-rays increases with increasing pressure indicates that the bonding character of the highest energy molecular orbitals is changing, as illustrated in Fig. 4c. Theoretical studies of the energetics of formation of the $(O_2)_4$ clusters provide a rationale for the formation of the tetramolecular unit as opposed to the dimer $(O_2)_2$. The work suggests that interactions of a similar nature, which are well known in organic chemistry, could occur between $(O_2)_4$ clusters at higher pressures, leading to still other, as yet undiscovered phases.

<u>High Pressure Melting Behavior of Oxygen</u> – Melting-curve maxima as a function of pressure have been observed in elements such as sodium, nitrogen, cesium, barium, europium, phosphorus and carbon. It is of interest to experimentally measure if other elements such as oxygen exhibit a maximum in the melting temperature at some high pressure. There are reports from shock wave measurements and first principles simulations, of oxygen transforming into a liquid metal when melted at pressures in the range of 50-60 GPa. Melting experiments reported in the literature up to 20 GPa using a resistive heating arrangement show a nearly linear increase in the melting point as a function of pressure. **Ravindran Thoguluva** (**Carnegie**) has started Raman spectroscopic measurements at using a modified DAC. Ruby and $SrB_4O_7:Sm^{2+}$ were used as pressure markers, the advantage of the latter being that its pressure coefficient is nearly independent of temperature. In the liquid state the low frequency Raman modes (lattice modes) disappear, the width of the vibron mode increases by 30-50%, and the sample becomes transparent to visible light, as indicated in Fig 5. Measurements at 26 GPa and 40 GPa indicated a still rising melting point. The highest temperature that has been reached so far is 950 K at 69 GPa, and at this pressure and temperature

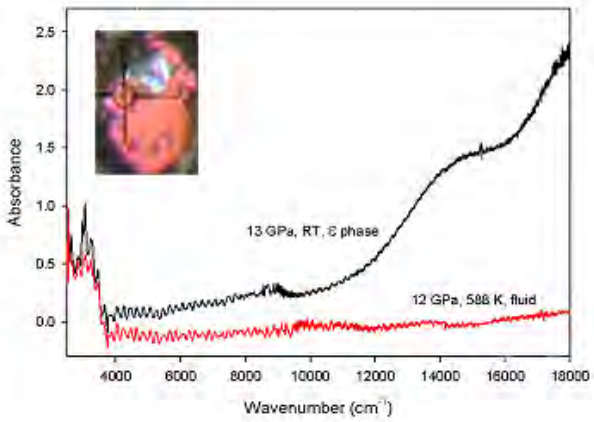


Figure 5. *Optical absorption spectra of fluid O_2 (red) and solid e-O_2 at 13 GPa. The characteristic absorption spectrum is observed for the solid phase at room temperature, and disappears at ~575 K, with a slight drop in pressure. Inset: Solid + fluid coexistence is observed at 20 GPa and 785 K.*

Carnegie post-doctoral associate ***Amy Lazicki****. Dr. Lazicki carried out her thesis research at* ***LLNL.***

oxygen is still a solid. Laser heating is planned in the near future to explore higher *P-T* regions.

High Pressure Behavior of Simple Elements – Elemental lithium, the simplest metal in the periodic table, develops unexpected and fascinating features under pressure, such as novel low-symmetry crystal structures, superconductivity and decreased metallic character. Postdoctoral fellow **Amy Lazicki** at **Carnegie** has been carrying out high pressure investigations of melting behavior of lithium using a multianvil apparatus using differential thermal analysis (DTA) (Fig. 6), as well as in a DAC using a variety of techniques including monochromatic and white beam synchrotron x-ray diffraction at **HPCAT**, optical and IR reflectivity at **NSLS-U2A**, and electrical conductivity. New features so far revealed include a flattening of the melting curve between 8 and 12 GPa, and an indication of the onset of a drop in melting temperature with pressure by 15 GPa.

Sodium, while quite a simple metal at ambient conditions, displays significant complexity at high pressure. The melting temperature drops above a critical pressure, nearly reaching ambient temperature by 120 GPa. In the same pressure regime, phase transitions to low-symmetry structures, some with hundreds of atoms per unit cell, are observed. Computational studies also predict a decrease in the metallic character of Na, and observations by experimentalists indicate this as well. **Amy Lazicki** has examined the changing metallic character of Na up to 190 GPa in the DAC. Results from recent experiments indicate a significant drop in reflectivity between 120 and 130 GPa while transmission remains negligible, indicating a large reduction in electrical conductivity but no metal-insulator transition within the pressure regime examined. This ongoing work provides important feedback for theoretical models of melting, enhancing our fundamental understanding of phenomena in simple elemental systems at high densities.

Polyamorphism in Elemental Solids and Related Materials – In the **Yarger** group at **Arizona State**, elemental systems such as germanium, silicon and tin alloys are the focus of current research, Efforts are directed at formalizing a developing idea that a low temperature melting point minimum in a single-component system is a property analogous to a eutectic point in a multi-component system, and can be used to increase the glass-forming ability of a material. The group is currently testing the idea of pressure-tuned glass formation in elemental germanium, which has a well-defined melting point minimum at 775 K and 9.5 GPa. Quenching liquids above this point has allowed, for the first time, the quenching of a monoatomic glass from liquid germanium. Figure 7 shows an example of the regions in the phase diagram in which glasses can be thermally quenched from liquid germanium. As expected, it is only close to the melting point minimum where glass formation is experimentally possible. At

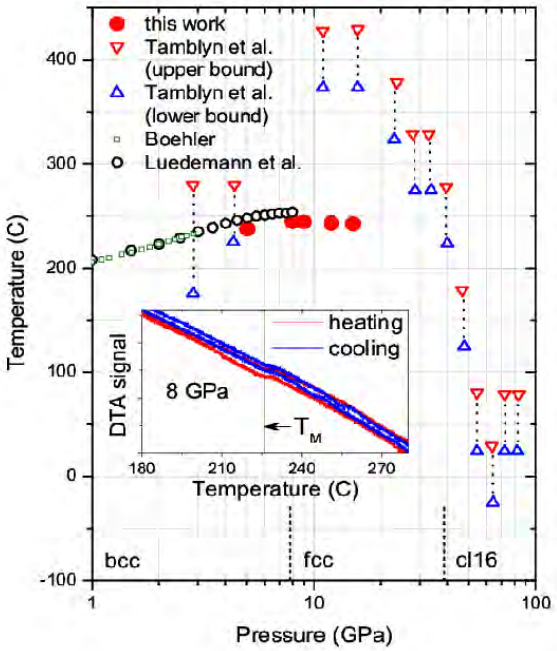


Figure 6. *Phase diagram of Li with theoretical predictions[25] and experimental data[26]. Inset: representative DTA signal showing melting (T_M).*

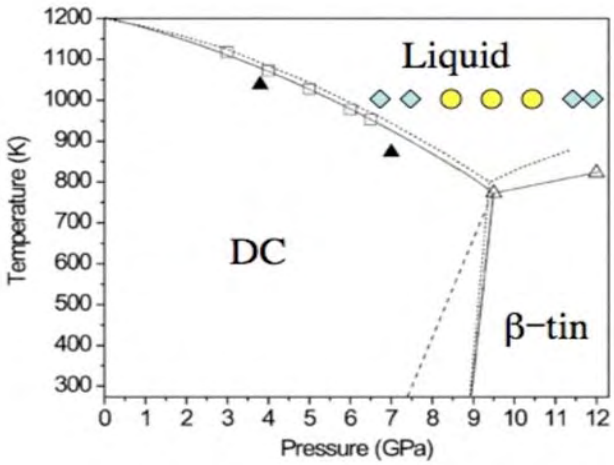


Figure 7. *Schematic phase diagram of Ge. The yellow circles represent regions where glass could quenched. The blue pyramids represent regions where crystalline material was quenched.*

regions away from this minimum, the viscosity at the melting point (ΔG_{fus}=0) is too low and the process of nucleation and growth happens faster than normal thermal quench rates for glass formation. A high-pressure melting point minimum is common in a large variety of materials including H_2O, Si, GaSb, InSb, Na, KNO_2, among many others. Efforts are underway in the lab to perform similar temperature-quenched DAC experiments, as shown in Fig. 7, to test the glass-forming properties of a range of different materials near their melting point minima.

The overall goal of this work is to find a general trend for better glass-formation properties near the triple point in all phase diagrams. Currently, most of the emphasis placed on laser heating of elemental silicon under pressure in the DAC. In a series of experiments similar to those on elemental Ge, an attempt to quench monoatomic elemental silicon (Si) glasses from the high-pressure liquid represented in the vicinity of the melting point minimum (1100 K and 14 GPa) is also underway. While developing the systematics of pressure-tuned glass formation is a primary goal of ongoing CDAC research, the work is also a part of growing effort through the community in polyamorphism and the nature of amorphous-amorphous transitions.

In recent studies, it has become evident that there is an urgent need to develop better DAC methods for characterizing the structure and dynamics of liquids and glasses at pressure. This has led to the development of perforated DACs for *in-situ* x-ray diffraction of liquids and glasses at high-pressure and temperature. The x-ray structure factor of vitreous As_2O_3 has been measured at 32 GPa in a laser-perforated DAC using a monochromatic, micro-focused high energy x-ray beam.[17] The results of this work are techniques for x-ray diffraction on DAC samples, as well as methods for data analysis and filtering that have greatly improved our 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. Figure 8 compares the scattered intensity of Ge-Se glasses using a normal DAC and perforated DAC. The signal to noise ratio can be improved substantially by using a perforated DAC for chalcogenide glasses. Utilizing a perforated DAC in high-energy x-ray experiments is even more important in elucidating glass structures for oxide glasses and other light element systems. A schematic of the perforated DAC used by our group is shown in the inset of Fig. 8. Further technique development is concerned with the use of dual-

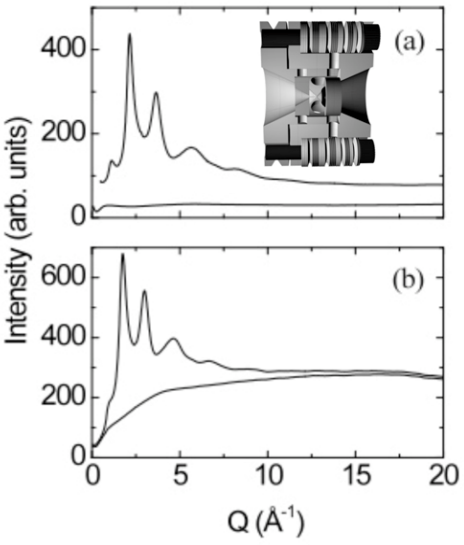


Figure 8. *a) The raw intensity measured using high-energy x-rays for glassy $GeSe_2$ in a perforated DAC at 5.3GPa (upper curve) and for the empty DAC at ambient pressure (lower curve); Inset: schematic diagram of the perforated DAC. b) The raw intensity measured using high-energy x-rays forglassy $GeSe_4$ in a diamond anvil cell at 6.0 GPa (upper curve) and for the empty DAC at ambient pressure (lower curve).*

perforated diamonds and exploring possibilities for the use of pressure-transmitting media to ensure hydrostatic pressure on the glasses in these experiments. This work follows up on earlier experiments on SbF_5,[27], As_2O_3,[28]SiO_2,[29] and beryllium hydride-based materials.[30]

Nanocrystals in Zirconium-Based Bulk Metallic Glass – Bulk metallic glasses (BMGs) are a newly developed class of materials that exhibit unusual corrosion resistance, high hardness, enhanced mechanical ductility and yield strength not found when the same alloys are in their stable crystalline states. Recently, multi component Zr- and Pd-based BMGs have been fabricated with a conventional casting process with a low cooling rate. High pressure studies taking place in the **Alabama-Birmingham** group are geared towards understanding the phase stability of nanocrystalline and amorphous phases that are present in BMGs and investigating stress-induced crystallization under extreme environments. Recent work at the BM-D station at HPCAT has revealed the existence of nanocrystals in a BMG based on $Zr_{57}Nb_5Cu_{15.4}Ni_{12.6}Al_{10}$; this nanocrystalline phase was observed to be stable up to 74 GPa (Fig. 9a). The origin of these nanocrystals in bulk metallic glasses remains an issue of considerable scientific interest and is likely related to shear deformations in these materials. Current studies indicate that these nanocrystals belong to the tetragonal Zr_2Ni phase (*I*4/*mcm*, Ni occupying 4a positions and Zr occupying 8h positions) and show broad diffraction peaks characteristic of nanocrystalline materials. The measured EOS at room temperature is shown in Fig 9b. The Birch-Murnaghan fit to the EOS resulted in a bulk modulus of 54 GPa and a pressure derivative of 4.94. Ongoing work is aimed at examining the existence of nanocrystalline phases in other Zr-based and Pd-based bulk metallic glasses and studies of their stability under high pressures.

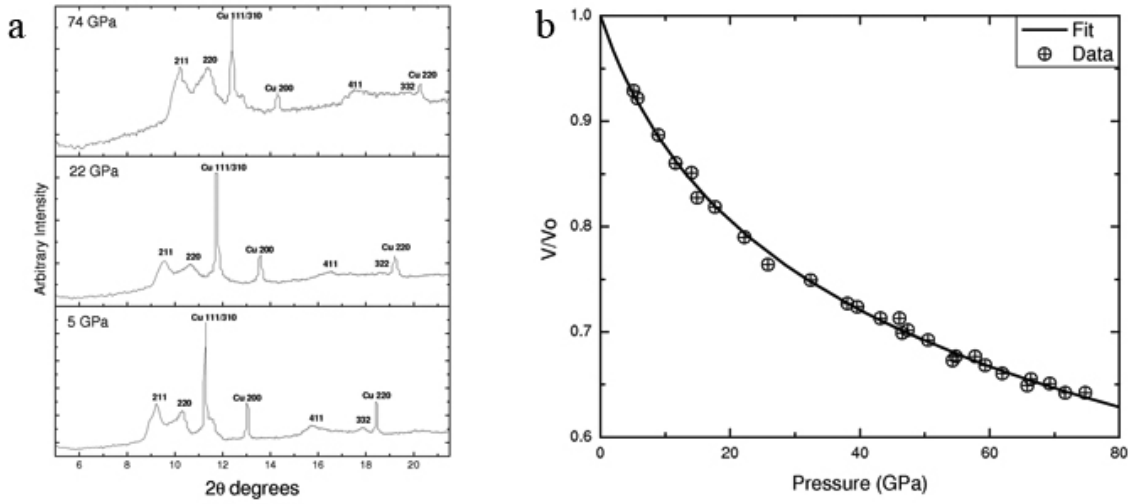


Figure 9. *a) Angle dispersive XRD spectra of a $Zr_{57}Nb_5Cu_{15.4}Ni_{12.6}Al_{10}$ metallic glass to a pressure of 74 GPa obtained at the HPCAT, beamline BM-D. The broad diffraction peaks are due to a tetragonal nanocrystalline Zr_2Ni phase and sharp peaks are due to a face-centered cubic phase of pressure marker copper (Cu) employed in this experiment. The X-ray wavelength is $\lambda = 0.40962$ Å. b) The measured equation of state of nanocrystalline Zr_2Ni tetragonal phase present in a $Zr_{57}Nb_5Cu_{15.4}Ni_{12.6}Al_{10}$ metallic glass to 74 GPa at room temperature. The solid curve is the Birch-Murnaghan equation of state fit to the data.*

High P-T Phase Equilibria and Melting in the Fe-S System – The **Heinz** group at **Chicago**, led by CDAC graduate student **Chris Seagle**, continues extend measurements of melting behavior in the Fe-S alloy system to higher pressures and temperatures. An Fe-10 wt. % sulfur sample heated at 160 GPa revealed a previously unknown phase by reaction of the iron with sulfur. A single phase (Fig. 10a) was formed from the mixture and could be indexed on a cubic unit cell. Following the synthesis of this phase, the sample was decompressed to watch for phase transitions and monitor the volume of the cubic phase as a function of pressure. Below 100 GPa, the volume of

this phase rose rapidly with decreasing pressure and subsequently disappeared below ~85 GPa. At 1 bar, no sample peaks could be detected in the laser heated region, suggesting that a transition to an amorphous phase upon decompression may be responsible for the sharp change in the bulk modulus (Fig. 10 b).

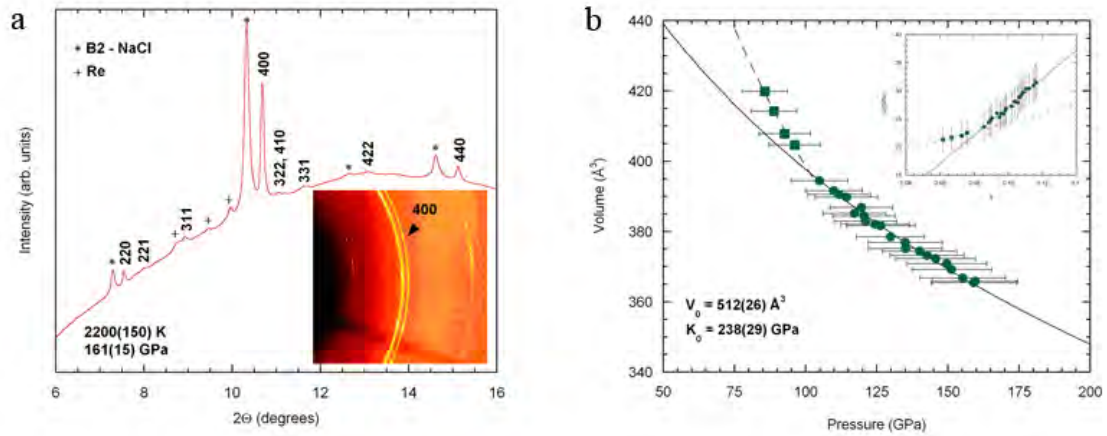


Figure 10. *a) XRD pattern at 161 GPa and 2200 K showing the indexing of the new Fe-S phase on a cubic unit cell. The inset shows a portion of the 2d diffraction pattern with the (400) peak of the new phase clearly marked. b) EOS of the cubic Fe-S alloy. Volume data was collected on decompression from ~160 GPa. The first pressure derivative of the bulk modulus has the assumed value of 4. Below 100 GPa the volume of the phase began to rise rapidly with increasing pressure and the XRD pattern of this phase completely disappeared below ~80 GPa. This is interpreted as a glass transition on decompression and indicated by squares on the figure. The inset shows the normalized pressure (G) vs. normalized strain (g) plot used in the fitting of the EOS.*

Triclustered $MgSiO_3$ Melts at High Pressure – **Jung-Fu Lin**, a Lawrence Fellow at **LLNL**, has investigated the local electronic structures of $MgSiO_3$ glass, a precursor to Mg-silicate melts, using x-ray Raman spectroscopy in a DAC up to 39 GPa at HPCAT and other synchrotron facilities. High-pressure oxygen K-edge spectra suggest the formation of triclustered oxygens (oxygen coordinated with three framework Si; $^{[3]}$O triclusters) between 12 and 20 GPa. The results (Fig.11) indicate that the formation of triply coordinated oxygens in $MgSiO_3$ melts would be accompanied by the densification and the formation of highly coordinated Si in the Earth's mantle, in addition to a reduction of non-bridging oxygens as previously suggested.[31] The continuous increase

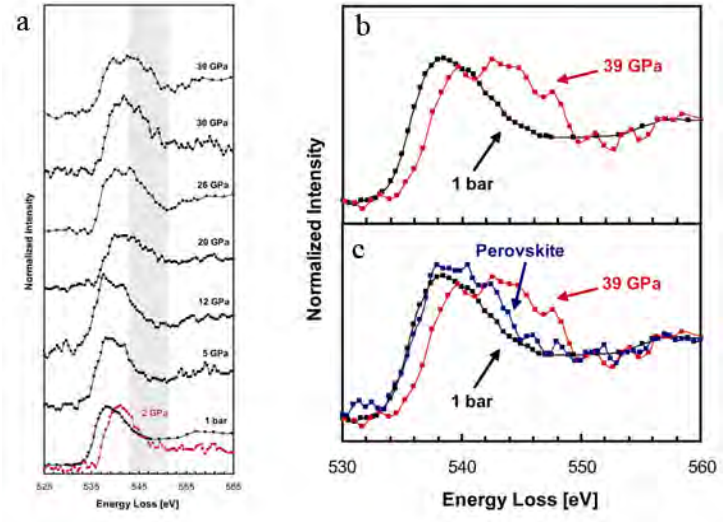


Figure 11. *a) Oxygen K-edge x-ray Raman spectra for $MgSiO_3$ glasses at high pressures [plotted as energy loss (incident energy – elastic energy) vs. normalized scattered intensity]. Grey area represents energy range from 543 eV to 551 eV. b) Comparison of the oxygen K-edge spectra for amorphous $MgSiO_3$ at 1 atm and 39 GPa. c) Oxygen K-edge x-ray Raman spectra for $MgSiO_3$ glasses at 1 atm, 39 GPa, and perovskite. Spacing of refer to the step size of the energy scan of the experiments.*[31,32]

in the fraction of oxygen triclusters at high pressure would thus result in enhanced density, viscosity, and crystal-melt partitioning, and reduced element diffusivity in $MgSiO_3$ melts above 20 GPa toward the deeper part of the Earth's lower mantle.

Transition Metal Chalcogenides at High Pressure – The high pressure behavior of transition metal compounds with practical applications as solid lubricants has been an ongoing research focus in the **Texas Tech** group, where the interest is in how these compounds perform under conditions of heavy wear. In the current year, a high pressure angle dispersive synchrotron x-ray diffraction study of TiS_2 was carried to pressures of 45.5 GPa in a DAC. At about 20.7 GPa, there is evidence of a phase transformation, but the structure of the high pressure phase remains unsolved. The compression behavior of TiS_2 is anisotropic along the different axes, with the *c*-axis is about nine times more compressible than the *a*-axis when pressures are lower than 1 GPa; the *c*-axis suddenly becomes just three times as compressible as the *a*-axis at about 3 GPa. A fit to the third-order Birch-Murnaghan EOS gives K_{0T}, was determined to be 45.9 ±0.7 GPa with its pressure derivative, K'_{0T}, 9.5 ± 0.3.

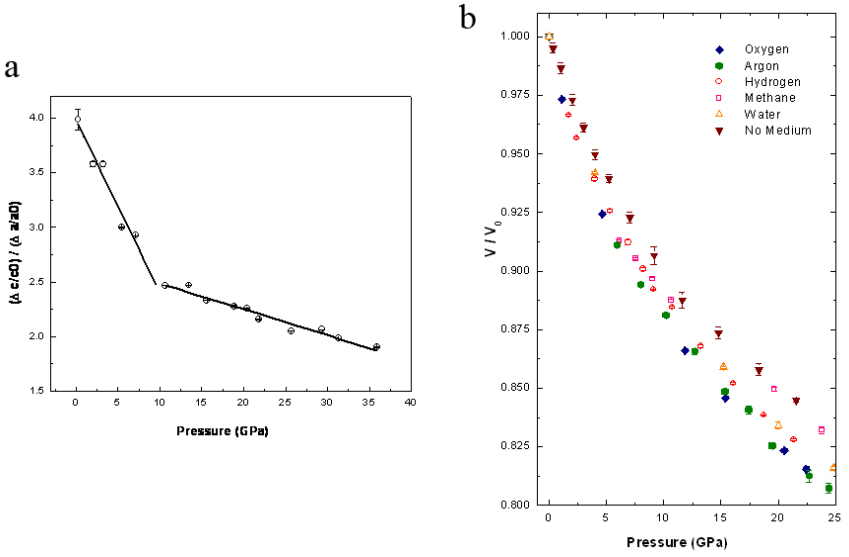


Figure 12. *a) Ratio of reduced lattice parameters for $MoSe_2$ with increasing pressure. The error bars are within the open circle symbols. The linear decrease to 10 GPa and 35.9 GPa is shown with two different solid lines. b) Comparison of pressure dependence of relative unit cell volume of WS_2 obtained with different pressure media.*

In contrast, phase transitions were not encountered in WSe_2 up to or $MoSe_2$ up to similar pressures, despite the overall similarities in their EOS. Synchrotron x-ray diffraction experiments yield K_{0T} = 85 ± 1 GPa and K'_{0T} = 3.4 ± 0.1 GPa for WSe_2 and K_{0T} = 45.7 ± 0.3 GPa and K'_{0T} = 11.6 ± 0.1 for $MoSe_2$. As shown in Fig. 12a, however, the compression mechanism clearly changes in $MoSe_2$ at approximately 10 GPa, where the ratio of reduced lattice parameters changes abruptly with pressure. In a study of the compressibility of WS_2 using different pressure media, it was found that the nature of the pressure medium in the DAC can have an effect on the compressibility. Fig. 12b shows the *P-V* data for a series of pressure media, and indicates that the differences in the EOS obtained using different media are clearly non-negligible, particularly at higher pressures.

Nanomaterials under Pressure – The compression behavior of nanostructured materials is an emerging area of research and further emphasizes the differences between the nanoscale and the bulk. In the **Ma** group at Texas Tech, a number of different systems are under current investigation.

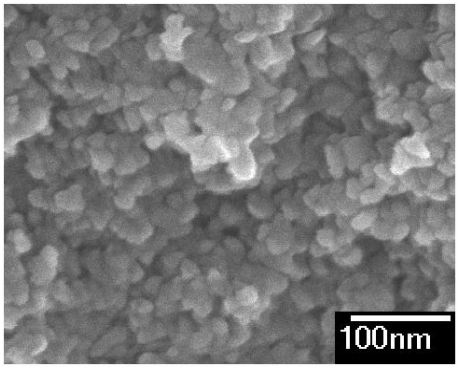


Figure 13. *SEM images of SiC nanoparticles*

SiC – Silicon carbide (SiC) nanocrystals were synthesized by an electrical explosion method. (Fig. 13) High pressure synchrotron x-ray diffraction was then used to investigate the properties of SiC to 15.8 GPa at room temperature, and shows that the nanocrystalline SiC has a larger cell parameter than the bulk material. The bulk modulus was determined to be K_{0T} = 178 ± 22 GPa with its pressure derivative K'_{0T} = 14.7 ± 5.3.

W and W_2N – X-ray diffraction measurements also show that a synthesized nanocrystalline tungsten nitride (W_2N) has a substantially larger cell parameter than its bulk material, and yet the lattice of nanocrystalline tungsten remains unchanged. High-pressure diffraction to 31 GPa resolved a much lower bulk modulus of 240 GPa for nanocrystalline W_2N, and a relatively unchanged bulk modulus of 307 GPa for nanocrystalline W compared to their respective bulk materials. This result suggests that the metallic bonding of a metal is not affected by reduction in grain size. The enlarged cell parameter and the relatively lower bulk modulus of W_2N reflect the nanocrystalline size effect in this material.

ZnO Nanowires – The high-pressure behavior of zinc oxide (ZnO) nanowires has been investigated to 38.7 GPa at room temperature by synchrotron x-ray diffraction. A transformation from a hexagonal wurtzitic structure to a cubic rocksalt structure was observed between 7. 9 and 10.5 GPa. The bulk modulii of the hexagonal wurtzite and cubic rocksalt phases were determined as 99.3 GPa and 164.8 GPa, respectively.

Mo_2N Phases – The structure and size of molybdenum nitride nanoparticles were investigated using high resolution transmission electron microscopy (HRTEM). Typical sizes of the particles were between 3 - 5 nm (Fig. 14). High resolution lattice imaging shows that the particles are single crystals and defect free. Two different phases of molybdenum nitride, γ-Mo_2N (cubic) and δ-MoN (hexagonal) were identified. In addition, the body-centered cubic molybdenum phase was also present. It is anticipated that molybdenum is formed because of an insufficient N_2 supply or slow reaction rate. A mixture of γ-Mo_2N and δ-MoN suggests the existence of a temperature gradient in the chamber leading to formation of γ-Mo_2N at lower temperature (500 to 700°C) and δ-MoN at higher temperature (850°C).

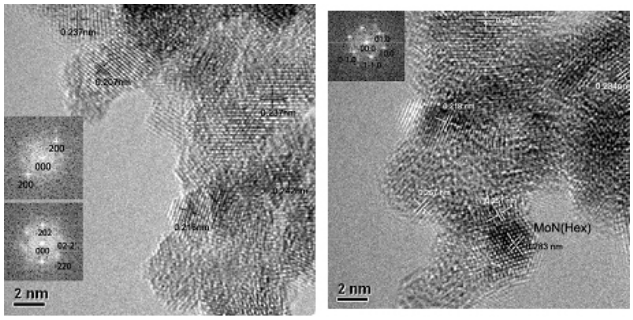


Figure 14. *High-resolution transmission electron micrographs with inserted fast Fourier transform (FFT) images showing that individual nanoparticles are single crystals with sizes 3 to 5 nm and without any defects. The upper and lower FFTs in the left figure are from bcc Mo and fcc Mo_2N, respectively. The FFT in the right figure is from a hexagonal MoN particle. The interplanar spacing of different particles has been clearly identified in these figures (d_{111} of fcc or γ-Mo_2N varies between 0.23 and 0.257 nm, d_{110} of Mo varies between 0.207 and 0.218 nm, and d_{100} of hexagonal or δ-MoN is 0.283 nm).*

2.2 *P-V-T* EOS Measurements

Obtaining accurate *P-V-T* EOS data is critically important to the CDAC mission, as this information provides the framework for predictions of material behavior at extreme conditions undertaken in a wide variety of stewardship science applications. Static methods such as x-ray and neutron diffraction and sound velocity measurements provide key information that complements the data obtained from dynamic compression studies. CDAC scientists are working on EOS data for low-Z materials,[33-36] detonation products, polymers high energy density materials,[33, 34, 36, 37] and a variety of different crystalline solids. Detailed computational studies also complement this experimental work and provide evidence as to the importance of complex, many-body effects even in simple systems.[38]

High P-T Materials Science at LANL – The CDAC Program has allowed **LANL** to study several key materials in order to gain fundamental knowledge and provide data applicable to national security matters. In the past year, for example, detailed studies of zirconium have resulted in an understanding of the effects of impurities on phase boundaries and grain growth. X-ray diffraction studies on high explosives have provided valuable static data, which has been incorporated with dynamic results to produce a better understanding of these materials. The information obtained in these studies continues to support the Stewardship Science program throughout the Department of Energy Complex.

Zirconium – Group IV metals, including Zr have a number of industrial applications, however limitations can be caused by the α → ω phase transition. Many factors influence the phase boundaries, such as elevated temperatures, non-hydrostatic stress, and impurities. **Neal Chesnut** and **Nenad Velisavjevic** have been exploring how impurities and non-hydrostatic stresses affect phase boundaries and other material properties. Three samples were obtained of varying purity as shown in Table 1. The Material Science and Technology Division at **LANL** characterized the samples.

Sample	**Hf**	**Fe**	**Al**	**V**	**O**	**N**	**C**	**$P_{\alpha\rightarrow\omega}$ (non-hydro.) (GPa)**	**$P_{\alpha\rightarrow\omega}$ (hydro.) (GPa)**
ZrI	35	<50	<20	<50	<50	<20	22	4.6	6.4
ZrII	350	125	<20	<25	390	15	70	5.5	7.5
ZrIII	14,000	2,400	-	-	1,200	80	270	10.8	11.6

Table 1. *Sample purity of Zr samples studied (Wt ppm). All three samples have initial grain size of 25 μm. Also included is the measured pressure at the start of the α→ω transition under both non-hydrostatic and hydrostatic conditions.*

In group IV metals, room temperature compression leads to a martensitic transformation from a ductile α to a brittle ω phase at ~8 GPa for Ti, ~8 GPa for Zr, and 38 GPa for Hf. The α → ω phase boundary decreases to lower pressures at high temperatures and can severely limit the use of group IV metals in industrial applications. Impurities also play an important role in determining the phase boundary as they can either aid or suppress the α → ω transition. Substitutional impurities such as aluminum can decrease *d*-electron concentration and increase the stability of the α phase to higher pressures, on the other hand *d*-electron rich impurities like molybdenum increase *d*-electron concentration and decrease the α → ω transition pressure. In the case of interstitial impurities, results of *ab initio* calculations show that oxygen, nitrogen and carbon occupying the hexahedral and octahedral sites increase the energy barrier and block the α → ω transformation.

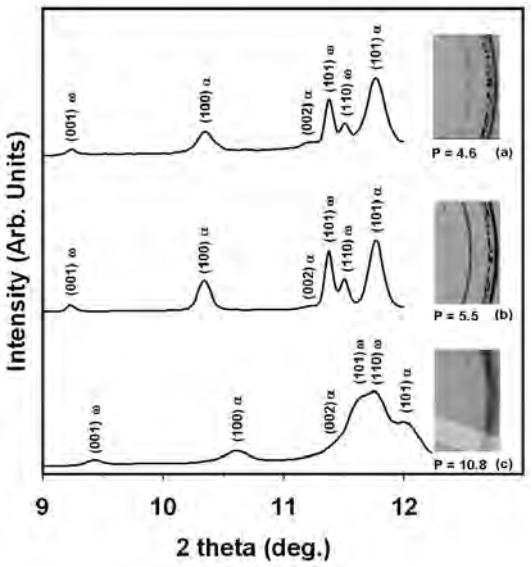


Figure 15. *X-ray diffraction patterns at the α→ω transition for the Zr samples. Large grain growth is observed for the two highest purity samples ZrI (a) and ZrII (b), but not the lowest purity sample, ZrIII (c).*

Multiple x-ray diffraction experiments on the well-characterized Zr samples revealed the effects of varying impurity levels as shown in Table 1. These experiments were performed in hydrostatic and non-hydrostatic conditions, which also demonstrate the effects of shear stress on a phase transition. Another interesting phenomenon that was observed with respect to the α→ω transition was grain growth as shown in

Fig. 15. The room temperature grain growth in the present experiments occurs at a much lower temperature, and during the α → ω transition compared to the grain growth observed in Zr by Hattori *et al.*[39] at 8.3 GPa and 650°C at the onset of the ω → ß transition. No information is given about the initial sample texturing, which could be responsible for the room temperature grain growth observed in our experiments. ZrIII was heated to 1279 K at 10.8 GPa and undergoes the ω → ß transition; however, no significant grain growth is observed. This series of experiments has helped improve the understanding of the effects of impurities and shear stress on the phase boundaries, which provides a greater understanding of the underlying physics and contributions to potential applications.[40, 41]

High Explosives – Investigation of the high pressure behaviors of high explosives plays a critical role in supporting national and global security and safety needs. Understanding the high pressure phase behavior, compressibility, and chemistry of explosive molecules is paramount to predicting their initiation behavior, both in the presence and absence of hot spots, where either local or global pressure and temperature rises couple to dynamic compression, heating, and eventual onset of chemistry. Static high pressure x-ray diffraction experiments have been essential for probing the accessible states in these materials, and, when combined with optical spectroscopies, may give insight into how energy may couple into them to initiate the first stages of chemical reaction leading to deflagration and detonation. In the past year, **Dana Dattlebaum** has examined the high pressure behavior of the organic explosive materials triamino-trinitrobenzene, nitromethane, ammonium nitrate, DAAF, and trinitrotoluene (TNT) using the 16-ID-B (HPCAT) beamline at the APS.[42, 43] In our experiments, the materials were loaded into DACs, and pressurized to > 25 GPa, while probing their inherent phase diagrams, at room temperature.

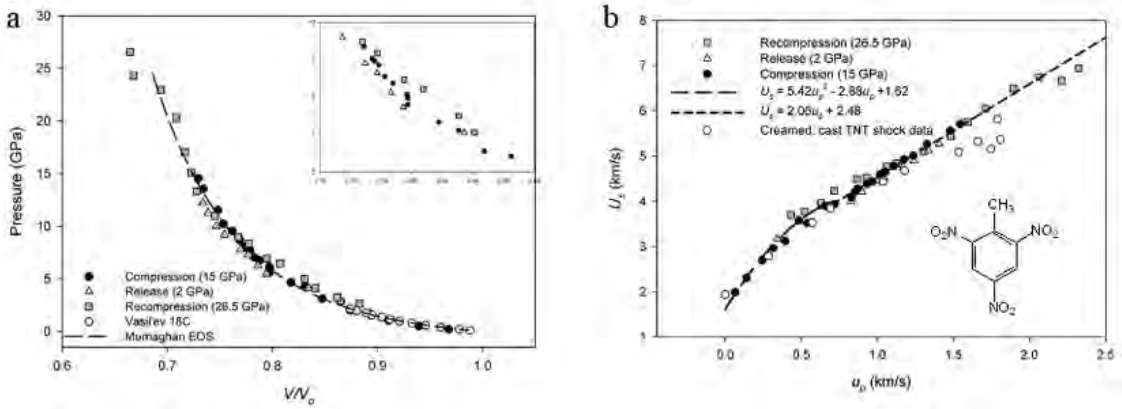


Figure 16. *(a) Room temperature isotherms from compression, release and recompression cycles for TNT derived from ADXD experiments. (b) Calculated pseudo-U_s-u_p data from ADXD experiments compared with shock data on creamed cast TNT (LASL Shock Handbook).*

Of particular interest has been the work on TNT, which is known by historical dynamic experiments to have a possible phase transition above 10 GPa. It has also been shown by dynamic mass spectrometry that TNT may dimerize when shocked to pressures within this range.[44] Similar reactions have also been observed in the multi-ring-structured anthracene[45] suggesting that the reaction mechanisms to be elucidated may be universal to these types of molecules (such as the proposed Diels-Alder reactions that may be facilitated by shear). The first isotherm for TNT to pressures exceeding 250 kbar has been measured. *P-V* isotherms derived from the high-pressure x-ray spectra displayed a slight density hysteresis around 4.0 GPa and a sharp discontinuity at ~20.0 GPa, as shown in Fig. 16a. The latter transition is ascribed to a monoclinic-to-orthorhombic, first-order phase transition in TNT. The isothermal bulk modulus (K_o) and its pressure derivative (K_o') were determined for monoclinic TNT to 20 GPa through a Murnaghan EOS analysis giving K_o = 8.52 GPa and K_o' = 8.0. The zero-pressure isothermal bulk modulus is slightly lower than the ~ 8.7 GPa isentropic bulk modulus determined from ultrasonic, sound speed measurements.[46] Conversion of the isothermal *P-V* data to the shock velocity-particle velocity plane revealed a deviation from

linearity at low u_p, a cusp associated with the phase transition at high u_p, and general agreement with the wealth of unreacted Hugoniot data on TNT (Fig. 16b). There was no evidence of dimerization of TNT molecules at high pressures, including through the pressure regime of the known cusp in the shock Hugoniot, 12-14 GPa.

Additional room temperature isotherms have been determined for the explosives ammonium nitrate, nitromethane, and DAAF, measured to Chapman-Jouguet (CJ) pressures. This information at high pressure will be valuable in constructing chemical potentials for input into molecular dynamics simulations of shocked response and chemistry onset. Ongoing work concerns the correlation of electronic and molecular structures at high pressure for these and related materials.

Polymers – X-ray diffraction experiments on fluoropolymers used as binders in plastic bonded explosives and related polymers continued during this year. The high pressure phase behavior of THV 500, a co-polymer of tetrafluoroethylene, vinylidene fluoride and hexafluoropropylene was probed by ADXD to over 10 GPa.[47] In this work, carried out by **Dana Dattlebaum**, it was determined that only ~ 25% of the 60 wt% tetrafluoroethylene domains were found to exist in a crystalline form. More importantly, it was found that co-polymerization of tetrafluoroethylene with the other two co-monomers inhibited the existence of a high pressure phase transition from a helical to planar zig-zag phase that is commonly observed for the homopolymer polytetrafluoroethylene, even at nearly comparable crystallinities.

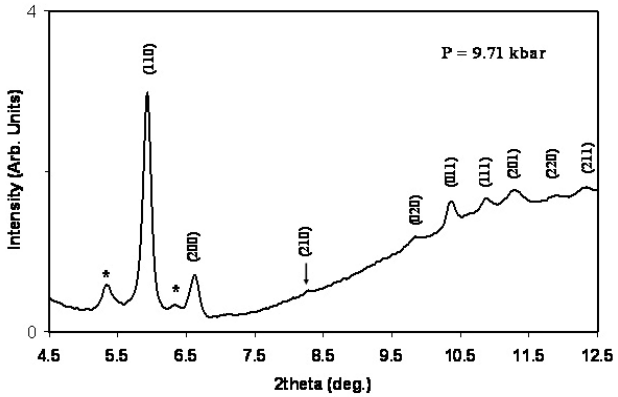


Figure 17. *High-density polyethylene x-ray diffraction spectrum at 9.7 kbar. Peaks corresponding to the orthorhombic phase are indexed accordingly.*

A second study completed this year was a combined high-pressure x-ray diffraction and vibrational spectroscopy investigation of the high pressure properties of three different types of polyethylene (HDPE, UHMWPE, and XPE). Evidence of a structural phase transition from the common orthorhombic *Pnam* phase (Fig. 17) to another as yet undetermined phase was found in the x-ray diffraction data. No clear evidence of the transition is found in the vibrational spectroscopy data. However, since the vibrational modes have the same splitting pattern at higher pressures, it is believed that the high pressure phase has two chains per unit cell as does the orthorhombic *Pnam* phase. Further detailed study of this phase transition would help to elucidate the nature of the transition. The correlation splitting of the infrared active C-H stretching modes was also observed for the first time in this study.

EOS of Alkaline Earth Fluorides to 95 GPa – The alkaline earth fluorides are a fundamental class of materials that exhibit extensive polymorphism at high pressures, and serve as model systems for understanding highly coordinated structures and phase transition pathways in other AX_2 compounds such as SiO_2. Shock compression studies show that fluorites transform to remarkably incompressible phases above 100 GPa. Other phenomena observed or predicted in fluorites at high pressures include ferroelastic behavior, metallization, and superionic conductivity. Technical applications of fluorites include their use as windows and lenses, scintillators, optical coatings, luminescent materials, and as pressure standards.

CDAC student **Susannah Dorfman** has examined phase transitions and EOS of the alkaline earth fluorides CaF_2 and SrF_2 to 95 GPa,[48] and has found that both materials undergo a phase transition from the cubic fluorite structure to the orthorhombic cotunnite-type structure at pressures less than 10 GPa. Both materials further transform to a hexagonal Ni_2In-type structure at 84 and 36 GPa, respectively, following laser heating. This finding is consistent with theoretical

calculations and the behavior of the analog compound BaF_2. For SrF_2, the Ni_2In-type phase was confirmed by Rietveld refinement. On decompression with heating, Ni_2In-type SrF_2 passes through an intermediate orthorhombic phase at 28 GPa before returning to cotunnite structure at 22 GPa. This transition appears analogous to the isosymmetric phase transition to the Co_2Si-type structure reported previously in PbF_2. Unit cell parameters and volumes were determined as a function of pressure for the new phases, and the EOS of the cotunnite phase of CaF_2 constrained to 82 GPa (Fig. 18). Fitting the data to a Birch-Murnaghan EOS yields a zero-pressure bulk modulus of 97.9 GPa with a pressure derivative of 5.6. This work represents the first synthesis and characterization of the Ni_2In-type phase for these compositions and the first report of Co_2Si structure in an alkaline earth fluoride.

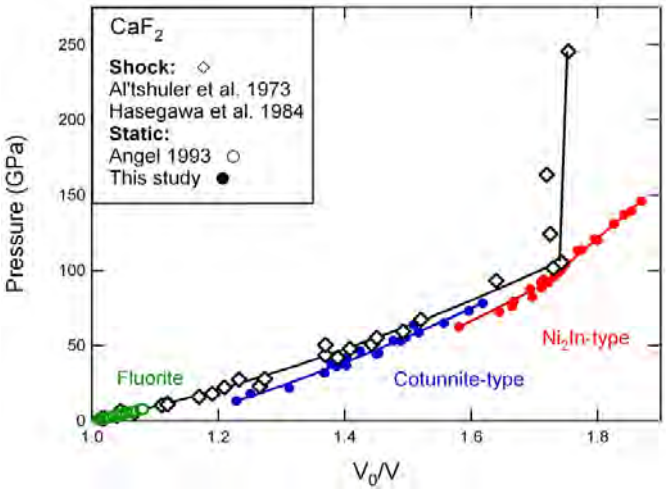


Figure 18. *Comparison of static compression data for CaF_2 to existing shock compression data.*[48]

Pressure Calibration at High Temperatures – The EOS of cubic boron nitride (c-BN) has been determined to a maximum temperature of 3300 K at a simultaneous static pressure of up to more than 70 GPa, and supporteed by *ab initio* calculations to 80 GPa and 2000 K. The experimental data can be reconciled with theoretical results and with the known thermal expansion at 1 bar if a small increase in pressure during heating relative to that measured at ambient temperature is assumed. This data combined with Raman measurements form the basis of a high-temperature pressure scale that is good to at least 3300 K.[18] In further work on the c-BN pressure scale, the thermal EOS and elastic properties of c-BN were determined.[19] The c-BN pressure scale is therefore derived from simultaneous measurements of density and sound velocities at high pressure and temperature and is independent of any previous pressure scale. These results, obtained at room temperature to 27 GPa suggest the validity of the current ruby scale (within ±4% at 100 GPa). At high temperature, data obtained at 16 GPa to 723 K are in fair agreement with the thermal EOS of c-BN reported in previous work, and establish that c-BN can serve as a convenient pressure gauge in x-ray and optical studies using the laser heated DAC.

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

Studies of the vibrational properties of both model compounds and complex materials continue to be an active area of study in several CDAC groups. Facilities at **LANSCE**, **HPCAT** and **NSLS**, in addition to laboratory-based Brillouin scattering methods, provide key thermodynamic data that also serve as tests for evolving theoretical methods.

Pressure-Induced Invar Effect in Pd_3Fe – The Invar effect has been of interest since Guillaume discovered the low thermal expansion of Fe-Ni alloys in 1897. Today "Invar behavior" has come to mean a broad range of anomalies in magnetic and mechanical properties, including molar volume, elastic moduli, pressure derivatives of the bulk modulus, heat capacity, thermal trends of electrical resistivity, magnetization and high field susceptibility, and others. Although the classic Invar phenomenon involves temperature as the intensive thermodynamic variable, pressure-induced Invar behavior has been found in the Fe-Ni system.[49] Pressure-induced Invar behavior can be simpler to understand than thermal Invar behavior because volume, as opposed to entropy, is the conjugate extensive variable for the thermodynamics of the transition. The Fe-Pd system has long been known for thermal Invar behavior for compositions around $Fe_{70}Pd_{30}$, but has received relatively little attention compared to Fe-Ni and Fe-Pt alloys. Increasing the Pd concentration stabilizes the

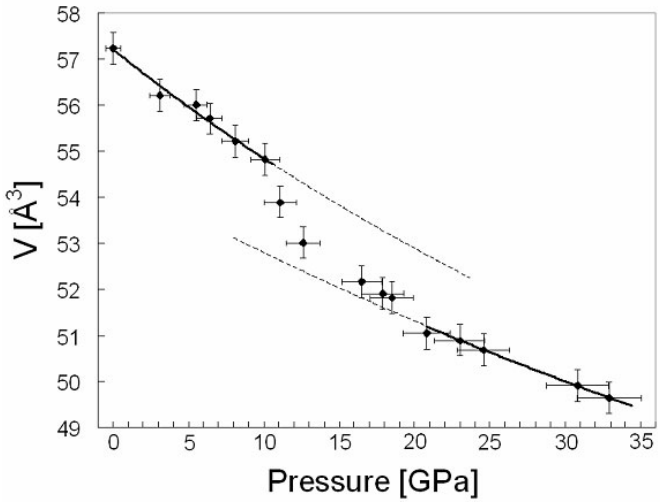


Figure 19. *Volume-pressure data for Pd_3Fe obtained from synchrotron x-ray diffraction measurements (symbols) together with least-squares-fits to two EOS. Solid lines show fitted points; dashed lines are extrapolations.*

ferromagnetic state, however, suppressing thermal Invar behavior. The composition Pd_3Fe does not show thermal Invar behavior.

In CDAC-funded work, graduate student **Mike Winterrose** discovered pressure-induced Invar behavior in Pd_3Fe with the ordered $L1_2$ structure. The pressure-induced anomaly in the bulk modulus was discovered in the **Caltech** group a few years ago, but only in the last year did computational work and new experiments at **HPCAT** allow for a full explanation. Figure 19 shows the volume as a function of pressure for ordered Pd_3Fe from the energy-dispersive x-ray diffraction (EDXD) measurements at beamline X17C of the **NSLS**. A significant volume collapse is found between 10 and 20 GPa, and a change of slope in the V vs. P data is found above 20 GPa. To assess the change in bulk modulus between 10 and 20 GPa, the EDXD data were fit separately to two third-order Birch-Murnaghan EOS in the two pressure regions, the first from 0 to 10 GPa giving a zero-pressure bulk modulus of 217 GPa, and the second from 20 to 33 GPa giving a bulk modulus of 293 GPa.

The Vienna Ab-initio Simulation Package (VASP) was used to treat ordered Pd_3Fe within the framework of density functional theory (DFT) in the local spin-density approximation (LSDA) for the electronic exchange and correlation potential. We found an abrupt magnetic collapse in the spin-polarized ferromagnetic DFT calculations at a volume compression corresponding to 49 GPa. The abrupt magnetic collapse was accompanied by a sudden change of slope in the calculated volume vs. pressure data. To facilitate a comparison to the EDXD results for the bulk modulus, the volume vs. pressure data from the DFT calculations were also fit to two third-order Birch-Murnaghan EOS; one for the high-volume high-moment (HM) state for pressures between 0 and 10 GPa, and one for the low-volume low-moment (LM) state for pressures between 20 and 35 GPa. This procedure gave values of B_0 of 218 and 279 GPa for the HM and LM states, respectively.

Nuclear forward scattering (NFS) spectrometry offers a more direct measure of the magnetic state under pressure, and was performed at the x-ray spectroscopy beamline 16-ID-D at **HPCAT**. Figure 20 shows NFS spectra from ordered Pd_3Fe at pressures up to 25.3 GPa. At low pressures, Pd_3Fe is ferromagnetically ordered with a Curie temperature of 499 K.[50] Quantum beats, expected from a magnetically-ordered material, are prominent in the NFS spectra up to 8.9 GPa. The quantum beats decrease significantly in strength at 12.3 GPa and

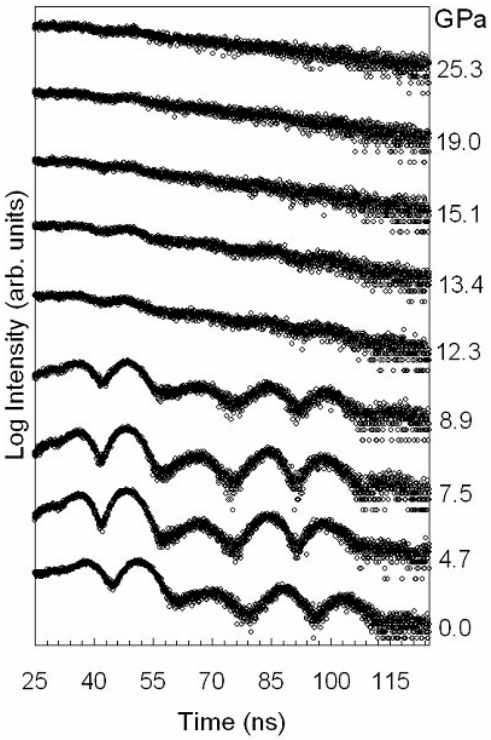


Figure 20. *Nuclear forward scattering spectra from ordered Pd_3Fe showing a sudden and significant decrease in the hyperfine magnetic field strength between 12 and 19 GPa.*

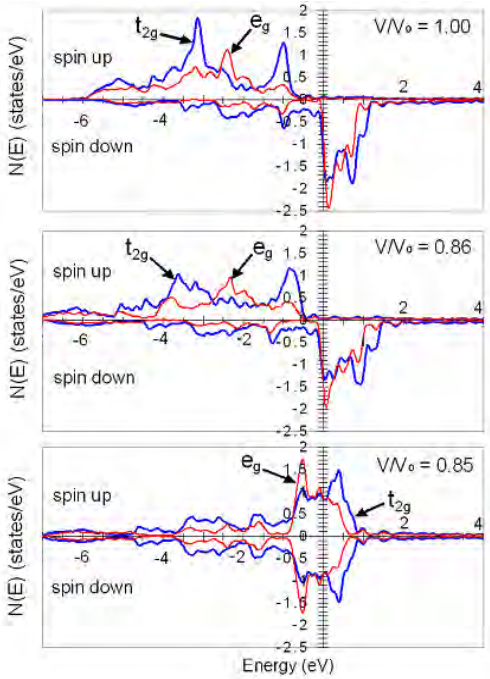


Figure 21. *Electronic density of states at the Fe site decomposed into t_{2g} and e_g symmetry at various cell compressions. E_F=0 eV.*

disappear by 19 GPa, indicating a pressure-induced collapse of the hyperfine magnetic fields in ordered Pd_3Fe. The change in bulk modulus found through the EDXD measurements between 10 and 20 GPa is accompanied by an abrupt pressure-induced collapse of the magnetic order.

The electronic densities of states (DOS) at the Fe site for $L1_2$ Pd_3Fe, decomposed into states of t_{2g} and e_g character, is shown in Fig. 21. The volume $V/V_0 = 0.85$ is just after the magnetic collapse to a state of very low moment (LM) of 0.006 μB at the Fe atoms. These features of the electronic structure are similar to those proposed by Entel, *et al.*[51] for thermal Invar alloys. In an fcc lattice of transition metals, the t_{2g} orbitals form strong dds bonds with first-nearest neighbor (1nn) atoms, owing to their large charge density in the [110] direction. This causes the t_{2g} DOS to split into a high-energy sub-band with anti-bonding character and a low-energy sub-band with primarily bonding character. The e_g orbitals, with maximum charge densities between the more distant 2nn atoms along the [100] direction, form weaker ddp bonds. (Fig. 21).

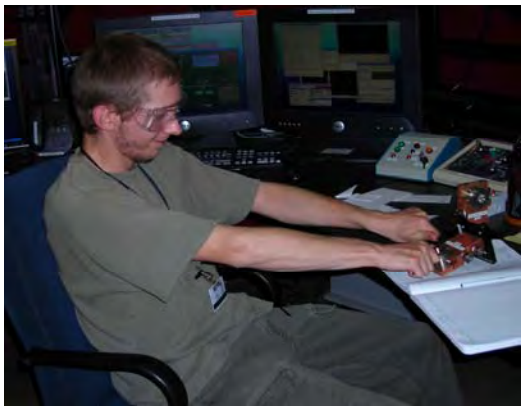
In the ferromagnetic state the t_{2g} levels, which lie along the nearest-neighbor bond directions, show the largest change under pressure, and the t_{2g} anti-bonding levels increase in energy relatively more rapidly than the e_g anti-bonding states. This trend is more pronounced for the states projected onto Pd sites than on Fe sites, demonstrating a connection between size effects and electronic structure in ordered Pd_3Fe. Across the magnetic transition, calculated at a change in relative volume from 0.86 to 0.85, t_{2g} anti-bonding majority spin states move above the Fermi energy (E_F), so there is a transfer of electrons from the higher-energy t_{2g} states to e_g states. Since the majority spin levels at Fe atoms are full, this electron transfer is coupled to a change in magnetic moment, and the electronic rearrangement occurs with the transition to the LM state.

Under pressure, the overlap of the t_{2g} states involving the Pd-Pd 1nn pairs becomes increasingly unfavorable, and the preferred states are the e_g levels in the interstitial regions, especially about Fe atoms. The systematics can be understood in part from the relatively large atomic size of Pd compared to Fe (1.376 vs. 1.274 Å). The fcc structure is close-packed for atoms of equal size, so in the $L1_2$ structure, which has a lattice parameter of 3.85 Å, similar to Pd 3.89 Å, the smaller Fe atoms have excess volume. With pressure it becomes favorable to put more electron density at the smaller Fe atoms. Across the transition to the LM state the charge density throughout the unit cell increases as the volume is compressed, but this increase does not occur uniformly. The total charge density between 1nn Fe-Pd pairs increases by 2.93 % through the transition, compared to a 0.08 % increase between 1nn Pd-Pd pairs. By integrating the electron density around fixed spheres, we find that the pressure-induced HM to LM transition coincides with a transfer of approximately 0.13 electron to each Fe atom from the neighboring Pd atoms.

Ultimately, pressure drives an electronic charge transfer and a magnetic transition in ordered Pd_3Fe, causing a small expansion of Fe atoms and contraction of Pd atoms. After the transition to the LM state, the Pd-Fe 1nn pairs contribute more significantly to the bulk modulus. It has been suggested[49] that pressure-induced Invar phenomena should be properly understood in the framework of non-collinear magnetic states at low volume, as recently predicted for Fe-Ni Invar alloys.[52, 53] The behavior in Pd_3Fe is different, being a more abrupt collapse, perhaps because it is

chemically ordered. The suggestion that non-collinear magnetism lies at the root of Invar behavior has proven controversial.[54]

Infrared-Active Phonons in Simple Oxides – Continuing the work begun in the **Heinz** group at **Chicago** during Year 4, CDAC graduate students **Chris Seagle** and **Wenxuan Zhang** have been using the synchrotron infrared beamline U2A at the **NSLS** to carry out infrared reflectivity measurements on a series of simple oxides. Non-stoichiometric wüstite, $Fe_{1-x}O$; periclase, MgO; and two magnesiowüstites, $(Fe_{0.75}Mg_{0.25})O$ and $(Fe_{0.90}, Mg_{0.10})O$, were studied because of their relevance as model compounds for more complex materials. The measurements yield the pressure dependence transverse optic (TO) and longitudinal optic (LO) phonon mode frequencies, and the resulting data can be used to constrain the optic and thermal Grüneisen parameters, as well as elastic and dielectric properties as functions of pressure.



*CDAC student **Chris Seagle (Chicago).***

In the far IR, (~100-700 cm^{-1}), these rocksalt oxides possess phonon modes which can interact with the oscillating electric field of the synchrotron beam.[55] This interaction causes peaks in the reflectivity spectrum which may be used to calculate the dielectric and averaged vibrational properties of the oxide. An example of the reflectivity spectra obtained is presented in Fig. 22a. The main feature in these spectra arise from the TO phonon mode, an additional weak mode is also observed at higher wavenumber consistent with previous studies at 1 bar.[56-58] The origin of this mode has not been understood previously, but a simple one-dimensional spring model has been developed to include the effects of vacancies, in which the spring constants nearest the vacancies are allowed to vary from the bulk lattice. Although it is quite simple, the model does shed light on the fundamental vibrations that are possible in a rocksalt type lattice, and shows that the presence of vacancies gives rise to a new type of localized vibrational modes. In the case of stronger forces nearest the vacancy sites, the localized mode has a higher frequency than the TO mode.[59] The pressure dependence of the strength and position of this mode suggests that excess charge is preferentially localized near the vacancy sites with increasing pressure, initially causing a rapid rise in the electrical conductivity with pressure. Figure 22b shows the pressure dependence of the TO modes for these materials. This

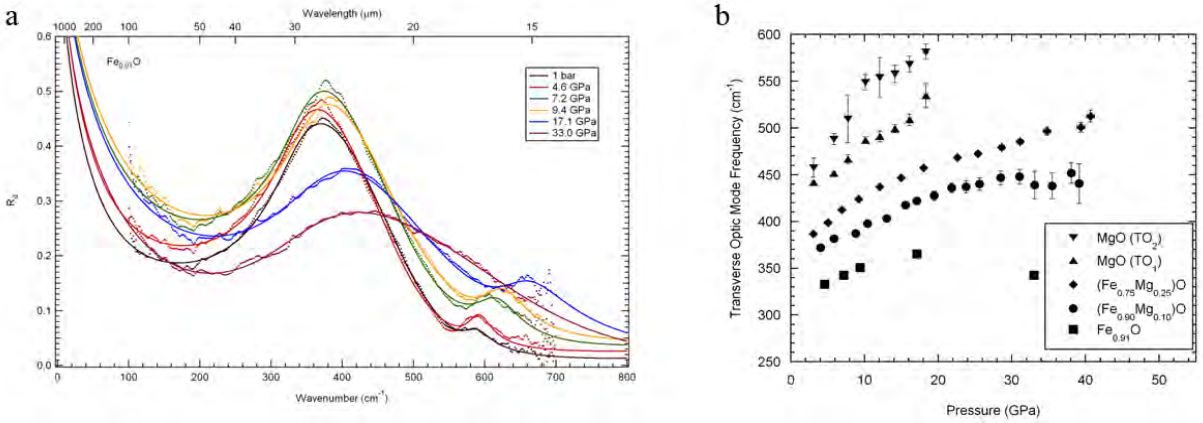


Figure 22. *a) Reflectivity of the $Fe_{0.91}O$-diamond interface as a function of pressure and wavenumber up to 33 GPa. The dots are the data collected and the lines are the best fits to those data based on a Lorentz oscillator model of the dielectric function. The main peaks in the spectra arise from the coupling of the synchrotron beam to the transverse optic phonon. A second weak peak near 600 cm^{-1} is due to localized vibrations near vacancy sites in the non-stoichiometric lattice. b) Transverse optic mode frequencies of rocksalt oxides as a function of pressure. Errors are smaller than the symbols when not shown.*

data will be used to constrain the optic and thermal Grüneisen parameters which are important properties in the in the theory of thermoelasticity.[60, 61]

Elasticity Across the Ferroelastic Phase Transition in MgF_2 – Magnesium fluoride has attracted interest due to its second-order phase transition from the tetragonal rutile-type to an orthorhombic $CaCl_2$-type phase at ~9 GPa. Because the transition occurs at relatively low pressure in this system, MgF_2 serves as an analog for understanding ferroelastic transitions that occur at higher pressures in other compounds such as SiO_2. Until recently, high-pressure measurements of the elastic constants in this system have been limited to 1 GPa. CDAC post-doctoral fellow **Fuming Jiang** has determined the full elastic constant tensor up to and across the soft-mode phase transition in this material, documenting for the first time the reduction in shear velocity and elastic constants as the transition is approached (Fig. 23). Further analysis, including a description of the evolution of the elastic constants using Landau theory, is in progress.

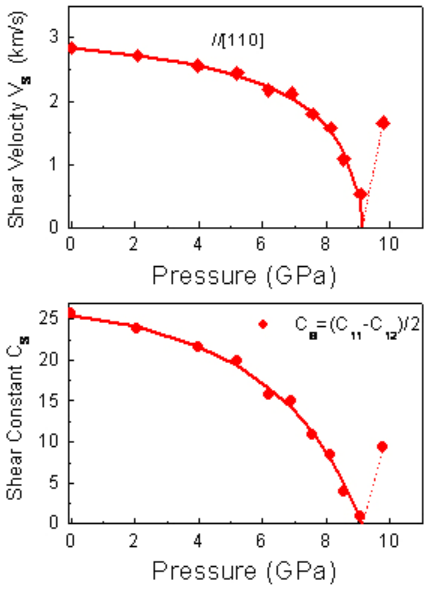
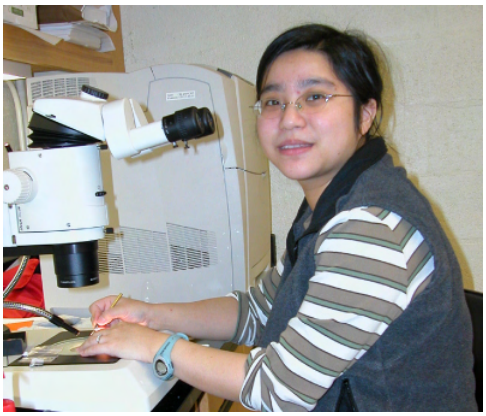


Figure 23. *Shear wave velocity along [110] direction in MgF_2 (upper panel) and associated shear constant $Cs = (C_{11}-C_{12})/2$ (lower panel): symbols (experimental data; solid lines: fit; dotted lines: guide to the eye).*

Elastic Properties of Complex Sulfates – Understanding the mechanical properties of cement paste and of hardened concrete is a longstanding problem in materials science and engineering. Our knowledge of the single-crystal elastic properties of the crystalline constituents of concrete is very limited and this makes it difficult to develop quantitative models able to predict the behavior and properties of such a complex multi-component system. Ettringite, $Ca_6Al_2(SO_4)_3(OH)_{12}\cdot 26H_2O$, is a complex trigonal sulfate and corresponds to one of the major hydration products of portland cement. It is both a primary crystalline product during cement paste consolidation and a secondary phase which crystallizes in hardened concrete, and plays an important role in concrete deterioration in humid environments. In a collaboration between the **Berkeley** and **Princeton** CDAC groups, including CDAC postdoctoral fellow **Fuming Jiang**, current CDAC graduate student **Zhu Mao** and former CDAC graduate student **Sergio Speziale**, the complete elastic tensor of ettringite was determined for the first time by Brillouin scattering at ambient conditions.[62] The results show that ettringite is much less stiff than portlandite. In addition, the elastic anisotropy of ettringite has a pattern with maximum stiffness along the *c*-axis and minimum along directions in the basal plane, reversed with respect to portlandite. The elastic anisotropy of ettringite is large both in terms of compressional and shear moduli. The large anisotropy of the Young's modulus, together with the observed crystalline morphology, suggest that fast growth of secondary fibrous ettringite in voids may be an important mechanism for deterioration of hardened cements in humid environments.

Elasticity of Hydrous Oxides by Brillouin Scattering: β-Mg_2SiO_4 – Wadsleyite, *β*-Mg_2SiO_4, is potentially a major hydrogen host in the Earth's transition zone (410-660 km depth) due to its large water solubility (up to 0.9 wt.% H_2O at 15 GPa and 1400 °C). In a previous study[63] it was found that the elasticity of wadsleyite decreases strongly with increasing water content at ambient conditions.CDAC graduate student **Zhu Mao** has measured the single-crystal elastic properties of *β*-Mg_2SiO_4, with 0.84 wt.% H_2O measured to 12 GPa by Brillouin scattering.[64] Pressure derivatives of the aggregate bulk modulus, K_{S0}, and shear modulus, G_0, of hydrous wadsleyite are 4.1(1) and 1.4(1) respectively. These values are indistinguishable within uncertainty from those of anhydrous wadsleyite. Given that the bulk seismic velocity increase at 410-km depth in the mantle is too large for dry pyrolite (60 vol% olivine), we estimate that ~1 wt.% H_2O in wadsleyite at 410-km depth is



*CDAC student **Zhu Mao (Princeton)**.*

required to reconcile seismic bulk sound velocities with a pyrolite-composition mantle by using our measured high-pressure elastic constants. If the H_2O content of the mantle is much less than this, then other factors such as other compositional or mineralogical variation need to be considered to explain the 410-km discontinuity. The variations in water content with depth under saturated conditions may also contribute to partial melting and the anomalously steep seismic velocity gradient in the transition zone.

AlOOH – Hydroxides are materials that readily form in natural environments in both the bulk state and on surfaces. These materials span a range of chemistries and possess diverse bonding and structural properties. Aluminum hydroxides and oxyhydroxides are widely found in soils and sediments and are industrially important as a major source of aluminum. Diaspore, α-AlOOH, is an aluminum hydroxide stable to at least 65 GPa at room temperature and to at least 14 GPa at 950 °C. Diaspore is isostructural with goethite, one of the most widespread iron oxides found in the natural environment. Hydrous phases in the Al_2O_3-SiO_2-H_2O system are also geologically relevant to understanding subducted pelitic sediments and Al-rich basalts.

The high-pressure elasticity of AlOOH has been determined by Brillouin spectroscopy to 12 GPa by CDAC postdoctoral fellow **Fuming Jiang** and former CDAC graduate student **Sergio Speziale**.[65] Acoustic velocities were measured in three approximately orthogonal principal planes at ambient and a series of eight elevated pressures, yielding the full elastic tensor as a function of compression. All individual C_{ij}s increase with pressure but C_{23} and C_{55} exhibit anomalously low pressure derivatives. From calculated linear compressibilities, the a-axis is the most compressible. The b-axis becomes the least compressible axis at high pressures. Over the examined pressure range, the azimuthal P-wave anisotropy decreased from 22% to 16%, while the azimuthal S-wave anisotropy increased from 15% to 21% (Fig. 24). Both volume and axial compression curves calculated using Brillouin results are in good agreement with the results from static compression studies. High-pressure sound velocities in diaspore exceed those of other hydrous minerals as well as many anhydrous phases relevant to Earth's upper mantle.

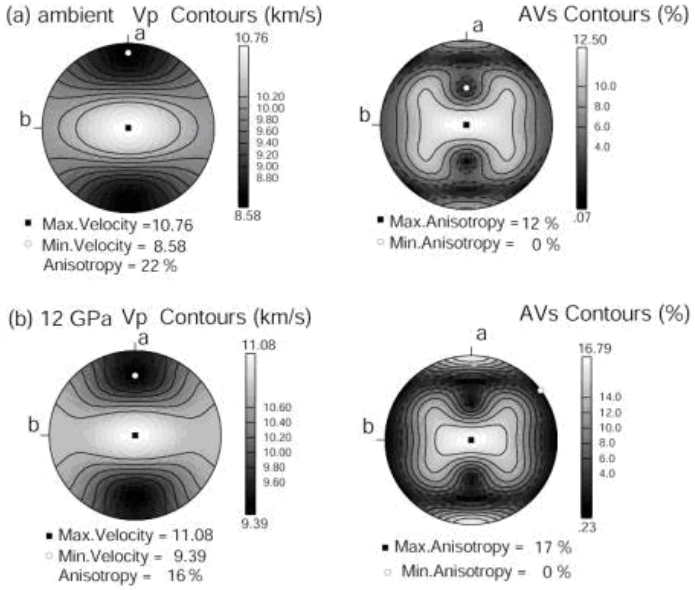


***Figure 24**. Stereogram showing distribution of P-wave velocities (left panel) and shear wave velocity splitting for diaspore at (a) ambient pressure and (b) 12 GPa.*

Ferroelectrics at High Pressure – The *in-situ* high pressure Brillouin scattering technique has been used at **Carnegie** to study a $Pb(Mg_{1/3}Nb_{2/3})O_3$ single crystal up to 10 GPa at 300 K. The pressure dependencies of the elastic constants and elastic anisotropy, as well as the bulk modulus were determined. The pressure dependence of the elastic anisotropy (Fig. 25) shows an abrupt jump

at 4.5 GPa, indicating a characteristic pressure-induced structural phase transition from the cubic Pm-3m to the rhombohedral R-3c phase.

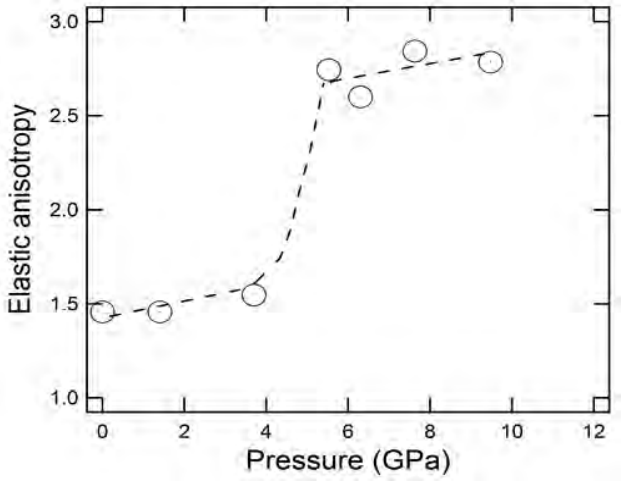


Figure 25. *Pressure dependence of the elastic anisotropy for $Pb(Mg_{1/3}Nb_{2/3})O_3$.*

A great deal of progress has been made recently in understanding ferroelectrics with the (1-x)$Pb(Mg_{1/3}Nb_{1/3})O_3$-x$PbTiO_3$ (PMN-PT) and $PbZr_{1-x}Ti_xO_3$ (PZT) compositions through temperature- and/or chemical composition-dependent investigations. For instance, careful structural investigations of the chemical substitution-temperature *(x-T)* phase diagram of PMN-PT have led to important advances in the understanding of their piezoelectric properties. In contrast to the large number of reported *x-T* investigations, reports of substitution-pressure (*x-P*), or temperature-pressure *P-T* phase diagrams are scarce. It is important to note that the limited number of high-pressure investigations on relaxors have nonetheless already revealed important pressure-instabilities on the local and average structure scale, in sharp contrast to the effect of temperature, which is known to lead generally to only small evolutions in the average structure of relaxors. The aim of these pressure-dependent studies is to extend the understanding of the PMN-PT system, regarded as a model for relaxor-based piezoelectrics. Furthermore, the work might well help to provide a structural basis for promising *ab initio* calculations, which are easier to perform on PMN-PT than on PMN via the so-called virtual crystal approximation.

To understand the pressure-composition phase diagram of PMN-%PT solid solutions, high-pressure Raman scattering and x-ray diffraction methods were used to investigate several different compositions: PMN-22%PT, PMN-30%PT, PMN-33%PT, PMN-35%PT, PMN-37%PT, and PMN-40%PT, all in powder samples. Preliminary results indicate that the morphotropic phase boundary persists up to 7 GPa between the compositions of 33% and 37%. A proposed preliminary phase diagram is presented in Fig. 26.

2.4 Plasticity, Yield Strength, and Deformation

High plastic strain (ε_p> 100%), over a broad range of strain rates (> 10^5) represent another set of extreme conditions that are important in the understanding of material properties relevant to stewardship science. Pressure- and temperature-induced phase transformations of materials produce systematic changes in texture patterns, which can allow a determination of transition mechanisms. During Year 5, CDAC groups continued to focus on data analysis techniques as well as new experimental methods, both with radial x-ray diffraction experiments at **HPCAT** and neutron diffraction at **LANSCE**.

Texture in Iron at High Pressure and High Temperature – The main goal of the **Berkeley** CDAC contribution is to study plastic and elastic deformation and the influence of non-hydrostatic stress, mainly at high and ultrahigh pressure and temperature, and investigate the

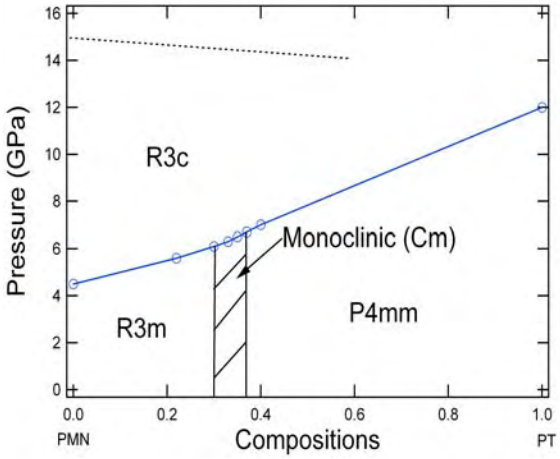


Figure 26. *Proposed composition-pressure phase diagram for PMN-x%PT solid solutions based on diffraction data.*

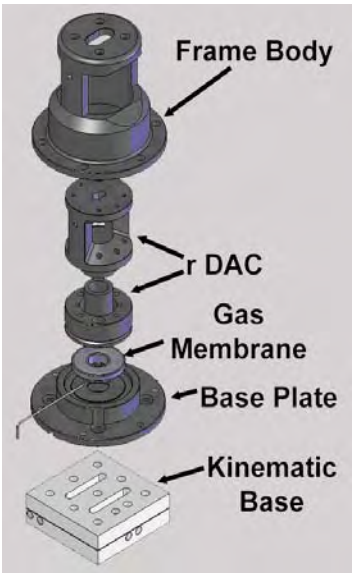


Figure 27. *Exploded view of the loading frame used for radial diffraction measurements. A frame body houses the DAC while a base plate holds the membrane against the DAC piston. Inflating the gas membrane applies force to drive the piston. The cap of the loading frame has a window to allow imaging and laser access.*

effects on deformation mechanisms and anisotropic elastic properties. The group has developed both laser and resistance-heated DACs with remote pressure and temperature control that are now available for the high pressure research community. Radial diffraction measurements on samples under pressure in the DAC is a useful technique to study the development of lattice strains and lattice preferred orientation (LPO), *in situ* at high pressures. However, previous work using the DAC and radial diffraction were performed at ambient temperature. It is questionable whether room temperature studies are appropriate for extrapolation to cases in which materials are deforming at both high pressure and high temperature. In order to address this limitation **Rudy Wenk's** group has developed a novel combination of remote pressure increase utilizing a gas membrane driven panoramic DAC and single sided *in-situ* laser heating for radial diffraction (Fig. 27). The device has been used to study bcc (α), fcc (γ) and hcp (ε) Fe at a range of pressures and temperatures up to 30 GPa and 1900 K.[16] Orientation relationships during phase transformations by *in situ* observation of textures (i.e. Burgers and Kurdjumov-Sachs) have also been documented. In addition, in contrast to room temperature measurements on hcp Fe, which indicate texture is developed primarily through basal (0001)⟨2-1-10⟩ slip (Fig. 28 Left), it appears that at high temperature pyramidal ⟨a+c⟩ {2-1-12}⟨2-1-13⟩ slip is activated and becomes dominant (Fig. 28 Right). This illustrates the importance of texture measurements at high temperatures where different slip systems may become active. It has also been observed that the high temperature fcc phase develops a (110) texture typical for fcc metals deformed in compression. This device is now installed and available to users at ALS beamline 12.2.2.

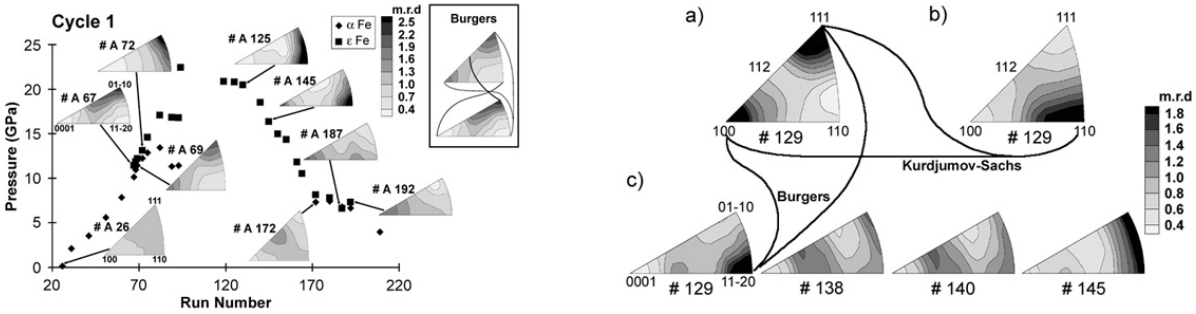


Figure 28. *Left: IPFs selected from the total of 40 images collected and analyzed from the high temperature run for a) bcc Fe, b) fcc Fe, and c) hcp Fe. Lines connecting IPFs show the Burgers relation for the bcc-hcp transformation, and Kurdjumov-Sachs relation for the bcc-fcc transformation. Right: Graph of pressure versus run number for room temperature deformation cycle, with inverse pole figures (IPFs) for selected points shown. Compression of the bcc phase yields maxima at 001 and 111 which are attributed to slip on {110}⟨111⟩. Upon completion of the phase transformation, hcp Fe develops a maximum at 11-20 consistent with Burgers' relationship. During decompression, the hcp phase develops a 0001 maximum. This is attributed to basal (0001)⟨2-1-10⟩ slip.*

Resistive Heating and Radial Diffraction of Iron – The **Berkeley** group is also collaborating with HPCAT staff in the development of a system for resistive heating and radial diffraction that will allow *in situ* measurements of stresses and textures in the DAC at simultaneously high pressures and temperatures. This new technique combines radial diffraction

geometry with external heating using a graphite heater and membrane pressure control, with current coverage in pressure and temperature to ~30 GPa and 1100 °C. This technique has the advantage over laser heating of more uniform temperatures in the sample, but temperatures are limited to a lower temperature range. This method was applied to collect *in situ* texture measurements on the high-pressure and temperature phases of iron. The experiment allowed the observation of (100) and (111) texture in bcc-Fe, and it was 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 (Fig. 29) was observed. This is consistent with observations using *in situ* laser heating, validating the new techniques. These techniques can be used in the future to expand the pressure temperature space over which radial diffraction experiments are performed.

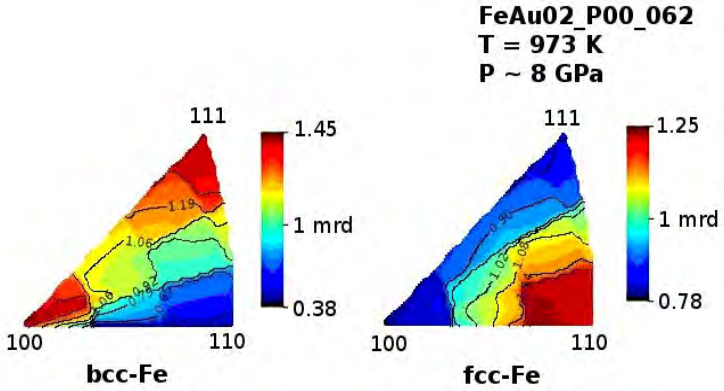


Figure 29. *Inverse pole figures for bcc and fcc iron at 8 GPa and 973 K. Bcc iron exhibits a texture characterized by {100} and {111} plane at high angle to compression, as is typical for compression of bcc metals. Fcc iron has {110} plane at high angles to compression as expected for compression of an fcc metal. This agrees with measurements obtained with in-situ laser heating.*

Experimental Determination of Elasticity in Iron – In an effort to resolve some unsettled questions concerning the elasticity of iron, the **Berkeley** group participated in an integrated study to determine the anisotropy of polycrystalline hcp-Fe at high pressure. Directional phonon measurements from inelastic x-ray scattering (IXS) on a textured sample at 52 GPa in a DAC were coupled with EOS results to determine the elastic tensor. Comparison of the results from this new method with the elasticity determined by lattice strain analysis of radial x-ray diffraction (RXD) measurements showed significant differences, highlighting the importance of strength anisotropy in hcp-Fe. It was found that a method which combines results from IXS and EOS measurements gives a smaller anisotropy and a shape close to sigmoidal with a faster *c* and slower *a* axis compared to the RXD lattice strain method.

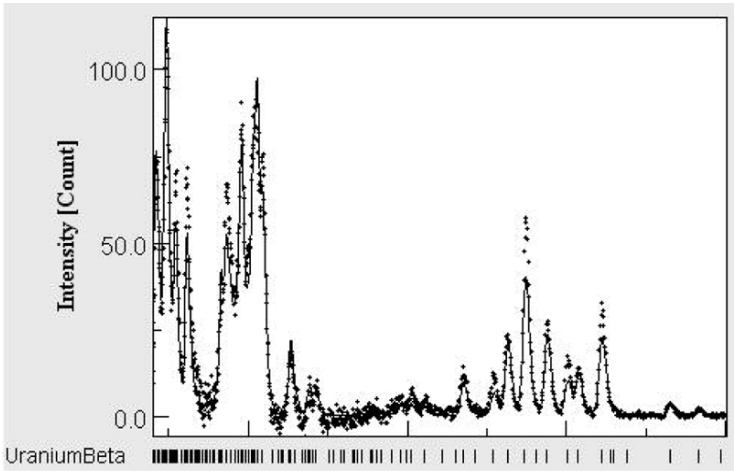


Figure 30. *Neutron diffraction spectrum of tetragonal uranium at 677°C.*

Texture Development During Phase Tranformations in Zr and U – Phase transitions in polycrystals have a profound impact on physical properties of materials, in particular on the anisotropy pattern, which is due to preferred orientation of crystals. Texture that forms as a result of dislocation glide and mechanical twinning is reasonably understood for many materials, but texture changes that occur during recrystallization are still much more enigmatic, particularly those taking place during phase transformations. This is due to the fact that until recently, it has been very difficult to measure textures *in situ* at temperature and pressure. In general, textures are measured at room

temperature, and the high-temperature texture is implied by modeling. This has changed with recent developments at the HIPPO diffractometer at LANSCE, which the **Berkeley** group has used to investigate texture changes during heating, both for recrystallization and phase transformations.

One of the first samples investigated with the HIPPO instrument at LANSCE has been Zircaloy-4 12. It was observed that a cold-rolling hcp texture recrystallized above 500 °C and transformed to bcc above 900 °C. The recrystallization does not affect the *c*-axis but interchanges $(10\bar{1}1)$ and $(11\bar{2}0)$ through preferential growth of orientations that are most susceptible to twinning. The same orientation component is preferred for transformation with distinct variant selection. The final texture is considerably stronger than the initial one. In this case, the transformation was complete with no bcc phase at low temperature and no hcp phase at the highest temperature; the two phases coexist only at the phase transition temperature. In impure zirconium, a small volume fraction of the bcc phase is present at room temperature and some hcp is still present at the highest temperature.

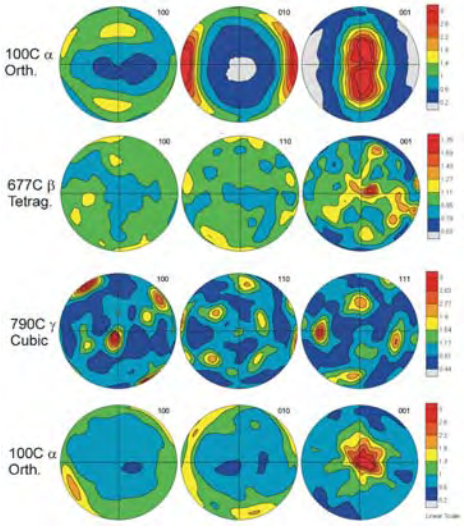


Figure 31. *Texture changes in uranium. Pole figures in equal area projection.*

In order to understand orientation selection and variant selection during phase transformations, low symmetry systems are most interesting since they are best constrained. Uranium is orthorhombic (α-phase, space group C*mcm*) up to 660°C, tetragonal (β, $P4_2/mnm$) from 668°C to 766°C, and becomes cubic (γ-phase, bcc) above 760°C. Interestingly, the tetragonal phase has a lower symmetry than the orthorhombic phase with a large unit cell and correspondingly a very complex diffraction pattern with many peaks as shown in Fig 30.

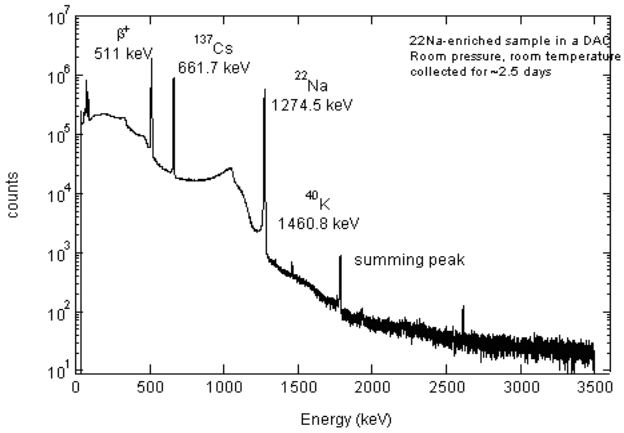


Figure 32. *Gamma-ray measurements of a ^{22}Na-enriched sample within a DAC without pressure applied. Spectra taken for ~2.5 days and used to benchmark high-P measurements. Major peaks are labeled and show significant positron (β^+) emission, both from the ^{22}Na sample as well from the background; calibrant ^{137}Cs; ^{22}Na sample peak; background ^{40}K peak and a summing peak from simultaneous β^+ and electron-capture decays (511 + 1275 keV).*

A cold-rolled sample of #520-1S uranium shows indeed a strong texture (Fig. 31). The texture changes slightly during heating to 500°C. Rapid grain growth occurs above 600°C and in most cases it was not possible to determine a meaningful texture pattern. When the sample was just barely heated above the β-transition (677°C) the 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 α-phase a cubic texture can be identified (790°C). So far only in one case a memory was observed after cooling. In the future experiments have to be repeated by choosing impure uranium with precipitates to avoid excessive grain growth.

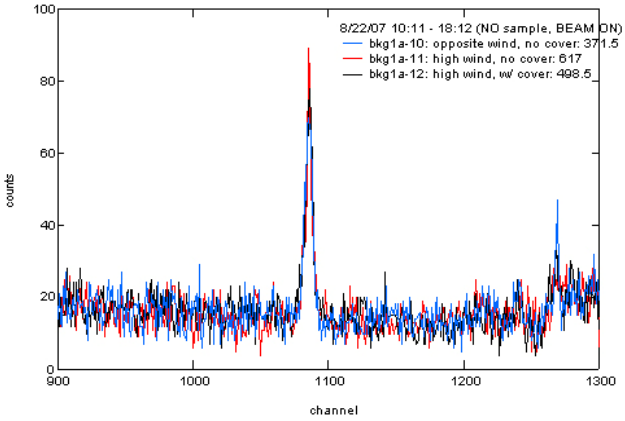
2.5 Electronic and Magnetic Structure and Dynamics

The effects of high *P-T* conditions on the electronic and magnetic properties of materials are studied in many CDAC groups. A productive interplay between experiment and theory is necessary to develop a full picture of

material behavior at extreme conditions. Elemental solids, molecular compounds, crystalline and polycrystalline materials and conventional and high-T_c superconductors are are among the systems under investigation in CDAC. With an increasingly sophisticated array of x-ray based techniques available at **HPCAT**, more complicated systems will be available for study in the near future.

Electron Capture in ^{22}Na With Pressure – **Kanani Lee (New Mexico State,** now at **Yale University)** has begun experiments at **LANSCE** designed to measure the effect of pressure on the decay constant of the electron capture isotope ^{22}Na. A sample of ^{22}Na-enriched NaCl (activity ~ 10 μCurie) is under pressure in a compact-cylinder DAC within a Re gasket pre-compressed to a thickness of 10-15 μm, with a 120 μm sample chamber. A small ruby grain that serves as a pressure marker and ^{137}CsCl (activity ~10 μCurie) is also added into the DAC, but not under pressure, and used as an internal γ-ray standard. To measure each ^{22}Na electron-capture decay and ^{137}Cs decay, two γ-ray detectors are arranged around the DAC to measure the characteristic γ-rays that are emitted with each decay: ~1275 and ~662 keV for ^{22}Na and ^{137}Cs respectively (Fig. 32).

Figure 33. *Background noise around the β^+ emission peak (511 keV, channel ~1090), taken without a sample in 2-hour increments when the LANSCE neutron beam was on. Comparing the blue (high wind speed from SW) and red (high wind speed from NE) spectra, the LANSCE emissions carried by the wind have a slight, but non-negligible, effect on the number of counts recorded: 371 vs. 617 respectively. The black trace indicates spectra taken after these effects are minimized with the addition of a plastic cover over the detectors (~499 counts).*



To support the first measurements on how pressure affects the half-life of ^{22}Na, careful considerations were necessary. LANSCE is the largest routine emitter of radionuclides at Los Alamos and has the potential to affect the results of the experiment if the wind blows in the right direction. As such, the effects on this experiment from the surrounding environment were considered by undergraduate research student **Shannon Pitcher** (Fig. 33). In order to minimize this interference, a plastic barrier was placed over the lead-enclosed detectors and special attention was paid to data corresponding to times when the wind was blowing in the direction of the experiment. Statistics were increased by collecting for 1-2 weeks (at two-hour intervals) to reduce the effects of interference. Data is also being collected at times when the neutron beam is off.

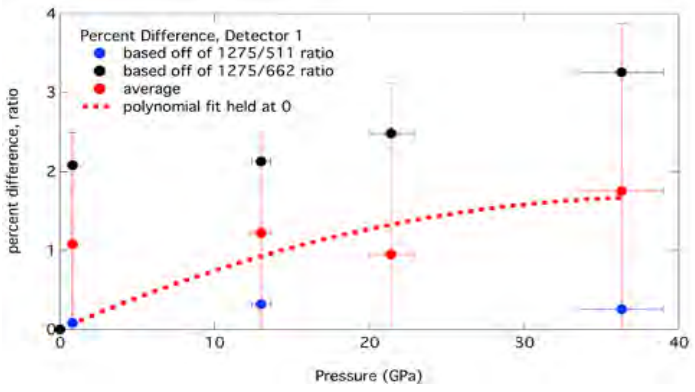


Figure 34. *The percent difference in the 1275/511 or 1275/662 ratios with their RPRT values vs. pressure. The average of the two ratios is shown in red with uncertainties. A polynomial fit to the average is shown as a guide for the eye.*

Due to the small changes predicted by *ab-initio* computations,[66] care had to be taken with the alignment of the detectors with respect to the sample. This proved difficult and is evident in the large uncertainties plotted in Fig. 34. Upon comparing the ratios of the 1275 keV/662 keV and 1275 keV/511 keV we find either a large change in the electron-capture decay constant or a negligible one. This inconclusive result is likely due to alignment problems as well as the need for more statistics.

Synchrotron Mössbauer Spectroscopy of Ferropericlase at High P-T – An electronic spin transition of Fe^{2+} from the high-spin state to the low-spin state has been recently reported to occur in lower-mantle ferropericlase. The effects of the spin transition are affecting the understanding of the mineral physics of the Earth's lower mantle. To understand the local electronic environment of the high-spin Fe^{2+} ions in ferropericlase, **Jung-Fu Lin** at **LLNL** has studied synchrotron Mössbauer spectra (SMS) of $(Mg_{0.75},Fe_{0.25})O$ in externally-heated and laser-heated DACs at high pressures and temperatures at **HPCAT**. The results show that quadrupole splitting (QS) of the dominant high-spin Fe^{2+} site decreases significantly with increasing temperature at a constant pressure. The QS values at a constant pressure are fitted to a temperature-dependent Bolztmann distribution model that permits an estimation of the separation of the crystal field splittings in the lower t_{2g} orbitals (Δ_3). The derived Δ_3 increases from approximately 36 meV to 95 meV between 1 GPa and 40 GPa, revealing that both high pressure and temperature have significant effects on the 3*d* electronic shells of Fe^{2+} in ferropericlase. The SMS spectra collected from the laser-heated diamond cells show no flat features within the time window of 146 ns (Fig. 35), indicating that the Δ_3 significantly decreases at very high temperatures. These results[67] provide new information on the hyperfine parameters and crystal-field splittings of the high-spin Fe^{2+} in ferropericlase at high pressures and temperatures.

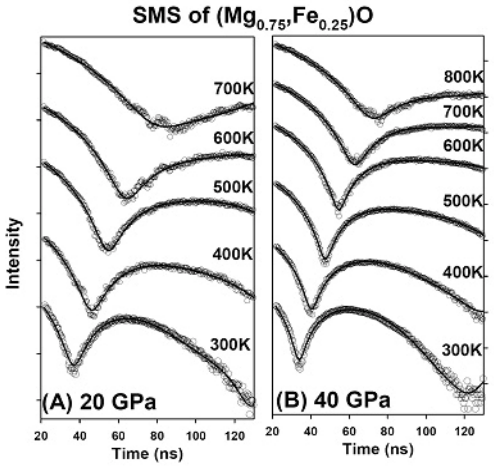


Figure 35. *Representative SMS spectra of ferropericlase [$(Mg_{0.75},Fe_{0.25})O$] at (A) 20 GPa and (B) 40 GPa as a function of temperature collected from an externally heated DAC. Open circles: experimental data; black lines: modeled spectra with two doublets. The sample thickness was approximately 1-3 μm.*

Pressure Effects on T_c in Cuprate Superconductors – Since the discovery in 1986 of high-temperature superconductivity in layered cuprates, the secrets of this remarkable phenomenon have steadily emerged. From the time of the earliest reports, it has been well recognized that the superconducting transition temperature is highly sensitive to the level of chemical doping, a necessary prerequisite to attaining the superconducting state in these materials. As a method of investigating the fundamental changes in physical properties characteristic of the superconducting state, however, doping is a rather coarse probe because a continuous variation in dopant concentration is difficult to achieve. **Tanja Cuk**, a graduate student at **Stanford University**, together with colleagues from **Carnegie**, the **University of Waterloo**, the **Naval Research Laboratory**, and the **Nanoelectronics Research Institute (Japan)** found for the first time that in addition to chemical manipulation, the superconducting state can be induced by applied pressure in high temperature, cuprate superconductors, as it has been for low-temperature, elemental superconductors. Using the Raman spectroscopy laboratory at Carnegie and the high-pressure synchrotron x-ray beamline at HPCAT, both CDAC-supported facilities, **Cuk** and colleagues have applied a unique combination of contact-free experimental techniques toward investigating the effects of pressure on superconducting properties.

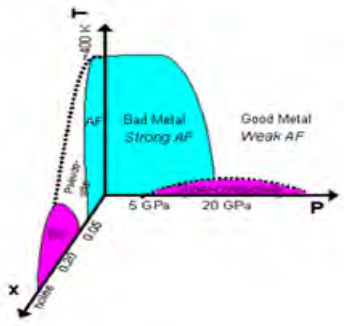


Figure 36. *3-D phase diagram in x (doping). Two distinct transitions take place as a function of both doping and pressure: the onset of superconductivity and the "insulator-to-metal" transition at higher doping, and at higher pressure. The phase line at 21 GPa is nearly vertical, given the similarity in the magnon and phonon behaviour at low and high temperatures.*

A slightly doped, non-superconducting sample of the insulating parent material $Bi_{1.98}Sr_{2.06}Y_{0.68}Cu_2O_{8+\delta}$ shows anomalies in electronic Raman background, electron-phonon coupling λ, spectral weight transfer, density dependent behaviour of phonons and magnons, and *c*-axis compressibility with pressure at 21 GPa, all of which are directly related to the changes in physical properties observed in the material at the critical doping level. The results suggest that compression along the *c*-axis brings CuO_2 layers closer together and leads to increased hole-doping to the optimal level, which would lead to the onset of superconductivity at the appropriate temperature (see Fig. 36). The work opens up new avenues of fundamental research aimed at understanding the phenomenon of high-temperature superconductivity and its response to applied pressure.

Metallization and Superconductivity in Compressed SiH_4 – At **Carnegie**, **Xiao-Jia Chen** and colleagues from Carnegie, in collaboration with scientists from the **Chinese University of Hong Kong** and **South China University of Technology**, have predicted from first principles the superconducting properties of the hydrogen-rich molecular compound silane (SiH_4). A gas at ambient conditions, solid silane adopts a structure with the SiH_4 molecules oriented so as to produce layers of hydrogen and silicon atoms. This newly-discovered superconducting phase, (Fig. 37). which forms at 60 GPa, has a structure belonging to the orthorhombic space group *Cmca*. With this layered structure, compressed SiH_4 at this pressure resembles a silicon-hydrogen alloy, and provides some insight into the long-predicted existence of metallization and superconductivity in dense hydrogen, a problem that has been an important driving force in the development of condensed matter physics and astrophysics for nearly a century.

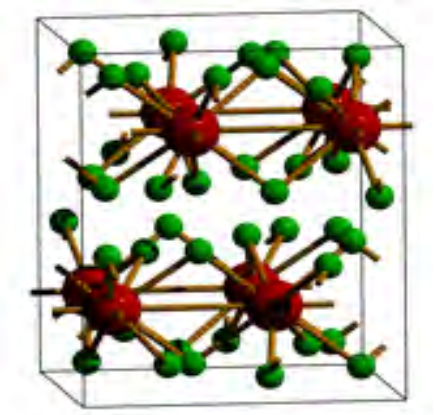


Figure 37. *Metallic Cmca SiH_4 structure, which is layered and favors superconductivity.*

The work suggests that the layered motif observed in the *Cmca* phase could be essential for superconductivity in other hydrogen-rich compounds.[9] This study confirms the experimental finding of pressure-induced metallization in SiH_4, which was reported by the team in January 2008.[10] At 60 GPa, silane has a superconducting transition temperature between 20 and 75 K in the layered metallic phase, demonstrating the potential to observe metallization and superconductivity in hydrogen within a potential silicon-hydrogen alloy at higher pressures, but still much lower than would be necessary for solid hydrogen, due to chemical precompression by the silicon. After submission of this work, evidence for superconductivity in metallic silane was reported by an international team led by former **Carnegie** visiting scientist **Mikhail I. Eremets**.[68]

2.6 High *P-T* Chemistry

Ongoing studies in the area of high *P-T* chemistry are central to the CDAC mission as the compositional basis of materials behavior at extreme conditions is more fully appreciated and understood. CDAC supports a wide range of research activities, including the study of a variety of potiential hydrogen storage materials, energetic materials, and novel elemental and binary phases, as well as the development of spectroscopic techniques for evaluating chemical reactions in the bulk and at interfaces.

Rhenium Reactivity with H_2O-O_2 Mixtures at High Pressure – Rhenium is commonly used as a gasket material in DAC experiments due to favorable materials properties such as high yield strength and plasticity, even at extreme pressures.[69] The Re gasket has been used in many high *P-T* studies of H_2O[70] and O_2.[71] Although Re is easily oxidized, no reaction has been reported separately with H_2O or O_2,[72] even with laser heating. In recent work on the chemistry of O_2 and H_2O at high pressure, **Raja Chellappa (Carnegie)** found that mixtures of H_2O-O_2 loaded in a Re gasket underwent a series of reactions to form a combination of rhenium oxide hydrates; $Re_2O_7 \cdot (H_2O)_2$ and $HReO_4 \cdot H_2O$. Such reactivity necessarily precludes the use of rhenium with aqueous samples with

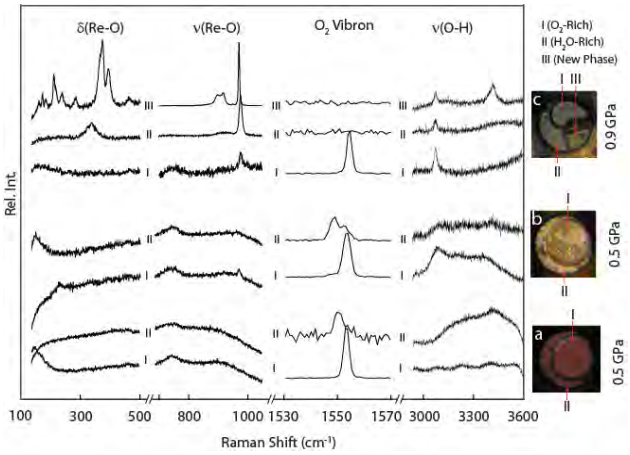


Figure 38. *Time lapse photomicrographs of Sample 1 showing the visual transformation of the Re-H_2O-O_2 system as reaction proceeds; a) H_2O with cavity and a small ruby ball. b) After cryogenic loading of O_2. c) Sample after heating to ~35 °C Region III is the fully crystallized mixture of rhenium oxide hydrates while region II is just perrhenic acid ($HReO_4$).*

high oxygen content (particularly relevant for hydrothermal synthesis studies) and understanding the reaction pathway provides some clues to the oxidation behavior of H_2O-O_2 system. Figure 38 shows the temporal evolution of the H_2O-O_2 sample in a Re gasket. The most dramatic signatures of the reaction are the appearance of the stretching and bending modes of Re-O. Further details of this study are soon to be published.[73]

SFG Spectra of Surfaces and Interfaces – In the **Dlott** group at **Illinois**, work is continuing on surface spectroscopy of energetic materials, particularly HMX, using vibrational sum-frequency spectroscopy generation (SFG). The third-generation SFG apparatus developed in Year 4 is now used routinely to generate high-quality spectra. A significant improvement was the implementation of the capabilty to use shaped pulses to suppress the nonresonant contributions which tend to overwhelm the HMX vibrational resonances. The better spectra obtained have shown that HMX surfaces were frequently of poor quality and contaminated. The surface contaminants are very interesting themselves, and work is ongoing to obtain very high quality spectra of the pristine crystal surfaces. At this point, it is now possible to produce clean and reproducible spectra of both pristine (Fig. 39) and contaminated crystal surfaces and therefore to characterize the crystals very accurately. Also under development are techniques for looking at the crystal-binder interface under pressure. A number of possible SFG geometries are possible and work is underway to determine the optimal one. The ultimate goal of this work is to better understand the interactions of surface nitro groups with polymers as a function of pressure. This series of studies is part of the dissertation research of CDAC graduate student **Aaron Lozano,** who will begin to investigate nitro-binder interactions at the crystal-polymer interface and will survey the properties of other energetic materials including RDX and PETN.

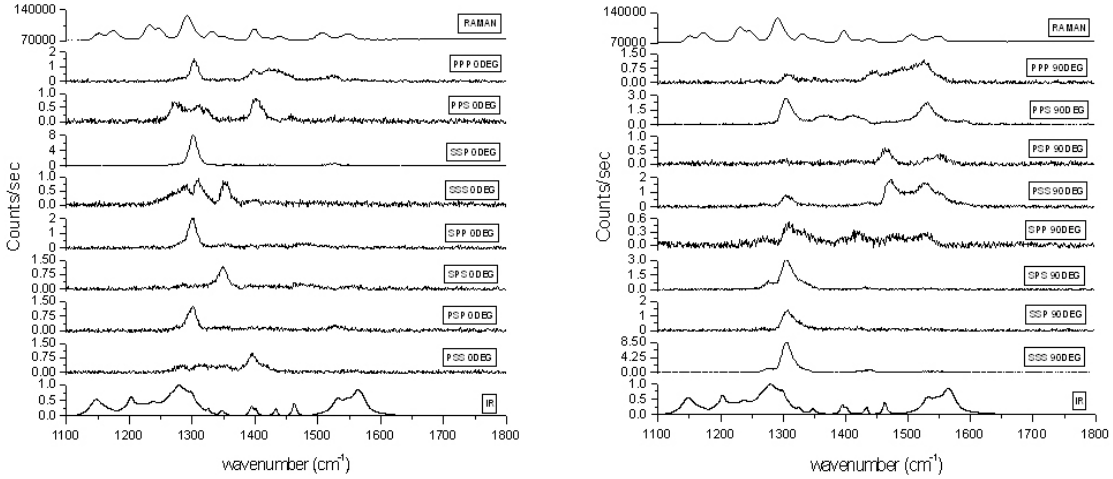


Figure 39. *SFG spectra of HMX crystal surfaces in the NO_2 region.*

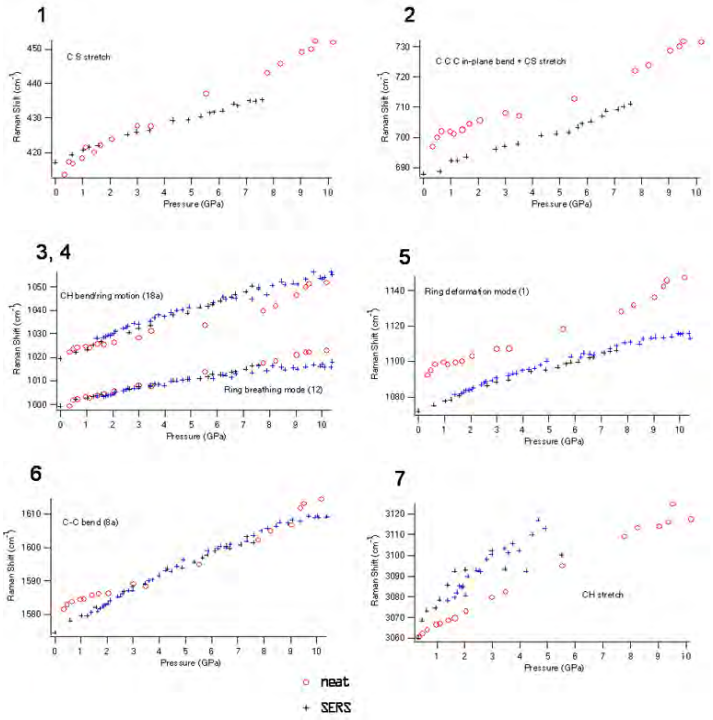


Figure 40. *Pressure-dependent shift data for the benzene thiolate monolayer.*

Molecular Monolayers at High Pressure – CDAC graduate student **Kathryn Brown** has recently completed studies of molecular monolayers at high pressure at **Illinois**, having developed the technology to fabricate surface-enhanced Raman (SERS) substrates that are compatible with the tiny sample volumes of the DAC. Using a 6 mm thick Mylar layer as the substrate and surface treating the Mylar with poly-vinyl alcohol to make the surface hydrophilic, she was able to then deposit a layer of 330 nm diameter polymer nanospheres and cover the spheres with 200 nm of Ag. This SERS substrate amplifies the Raman spectrum by a factor of 10^5. Two kinds of molecular monolayers, benzenethiol, S-C_6H_5 and benzene-methyl thiol, S-CH_2-C_6H_5, have been studied and high-quality Raman spectra have been obtained for both, as illustrated in Fig. 40, in addition to the spectra obtained for the corresponding bulk materials. There are several notable differences between the bulk and a monolayer. The substituted benzenes appear to have a liquid-solid phase transition below 1 GPa, as previous work on benzene would suggest, whereas the monolayers do not have this phase transition. In addition, the Gruneisen parameters for some modes are similar in the bulk and on the surface and others are different. Focusing on the differences will allow an understanding of how a molecular interactions are affected when molecules are bound to a metal surface. Quantum chemical calculations in support of this work are also ongoing. In a new collaboration, a method for making extremely robust wafer-scale SERS surfaces developed by V. Colvin at Rice University and P. Jiang at the University of Florida is being used to produce improved SERS materials on 5 mm thick Si wafers, which will be more suitable for DAC studies.

Shock Compression of Molecular Monolayers – During the early years of CDAC, **James Patterson** at **Illinois** developed techniques for shock compression measurements on molecular monolayers. With a monolayer and a femtosecond laser, he was able to achieve ultra-high time and spatial resolution of a shock front. With a major upgrade in laser facilities in the Illinois lab, the group will again be carrying out shock compression experiments. In the previous work, it was observed that long-chain alkanes, S-$(CH_2)_{17}$-CH_3, buckled under uniaxial shock compression to form gauche defects. Alkane thiols were studied because they were the simplest model monolayer available. The goal of this work now is to look at the shock compression behavior of molecules more relevant to NNSA missions, specifically energetic material simulants. **Aaron Lozano** is finishing a chemical synthesis of a simulant for nitramines such as RDX. This molecule will have the structure S-C_6H_5-NNO_2, which has a similar size and shape as RDX and also the critical nitramine moiety, but it will form a highly ordered self-assembled monolayer suitable for shock studies.

The new effort involves using laser-generated flyer plates to generate high pressure shocks in reactive materials. In principle it should be possible to launch 0.5 mm diameter flyer plates at a high velocity up to 10 km/s or more, in a reproducible manner, at a high repetition rate of 10 Hz using a YAG laser, but in practice this has not been realized. At this point, however, a fiber optic

CDAC student ***Kathryn Brown (Illinois).***

can be used to homogenize the beam and a chemically active thin layer under the metal flyer plate used to assist the launch. According to recent reports, such a technque has been used to generate up to 5 km/s launches with a very small laser power of 12 mJ. With modern YAG lasers operating with 600 mJ pulses, the two biggest issues are making a very flat profile laser beam and making a very reproducible array of flyer plates. The apporoach will be to use newly available aspheric beam shaping optics for the laser and advanced fabrication techniques for the flyer plate array. **Kathryn Brown** will also be working on this project and will combine the flyer plate launcher with some advanced diagnostic techniques already available.

The primary motivation for this project will be to investigate the impact-induced reactivity of nanotechnology "reactive materials" that include nanoparticle fuels with polymer oxidizers (e.g. nanoAl + Teflon) and bimetallic nanoparticle aggregates such as nanoAl + nanoNi that react to form intermetallic compounds and large quantities of heat. With ultrafast laser technology it will be possible study these impact-induced chemical reactions in real time.

H_2 Interactions with NH_3BH_3 – H_3NBH_3 (ammonia-borane, AB) is a very high hydrogen content (19.5 wt.% H_2) chemical hydride that is being considered for hydrogen storage applications, although there are many issues to be resolved. First and foremost is the establishment of reversible H_2 removal and addition. Although, partial H_2 release (5 wt.% H_2) can be accomplished by heating to ~100 °C, the thermal residue (considered polymeric NHxBHx) is considered inert to re-uptake of H_2. The presence of dihydrogen bonding (N-$H^{\delta+}$...$^{\delta-}$H-B) in AB dictates many of its unique properties when compared to its isoelectronic organic analogue ethane (CH_3CH_3). An understanding of the fundamental mechanisms of B-H and N-H bond cleavage and re-formation is important from a practical and basic science perspective. The goal of **Raja Chellappa's** work at **Carnegie** is to understand the nature of H_2 interactions with AB and its thermal polymeric residue at slightly elevated *P-T* conditions. DAC techniques provide a window to spectroscopic as well as structural characterization and all the experiments in this study are carried out using the DAC.

The evolution of Raman spectra for a heating and cooling cycle of a AB+H_2 mixture is shown in Fig 41. The as-loaded sample at 0.4 GPa contains two regions that are relatively rich in H_2 and AB. AB Raman spectra (at 0.4 GPa) are characterized by sharp signatures corresponding to BH (doublet: 2289 (s), 2382 (br, m) cm^{-1}) and N-H (triplet: 3173(sh, w), 3253 (s), 3319 (sh, w) cm-1) stretching modes. The B-N stretching modes appear at 733 (br, w), 794 (s) with shoulder at 809 (m) cm^{-1}). AB undergoes a series of pressure-induced phase transitions that were also determined (not discussed here) in this study. The AB+H_2 mixture was heated to (~150-170 °C) at ~3.5 GPa which resulted in the decomposition of AB. The polymeric residue is characterized by the loss of lattice modes, a very broad peak corresponding to B-H stretching and a singlet for the N-H stretching mode. The H_2 vibron appears as a doublet with a soft shoulder. After cooling down to room temperature, the pressure increased slightly to 5.6 GPa and a new N-H stretching mode appeared. In addition, the B-H stretching mode considerably weakened. The diffraction pattern obtained from this sample showed a single crystal pattern that was not fully resolvable. However, it can be stated with some certainty that at slightly

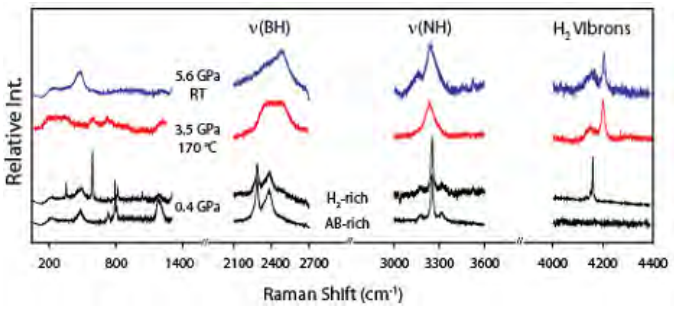


Figure 41. *H_2 re-uptake by (NH_xBH_x) residue (after decomposition of AB). Note the soft shoulder to H_2 vibron and reappearance & changes in peak profile of B-H and N-H stretching modes in the cool-down portion of the heating cycle.*

elevated pressure, H_2 exihibits a weak intermolecular interaction in manner similar to that observed in H_2-H_2O clathrates. A similar experiment was carried out with AB+Ne mixture (heating and then cooling) and a similar behavior (shouldered H_2 vibron) was observed.

In another experiment, a room temperature compression of an AB+H_2 mixture was carried out to very high pressures (upto 1 Mbar) to look for any dramatic changes in H_2 signatures. The results of this experiment (up to 59 GPa) are shown in Fig. 42a. Around 7 GPa, a soft H_2-vibron develops at 4149 cm^{-1} (main vibron at 4218 cm^{-1}) and at ~10 GPa, a stronger H_2-vibron appears at 4241 cm-1. Both these new vibrons persist upto 40 GPa when the softer vibron crosses over the main vibron and continues to strengthen with pressure. Figure 42b shows the H_2-vibron behavior in detail and Fig. 42c shows the Raman shift versus *P* for all the three vibrons plotted with literature values for Raman and IR for pure H_2 upto 1 Mbar. At this time, we have not established the exact nature of how H_2 is interacting with AB but it is expected that the changes in dihydrogen bonding with pressure play an important role. It is interesting to see that the NH stretching modes shift to lower frequencies while BH stretching modes move to high frequencies.

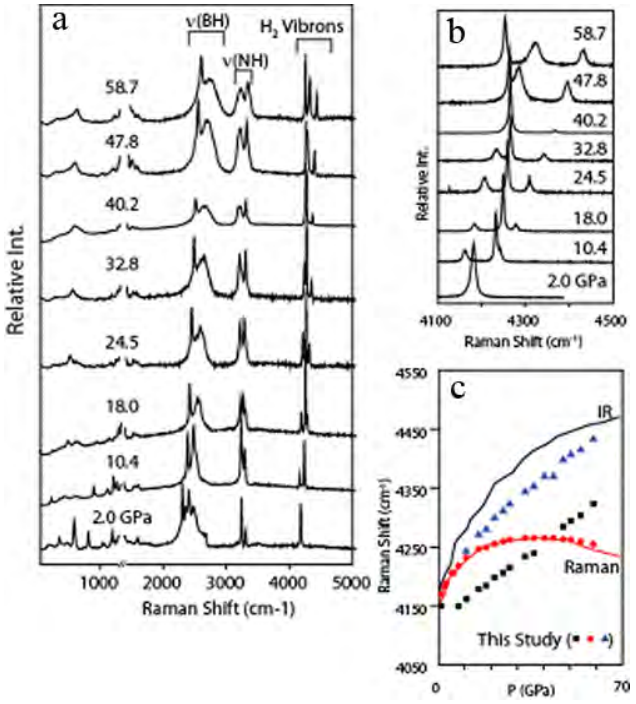


Figure 42. *a) AB+H_2 compressed at RT. b) and c) Raman shift vs P of H_2-vibrons interacting with AB.*

Experiments are in progress with deuterated analogues of AB that are loaded with H_2 and D_2 and subjected to heating/cooling cycles. These isotope substitution experiments will clearly establish the sequence and mechanism of bond cleavage and re-formation in AB and its derivatives. In addition, the observed interaction of H_2 with AB upto 59 GPa has been quite novel with the splitting of H_2 vibrons and exhibiting mutual crossover. The next step is go up to at least 1 Mbar; an experiment that will have great relevance to long standing high pressure frontier problems involving H_2, such as metallization.

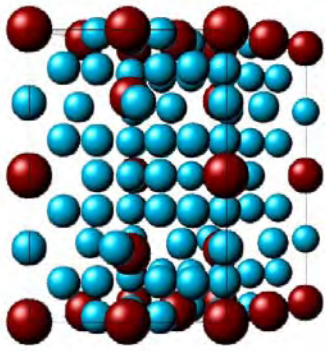


Figure 43. *Structure of Xe-H_2 compound. The blue spheres are molecules of hydrogen which can be visualized as freely rotating dumbbells while the red spheres are xenon atoms. The only other rare gas hydrogen compound known is $Ar(H_2)_2$, which also remains non-metallic at these pressures.*

Novel Xenon-Hydrogen Chemistry – The search for new molecular hydrides is driven by two predominant motivations: first, the quest for novel hydrogen storage systems, and second, the quest for metallic hydrogen. A number of approaches employing the concept of "chemical precompression" are currently under investigation in CDAC groups.

Hydrogen has been predicted to become a metal and superconductor at room temperature when pressurized sufficiently. Current estimates of this pressure are above 500 GPa, a pressure that is well beyond the technical capabilities of presnt day DAC designs. An alternate route to this metallization has been proposed, however, and involves populating the band gap of the solid, insulating hydrogen with impurity electronic states as in a semiconductor. This is predicted to aid metallization and also lower the pressures at which metallization actually occurs. Using rare gas

solids allows the formation of such alloys or molecular solids. *In-situ* characterization of such solids can be done only by using synchrotron sources.

Using these considerations, a new molecular compound has been discovered in the xenon-hydrogen binary system. In work by CDAC Research Scientist **Maddury Somayzulu**, it has been shown that compound formation between noble gases and molecular hydrogen is possible at high pressures. The molecular compound $Xe(H_2)_6$ whose structure is shown in Fig. 43 was characterized by a suite of synchrotron based techniques at HPCAT and NSLS-U2A. An unexpected stability of this compound to pressures of approximately 200 GPa is observed; at this pressure, the material continues to be non-metallic. These studies not only open avenues to discovering new compounds but also help explore metallization in alloys of hydrogen which are expected to be novel superconductors.

This new compound also offers a window into novel physics and chemistry of molecular solids. $Xe(H_2)_6$ provides an archetypal system with which to study metallization brought about by pressure-induced ionization of guest atoms (in this case Xe); such compounds can be classified as novel semiconducting *molecular hydrides*. From a technological point of view, this study opens the possibility of a whole new family of hydrogen storage materials as also a whole new class of rare-gas based hydrides.

Hydrogen Storage Materials at High Pressure and Temperature – CDAC graduate student **Lyci George** and postodoctoral associate **Vadym Drozd** at **Florida International University** have investigated the structural stability of $Mg(BH_4)_2$, a promising hydrogen storage material, under pressure up to 22 GPa with combined synchrotron x-ray diffraction at HPCAT and Raman spectroscopy. The analyses show a structural phase transition around ~ 3.5-5.0 GPa (Figs. 44 a and b) and again around ~15 GPa (Fig. 44c). At ambient conditions $Mg(BH_4)_2$ has a hexagonal structure (space group-$P6_1$, a = 10.1647(6) Å, c = 36.902(8) Å and V = 3301.9(8) Å^3), which agrees well with early reports. The high pressure phase is found to have a different structure from theoretically determined structures; the structure also does not match with that of the high temperature phase. Most importantly for energy storage applications, the high pressure phase is found to be stable on decompression, similar to the case of the high temperature phase.

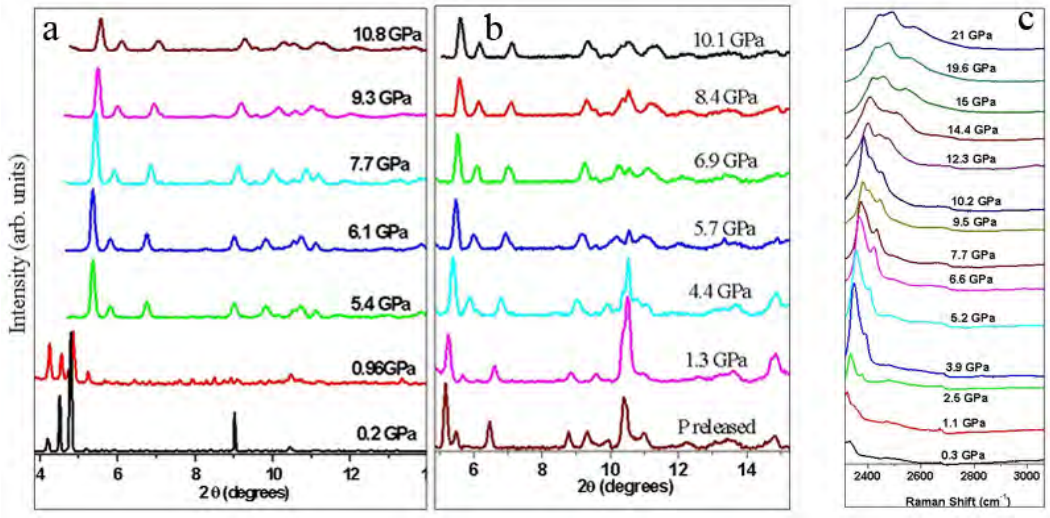


Figure 44. *a) Synchrotron x-ray diffraction patterns obtained for $Mg(BH_4)_2$ in the DAC during compression up to ~ 11GPa. b) Synchrotron x-ray diffraction patterns obtained for $Mg(BH_4)_2$ in the DAC during decompression at various pressures. c) Raman spectra of $Mg(BH_4)_2$ in the region of the B-H stretching modes. Spectra collected during compression up to 21 GPa.*

Noble Metal Nitrides – The thermodynamic stabilities of various phases of the nitrides of the platinum-metal elements have been systematically studied using density functional theory. In a collaboration between **Alexander Goncharov** at **Carnegie** and **Jonathan Crowhurst** and

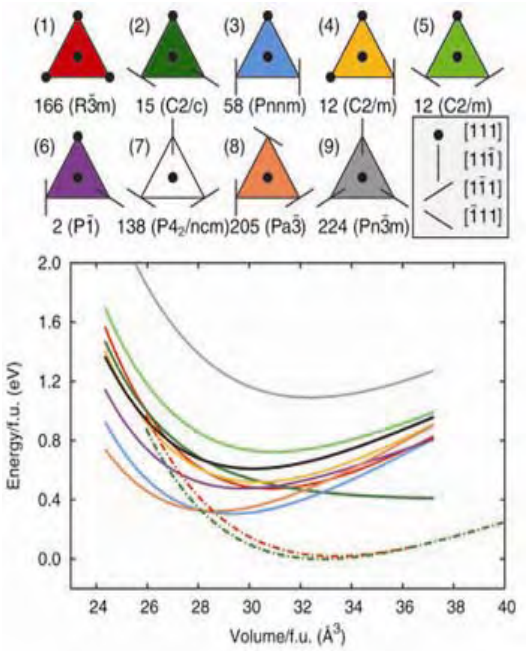


Figure 45. *Top: projections of all possible distinct nitrogen dimmer orientations derived from the 12-atom conventional unit cell, along with the space group number and Hermann-Maguin symbol of the corresponding structure. Bottom: energy/f.u. vs. volume curves from LDA for the above related structures (solid lines) in the case of PdN_2. Each structure can be identified by matching the line color to the corresponding triangle color.*

colleagues at **Livermore**, it has been shown that for the nitrides of Rh, Pd, Ir, and Pt two new crystal structures, in which the metal ions occupy simple tetragonal lattice sites, have lower formation enthalpies at ambient conditions than any previously proposed structures. The region of stability with respect to those structures extends to 17 GPa for PtN_2. Calculations (Fig. 45) show that the PtN_2 simple tetragonal structures at this pressure are thermodynamically stable also with respect to phase separation.

The chemical combination of noble (platinum group) metals with elemental nitrogen represents a significant synthetic challenge, due to the inert nature of both the metal and the nitrogen-nitrogen triple bond. Recent high pressure work has shown, however, that a number of MN_2 compounds (M = platinum group metal) are stable in the DAC at elevated pressures.[74] As a result of the difficulties involved in the solution and refinement of crystal structures from diffraction data that are dominated by scattering from the metal, the structures of the MN_2 compounds have been the subject of debate and controversy.

Stability of N_2 at High Pressure and Temperature – The N-N triple bond in molecular nitrogen is one of the strongest and most stable chemical bonds in nature, giving rise to the two most commonly observed states, the solid and liquid. Molecular nitrogen itself, however, has shown a surprising degree of polymorphism, leading to a complex phase diagram that is still incomplete in the high pressure and temperature regions. Particularly important is the region near the melting line at pressures higher than 50 GPa, where theoretical work and shock wave experiments have suggested the transition to a polymeric form, which occurs at much higher pressures at low temperatures, according to previous static compression experiments.

Alexander Goncharov and colleagues at **Carnegie** and **Livermore** have obtained Raman spectra up to 120 GPa and 2500 K for both solid and fluid nitrogen in an effort to clarify the behavior of this system at high pressures and temperatures. To probe the material directly at high pressure and temperature, a pulsed laser to the sample was combined with a second pulsed laser that excited the vibrational spectrum characteristic of the molecular state of the solid. This pulsed Raman spectroscopy technique allows the acquisition of spectra at precisely the peak temperature of the sample, and also reduces the background thermal radiation from a metallic laser light absorber. The spectroscopic data show that nitrogen in the fluid

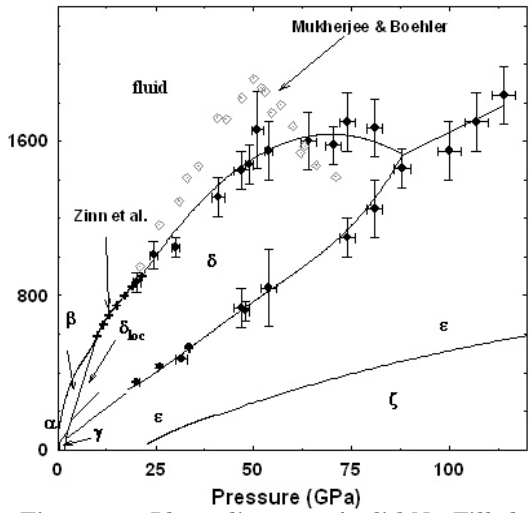


Figure 46. *Phase diagram of solid N_2. Filled symbols indicate data obtained in the present study.*

state remains in the molecular form throughout the pressure and temperature ranges investigated, and that there is no evidence to support a fluid-fluid transition.

The Raman spectra reveal that the melting line exhibits a maximum near 70 GPa, followed by a triple point near 87 GPa, after which the melting temperature rises again (Fig. 46). Fluid nitrogen remains molecular over the entire pressure range studied, and there is no sign of a fluid-fluid transition. Solid phases obtained on quenching from the melt above 48 GPa are identical to the recently discovered ι and ζ' phases. These results indicate that kinetics plays a major role in the experimentally observed phase changes and accounts for the metastability of various crystalline molecular phases and the existence of an amorphous single bonded h-N. This behavior suggests an explanation for the onset of amorphization at still higher pressures and lower temperatures as has been observed previously in SiO_2 and H_2O.[12]

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 reseach are acquainted with not only advanced experimental techniques and results, but also with state-of-the-art computational methods (*e.g.*, Refs.[75-77]).

CDAC graduate student ***Lyci George (Florida International)****.*

In Year 5 of the CDAC program, the 12 academic partners supported a total of 18 graduate students and two postdoctoral fellows. Three undergraduate students also participated in CDAC-related research.

Princeton:	**Susannah Dorfman**
	Zhu Mao
Caltech:	**Matt Lucas**
	Michael Winterrose
	Jorge Munoz
Chicago:	**Chris Seagle**
	Wenxuan Zhang
Berkeley:	**Lowell Miyagi**
Alabama:	**Gopi Samudrala**
	Andrew Stemshorn
Illinois:	**Kathryn Brown**
	Aaron Lozano
Arizona State:	**Erin Oelker**
	Samrat Amin
New Mexico State:	**Jeffrey Montgomery**
	Shannon Pitcher (Undergraduate)
Texas Tech:	**Resul Aksoy**
	Emre Selvi

	Jeff Aycock (Undergraduate)
	Russell Knudson (Undergraduate)
Florida International:	**Lyci George**
Nevada – Reno:	**Eric Emmons (Postdoctoral)**
Carnegie:	**Raja Chellappa (Postdoctoral)**

At this point, 11 graduate students have received their Ph.D. degrees with CDAC support. Four of them, **James Patterson,** (**Illinois**, 2004), **Wendy Mao** (**Chicago**, 2005), **Nenad Velisavljevic** (**Alabama-Birmingham**, 2006), and **Raja Chellappa** (**Nevada-Reno**, 2004) have continued working in the area of stewardship science. **Patterson** pursued a postdoctoral appointment at the **Institute of Shock Physics, Washington State University**. **Mao** was an Oppenheimer Fellow at **LANL** working in the **LANSCE** division and has gone on to a faculty position at **Stanford Universtity**, where she will continue work in the area of high-pressure materials science. **Velisavjlevic** is at **Los Alamos National Laboratory** working in the group of CDAC Laboratory Partners **Neal Chesnut** and **Yusheng Zhao**. **Chellappa** is now a CDAC postdoctoral fellow at **Carnegie**, working on both stewardship science and energy storage projects. The full list of graduate students who have received the PhD degree with CDAC support is as follows:

James Devine (Chicago, 2004)
James Patterson (Illinois, 2004)
Wendy Mao (Chicago, 2005)
Jenny Pehl (Berkeley, 2005)
Sergio Speziale (Princeton, 2005)
Tabitha Swan-Wood (Caltech, 2005)
Raja Chellappa (Nevada-Reno, 2004)
Joanna Dodd (Caltech, 2007)
Joel Griffith (Alabama-Birmingham, 2006)
Alexander Papandrew (Caltech, 2006)
Nenad Velisavjevic (Alabama-Birmingham, 2006)
Nicholas Cunningham (Alabama-Birmingham, 2007)
Emre Selvi (Texas Tech, 2007)
Matthew Lucas (Caltech, 2008)
Resul Aksoy (Texas Tech, 2008)

Publications and presentations involving CDAC-supported students and postdoctoral fellows in Year 5 are listed below.

Student Publications

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3.2 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, Trieste, Italy
S. Scandolo
Argonne National Laboratory
A. Atalas
C. J. Benmore
J. A. Cowan
D. Haskel
J. C. Lang
P. L. Lee
B. M. Leu
Y. Ren
A. H. Said
S. D. Shastri
H. Sinn
W. Sturhahn
N. M. Souza-Neto
Y. C. Tseng
J. Urquidi
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
A. El Goresy
D. J. Frost
Anastasia P. Kantor
I. Y. Kantor
Catherine A. McCammon
Beijing Institute of Spacecraft Environment Engineering, China
Z. Gong
Brookhaven National Laboratory
G. L. Carr
O. Gang
W. Q. Han
J. Hanson
C. C. Kao
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
J. C. Castillo
O. Delaire
Jennifer M. Jackson
S. Kung
H. Su
Case Western Reserve University
J. Van Orman
Chinese Academy of Science
M. Chen
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Institute of Crystallography, Moscow
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Institute of Geochemistry, Chinese Academy of Sciences
M. Chen
X. Xie
Institute of Metal Physics, Russia
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Northern Illinois University
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M. R. Frank
S. J. Maglio
Northwestern University
K. Brister
D. Brown
C. M. Holl
S. Jacobsen
Y. C. Tseng
Nuclear Research Center-Negev, Israel
I. Halevy
Oak Ridge National Laboratory
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G. E. Ice
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Okayama University, Japan
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G. Guenthrodt
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University of Tennessee
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L. A. Taylor
University of Texas, Arlington
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S. Sharma
University of Tokyo
K. Matsubayashi
S. Merkel
M. Takigawa
Y. Uwatoko
T. Yagi
University of Toronto
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University of Tsukuba
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University of Warsaw, Poland
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University of Warwick, UK
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J. J. Hamlin
K. M. Pitman
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3.3 Undergraduate Student Scholars

A number of university undergraduate students participating in the highly successful Carnegie Summer Intern Program (Fig. 47) have worked on projects directly related to CDAC goals during the past year. This NSF-funded program, which is run by CDAC coordinator **Stephen Gramsch**, seeks to identify students at smaller institutions who may not have the opportunity for front-line research during the academic year, or students without a significant research background. At **Carnegie**, such students experience a rigorous an introduction to scientific research, and within the structure of CDAC, are learning about the important problems in the field of high-pressure research (Fig. 48). During the summers of 2007-2008, the following students participated in this program wit the **Carnegie** high pressure group.

Figure 47. *2008 Carnegie Summer Scholars.*

2007:

Seth King, Purdue University
Investigation of the High P-T Phase Diagrams in the H_2-He System
Zachary Newman, Case Western Reserve University
Melting of Silicon at High Pressures

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

Figure 48. *2008 Summer Scholars* ***Violeta Castro (Bucknell University)***, ***Rohan Kundargi (UCLA)***, *and* ***Caitlin Farnsworth (UC Davis)*** *presenting their work at the Carnegie Institution of Washington Summer Scholars Research Symposium on August 6, 2008.*

3.4 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. 49). In 2007, two students from Washington, DC returned to Carnegie for a second summer after beginning in 2006 and working on their projects during the 2006-2007 school year. **Alexander Levedahl**, working with **Maddury Somayazulu**, used the research he completed on the preparation and characterization of a hydrogen clathrate hydrate to enter the 2007 Intel Science Talent Search. **Andrew Kung** worked with **Chang-Sheng Zha** on the development of resistive heating methods for hydrogen at high pressure. Kung measured the frequency of the H_2 vibron at 20 GPa, from 300 to 500 K (Fig. X). In 2008 (Fig. 48), **Jaqueline Rivera** worked on chemical synthesis methods for the preparation of Fe- and Al-containing solid solutions with **Stephen Gramsch**. **Maura James** investigated the NH_3-H_2O-H_2 system at high pressure and temperature with Gramsch and Somayazulu, and submitted her work to the Intel and Siemens competitions. **Manchali Madduri** was a semifinalst in the 2008 Siemens Competition for Math, Science, and Technology, placing her among the top 300 entrants throughout the country. She investigated hydrogen complexation studies in crown ethers.

Figure 49. *2008 High School Summer Scholars. Left:* ***Jaqueline Rivera (César Chávez Public Charter High School)****. Center:* ***Maura James (Convent of the Sacred Heart)****. Right:* ***Manchali Madduri (Thomas Jefferson High School)****.*

2007:

Andrew Kung, Winston Churchill High School, Potomac, MD
Temporal and Compressional Behavior of X-Ray Induced Dissociated Water
Alexander Levedahl, St. Anselm's Abbey School, Washington, DC
Stability of a H_2-H_2O Clathrate at High Pressures

2008:

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

3.5 2008 Stewardship Science Academic Alliances (SSAA) Program Symposium

As part of the meeting schedule, attendees at the conference toured the research facilities at the Broad Branch Road campus, home of **Carnegie's** Geophysical Laboratory and Department of Terrestrial Magnetism.

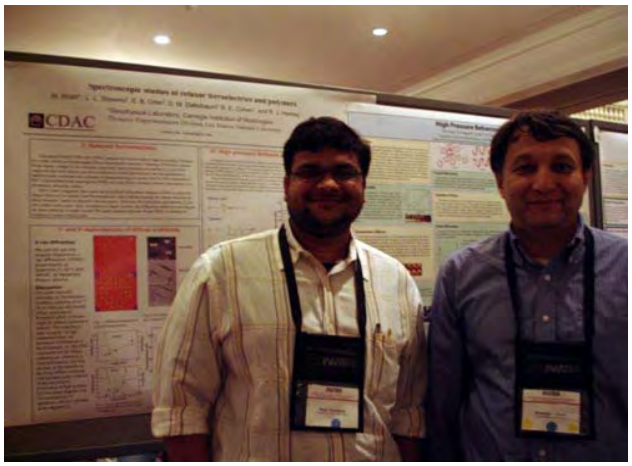


***Figure 50. Carnegie** CDAC Postdoctoral associate **Raja Chellappa** and **Carnegie** CDAC Research Associate **Muhtar Ahart** at the poster session during the 2008 SSAAP symposium in Wasihngton, DC.*

At the student poster session, CDAC graduate students were well represented, with 14 of the 18 students currently supported giving poster presentations (Fig. 50). In all, 30 posters were presented by CDAC students, postdoctoral fellows, collaborators and partners. The following is a list of CDAC related talks and posters:

Ahart, M., Spectroscopic studies of ferroelectrics and polymers, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Amin, S., High pressure behavior of As_2O_3 glass, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Brown, K., High pressure vibrational spectroscpy of molecules at interfaces, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Chellappa, R., Reactivity of water-oxygen system at high pressure, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC February 26-28, 2008).

Dorfman, S., Superhard phases in the alkaline earth flourides at high pressure?, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Ganesh, P., Exotic perovskites under pressure, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Garimella, S., High energy dense materials via high pressure decomposition of metal hexacarbonyls?, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

George, L., Principal component analysis on hydride database, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Goncharov, A. F., Melting of simple molecular solids in Mbar pressure range, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Guo, L., High pressure x-ray diffraction study of nanocrystlline AuCu alloy, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Hou, D., High pressure x-ray diffraction study of nanocrystalline zinc oxide, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Kulkarni, S., Synthesis and high pressure behavior of M_2SnC (M=Ti,Zr) MAX phases, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Lee, K., First measurements on how pressure affects the half-life of ^{22}Na: Comparison to theory and analog to 40 K, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Lerche, M., Grand challenges at HPSynC, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Lozano, A., Using nonlinear coherent vibrational spectroscopy to probe the surface of high explosives, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Lucas, M., High pressure study of Fe-Cr Alloys, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Luo, R. X., First-principles investigation of equation of state and phonon-dispersion of $Fe_xNi_{(1-x)}$ alloy at high pressure and temperature, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Mao, Z., Effects of hydrogen incorporation on elasticity of a mantle silicate to 12 GPa, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Miyagi, L., In-situ phase transformation and deformation of iron at high pressure and temperature, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Miyagi, L., Deformation and texture development in $CaIrO_3$ post-perovskite phase up to 6 GPa and 1300 K, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Oelker, E., High pressure structural investigation of glassy and crystalline BeF_2, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Phatak, N., Synthesis and structure stability of a new compound $(Cr_{0.5}V_{0.5})_2GeC$ and M_2GeC (M=Ti, V, Cr) at high pressure and temperature, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Pitcher, S., Weather paterns at LANL and their effect on measurements of electron-capture radioactive decay under pressure, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Samudrala, G., Growth chemistry for the fabrication of designer diamonds for high pressure research, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Seagle, C., Experimental determination of melting curves at high pressure, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Selvi, E., Interaction of tungsten disulfide with different pressure media, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Sharma, A., Hydrocarbon synthesis at extreme conditions: a window into the reaction pathways, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Shen, G., HPCAT facilities for high pressure research, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Shen, G., HPCAT science highlight I, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Shen, G., High pressure synergetic center at Advanced Photon Source, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Stemshorn, A., Electrical and structural studies of metallic glass under high pressure, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Weinberger, M., Rational design and characterization of ultra-incompressible superhard materials, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Winterrose, M., Pressure-induced invar behavior in Pd_3Fe, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Yang, W., HPCAT science highlight II, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Yarger, J. L., Polyamorphism & amorphous-amorphous transitions in BeF_2 and BeH_2 (invited), *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2008).

Zha, C. S., X-ray diffraction study of H_2O ice to 200 GPa, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

Zhu, H., Synthesis and high pressure x-ray diffraction study of nanocrystalline silicarbon carbide, *2008 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 26-28, 2008).

3.6 Workshop: Advances in High-Pressure Science using Synchrotron X-rays

The Workshop on "Advances in High-Pressure Science using Synchrotron X-rays," held on October 4th at the **NSLS**, was a tremendous success. The workshop was organized in honor of **Jingzhu Hu** and **Quanzhong Guo** in celebration of their retirement after up to 18 years of dedicated service to the high-pressure community. **Hu** was the beamline scientist of X17C, the first synchrotron beamline in the world dedicated to high-pressure research. The beamline, which was created and managed by **Carnegie** for many years, was later complemented by X17B, which was led by **Guo**. Forty-seven participants (Fig. 51) from 18 institutions were present at the workshop. CDAC partners **Yangzhang Ma** (**Texas Tech**) and **Jie Li** (**University of Illinois, Urbana-Champaign**), presented talks, along with **Carnegie** scientists **Ho-kwang Mao**, **Alexander Goncharov**, **Yingwei Fei**, and **Michelle Weinberger**, and **HPCAT** scientist **Wenge Yang**.

Figure 51. *Attendees of the "Advances in High-Pressure Science using Synchrotron X-rays" workshop.*

Lectures – Talks were given by 18 presenters on subjects related to the use of synchrotron radiation techiques in high pressure materials research. Lecturers supported by CDAC funds (staff, partners, postdoctoral fellows, or students) are designated by an asterisk (*)

Session I (Chair: Tom Duffy,* Princeton University**)**

Ho-kwang Mao* (Carnegie), *The legacy of X17*
Li Hua Yu (Brookhaven National Laboratory), *R & D towards x-ray free electron laser*
Gene Ice (Oak Ridge National Laboratory), *Some new directions for high-pressure research?*

Session II (Chair: Haozhe Liu, Harbin Institute of Technology**)**

Qun Shen (Brookhaven National Laboratory), *Opportunities for high-pressure research at advanced synchrotron facilities*
Ken Evans (Brookhaven National Laboratory), *X-ray kinoform optics for high pressure science: Status and opportunities*

Alexander Goncharov* (Carnegie), *Laser heating in the DAC: New pulsed techniques and recent results*

Session III (Chair: Lars Ehm, Stony Brook University)

Yangzhang Ma* (Texas Tech University), *Seeding the future: The high pressure program at Texas Tech*

Wenge Yang* (HPCAT), *Anomalous scattering study of crystal and amorphous materials under high pressure*

Luhong Wang (Harbin Institute of Technology), *Bridging stage from amorphous Se to crystal under compression*

Maik Lang* (University of Michigan), *Combining high pressure and heavy-ion irradiation: A novel approach*

Session IV (Chairs: Jiuhua Chen, Florida International University, and **Zhenxian Liu**,* NSLS)

Jie Lie* (University of Illinois, Urbana–Champaign), *Density and sound velocity of iron-rich alloys and nature of Earth's core*

Andy Campbell (University of Maryland), *Geochemical applications of high pressure, high temperature equations of state of metals and oxides*

Li Li (Stony Brook University), *Viscoelasticity of rocks at mantle P-T*

Sean Shieh (University of Western Ontario), *High-pressure x-ray diffraction and Raman study on $BaCrO_4$ and $SrCrO_4$*

Michelle Weinberger* (Carnegie), *Using X17C to study ultra-incompressible superhard materials*

Yingwei Fei* (Carnegie), *Progress on P-V-T measurements of solids using synchrotron x-ray diffraction techniques*

Trevor Tyson (New Jersey Institute for Technology), *Application of synchrotron-based high-pressure techniques to understand strongly correlated transition metal oxides*

Jiuhua Chen (Florida International University), *Pressure induced phase transition in ammonia borane*

3.7 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. 52).

Figure 52. *CDAC visitors to* ***Carnegie****. From left:* ***Bin Chen (University of Illinois), Dominik Kurzydlowski (Warsaw University), Hirokon Yokota (Waseda University),*** *and* ***Jianjun Dong (Auburn University).***

Visitors	Affiliation	Project	Date
J. J. Dong	Auburn University	Visiting Investigator with Russell Hemley	September 17-December 7, 2008
L. Zhiguo	Harbin Institute of Technology	Visiting Investigator with Yingwei Fei	October 12, 2007-October 12, 2008

A. Brieva	Newcastle University	Research experiments with Alexander Goncharov	October 23-26, 2007
Melike Abliz	Argonne National Laboratory	Research experiments with Alexander Goncharov	November 9, 2007
E. Gregoryanz	University of Edinburgh	Experiments	December 4, 2007
Katherine Crispin	Case Western Reserve University	Experiments with Yingwei Fei	December 6-20, 2007
B. Tattitch P. Pricoli Z. Zajack	University of Maryland	Work on drill with Yingwei Fei	February 14, 2008
Hirokon Yokota Y. Uesu	Waseda University	Research with Ronald Cohen	February 14-15, 2008
C. Howard A. Walters	University College London	Loading pressure cells	February 19-20, 2008
H. Liu L. Wang	Harbin Institute of Technology	Experiments with Russell Hemley and Ho-kwang Mao	February 20-26, 2008
A. Kolesnikov	Moscow State Academy	Research experiments with Alexander Goncharov	March 7-May 6,2008
D. Kurzydlowski	Warsaw University	Flouride experiments with Viktor Struzhkin	March 28-May 13, 2008
Y. Yu	Institute of Sciences, Beijing	Superconductivity in high T_c superconductors and related materials under high pressure in DACs	April 21-June 15, 2008
B. Chen	University of Illinois, Urbana-Champaign	Melting iron-rich alloys	May 5-31, 2008
P. Lazor	Uppsala University	Research with Viktor Struzhkin	May 5-23, 2008
A. Gavriliuk	Institute for High Pressure Physics	Research with Viktor Struzhkin	May 9-June 8,2008
Katherine Crispin	Case Western Reserve University	Experiments with Yingwei Fei	May 13-23, 2008
Jie Li	Univesity of Illinios – Urbana-Champaign	Talk on "Investigating planetary cores with photons"	May 21-23, 2008
M. Guthrie	HPSynC	Visit with Joe Lai	May 22-23, 2008
Yu Lin Shibing Wang Marina Baldini Wendy Mao	Stanford	Raman spectroscopy	July 7-11, 2008
A. Rush L. Gasparov	University of North Florida	Measurements with Viktor Struzhkin	August 19-22, 2008
M. Haske	Adams Gemology Laboratory	Work with Yufei Meng	August 27-29, 2008

3.8 High Pressure Seminars

Several times a month, CDAC holds informal seminars at **Carnegie**. These seminars are open to the high-pressure community and cover new and exciting topics in the world of high-pressure science and technology. Speakers come from within CDAC as well as from around the world.

Speaker	**Affiliation**	**Topic**	**Date**
S. Sinogeikin	HPCAT	New developments at HPCAT, IDB, and supporting facilities	October 2, 2007
B. Burton	NIST	First principles based modeling of dielectric properties in relaxor ferroelectrics	October 18, 2007

Jörgen Rosenqvist	Oak Ridge National Laboratory	Surface charge, ion adsorption and molecular dynamics at the SnO_2/water interface	November 6, 2007
Li Zhang	Carnegie	Melting behavior of (Mg,Fe)O solid solutions at high pressure	November 8. 2007
Z. Chi	University of California – Berkeley	Energy-dispersive synchrotron x-ray diffraction in DAC & heat capacity of DAC sample on chip calorimeter	November 14, 2007
R. Jeanloz	University of California – Berkeley	Scaling relations for high-density high-pressure impacts	November 15, 2007
D. Foustoukos	Carnegie	Kinetics of H_2(aq)-O_2 (aq) redox equilibria and the metastable formation of H_2O_2 (aq) under low-temperature hydrothermal conditions	November 29, 2007
Caroline Jonsson	Carnegie	Speciation of the herbicide Glyphosate in aqueous solution and at mineral surfaces: An experimental and modeling approach	December 4, 2007
J. Yang	United States Patent Office	High quality diamond and its electronic applications	December 5, 2007
E. Gregoryanz	University of Edinburgh	Structural diversity of sodium	December 5, 2007
H. Yokata	Waseda University	Ordering of polar state and critical phenomena in the quantum relaxor potasium lithium tantalite $K(1-x)LixTaO_3$	February 15, 2008
D. Spaulding	University of California – Berkeley	Exploring the mantle with laser-driven shock waves	February 29, 2008
T. Sun	SUNY – Stony Brook	Lattice dynamics and thermal EOS of platinum	March 27, 2008
L. Shulenburger	University of Illinois – Urbana-Champaign	Correlation effects in quasi one dimensional wires	April 17, 2008
M. Ouyang	University of Maryland	Tailoring spin and phonon properties of quantum dots	April 18, 2008
Felisa Wolfe-Simon	Harvard University	Did nature also choose arsenic?	May 28, 2008
F. Zhang	University of Michigan	Structural changes of pyrochlore oxides($A_2B_2O_7$) at extreme conditions	July 18, 2008
J. G. O. Ojwang	Eindhoven University of Technology	Modeling the sorption dynamics of complex metal hydrides using a reactive force field	August 19, 2008

3.9 Carnegie CDAC Group Meetings

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

Speaker	Affiliation	Topic	Date
R. Thoguluva	Carnegie	Phonons in $Zn(CN)_2$, studied by vibrational spectroscopy and first principles calculations	January 11, 2008
R. Chellappa	Carnegie	Unusual reactivity of H_2O-O_2 mixtures with rhenium and its implications for high pressure research	January 18, 2008
Maureen Long	Carnegie	Mantle flow in subduction zones from seismic anisotropy	January 25, 2008
Adrienne Kish	Carnegie	Survival in the extreme: what molecular-level studies can tell us about the survival of extremophiles	February 1, 2008
P. E. Janolin	Carnegie	Ferroelectricity under hydrostatic pressure and questions that might be solved by dielectric measurements	February 22, 2008
P. Griffin	Carnegie	High pressure microbiology	March 20, 2008
S. Newsome	Carnegie	Biological geochemistry	April 4, 2008
P. Ganesh	Carnegie	A first-order liquid-liquid phase transition in supercooled silicon	April 11, 2008
M. Ahart	Carnegie	Pressure-temperature effects on diffuse scattering in relaxor ferroelectrics	May 2, 2008
A. Sharma	Carnegie	Hydrocarbon synthesis at geobiotic extremes	May 9. 2008
Katherine Crispin		Diffusion of trivalent cations in MgO: Implications for diffusion in earth's lower mantle	May 23, 2008
S. Natarajan	Carnegie	Recent trends in hydrogen metallization research	June 16, 2008
Amy Lazicki	Carnegie	Lithium at high pressure and temperature	June 27, 2008
T. Kuribayashi	Carnegie	System development of single crystal s-ray diffraction facility at 16-BM-D in APS and its applications	July 25, 2008
X. J. Chen	Carnegie	Uncovering hidden superconductivity in inner CuO_2 plane of $Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$	August 1, 2008
M. Weinberger	Carnegie	Hydrogen storage in covalent organic frameworks under high pressure	August 8, 2008
J. Montoya	Carnegie	High pressure structural search: an *ab-initio* approach	August 15, 2008
R. Chellappa	Carnegie	Hydrogen interaction with ammonia borane (H_3NBH_3) and its derivatives	September 5, 2008
L. Zhiguo	Carnegie	Components of solid oxide fuel cells: Pr-based electrolytes	September 12, 2008

4. TECHNOLOGY DEVELOPMENT

The development of high *P-T* experimental techniqes is a high priority in many CDAC groups, yielding improvements in measurement capabilities for a wide variety of sample types. In Year 5, a number important advances have taken place in the area of diamond cell sample preparation as well as at CDAC-supported facilities.

4.1 High *P-T* Experimental Techniques

c-BN and Kapton Composite Gaskets for DACs – One of the challenges of DAC deformation experiments that the **Berkeley** group has been tackling is that of the gasket material. Ideally, high-strength metals such as Be or Re have been used, but in the radial geometry this produces interference with the diffracting beam. The group is currently developing new gasket technology in collaboration with former CDAC research scientist **Jung-Fu Lin**, a Lawrence Fellow at **LLNL**, and currently at the **University of Texas-Austin**. For pressures up to 70 GPa, the current choice is a two-stage boron-kapton composite gasket. These gaskets have the advantage of low background for ease of data analysis. They are, however, limited in pressure range and sample stability. For pressures above 70 GPa and up to 200 GPa, beryllium gaskets have been utilized. While these gaskets have an extended pressure range, they have the drawback of high background and peak overlaps which complicate data analysis, in addition to the health hazards posed by use of the metal. To overcome these drawbacks, a modification of the boron kapton gasket, utilizing cubic boron nitride for an extended pressure range and sample stability, is under development. Gaskets must be strong enough to maintain stresses and yet sufficiently compressible to allow deformation to significant strains. Testing and gasket improvements are currently underway.

Development of Isotopically Enriched C-13 Diamond – Work in **Yogesh Vohra's** group at **Alabama-Birmingham** is focused on the continued development of homoepitaxial C-13 diamond layers for pressure sensing as well as for monitoring the growth rates in chemical vapor deposited diamond. In a series of experiments, (100) oriented, 0.3 carat brilliant cut diamonds were used as substrates in homoepitaxial growth experiments. All diamond anvil substrates had a flat (100) surface of approximately 300 microns in diameter on which homoepitaxial diamond was deposited. Homoepitaxial diamond deposition was carried out in a 1.2 kW microwave plasma chemical vapor deposition chamber with isotopically enriched methane in a hydrogen-oxygen plasma where a small amount of nitrogen was added. The plasma was maintained with a gas flow rate of 390 standard cubic centimeters per minute (sccm) of H_2, 8 sccm of $^{13}CH_4$, and 0.8 sccm of O_2. The group has investigated the role of substrate temperature ranging from 950° C to 1200 °C as well as the nitrogen flow rates ranging from 0.2 sccm to 1.4 sccm, and has found that the diamond growth rate is directly proportional to the intensity of the Raman mode for C-13 diamond at 1281 cm^{-1}, which provides a reliable estimate of change in growth rate with change in growth conditions. The optimal growth rates were obtained at a nitrogen flow-rate of 0.5 sccm and for a substrate temperature of 1200 °C. These optimized conditions are now used for the fabrication of C-13 diamond layers deposited on the top of diamond anvils as part of the effort to create an improved pressure sensor.

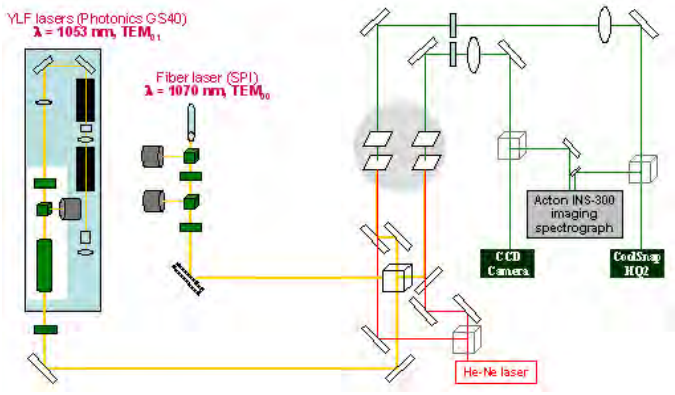


Figure 53. *Schematic diagram of the laser heating apparatus currently in use at station 16-ID-B of HPCAT.*

4.2 Technical Improvements at HPCAT

Technique development continues on the four beamlines at the HPCAT sector, despite the fact that all four stations are fully commissioned and have been accepting users from the APS General User Proposal (GUP) system since 2005. The following

sections describe enhancements on the individual beamlines which have resulted in significant improvements in the user experience, particularly on the bending magnet stations 16-BM-B and 16-BM-D, the last of the four stations to be completed.

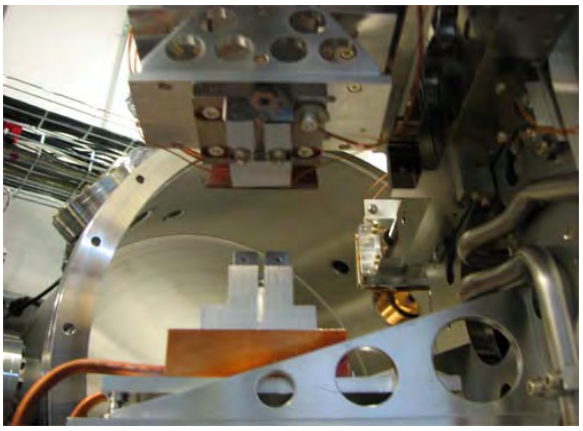


Figure 54. *Double crystal monochromator improvements in 16-ID-A, the first optics enclosure. The first crystal holder is shown in the middle bottom and second crystal holder is in the middle upper.*

Enhanced Fiber Laser Heating Capability at 16-ID-B – The application of fiber lasers in the heating of DAC samples has drawn attention in recent years, due to some important advantages, including improved power stability, and a small size and light demand on utilities. The fiber laser is now considered as an ideal option for *in-situ* laser heating in a micro-focused synchrotron x-ray diffraction system. Fiber lasers do, however, exhibit several key differences in optical characteristics from the commonly used Photonics IR laser, and its application therefore requires the development of a new optical system, particularly if one fiber laser is used for double-sided laser heating.

During the past year, **Yue Meng**, **Eric Rod** and **Arun Bommannavar** at HPCAT have tested three different fiber lasers to evaluate different aspects of the application including power stability, polarization, and control software. The fiber laser heating capability has been established and successfully applied in user operations during run 2007-3. Figure 53 shows the configuration used in station 16-ID-B. This design allows users to choose conventional laser, fiber laser or both simultaneously with combined TEM_{01} and TEM_{00} modes, providing flexibility and the state-of-the-art capability.

X-Ray Spectroscopy on Beamline 16-ID-D – Current techniques available on the x-ray spectroscopy beamline 16-ID-D at HPCAT include x-ray emission spectroscopy (XES, also RXES), inelastic x-ray scattering (IXS, also XRS, x-ray Raman spectroscopy) and nuclear resonant scattering (NRIXS and NFS, also known as synchrotron Mössbauer spectroscopy).

In 2008, a new holder for first the DCM diamond crystal was installed (Fig. 54); the cooling efficiency and beam stability were greatly improved, and the flux at the sample position increased significantly. A challenging experiment on the electron density of sodium metal up to 50 GPa was carried out using small KB mirrors (200mm each, replacing the large, 1 m KB mirrors) during run 2008-2. With the small KB mirrors, the beam focus at the sample position improves to 12μm (V) x 12 μm (H) instead of the typical 30μm (V) x 50 μm (H) focus that was possible with the large mirrors. A vacuum box for low energy x-ray emission spectroscopy was designed and built, and will be tested in run 2008-3.

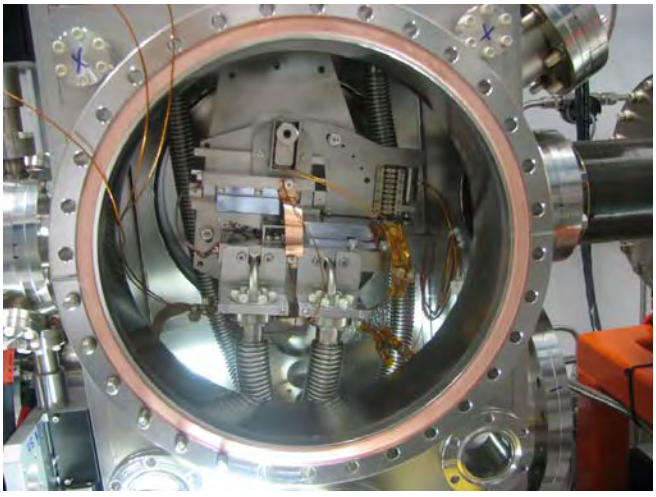


Figure 55. *Channel-cut monochromator installed on 16-BM at HPCAT.*

Bending Magnet Beamline Improvments – In the past year, both 16BM stations have been underdoing significant re-configurations. As a result, several new techniques have been established and are now offered to users.

A wide energy range, artificial channel-cut monochromator (Fig. 55) has been installed, commissioned and routinely used since Run 2007-2. This newly installed monochromator has several unique characteristics optimized for high pressure research: a wide energy range (6-70 keV), high energy resolution, a high-precision nanomotion stage that is capable of energy changes on the sub-eV level, a fixed-exit monochromatic beam position, a short warm-up time and high stability, and the capability to change energy at any time.

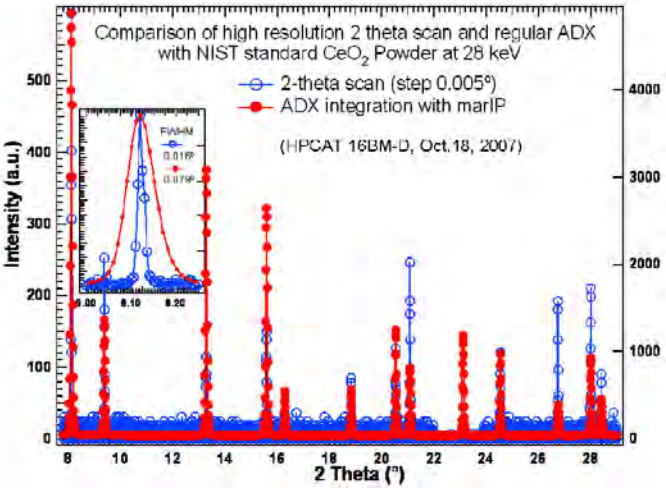
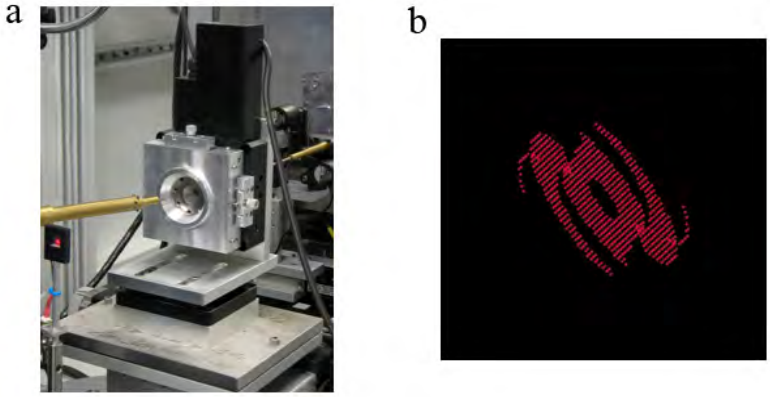


Figure 56. *Comparison of high-resolution 2theta scan and regular ADX with NIST standard CeO_2 at 28 keV. Blue trace: 2theta step scan (step size 0.005°). Red trace, standard ADX pattern with MarIP integration.*

A large, vertical focusing K-B mirror (1.2 m long) has been installed in station 16-BM-C downstream from the monochromator. This mirror accepts up to a 2 mm beam in the vertical direction. Compared to the 200 mm vertical focusing mirror used previously, flux has increased by a factor of 5 in the vertical direction, which is very important for the monochromatic beam mode, since the flux is two orders of magnitude lower than on the ID lines. Progress is being made on the optimal focusing.

<u>High resolution monochromatic powder diffraction capability</u> – The high demand for powder diffraction capabilities among users has resulted in the commissioning of a monochromatic operation mode on 16-BM-D. In 2007, the group at HPCAT demonstrated the capability of scanning angle powder diffraction with the monochromatic beam. With the eccentricity of about 5 μm and collimations in front of the point detector (Ge solid state detector), it is now possible to collect the diffraction intensity while scanning the 2theta angle. Preliminary results indicate that a factor of five to eight better angular resolution is achievable (see the comparison figure with regular area detector in Fig. 56).

Figure 57. *a) Single crystal EDXD setup at consisting of a 3 circle diffractometer, and an EDXD detector with collimation for cell parameter determination of low Z materials. b) Reciprocal lattice for marokite in the DAC at 15 GPa collected with the single crystal EDXD setup at 16-BM-B.*



<u>Single crystal structure determination with ADX and EDX</u> – In 2007 the single crystal EDXD setup in station 16-BM-B was made available to general users for the determination of lattice parameters under pressures in the DAC. The setup consists of a 3-circle diffractometer (2theta, omega, and chi, Fig. 3). A Ge solid-state detector is positioned on the 2theta arm and works as a point detector. It is therefore possible to determine cell parameters by means of the energy/d-spacing as well as the angular position of the diffraction peaks. The three-circle diffractometer has a very small eccentricity of less then 5 μm in 2theta and omega (Fig. 57a).

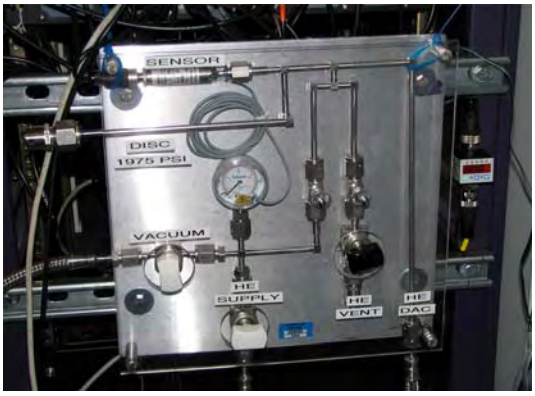


Figure 58. *Membrane control setup at station 16-BM-D.*

The eccentricity in chi can be adjusted manually to within 10 μm optically and less then 5 μm with an x-ray absorption map. The advantage of using the EDXD single crystal setup arises from the fact that a collimation in front of the detector is suppressing diffraction from the seats, the gasket and the diamonds, thus allowing the determination of cell parameters and possible lattice types of very low Z materials (Fig. 57b). Collection of reliable intensity data is still under development and expected to be available in 2009-2.

The single crystal ADXD system in 16-BM-D is still under commissioning but significant progress has been made through collaborations with **Przemek Dera** (GSECARS) and **Takamitsu Yamanaka** (Carnegie). It is now possible to reliably determine the structure of single crystals (NIST ruby sphere) at ambient pressure. Further benchmark experiments are planed for run 2008-3.

Membrane pressure control – Station 16-BM-D has been equipped with a dedicated membrane control system since early 2008 (Fig. 58). Users now can bring different types of DACs (symmetric or Mao-Bell type) to the beamline and use membranes and adaptors provided by HPCAT to modify the pressure on the sample remotely from the beamline control area. This will increase the productivity of the station, allow finer pressure control and decrease wear and tear on vital beamline components. The membrane control system is now also available for the He flow cryostat for temperatures down to 4 K.

5. INTERACTIONS WITH NNSA/DP LABORATORIES

5.1 Overview

From the very start of the program, and as a primary goal in its mission CDAC has sought to promote interactions between high-pressure groups at the National Labs (Laboratory Partners) and the Academic Partners. CDAC has therefore provided access to synchrotron beamlines at APS and NSLS, the CDAC high-pressure labs at Carnegie, as well as all of the facilities maintained by our academic partner groups. Laboratory Partners are also invited and encouraged to attend the regularly scheduled HPCAT meetings at the APS. The *CDAC Summer School* in 2005, and the *SSAAP Symposia* in Albuquerque (2004) and Las Vegas (2005) and Washington (2007 and 2008), the *Synergy of 21st Century High-Pressure Science and Technology Workshop* in 2006 and the SMEC meeting in 2007 have all been highly successful ventures in terms of promoting interaction between CDAC students and scientists from the NNSA Labs. The CDAC Winter Workshop, to be held in February 2009, is in the planning stages and will provide another venue for CDAC students, partners and lab scientists to interact and discuss research opportunities. In addition, the following features of the CDAC program enhance opportunities for interaction and collaboration on a continuing basis:

- ***Beam time for experiments at HPCAT.*** Each year, groups from **LLNL** and **LANL** take advantage of discretionary beam time provided by CDAC to carry out experimental work in one or more of the sectors now on-line at HPCAT. Over the past year, approximately 20% 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. Records of visits by NNSA Lab scientists, CDAC academic partners, CDAC collaborators, and other users are listed below in Appendix II. In addition, we made available beam time for groups from **SNL** and **WSU** to carry out the first synchrotron measurements of dynamic compression events at **NSLS** and **HPCAT,** respectively. CDAC will continue to assist in facilitating these emerging and highly important experiments.

Figure 59. *Screen shot of the CDAC website, http://www.gl.ciw.edu .*

- ***Carnegie high-pressure facilities.*** During Year 5, we have interacted 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 5, 31 different people visited **Carnegie** for work at CDAC facilities.

- ***Academic Partner Participation at NIF.*** As the academic use of NIF becomes closer to a reality, CDAC has been active in promoting this opportunity amongst interested Academic Partners. There will be potentially five to seven CDAC Academic Partner groups applying for time at the facility.

- ***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. 59). The site presents an array of scientific and technical developments, meeting announcements and links, beam time updates, the site serves as gateway to high-pressure research not only at CDAC, but throughout the US and around the world. Publication records and abstracts for the CDAC community are updated regularly. Research highlights detailing information on new papers or research breakthroughs that have been supported by CDAC are also featured and updated on monthly basis.

5.2 HPCAT Membership and Beam Time Allocation

HPCAT is a member-owned facility with ownership proportional to member contribution. Originally, 30% of the ownership was associated with stewardship science (H-Division of **LLNL** 10% and University of Nevada, Las Vegas, 20%). With construction completed at the facility, and with the increase in the CDAC budget following Year 3, CDAC now is a 30% member based solely on the contribution from the core CDAC budget. This gives participating NNSA/DP Lab divisions and university partners representation on the HPCAT Council. Moreover, the stewardship science interest in HPCAT has been lifted from a minority to 75% (LLNL H-Division, 20%, CDAC, 30%, UNLV, 25%), thereby significantly increasing the ability of NNSA/DP to steer future developments at the facility.

CDAC beam time is allocated based on the membership shares of each of the contributing members. For each beamline, the available shifts (three per day) during a beam time run period are totaled. After subtracting shifts for the General User Proposal (GUP) program of the APS (25% of beam time) and HPCAT time for technique development, beamline upgrades and staff research (25%), the available shifts are distributed among the HPCAT partners: **Carnegie** (25% of remaining time), CDAC (30%), **LLNL** H-Division (20%), and **University of Nevada-Las Vegas** (25%). At this

point, that means approximately 35-40 shifts per beamline in a typical run period (three run periods per year) will go to CDAC academic partners, their students, and National Laboratory partners. During Year 5, 32 proposals were submitted for beam time through CDAC (12 from National Lab scientists and 20 from Academic Partners). Some of these proposals were granted beam time through the GUP process, allowing other users from within CDAC to benefit from the extra time allotted. In all cases, however, CDAC users who requested beam time were able to receive it. A detail of those who obtained beam time at HPCAT and the experiments they performed is given in Appendix II.

Notably, a large number of former students and post-doctoral fellows from CDAC academic groups have established new research programs in high-pressure science in academia. In the past four years, the following former postdoctoral fellows have set up teaching programs as new assistant professors (or the equivalent). Each of these young scientists is an active collaborator and is training new students.

Jung-Fu Lin (University of Texas; from Carnegie and LLNL)
Steve Jacobsen (Northwestern University; from Carnegie)
Wendy Mao (Stanford University; CDAC graduate student from Chicago, postdoctoral fellow from LANL)
Jennifer Jackson (California Institute of Technology; from Carnegie)
Tabitha Swan-Wood (CSU-Channel Islanads; from Caltech)
Olga Degtyareva (University of Edinburgh; from Carnegie)
Jie Li (University of Illinois; from Carnegie)
Eugene Gregoryanz (University of Edinburgh; from Carnegie)
Boris Kieffer (New Mexico State; from Princeton)
Mark Frank (Northern Illinois University; from Carnegie)
Yanzhang Ma (Texas Tech; from Carnegie, now a CDAC academic partner)
Sebastien Merkel (Lille, France; from Berkeley)
Henry Scott (Indiana University South Bend; from Carnegie)
Anurag Sharma (Renssalear Polytechnic Institute; from Carnegie)
Sean Shieh (University of Western Ontario; from Princeton)
Yang Song (University of Western Ontario; from Carnegie)
Sergio Speziale (GFZ Potsdam, Germany; CDAC graduate student from Princeton, postdoctoral fellow from Berkeley)
Sarah Stewart-Mukhopadhyay (Harvard; from Carnegie)

6. MANAGEMENT AND OVERSIGHT

The management and oversight of CDAC, including the organizational structure and managerial activities of the past year, are reviewed below. Leading scientists from the University and National Laboratories provide oversight as part of the Advisory and Steering committees.

6.1 CDAC Organization and Staff

Managed at **Carnegie**, the group leaders from each academic node of CDAC together with representatives from directorates (or divisions) at NNSA/DP Labs form an Executive Committee to direct and coordinate research, development, and access to facilities. The organizational structure of CDAC is shown in Fig. 60. CDAC directly supports the HPCAT facility and graduate students in the groups of the Academic Partners. Beam time at HPCAT and NSLS is awarded to the academic partners, laboratory partners and university collaborators. Coupled with beam time at **Carnegie**-managed facilities at the NSLS and interactions with National Lab Partners at its unique NNSA Lab facilities, CDAC has put in place a proven structure that promotes collaboration and interaction and a sharing of a broad range of unique experimental and theoretical capabilities.

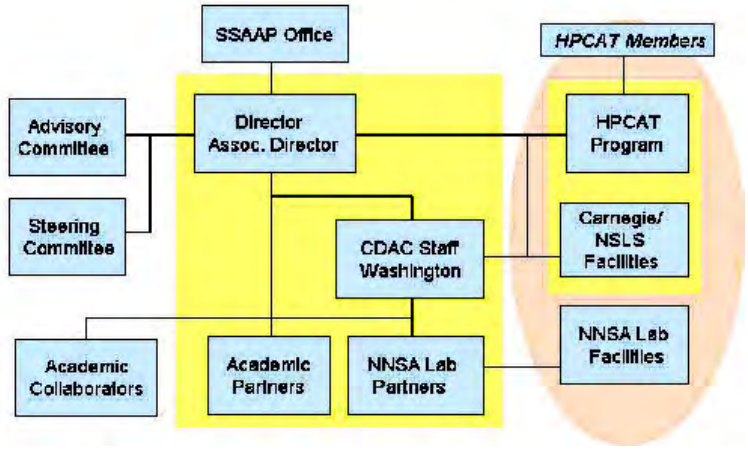


Figure 60. *CDAC organizational chart. The yellow area designates the principal components of CDAC. The oval area encompasses the three different groups of experimental facilities associated with CDAC.*

At **Carnegie** the CDAC staff includes **Russell Hemley**, Director, and **Ho-kwang Mao**, Associate Director. 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

Takamitsu Yamanaka came to **Carnegie** in April of 2007 from **Osaka University** as a Visiting Fellow. He is collaborating with CDAC researchers and personnel at HPCAT on high pressure crystal chemistry and working on improving methods for synchrotron-based high-pressure crystallography utilizing white-beam Laue at HPCAT.

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

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

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

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

In 2006, oversight for the x-ray beamlines X17B and X17C at NSLS was turned over to the University of Chicago. CDAC continues to provide support for the U2A infrared spectroscopy beamline, and a number of CDAC users take advantage of the facility each year, as listed in the Appendices.

A number of predoctoral and postdoctoral fellows at **Carnegie** supported by the Institution, other grants, or outside fellowships worked on CDAC tasks during Year 5. 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**
- **Patrick Griffin**
- **John Janik**
- **Joseph Lai**
- **Amy Lazicki**
- **Yufei Meng**
- **Subramanian Natarajan**
- **Tim Srobel**
- **Ravindran Thoguluva**
- **Michelle Weinberger**

6.2 CDAC Oversight

In order to complement SSAAP oversight of CDAC, Steering and Advisory Committees have also been assembled to guide the research efforts in the long term. The tasks of the Steering Committee are to advise on monthly operational issues, attend monthly HPCAT meetings to serve as the member representatives of CDAC on the HPCAT council, and to serve as points of contact between CDAC and the participating divisions and directorates of the NNSA Labs. Members of the Steering Committee are:

- **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)
- **Joe M. Zaug** (LLNL)
- **Yusheng Zhao** (LANL)

The Advisory Committee is charged with assisting with strategic planning, providing guidance on scientific issues and programmatic needs, and acting as liaisons between CDAC and the NNSA Labs, other SSAAP Centers, and the broader academic community. The Advisory Committee consists of

- **Neil W. Ashcroft** (Cornell)
- **Robert Cauble** (LLNL)
- **Yogendra M. Gupta** (WSU)
- **Alan J. Hurd** (LANL)
- **Chi-chang Kao** (Brookhaven)
- **Christian Mailhiot** (LLNL)
- **Tom Melhorn** (SNL)

Members of the committees are invited to attend the monthly CDAC/HPCAT meeting and many interact frequently with the Director and Associate Director. Each of the members of the two CDAC committees renewed their commitment to serving through Year 5 and into Year 6 of the CDAC program. The CDAC Steering Committee will take on a critical role in the evaluation of proposals from prospective Academic Partners beginning with Year 6.

7. PLANS FOR YEAR 6 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, we have added several new partners to the CDAC group as of the beginning of Year 6. At the writing of this report, these partners and students have begun their work on high *P-T* materials science, as outlined below.

Abby Kavner, UCLA

Abby Kavner (UCLA).

The goals of the CDAC-supported work of new Academic Partner **Abby Kavner** at **UCLA** are to understand the principles governing the mechanical behavior of materials at high pressure, with emphasis on (1) high pressure lattice strength systematics of a variety of materials, including elements, and oxides, (2) thermoelastic properties of materials with applications covering fields of condensed matter physics, materials engineering, and geophysics, and (3) design and evaluation of superhard materials. CDAC graduate student **Richard Armentrout** uses radial x-ray diffraction measurements of DAC samples to examine the lattice-dependent strain of halide pressure markers (e.g. NaCl, CaF_2, AgI) in their low and high pressure phases, and as they undergo phase transformations. This information is useful for understanding mechanical properties of aggregates as they are subject to large strains. The results will continue to establish the use of halides as internal pressure calibrants to measure high pressure and temperature thermoelastic properties in the DAC.

High Pressure Strength and Elastic Behavior of CaF_2 – The radial diffraction lattice behavior of CaF_2 was analyzed in its low pressure (fluorite) and high pressure phases up to 11.5 GPa. Between 3.5 and 7.1 GPa, fluorite develops a radial diffraction strength of ~0.8 GPa. The corresponding lattice anisotropy of the fluorite phase was measured to be equal to 0.73, in good agreement with previous Brillouin spectroscopy measurements. By 8.8 GPa, CaF_2 has undergone a phase transformation to its high pressure (orthorhombic) phase, with a corresponding volume

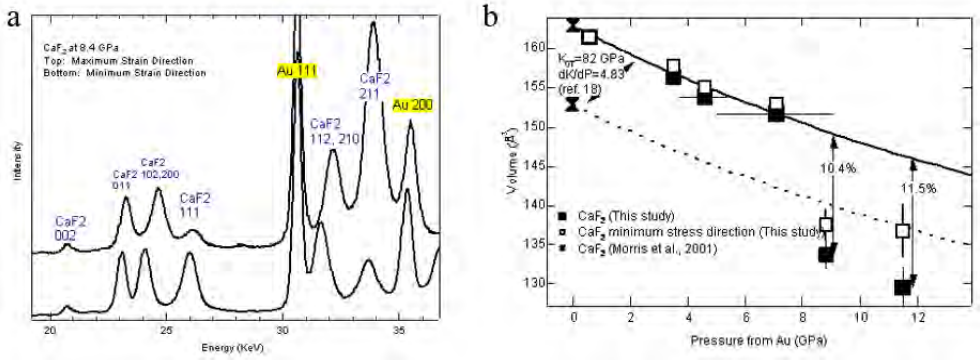


Figure 61 *a) Portion of diffraction patterns in the minimum and maximum stress directions for high pressure orthorhombic phase of CaF_2 and gold at 8.4 GPa. Diffraction peaks for both phases are indexed. b) Measured unit cell volumes as a function of pressure for CaF_2. Solid squares are volumes at the hydrostatic conditions. Open squares are volumes inferred from strains in the minimum stress direction. Pressure is determined by using the lattice parameters of Au, added as a pressure calibrant in the diamond anvil cell. The measured $DV=(V_2-V_1)/V_1$ for the transition between the high pressure phase and low pressure phase are shown at the two highest pressure steps.*

decrease of 10.4%. By 11.5 GPa, the volume drop between the low pressure and high pressure phase has increased to 11.5% (Fig. 61). In addition, the high pressure phase is found to withstand a significantly larger differential stress than the low pressure fluorite phase, with a large degree of lattice anisotropy. In the maximum stress direction at 8.8 GPa, we observe a time-dependent evolution of the lattice parameters of CaF_2, indicating that the high pressure structure is still undergoing deformation on timescales of hours after the phase boundary has been crossed (Fig. 62).

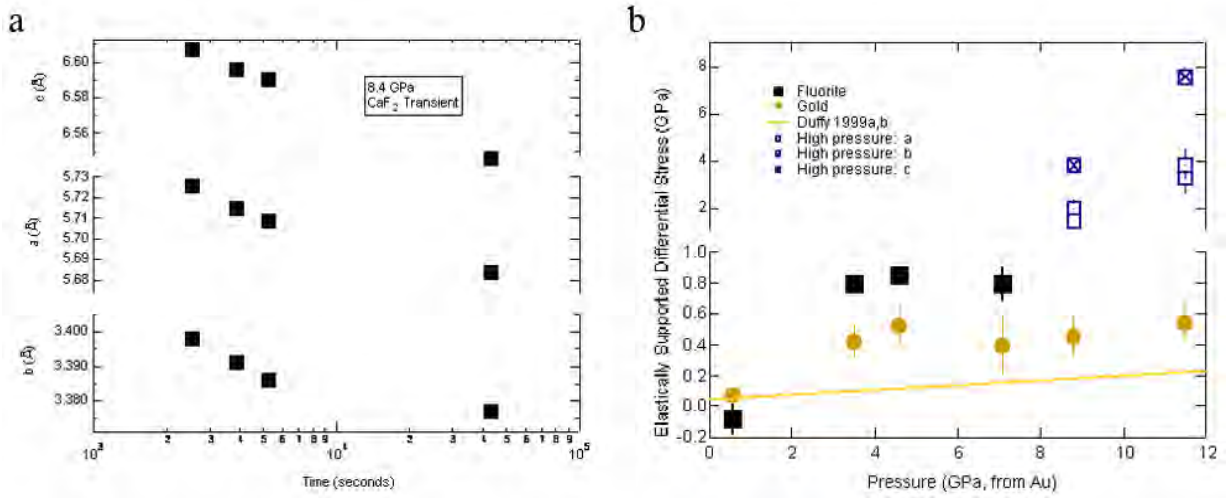


Figure 62. *a) High pressure CaF_2 lattice parameters in the maximum stress directions as a function of time for P=8.4 GPa). The lattice parameters indicate a time-dependent shrinking of the lattice. b) Differential stress as a function of pressure for CaF_2 and Au. The high pressure phase of CaF_2 appears to be much stronger than the fluorite phase.*

<u>High P-T EOS of Osmium Metal</u> – Since Os metal is known to be a mechanically strong elemental metal and is therefore used as a host material to generate ultrahard materials,[78-84] the high pressure, high temperature behavior of Os metal in the DAC has been examined. A series of experiments to examine the structure and EOS of Os at pressures up to ~50 GPa, and temperatures up to the melting temperature was carried out. Preliminary results show that Os appears to be stable in its hexagonal-close-packed phase up to ~ 50 GPa and at high temperature (Fig. 63).

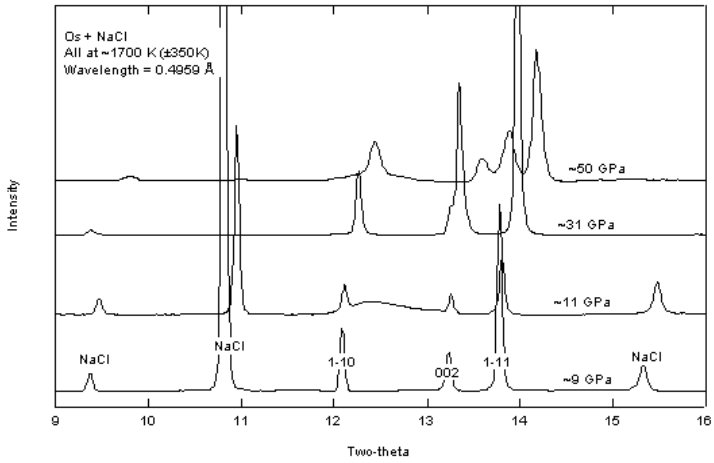


Figure 63*. X-ray diffraction patterns for Os metal obtained in situ at high pressures and temperatures (during laser-heating) in the diamond anvil cell. Data obtained at beamline 12.2.2 at the Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA.*

Steven Jacobsen, Northwestern University

Steven Jacobsen (Northwestern).

Research in **Steven Jacobsen's** group focuses on the elastic properties of a variety of different materials. X-ray diffraction and Brillouin spectroscopic methods, as well as evolving GHz interferometry methods are employed for ultrahigh pressure investigations of key material properties.

Compression of Single-Crystal MgO – Magnesium oxide (MgO, periclase) is among the most widely studied standard materials for testing experimental and theoretical methods for determining elastic properties at high pressures. MgO maintains the B1 (halite) structure to multi-megabar pressures and is geophysically important as the end-member of ferropericlase, (Mg,Fe)O, thought to be the major non-silicate oxide of the lower mantle. Because of its simple structure and geophysical relevance, knowledge of accurate elastic properties of MgO pertains to problems ranging from experimental pressure scales to interpreting Earth's seismic structure. At **Northwestern**, new CDAC Academic Partner **Jacobsen**, along with postdoctoral researcher **Christopher M. Holl**, graduate student **Kimberly Adams**, and undergraduate student **Rebecca Fischer**, are investigating the compression behavior of MgO single-crystals in quasi-hydrostatic helium pressure media to megabar pressures. As shown in Fig. 64, these Mbar single-crystal equation-of-state studies of MgO have revealed significant differences in pressure calibrations between the former quasi-hydrostatic ruby fluorescence gauge and the absolute pressures determined from the primary MgO pressure scale[85].

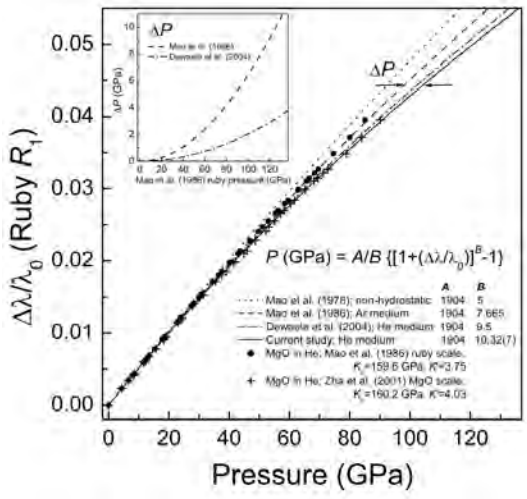
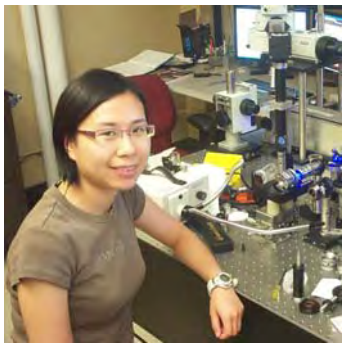


Figure 64. *Ruby pressure gauge for experiments in diamond cells ranging from non-hydrostatic conditions (dotted curve) to helium quasi-hydrostatic conditions (solid line, current study against MgO pressure scale). The calculated pressure difference (ΔP) between the former quasi-hydrostatic pressure gauge (in argon, dashed curve) and the new calibration for helium against MgO pressures (solid curve) is about 8 GPa at 100 GPa, shown in the inset.*



*New CDAC graduate student **Yun-yuan Chang** will be developing the GHz-ultrasonic system to study high-pressure elastic properties of metals and glass materials with CDAC partner **Steven Jacobsen** at **Northwestern**.*

Effects of Hydration on Elastic Properties – Water, dissolved as hydroxyl (OH-) into the solid silicate minerals of the upper mantle can reduce adiabatic wave speeds through associated defects. The role of deep-mantle water in Earth processes such as plate tectonics has recently gained attention in the geophysical community, but understanding why hydration influences the physical properties of silicate minerals requires an interdisciplinary approach including high-pressure chemistry and physics of defects.[86] At **Northwestern**, **Steven Jacobsen** and **Chris Holl**, in collaboration with CDAC partner **Thomas Duffy,** postdoctoral associate **Fuming Jiang**, and graduate student **Zhu Mao** at **Princeton**, have conducted Brillouin spectroscopy measurements (at **Princeton**) of the sound velocities and single-crystal elastic constants of hydrous forsterite (hy-Fo100) and hydrous olivine (hy-Fo97) containing 0.8-0.9 wt% H_2O (Fig. 65). The samples, synthesized at 12 GPa and 1250°C,

represent nearly the maximum storage capacity of water in olivine at conditions of 350-400 km depth. The adiabatic bulk and shear moduli of hy-Fo100 are 125.7(±0.2) GPa and 79.8(±0.1) GPa, respectively. For hy-Fo97, K_{S0} = 124.4(±0.4) GPa and G_0 = 75.3(±0.3) GPa. Compared with anhydrous forsterite, the combined effects of 3 mol% Fe and 0.8 wt% H_2O reduce bulk and shear moduli by 3.5(±0.3)% and 7.5(±0.4)% respectively, with greater reductions expected for more iron-rich mantle compositions. Together with seismological observations from colleagues at **Northwestern** and **Princeton**, the new mineral physics data on the effects of hydration on the elastic properties of olivine, the most abundant mineral phase in the Earth's upper mantle, are being applied to evaluate seismic anomalies in the upper mantle that are not easily explained by temperature alone.

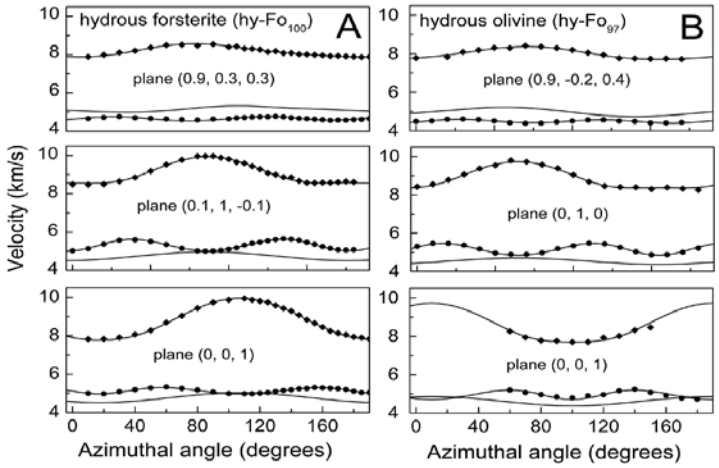


***Figure 65**. Brillouin spectroscopy measurements of acoustic velocities in hydrous forsterite and hydrous olivine as a function of azimuthal angle perpendicular to each specified plane. These data are being used to evaluate the effects of water, or hydration, on the single-crystal elastic constants of olivine, the most abundant phase in Earth's upper mantle. Comparison to seismological data provides constraints on potential hydration of the Earth's mantle.*

Jie Li, University of Illinois

Jie Lie (University of Illinois).

In a fruitful collaboration with colleague **David Cahill** in the Department of Materials Science and Engineering at **Illinois**, new CDAC academic partner **Jie Li** is extending Cahill's time-domain thermo-reflectance technique so that it may be used for thermal conductivity measurments in the DAC.

Thermal Conductivity of Materials With Time-Domain Thermo-Reflectance – In the group of **Jie Li** at **Illinois**, fourth-year graduate student **Bin Chen** has been investigating the thermal conductivities of compressed water ices using the time-domain thermo-reflectance method developed in the group of colleague David Cahill in the Materials Science and Engineering department (Fig. 66a). Initial measurements have been conducted at ambient temperature. These thermal conductivity measurements involve the use of a piece of aluminum-coated kapton tape that was pressed onto one of the anvils (Fig. 66b). Since the thermal effusivity of water ice is nearly a factor of 10 larger than the thermal effusivity of kapton, heat flow was dominated by the thermal properties of water ice in contact with the Al film. Preliminary measurements on water, tetragonal ice VII and cubic ice VIII are in good agreement with existing data.

High-Pressure Ices – Thermal conductivity of high-pressure polymorphs of water is of fundamental interest to materials science, condensed matter physics, and Earth and planetary sciences. In our solar system, water ice is present under a wide range of pressure and temperature conditions. X-ray diffraction, optical and spectroscopic investigations have revealed a series of pressure-induced phase transitions in H_2O.[87-89] Some of the high-pressure polymorphs of water are expected to exist in the interiors of giant planets, icy planetary satellites, and Kuiper Belt Objects

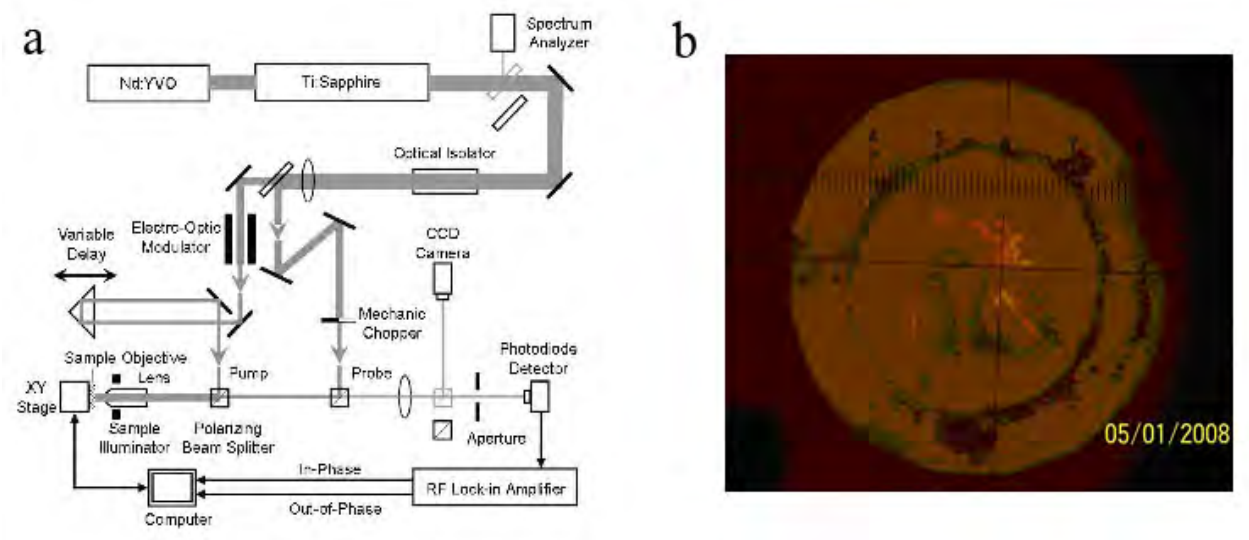


Figure 66. *a) Schematic of the time-domain thermo-reflectance and picosecond acoustics apparatus in use at the Laser Facility of the Frederick Seitz Materials Research Laboratory, University of Illinois. b) Image of cubic ice VIII and Al-coated mica in a diamond-anvil cell at 3.2 GPa and 300 K.*

(KBOs). Computer simulations suggest that at high pressures and moderate temperatures, the phase diagram of H_2O exhibits a super-ionic solid phase under *P-T* conditions inside Neptune and Uranus.[90] Thermal conductivity of high-pressure ices is a critical property that influences the thermal evolution of icy bodies. In the field of material science and condensed matter physics, a large number of experimental investigations have focused on understanding the symmetrical hydrogen bonded form ice (ice X).[88] The high-pressure phases of ice provide a unique opportunity to systematically study the effects of disorder, crystal symmetry, and anharmonicity in controlling the thermal conductivity of materials.

The experimental data on the thermal conductivity of water ices are limited to a few GPa so initially the main goal will be to continue to investigate thermal conductivity of water ices under higher pressures. Measurements at higher temperatures or under cryogenic conditions are planned as the next step of the project. An external heating method will be used to achieve temperatures up to about 1000 K Thermal conductivity at temperatures down to 80 K will be studied using a liquid-nitrogen cryostat.

Raymond Jeanloz, UC-Berkeley

Raymond Jeanloz (Berkeley).

Arianna Gleason, a new CDAC graduate student in **Raymond Jeanloz's** group at **Berkeley**, has been carrying out exploratory Brillouin spectroscopy experiments at the **Lawrence Berkeley National Laboratory**. Wave velocities at room temperature on polycrystalline NaCl and argon have been measured to 8 and 26 GPa, respectively. Multiple orientations and points across the sample were measured to ensure reliable averaging of the velocities; these data are in excellent agreement with previous work. The initial focus on simple materials (Ar and NaCl) benchmarks the system and approach before combining the diamond-anvil cell, resistance heating and Brillouin spectroscopy to assess more complex minerals relevant to the deep Earth.

Gleason's main focus will be to investigate the role of water in the transition zone[91] of the Earth's mantle as influencing seismic tomography,[92] comparing that with the role of temperature variations. Using the Brillouin scattering technique,[93], it will be possible to

systematically determine average compression- and shear-wave velocities of well-characterized natural or synthetic aggregates of hydrous and anhydrous mineral assemblages. These velocity measurements will be compared with seismological data to quantify the degree of hydration required to explain observed seismic-velocity variations within the upper mantle and transition zone. A suite of materials ranging in their degree of hydration will be measured, from serpentinite – the hydrous end-member – to dunite as the anhydrous end-member of a model mantle composition. The overall goal will be to document the percent velocity change as a function of hydration and quantitatively assess the degree to which water variations could explain variations in the seismological wave velocities. It is expected that the retardation of the shear-wave velocities to be more pronounced with increased hydrogen content than that of the compression-wave speeds.

Wendy Panero, Ohio State University

Wendy Panero (Ohio State University).

A series of experiments is underway in the research group of **Wendy Panero** at **Ohio State University** to examine electronic transitions in K and Rb using the reactivity with transition metals as a marker. In this way, 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. It is necessary to investigate the influence of sample preparation on the results. If the hypothesis that an electronic transition in the alkali metals is causing solubility in iron is indeed correct, then the experiments should be reproducible with rubidium in place of potassium.

s-d Transitions in Heavy Alkali Metals – Experiments have been performed by CDAC graduate student **Sabrina Whitaker** using a laser-heated DAC (LHDAC) at pressures of 10-90 GPa, heated to the melting temperature of iron. Samples were constructed with layers of high purity, natural potassium feldspar, $KAlSi_3O_8$, or high purity rubidium feldspar, $RbAlSi_3O_8$, with iron foil between the silicate layers. 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 above the s-to-d transition pressure is expanded by 1-2% relative to pure iron (Fig. 67a). The expansion is only observed at high pressure, which indicates that the expansion is not due to Si or O. However, the chemistry of the iron metal needs to be analyzed directly. To test this,

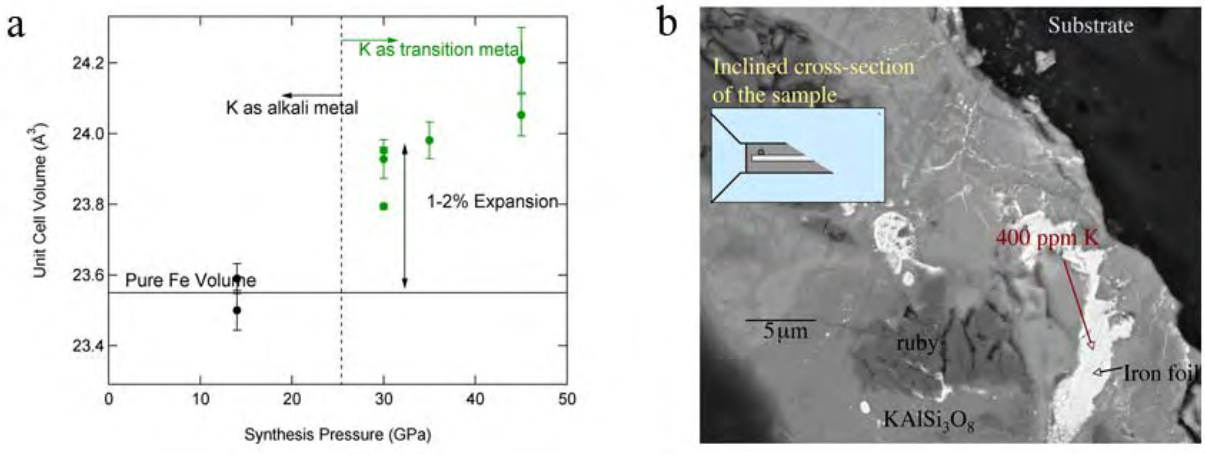


Figure 67. *a) The unit cell volume of iron quenched from high pressure and temperature in equilibrium with $KAlSi_3O_8$ as a function of the synthesis pressure. Assuming Rault's Law and that oxygen and silicon do not participate in the process, the volume expansion is consistent with ~8000 ppm K. b) Sample synthesized at 35 GPa and 2700 K, polished on a cross section (inset) to reveal the imbedded iron foil. Preliminary SEM shows a K concentration of ~400 ppm, but this will need to be tested fully after extraction of a TEM foil from the cross section to avoid problems with the sampling volume of the SEM.*

initial work has been done to expose the iron layer through polishing (Fig.67b) and extraction of a foil across the sample.

To gain quantitative results on the composition of the metal phase, conclusions based on the x-ray diffraction will be quantified *ex-situ* with ATEM on cross sections of the sample extracted with Focused Ion Beam Milling (FIB). This will result in quantitative measurements of K and Rb in the metal phase, as well as establish the oxygen content in the metal and metal content in the silicate for approximation of the oxygen fugacity of the samples and determine the degree of equilibration in the sample. Also working on this project is an undergraduate, **Eugenia Hyung**, who is using the x-ray diffraction data to examine the elasticity and phase stability of the high-pressure phases of K- and Rb- feldspar. Preliminary results were presented at the 2008 annual COMPRES meeting in Colorado Springs, CO.

James Schilling, Washington University-St, Louis

James Schilling (Washington State University).

In order to investigate the magnetic properties of rare earth metals at pressures over 100 GPa, CDAC graduate student **Wenli Bi** at **Washington University** is preparing DACs for high pressure electrical resistivity measurements and synchrotron x-ray diffraction experiments. She has designed an exposure mask to allow the placement of tiny (2 micron wide) electrical leads and ac susceptibility coil systems directly on the diamond anvils via photo-lithography techniques. A substantial further decrease in lead size (or coil size) will be possible through the use of a recently purchased electron beam photolithography apparatus in the **Center for Materials Innovation**. Initial metals for investigation include Pr, Nd, Eu, Tb and Yb.

Robert Downs, University of Arizona

Robert Downs (University of Arizona).

New CDAC graduate student **Madison Barkley** is working on the development of new approaches to ultrahigh pressure single crystal structure determination using diffraction facilities at the APS (**HPCAT** and **GSECARS**). In particular, the synchrotron facilities will be capable of examining very small crystals that can be subjected to very high pressure. **Robert Downs's** group has partnered with **Malcolm Nicol** (**UNLV**), and **Mark Rivers** and **Przemek Dera** (**GSECARS**) in this development project.

Wendy Mao, Stanford University

Wendy Mao (Stanford).

At **Stanford**, the research group of new academic partner **Wendy Mao** has started work in two research areas: the high-pressure behavior of hydrogen in low-Z molecular systems, and the study of iron and transition elements at high pressure. Both the behavior of light elements under extreme conditions, and the physics of 3*d* elements, including the electronic, magnetic, phonon, and structural properties are key research topics in the overall mission of the NNSA.

Behavior of Hydrogen in Low-Z Molecules at High Pressure – The effect of pressure on the bonding of hydrogen with second-row elements in low-Z hydrides (*e.g.* LiH, BH_3,CH_4, H_2O, and NH_3) will be a central focus of the work of CDAC graduate student **Yu Lin.** Exploration in the vast *P-T-X* field for promising structures, compounds, and reaction processes have barely scratched the surface for even the two most elementary, hydrogen-rich compounds, H_2O and CH_4. Pressure induces dramatic changes in the chemical bonds of these compounds, opening up rich possibilities for different *s-p* hybridization, the transition of covalent and hydrogen bonding to ionic and even superionic states at high *P-T*, metallic bonding, and superconductivity at extreme pressures. The nature of the bonding of hydrogen in these materials as a function of *P-T-X* will be investigated using a number of *in-situ* probes. Element-specific, near *K*-edge spectroscopy reveals the nature of bonding between the element and its surrounding atoms. Recent coupling of XRS with a DAC has enabled a full range of high-pressure investigation of light element bonding, as demonstrated by the successful XRS studies of second-row elements and compounds. High pressure XRS experiments will be conducted at the **HPCAT** facility at APS, and neutron scattering studies for elucidating the structural features and dynamics of hydrogen will be conducted at **LANSCE** as well as the newly built **Spallation Neuron Source** and will be complimented by Raman spectroscopy. Thus far, the ammonia-borane and ammonia-borane + H_2 systems have been investigated, both to above 20 GPa using Raman spectroscopy. Preliminary work on the decaborane + H_2 and boric acid + H_2 systems has also been started.

Iron and Transition Row Elements at High Pressure – To investigate the electronic properties of materials, the **Stanford** group will adapt a suite of complementary x-ray based techniques that have been well demonstrated for iron at ambient conditions, in new high-pressure applications. These include XANES for electronic states, EXAFS for structural information, RIXS for local electronic structure and spin states and XES for high- to low-spin transitions. These experiments will be conducted at **HPCAT** as well as appropriate beamlines at **SSRL** and **ESRF**. These emerging high-pressure techniques will be used to study the electronic behavior of iron-bearing compounds, where definitive characterization of the iron at high *P-T* will greatly enhance the understanding of material behavior at high *P-T*. A similar approach can

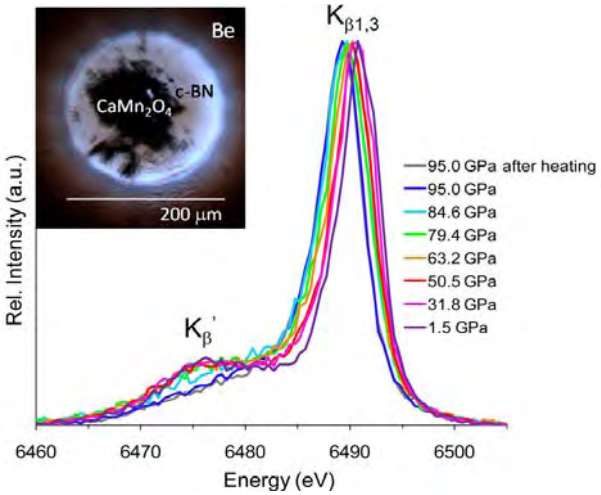


Figure 68. *XES results for $CaMn_2O_4$. A spin transition was observed at approximately 85 GPa as indicated by the loss in intensity in the Kβ'satellite peak and a shift in the position of the main peak to lower energy. XRD results suggest that a structural transition may also occur in this pressure region. Insert: photomicrograph of sample at 95 GPa.*

also be applied to fundamental physics and chemistry of other transition row elements and compounds. CDAC graduate student **Shibing Wang** will undertake this experimental effort for her thesis work.

Detailed studies of phonon dynamics in highly compressed materials are necessary for understanding vibrational thermodynamic properties, elasticity, and phase transition mechanisms of materials, but until very recently have eluded high pressure experimental investigation. Non-resonant phonon inelastic x-ray scattering (PIXS) is a powerful method which holds great promise for studying phonon dynamics of materials at high pressure. Preliminary arrangements have been made with personnel at the HRIXS beamline at APS for collaborative development of high-pressure programs.

Synchrotron nuclear resonant inelastic x-ray scattering (NRIXS) spectroscopy allows for the determination of the phonon DOS related to the ^{57}Fe isotope in a high-pressure sample. The phonon DOS is extracted from the phonon excitation spectrum associated with the nuclear resonant isotope. The Debye sound velocity (V_D) is determined from a fit to the low energy (long wavelength) portion of the DOS; V_D is heavily weighted in V_S and therefore provides a good constraint on V_S. In addition, the resonant isotope-related portion of different thermodynamic parameters can be calculated by integration of the phonon DOS The expected results of an accurate constraint of V_S, however, will be quite rewarding and will provide a complement to a hydrostatic *P-V* EOS study for determining both V_P and V_S. Incorporation of the textural analysis and the PIXS and NRIXS results allow for a more accurate determination of the elastic parameters. This would also provide a test of the elasticity results determined from radial XRD. Thus far, Fe_2O_3 has been investigated using NRIXS, XAS, and XRD in helium to over 50 GPa. Also, XRD and XES have been used to study structural and electronic transitions in the 3d transition metal compounds $FeGeO_3$, $CaMn_2O_4$ (Fig. 68) and Mn_2O_3 and observed phase transitions and spin transitions in all three materials have been observed.

7.2 Major New Initiatives

In its second five year period, CDAC will take advantage of new opportunities and initiatives in DOE to facilitate advances in the above science areas while at the same time providing NNSA/DP with critical input needed for important decisions regarding the future of the weapons complex. The following sections summarize key areas identified in the CDAC renewal proposal, submitted in May 2007.

7.2.1 HPSynC: Coordination of High Pressure Activities at APS

The High Pressure Synergetic Center (HPSynC) at the APS begun its operations near the close of Year 4 of the CDAC program with the goal of coordinating high pressure activities at the APS and promoting high *P-T* technique development at multiple beamlines so that the particular strengths of a number of different beamlines could be utilized for specific methods. HPSynC therefore becomes a convenient point of contact for users interested in getting started in high pressure work as well as established users looking for assistance in extending existing techniques. HPSynC began its first year of operation with a Board of Governors meeting at which some guiding principles were established and initial plans formulated. Under the direction of **Ho-kwang Mao** (Director) and **Guoyin Shen** (Project Manager), HPSynC has already established some fruitful collaborations, as outlined in the sections below.

Pressure-Induced Magnetic Transition and Sound Velocities in Fe_3C – In a collaboration between HPSynC, APS/XOR Sector 3 and the University of Illinois, and facilitated by **Michael Lerche**, the iron-rich alloy Fe_3C was investigated up to 50 GPa using nuclear resonant x-ray scattering techniques. Synchrotron Mössbauer spectra reveal a pressure-induced magnetic transition in Fe_3C between 4.3 and 6.5 GPa, while nuclear resonant inelastic x-ray scattering spectra and existing equation-of-state data allow the derivation of the compressional wave velocity V_P and shear wave velocity V_S for the high-pressure nonmagnetic phase. The addition of carbon to an iron-nickel alloy brings the density, V_P and V_S closer to seismic observations, supporting the inclusion of carbon as a principal light element in the Earth's inner core.

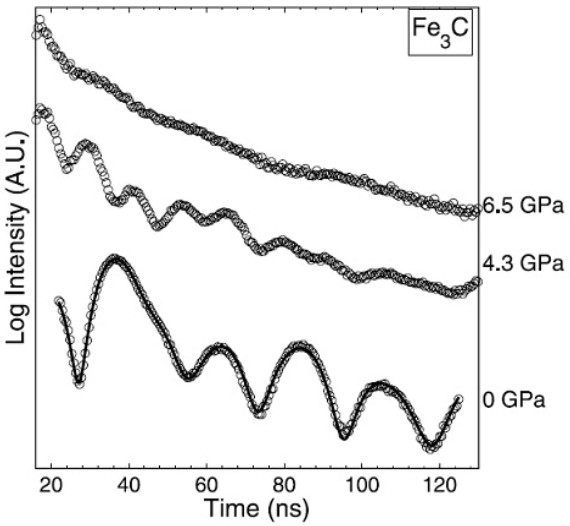


Figure 69. *Synchrotron Mössbauer spectra of Fe_3C (open circles) and fitting results for the 1-bar data (solid curve). The loss of fast oscillations between 4.3 and 6.5 GPa indicates the occurrence of a pressure-induced magnetic transition.*

At 1 bar and 300 K, Fe_3C is ferromagnetic. The SMS spectrum at 1 bar can be fitted assuming one iron site with a hyperfine field of 20.0 (±2.4) T, consistent with the known value of ~20.5 T. A loss of magnetism was observed between 4.3 and 6.5 GPa, as indicated by the disappearance of fast oscillations in the SMS spectra (Fig. 69).

For direct comparison with previous studies, the density of Fe_3C was calculated at an average inner core pressure of 338 GPa and a likely inner core temperature of 5300 K, using the third-order Birch-Murnaghan EoS and estimated thermal expansion coefficients at 338 GPa. The results suggest that Fe_3C is 2.4% lighter than the inner core at these pressure and temperature conditions. The density of Fe at core conditions is 2.9% higher than that of the inner core. Indeed, Fe_3C alone cannot reproduce the inner core density. To account for the density deficit in the inner core, ~3 wt.% carbon (equivalent to about 50% Fe_3C) is needed.

From the NRIXS spectra collected at 300 K and up to 50 GPa, the partial phonon DOS of Fe in Fe_3C was calculated (Fig. 70). At each pressure, the Debye velocity (V_D) of Fe_3C is extracted from a parabolic fitting of the low-energy portion of the PDoS. Known EoS parameters and the values obtained for V_D allow the calculation of compressional velocity V_P and shear wave velocity V_S. V_P and V_S of Fe_3C do not increase smoothly with density. The V_P of the low-pressure magnetic phase plots slightly below the linear trend of the high-pressure non-magnetic phase, whereas the V_S of the magnetic phase plots well below the linear trend of the non-magnetic phase, reflecting a significant increase in shear modulus across the magnetic transition boundary.

<u>Iron in (Mg,Fe)SiO_3 Post-Perovskite at Megabar Pressures</u> – The electronic environments of the iron sites in post-perovskite (PPv) structured (^{57}Fe,Mg)SiO_3 have been measured *in situ* at 1.12 and 1.19 Mbar at room temperature, using ^{57}Fe synchrotron Mössbauer spectroscopy. Evaluation of the time spectra reveals two distinct iron sites, which are well distinguished by their hyperfine fields. This work is a collaboration between HPSynC, Caltech, APS/XOR Sector 3 and Carnegie.

The dominant Fe site in this material is consistent with an Fe^{3+}-like site in a high spin state. The second site is characterized by a small negative isomer shift with respect to alpha-iron and no quadrupole splitting, consistent with a metallic iron phase which has disassociated from the PPv. *In situ* Mössbauer measurements and SEM/EDS analyses of the

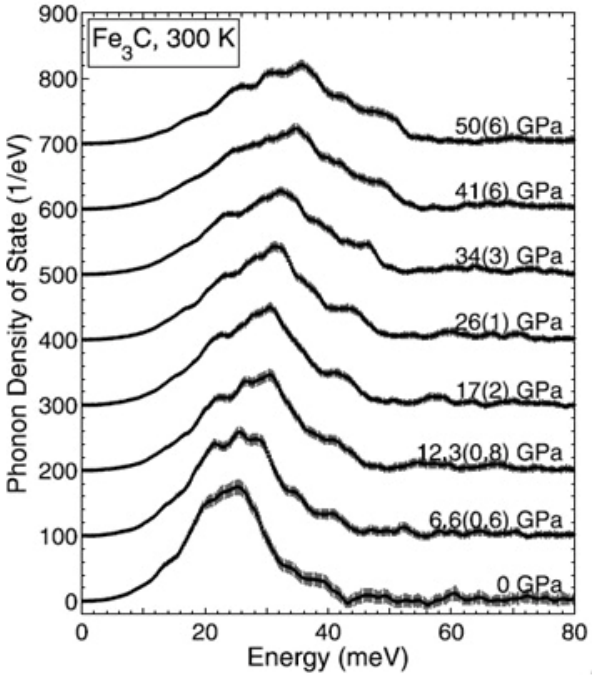


Figure 70. *Fe partial phonon density of states (PDoS) of Fe_3C extracted from NRIXS spectra between 1 bar and 50 GPa, at 300 K. High-pressure spectra are shifted vertically for clarity.*

quenched assemblage strongly support the presence of a metallic iron phase co-existing with a ferric-rich PPv. If such a reaction occurs at the core-mantle-boundary region within Earth, the resulting phase assemblage would have unique physical and chemical properties, consisting primarily of PPv, (Mg,Fe)O, $CaSiO_3$ perovskite, α-PbO_2-type SiO_2, and a metallic iron phase.

Michael Lerche has also assisted users from the **GE Research Laboratory** with the first high-pressure diffraction experiment on the hydrogen storage material $Mg(BH_4)_2$, as well as users from the **University of Notre Dame** in the first high pressure diffraction experiment on FeTPPNO porphyrin, a heme protein. With the IXN group at APS, Lerche has established an ongoing collaboration on the investigation of high-pressure liquid dynamics, and has assisted in instrumental design and setup.

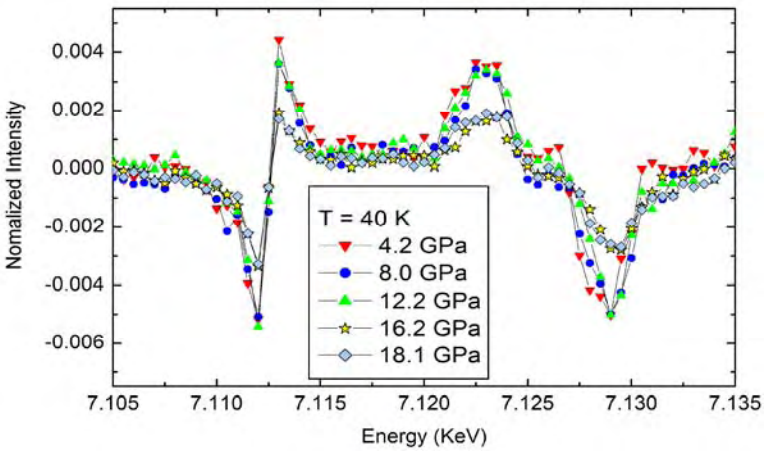


Figure 71. *XMCD measurement. The normalized XMCD of magnetite collected at 40 K from 4.2 GPa to 18.1 GPa.*

Novel Mangetic Transition in Fe_3O_4 – X-ray magnetic circular dichroism (XMCD) has been applied to study the electronic states of mixed valence compound Fe_3O_4 at high pressure. In a collaboration betweeen HPSynC and APS/XOR Sector 4, HPSynC staff scientist **Yang Ding** and co-workers have been working to develop the technique of high pressure XMCD, in which high-brilliance, circularly polarized x-rays are used probe the magnetic state of a material in the DAC. Results of XMCD experiments (Fig. 71) show that between 16 and 18 GPa, the Fe^{2+} in the inverse spinel structure changes from a a high-spin state to an intermediate-spin state, while the two Fe^{3+} in remain in the high-spin state.[94]

Local Structure in Disordered Systems – In the case of crystalline matter, the most powerful probe of structure in disordered systems is diffraction. However, this technique is challenging when applied to non-crystalline matter and becomes more so at high pressure. In particular, traditional DACs are not optimised for such measurements. Building on existing expertise at the APS, **Malcolm Guthrie** of HPSynC has begun to develop and test novel high-pressure anvils for non-crystalline diffraction.

Anvils for X-ray Diffraction – The principle elements of the design are to maximise sample signal while minimising background levels. Such considerations are vital for studies of fundamental systems such as H_2O, the alkali metals, O_2 and CO_2 which are comprised of low-Z elements, which scatter x-rays poorly. Pioneering work at the APS has lead to the development of "perforated" diamond anvils for diffraction measurements. Here, a laser-cut channel running parallel to the incident and transmitted beam direction vastly reduces the dominant background contribution: Compton scattering from the diamonds themselves. HPSynC has begun to continue the evolution of this design, introducing culet indents to maximise sample volume (Fig 72a). Finite element analysis techniques will also assist in optimization of the shape and depth of the perforations.

In addition to linear developments of existing technology, HPSynC has also begun to design micro-toroidal anvils for x-ray diffraction at high pressure (Fig. 72b). The principle of the design (initially developed for conductivity and neutron-scattering measurements) is to use a toroidal groove to support gasket extrusion, permitting a greatly enhanced sample volume, as shown Fig. 72b. The ability to machine features of the relevant (<100μm) size into ultra-hard materials such as diamond

and polycrystalline BN and B_4C is a significant challenge. HPSynC has conducted preliminary tests of laser ablation techniques and is in the initial stages of collaboration with a team at **Western Michigan University** to investigate the possibilities of a laser-assisted machining approach.

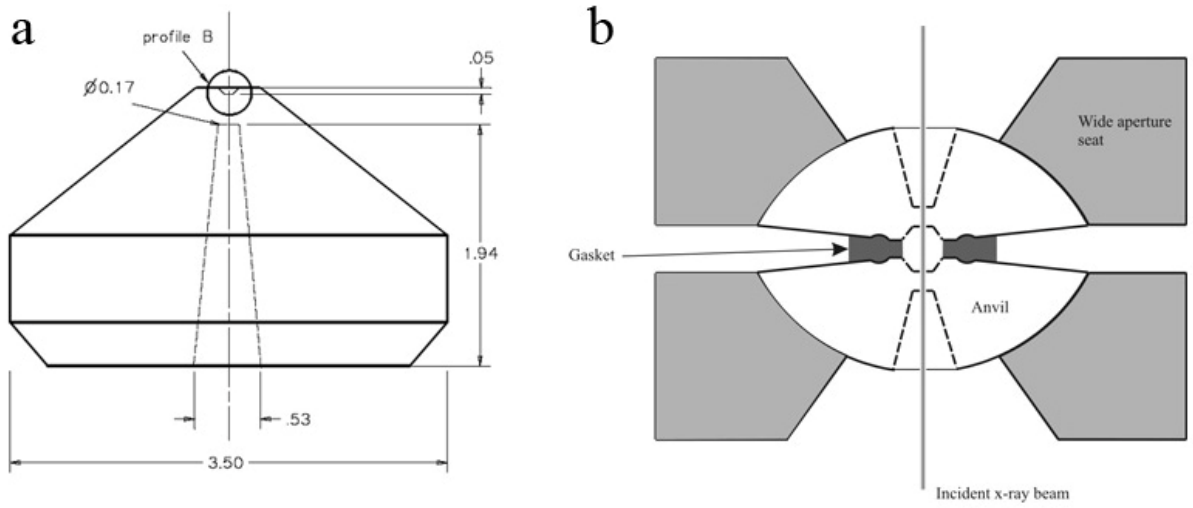


Figure 72. *a) Perforated diamond with culet indent. b) Micro-toroidal anvil with wide-aperture seats used in transmission geometry.*

Complementary Neutron Studies – For diffraction studies of disordered matter, it is vital to develop neutron techniques to complement x-ray capabilities. Not only are neutrons sensitive to the location of H atoms (which are nearly invisible to x-ray techniques), but the point-to-point nature of the inter-nuclear scattering yields access to exceptionally high values of momentum transfer. Furthermore, a complex dependence of scattering strength on atomic number can often yield additional contrast between species not available to x-ray measurements. In collaboration with **Chris Tulk** (**ORNL**), beamline scientist of the SNAP high pressure instrument at the SNS, HPSynC has initiated a project to develop micro-toroidal anvils for neutron diffraction. In contrast to the x-ray case, it is anticipated that these anvils will be used in a 'through gasket' geometry. The new neutron anvils will be coupled with focusing optics with the aim of significantly enhancing the maximum sample pressures available for neutron diffraction from non-crystalline systems.

7.2.2 Anticipated New Facilities

In addition, new extreme conditions facilities are in the planning stages, and these will provide additional platforms for the combination of static and dynamic compression studies, as well as unique opportunities for student training. The **MaRIE** (Matter-Radiation Interactions in Extremes) facility at LANL would be a new signature facility expanding on capabilities already in place at LANSCE. **DC-CAT** (Dynamic Compression-Collaborative Access Team) a dynamic compression sector at the APS, would allow x-ray diffraction and spectroscopic studies of shock compression events. CDAC will continue to play a leading role in coordinating efforts on the part of our academic groups to access anticipated new facilities. The composition of the CDAC program will be evaluated on a consistent basis and designed to take advantage of new opportunities to support DOE/NNSA needs.

7.3 HPCAT Upgrade

7.3.1 Proposed Mid-Scale Upgrade Program

Designed in 1998, the HPCAT sector (Fig. 73) at the Advanced Photon Source has been exceedingly successful in scientific impact, technological advances, and user community development. Within five years of its commissioning, HPCAT has surpassed all high-pressure synchrotron sectors in the world in terms of impact and quantity of scientific publications, and has emerged as one of the most productive sectors at APS. In addition, HPCAT has made significant contributions to DOE/NNSA research programs.

Figure 73. *User area at the HPCAT sector at the Advanced Photon Source.*

Ten years of scientific exploration made possible by HPCAT has revealed clear directions for the next generation of HP-SR advances. Meanwhile, the facility developed a decade ago is aging and facing steep competition from newly established high pressure beamlines in Europe and Asia, many of which have adopted HPCAT innovations. The great demand and shortage of the very limited HPCAT beam time also severely restricts our ability in community outreach. We have reached a critical stage for a major upgrade to stay competitive and remain at the cutting edge. The proposed upgrade will accomplish three goals at the same time: (1) advancing to the next generation of HP-SR science, (2) optimizing the present mainstream high pressure-synchrotron radiation experimentation, and (3) resolving beam time shortage issues. The upgrade will lead to discoveries of novel hydrogen storage materials, superconductors, electronic materials, magnetic materials, superhard materials, optical materials, high-energy-density materials, and in stewardship science - all of which are central to DOE long-range goals; the upgrade will also have far-reaching impact on fundamental research in physics, chemistry, geoscience, and astrophysics.

HPCAT has four simultaneously operating beamlines; two share the same insertion device (16ID) source by splitting the energy, while the other two share the bending magnet (16BM) source by dividing the radiation fan. Five x-ray optics hutches deliver beams into four experimental end stations for a full range of x-ray diffraction and spectroscopy experiments optimized for HP samples. The source of x-rays is a single, old type-A undulator which was designed conservatively before the start of the APS in the early 1990's. Most of the current HPCAT x-ray optics components were designed in 1998 based on the undulator-A parameters with an allowance for twice the power. To stay competitive, they need to be upgraded for the anticipated higher power and brilliance. It is equally important to consider numerous unexpected advances in x-ray optics and detectors during the past decade that can potentially bring a new revolution into the HP-SR program.

Double Undulators and Optimized Beamline Optics – As a part of an overall long-range facility renewal/upgrade plan, the APS has been gradually replacing old single undulators with new long or double undulators at APS-owned sectors, and has called for proposals from CAT-owned (non-APS) sectors that can benefit from new undulators. HPCAT submitted a proposal which was very highly rated by the APS. APS management has promised to replace our archaic single undulator-A with the latest design of double undulators and cover the cost of the new undulators and front-end components inside the shielded wall, on the condition that HPCAT upgrade the beamline x-ray optics to utilize the much more intense source.

We therefore plan to upgrade the 16ID x-ray optics train for higher brilliance to keep HPCAT at the leading-edge of high pressure research and allow us to develop novel high pressure

synchrotron techniques. We have investigated and identified the key components that need to be strengthened, improved, or replaced for robust operation with maximum brilliance. We propose to upgrade the insertion device to have two undulators in canted mode at optimized magnetic periods. The upgrade will free the two 16ID lines for totally independent operations. The upgrade also will involve modification or replacement of high heat-load beamline optics, including front end slits, two thermal apertures, and two monochromators. HPCAT currently has a diamond double-crystal monochromator (DCM) to reflect vertically a monochromatic segment of the x-rays at 16ID into the 16ID-C-D-E stations for HP scattering and spectroscopy studies, and a branching DCM to divert horizontally the transmitted x-ray beam (at a higher energy) to the 16ID-B station for HP XRD studies, thus creating two simultaneously operating ID lines, but the two lines constrain and interfere each others operations. With the proposed two canted beamlines, these two monochromators can be optimized for individual applications and independent operations. The existing water cooled thin diamond crystals in the DCM will be replaced by cryogenically cooled silicon crystals. The branching DCM will be upgraded for a larger energy range and better efficiency with cryogenic cooling. Upgrading these components will immediately benefit the present operation as well as the proposed new high pressure x-ray techniques. Moreover, the x-ray optics upgrade will provide sufficient margin for HPCAT to handle the anticipated higher brilliance due to the source upgrades: first, a local enhancement at 16ID by adding the second undulator in the next couple of years, followed by a facility-wide upgrade of the APS storage ring and lattice in the next five years.

Optimized Submicron Probe – Extreme conditions are achieved at the cost of sample volume. It took three decades to reduce the x-ray beam size from 50 μm to the current standard of 5 μm in high pressure research. Yet, the impact of this one order of magnitude reduction is tremendously significant. While beam sizes of a few tens of nm have been reached in specialized beamlines, a beam size of 5-10 μm is still typical in all state-of-the-art high pressure synchrotron beamlines in the world. Sub-micron probes will discriminate the weak high pressure sample signals from the very strong background due to the pressure chamber materials. This should be the most important consideration for high pressure experiments, yet it is least explored and developed. Reducing the incident beam size from 5 to 0.5 μm and depth probe from 300 to 3 μm will undoubtedly revolutionize HP synchrotron science in general, and will increase the counting efficiency by a factor of 100 since S/N only improves with the square root of the counting time.

Improving Depth Resolution – While the spatial resolution in a plane perpendicular to x-ray beam has been effectively improved by reducing the probe size, the spatial depth resolution along the x-ray beam remains an under-developed area. Yet, this is particularly important to high pressure research because HP samples are always surrounded by chamber materials which often cause strong background signals. Improving depth resolution not only will greatly increase the counting efficiency due to the improvement of S/N ratio, but will make a number of cutting edge projects feasible. The conventional pinhole collimator is often used on the detection side in high pressure studies, which typically provides a depth resolution of 300-500 μm. We propose to use the newly developed x-ray microscope for collecting the scattered signal. The use of an x-ray microscope on the detection side will improve the depth resolution by at least an order of magnitude, and will significantly reduce the background from surrounding materials and enhance the detection sensitivity by two orders of magnitude. The depth resolution gain through the use of an x-ray microscope is particularly beneficial in high pressure IXS and high pressure emission experiments.

High Pressure Inelastic Scattering at 70-200 meV Resolution – Pressure has drastic effects on the energy and dispersion of electronic bands and is an ideal tuning variable for directing and controlling matter at the electronic level. The IXS technique developed at HPCAT has an energy resolution of 0.7-1 eV for investigating fundamental properties of the electron gas, chemical bonding, and high-energy electronic excitations in energy and momentum space. However, many interesting properties occur for electronic excitations within a small fraction of an eV to several eV of the Fermi surface. There is a great need for improving the energy resolution in IXS to obtain more detailed information on electronic excitations and plasmons, and finer features in x-ray Raman spectra. Count rates become a challenging issue because higher resolution means a smaller slice of both the

incident spectrum and the scattered photons, in addition to the small inelastic scattering cross-section. With the source and optics upgrade, the increase in brilliance and efficiency will allow for the development of high resolution IXS in the 100 meV region at HPCAT. We propose to construct a set of medium resolution (MR) monochromators with 70 meV to 200 meV resolution and an analyzer array matching (and slightly higher than) the energy resolution of the monochromator. We propose to establish a KB mirror system that will collect most of the undulator beam and focus it down to 5 μm. Flat-pixel analyzers, together with the newly developed Pilatus area detector, will be used for high energy resolution, low background, and high efficiency MR-IXS measurements. Particular effort will be devoted to minimizing scattered signals from surrounding materials (anvils and gaskets), by using a confocal x-ray microscope for background rejection.

7.3.2 Supplementary Material Available

For a complete description and details of the HPCAT proposed upgrade, please go to http://cdac.gl.ciw.edu/images/stories/HPCAT%20Overview.pdf.

APPENDIX I: CDAC Publications and Presentations for Year 5*

A. CDAC Publications

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APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for Year 5

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. Asterisks denote work done with beam time available through CDAC.

User Name	Affiliations	Project	Dates
W. Yang Olga Shebanova	HPCAT	Commissioning of monochromator and large KB mirror. High energy diffraction of amorphous materials	October 2-12, 2007
N. Velisavljevic	LLNL	Emission, zirconium	October 5-9, 2007
T. Komabayashi Angele Ricolleau	Carnegie	Phase relations and *P-V-T* EOS of iron	October 7-9, 2007
M. Somayazulu	Carnegie	Single crystal EDXD on Xe/H and N/H	October 10-11, 2007
H. Cynn Z. Jenei	LLNL	Laser heating of simple metals under pressure to measure plastic deformation	October 10-12, 2007
H. K. Mao Y. Ding	Carnegie	Emission, Fe and Mn	October 10-15, 2007
F. Peng	HPSynC	Radial diffraction of powdered Möissanite (SiC)	October 11-15, 2007
Melike Abliz	HPSynC	Compression of Fe_2P	October 12-13, 2007
J. McClure	University of Nevada – Las Vegas	High pressure phase transitions in lanthanide sesquioxides	October 12-14, 2007
M. Somayazulu C. S. Zha	Carnegie	EOS study of Ni under multple megabar	October 14, 2007
H. K. Mao J. Shu T. Yamanaka W. Mao	Carnegie Stanford University	X-ray diffraction of $CaMn_2O_4$ and Mn_2O_3 under high pressure	October 14-16, 2007
O. Tschauner J. McClure E. Romano	University of Nevada – Las Vegas	High-resolution diffraction scanning with the 2theta huber circle and the EDXE detector as point detector	October 14-22, 2007
H. Liu Luhong Wang	Harbin Institute of Technology	Pressure-induced phase transition of ZnO	October 15-16, 2007
T. Yamanaka	Carnegie	Emission, Mn	October 17-19, 2007
Zhu Mao T. Duffy F. Jiang Susana Dorfman S. Shieh	Princeton University University of Western Ontario	X-ray diffraction study of $Gd_3Ga_5O_{12}$ and $(Fe,Mg)_3(Al, Si)_5O_{12}$ under megbar pressures and high temperature by laser heating	October 17-20, 2007
S. Maglio Kelly Robertson A. Simon	University of Nevada – Las Vegas	Fluorescence measuremnts of La_2O_3, Ce_2O_3, Nd_2O_3 in 10000 ppm solution and insitu dissolution of collomite crystals	October 18-21, 2007
R. Kumar	University of Nevada – Las Vegas	Emission, Yb non resonant	October 19-22, 2007
Kanani Lee Y. Al Khatabeh	New Mexico State University	High-pressure investigation of TiO_2 and pyroxenites using laser heating of DAC	October 20-22, 2007

M Lerche Y. Gao	HPSynC GE Global Research Center	High Pressure Studies on Hydrogen Storage in $Mg(BH4)_2$	October 24-25, 2007
M. Lipp	LLNL	Emission, cerium	October 24-26, 2007
C. Gao W. Yang	Texas Tech University HPCAT	Effect of electrical field on the pressure induced phase transition of dielectric powder	October 24-27, 2007
L. Miyagi	University of California – Berkeley	Texture development in perovskite at conditions in the Earth's lower mantle	October 24-27, 2007
D. Ikuta H. P. Liermann P. Dera	HPCAT GSECARS	Single crystal thin sections project	October 25-26, 2007
V. Iota	LLNL	Emission, actinide, and gallium	October 26-28, 2007
M. Lipp D. Jackson	LLNL	Metling of cerium	October 26-30, 2007
Q. Zeng	HPSynC	EDXD study of CeAl under high pressure in DAC	October 28-29, 2007
A. Goncharov A. Brieva	Carnegie Newcastle University	X-ray diffraction study of Au nitride, Ir nitride, Pt nitride, and CeSe	October 28-30, 2007
Q. Zeng W. Yang	HPSynC HPCAT	Amorphous with scanning angle EDXD	October 31-November 1, 2007
H. K. Mao C. S. Zha W. Mao Yue Meng	Carnegie Stanford University HPCAT	High *P-T* phase transitions and EOS of FeO	October 31-November 2, 2007
V. Struzhkin	Carnegie	Emission, Mn and Fe	November 1-7, 2007
D. Ikuta H. P. Liermann P. Dera	HPCAT GSECARS	Single crystal thin sections project	November 2-4, 2007
M. Somayazulu	Carnegie	*P-V-T* EOS of B_4C and x-ray diffraction studies of $MoF+H_2$, MoF-W, and CoF_{102}	November 2-4, 2007
M. Pravica E. D. Romano S. Tkachev	University of Nevada – Las Vegas	Studies of energetic materials and hydrocarbons subjected to extreme conditions	November 2-5, 2007
L. Wang	HPSynC	Radial diffraction of carbon nano rods	November 4-5, 2007
Svetlana Kharlamova V. Sruzhkin S. Sinogeikin	Advanced Photon Source Carnegie HPCAT	Structural transitions in $GdFe_3(BO_3)_4$ at high pressures and low temperatures	November 5-8, 2007
V. Struzhkin	Carnegie	RIXS, Ge	November 7-9, 2007
P. Dera Barbara Lavina Lauren Borkowski H. P. Liermann W. Yang	GSECARS University of Nevada – Las Vegas HPCAT	Calibration of the single crystal energy dispersive x-ray diffraction technique	November 7-9, 2007
S. Jacobsen C. Holt C. Ebeling Kimberly Adams Emily Martin	Northwestern University	Compressibility of mantle oxide materials	November 7-9, 2007
H. K. Mao Yue Meng	Carnegie HPCAT	High *P-T* phase transitions and EOS of FeO	November 9-10, 2007

R. Kumar	University of Nevada – Las Vegas	Emission of Yb, resonant L_3	November 9-12m 2007
G. Chesnut	LANL	Radial diffraction of ^{239}Pu	November 9-12, 2007
Lauren Borkowski Barbara Lavina P. Dera H. P. Liermann	University of Nevada – Las Vegas GSECARS HPCAT	Determination of the crystal structure of phases II' and IV' of $CuGeO_3$	November 10-11, 2007
H. Cynn H. P. Liermann	LLNL HPCAT	Simultaneous high *P-T* study on the EOS of metals	November 14-16, 2007
M. Ahart	Carnegie	Pressure induced ferroelectric to relaxor crossover in $Pb(Sc_{0.5}Nb_{0.5})O_3$ (III)	November 15-16, 2007
H. Cynn W. Evans B. Baer Chantel Aracne	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	November 16-19, 2007
Jennifer Ceizak H. P. Liermann	Carnegie/ANL HPCAT	EDXD single crystal structure on N_2/H_2 mixtures	November 17-20, 2007
W. Yang	HPCAT	Angle-dispersive scattering on amorphous structure with nulti-energies in DAC	November 18-24, 2007
M. Jacobsen J. Baker	University of Nevada – Las Vegas	High pressure studies of $CaRuO_3$, Sb_2Te_3	November 19-21, 2007
S. Tkachev	University of Nevada – Las Vegas	Single crystal studies of energetic materials at high pressure	November 21-15, 2007
H. P. Liermann	HPCAT	EDXD single crystal structure determination on marokite with Al as a pressure medium	November 21-26, 2007
M. Ahart	Carnegie	Pressure induced ferroelectric to relaxor crossover in $Pb(Sc_{0.5}Nb_{0.5})O_3$ (III)	November 24-28, 2007
J. Howard	University of Nevada – Las Vegas	Single crystal x-ray diffraction of Fe_3P (iron phosphide) under pressure	November 25-27, 2007
O. Tschauner	University of Nevada – Las Vegas	X-ray diffraction, powder and single crystal	November 28, 2007
S. Maglio A. Bell A. Simon	University of Nevada – Las Vegas	Quantifying element mass transfer at subduction zone conditions by using the hydrothermal DAC and *in-situ* x-ray fluorescence	November 28-30, 2007
H. K. Mao	Carnegie	backscattering setup, sodium, water exposure	November 28-December 2, 2007
R. Kumar	University of Nevada – Las Vegas	High pressure diffraction studies on $YbFe_2Ge_2$, $CdAl_2Se_4$, B_4C compounds	November 29, 2007
R. Kumar H. P. Liermann	University of Nevada – Las Vegas HPCAT	Low temperature x-ray diffraction studies on $CeCu_2Si_2$ and $CeCu_2 (SiGe)_2$ compounds at high pressures	November 30-December 1, 2007
W. Yang	HPCAT	X-ray absorption spectroscopy study with a Laue diffraction method	November 30-December 3, 2007
H. Cynn W. Evans B. Baer Chantel Aracne	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	November 30-December 3, 2007
H. P. Liermann	HPCAT	High *P-T* EOS of fcc iron in the resistive heated membrane DAC	December 2-3, 2007

M. Pravica	University of Nevada – Las Vegas	Backscattering setup, acetone and cyclo-octo-tetraene, carbon x-ray Raman	December 2-4, 2007
T. Jenkins	NIST	High pressure/low temperature powder diffraction on hydrogen clathrate	December 3-4, 2007
Y. Wang J. Zhang	LANL	The phase transition, bulk modulus, and strengths of Si, Ge nanowires under high pressure	December 5-6, 2007
F. Peng	HPSynC	The researching of SiC by radial x-ray diffraction under nonhydrostatic compression	December 5-7, 2007
L. Wang	HPCAT	Phase transition of YAG:Ce under high pressure	December 5-9, 2007
A. Goncharov L. Lundegaard E. Gregoryanz	Carnegie University of Endinburgh	Structural properties of H_2 up to 200 GPa by single crystal x-ray diffraction	December 6-8, 2007
S. Gramsch	Carnegie	X-ray Raman, B_6O	December 6-9, 2007
M. Pravica S. Tkachev	University of Nevada – Las Vegas	X-ray diffraction studies of energetic materials	December 7-8, 2007
H. P. Liermann	HPCAT	Radial diffration of Nb and Ta in amorphous boron gaskets	December 8-9, 2007
L. Wang Q. Zheng F. Pang	HPSynC	Phase transition of Y_2O_3 under high pressure	December 9-10, 2007
R. Kumar	University of Nevada – Las Vegas	X-ray Raman, boron	December 9-14, 2007
L. Sun	Chinese Academy of Science	Crystal structure studies of solid methane (CH_4) at megabar pressure	December 10-11, 2007
H. Cynn W. Yang	LLNL HPCAT	Microstructure analysis using a Laue method at high pressure, setup and test	December 10-15, 2007
W. Evans M. Lipp H. Rhee	LLNL	Ambient and high-temperature crystal structures, phase transitions, and EOS of materials at high pressures	December 10-15, 2007
E. Soignard	Arizona State University	High pressure phase transformation in BeF_2 and BeH_2	December 12-13, 2007
L. Stevens N. Velisavljevic	LANL	Compressive properties of high explosives and metals at high pressures for EOS determination	December 14-15, 2007
L. Sun	Chinese Academy of Science	Crystal structure studies of solid methane (CH_4) at megabar pressure	December 16, 2007
L. Wang	HPSynC	Phase transition of Y_2O_3 under high pressure	December 16-18, 2007
T. Yamanaka T. Kuribayashi P. Dera W. Yang	Carnegie GSECARS HPCAT	Single crystal determination of $FeCr_2O_4$ under high pressure in DACs	December 16-18, 2008
H. K. Mao J. Shu L. Wang W. Zeng Y. Ding Melike Abliz	Carnegie HPSynC	Various high pressure diffraction experiments	December 16-19, 2007
M. Klepeis	LLNL	X-ray Raman, nitrogen	December 17-19, 2007
S. Jacobsen	Northwestern University	EOS of hydrous wadsleyite	February 2-3, 2008

M. Pravica S. Tkachev E. Romano	University of Nevada – Las Vegas	X-ray diffraction studies of organic materials	February 2-4, 2008
O. Tschauner S. Tkachev E. Romano	University of Nevada – Las Vegas	High resolution powder diffraction	February 2-10, 2008
Amy Lazicki	Carnegie	Structural investigation of potential high pressure superconducting phase of LiB	February 3-4, 2008
R. Greene C. Rotundu	University of Maryland	Very high pressure study of $Pr_{1.85}Ce_{0.15}CuO_{4-\delta}$	February 4-5, 2008
Amy Lazicki	Carnegie	Single crystal of Li	February 4-5, 2008
Q. Zeng	HPSynC	High pressure induced phase transition in metallic glasses	February 6-9, 2008
O. Tschauner O. Grubor-Urosevic S. Tkachev P. Dera	University of Nevada – Las Vegas GSECARS	Single crystal diffraction in DAC	February 6-10, 2008
H. Cynn W. Evans Y. Xiao	LLNL	NFS studies of Fe compounds	February 6-11, 2008
Melike Abliz	HPSynC	Phase transition of $YbIr_2Zn_2O$ alloy under high pressure	February 9-11, 2008
T. Yamanaka T. Kuribayashi	Carnegie	Structure determination of chromite	February 10-11, 2008
M. Somayazulu C. S. Zha	Carnegie	Single crystal diffraction of Ice VII	February 10-11, 2008
R. Kumar	University of Nevada – Las Vegas	Low temperature x-ray diffraction studies on heavy fermion compounds $CeCoIn_5$ and $CeIrIn_5$	February 13-16, 2008
Elizabeth Tanis D. Sauter	University of Nevada – Las Vegas	NRIXS and NFS on alpha-Fe alloys	February 13-17, 2008
M. Lipp	LLNL	EOS and phase transition of Ce	February 13-17, 2008
W. Yang	HPCAT	Dispersive EXAFS measurement of metal alloys	February 13-22, 2008
H. Liu Luhong Wang	Harbin Institute of Technology	Pressure induced phase transition on ZnO	February 16-18, 2008
Svetlana Karlamova	Carnegie	Effects of broadening of spin cross-over tuned by pressure in transition metal oxides	February 17-22, 2008
H. P. Liermann	HPCAT	Radial diffraction of Fe and MgO	February 17-23, 2008
C. Zeng F. Peng L. Wang	HPSynC	High pressure behavior of metallic glass in He pressure medium	February 18-19, 2008
H. K. Mao J. Shu F. Peng L. Wang	Carnegie HPSynC	Powder diffraction of Fe, Pt and W at pressure over 300 GPa	February 20-21, 2008
H. Cynn K. Visbeck B. Baer	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	February 22-25, 2008
M. Lucas	California Institue of Technology	Study of ^{57}Fe PDOS as a function of alloying and temperature	February 22-26, 2008
M. Pravica S. Tkachev E. Romano	University of Nevada – Las Vegas	Studies of cyclooctatetraene at high pressures using energy-dispersive x-ray diffraction	February 22-26, 2008

M. Lerche	HPSynC	Strucutre determination of $Mg(BH_4)_2$	February 23-25, 2008
Olga Shebanova	HPCAT	Alkali metal-transition metal alloys	February 25-26, 2008
Dana Dattlebaum L. Stevens N. Velisavljevic	LANL	High pressure behavior of explosive molecules toward understanding hot spot related sensitization	February 25-28, 2008
L. Wang	HPSynC	Single crystal diffraction of C_{60} nanorod	February 27-28, 2008
P. Dera H. P. Liermann	GSECARS HPCAT	Single crystal project development	February 27-29, 2008
Dana Dattlebaum L. Stevens N. Velisavljevic	LANL	High pressure x-ray diffraction of metals and explosives	February 28-29, 2008
D. Ikuta	HPCAT	Structure determination of Pb feldspar	February 29-March 1, 2008
J. Zhang Z. Lin	LANL	Phase transition, bulk modulus, and strengths of Si and Ge nanowires under high pressure	March 3-6, 2008
F. Peng	HPSynC	Stress and strain of SiC	March 1-4, 2008
V. Struzhkin	Carnegie	XES studies of Co compounds under high pressure	March 1-6, 2008
P. Dera	GSECARS	Single crystal project development	March 3-7, 2008
E. Gregoryanz C. Guillaume J. Proctor	University of Edinburgh	EOS and phase transitions in Li metal at cryogenic temperatures and high pressures	March 6-8, 2008
J. F. Lin	LLNL	Spin states of Fe in silicate perovskites in the Earth's lower mantle	March 6-9, 2008
D. Ikuta	HPCAT	Structure determination of Pb feldspar	March 7-10, 2008
Kristina Lipinska-Kalita Patricia Kalita	UNLV	High-pressure x-ray diffraction of a ceramic	March 8-9, 2008
M. Pravica S. Tkachev E. Romano	UNLV	High pressure studies of cyclooctatetraene	March 8-10, 2008
S. Gramsch	Carnegie	XES of $FeAlO_3$ at high pressure	March 9-10, 2008
C. Zeng F. Peng L. Wang	HPSynC	High pressure behavior of CeAl metallic glasses	March 9-10, 2008
W. Yang	HPCAT	Buffer for dispersive EXAFS measurement of metal alloys	March 12-13, 2008
T. Yamanaka Y. Xiao	Carnegie LLNL	X-ray Emission spectroscopy of $CaMn_2O_4$, $CaFe_2O_4$ and $CaFe_2O_4$ under high pressure	March 12-15, 2008
T. Yamanaka T. Kuribayashi	Carnegie	Single crystal of Ice and oxides	March 12-16, 2008
W. Yang	HPCAT	Dispersive EXAFS measurement of metal alloys	March 13-16, 2008
A. Goncharov R. Thoguluva K. Litasov	Carnegie	High-pressure study of oxygen, post-perovskite, and sodium azide	March 14-16, 2008
H. K. Mao Y. Ziao W. Mao	Carnegie LLNL Stanford University	XAS and XES of Fe in Fe_2O_3, Fe_3O_4, and $FeGeO_3$ at high pressure	March 15-31, 2008

T. Komabayashi Y. Fei K. Litasov	Carnegie	Phase relation and *P-V-T* EOS of iron	March 16-18, 2008
G. Chesnut	LANL	High-pressure studies of metals	March 16-18, 2008
H. Cynn	LLNL	Dispersive EXAFS measurement of metal alloys	March 16-21, 2008
N. Velisavljevic L. Stevens	LANL	High pressure studies of metals and explosives	March 19-20, 2008
Yue Meng	HPCAT	Wavelength change and beamline issue resolution	March 19-21, 2008
Dana Dattlebaum	LANL	High-pressure study of explosive molecules	March 20-22, 2008
W. Yang	HPCAT	Buffer for dispersive EXAFS measurement of metal alloys	March 21-22, 2008
H. K. Mao L. Zhang	Carnegie	High-pressure melting of (Mg, Fe)O	March 21-24, 2008
G. Amulele	Stanford University	Compression of Fe_2O_3	March 21-24, 2008
X. J. Chen	Carnegie	High-pressure study of GeH_4	March 21-24, 2008
O. Tschauner	University of Nevada – Las Vegas	Micro Laue diffraction on thin sections	March 22-24, 2008
O. Tschauner S. Tkachev	University of Nevada – Las Vegas	Computon scattering	March 22-27, 2008
C. S. Zha T. Kuribayazhi	Carnegie	X-ray diffraction determination for single crystal ice VII	March 26-27, 2008
O. Tschauner O. Grubor-Urosevic	University of Nevada – Las Vegas	X-ray diffraction	March 27-28, 2008
W. Yang	HPCAT	EOS and phase transition of Ce	March 27-29, 2008
M. Somayazulu	Carnegie	High-pressure studies of hydrogen storage materials, ammonia, and B_4C	March 28-30, 2008
H. P. Liermann H. Yang	HPCAT University of Arizona	Single crystal compression experiments on pyroxenes with six-coordinated silicon	March 29-31, 2008
H. Cynn Z. Nie	LLNL Northern Illinois University	EOS of Nb	March 29-31, 2008
Barbara Lavina	University of Nevada – Las Vegas	High-pressure investigation of single-crystal hercynite	March 31-April 3, 2008
H. K. Mao L. Zhang	Carnegie	High-pressure melting of (Mg, Fe)O	March 31-April 4, 2008
R. Kumar	University of Nevada – Las Vegas	Resonant x-ray emission studies on YbTe, YbB_6 and $YbMg_2Ge_2$ at high pressures	March 31-April 5, 2008
Kristina Lipinska-Kalita Patricia Kalita	University of Nevada – Las Vegas	High-pressure study of ion-conductive ceramics	April 2-4, 2008
Michelle Weinberger	Carnegie	*P-V-T* behavior of MOF-120 and hydrogen	April 2-4, 2008
W. Yang	HPCAT	Amorphous structure study in DAC	April 2-8, 2008
R. Chellappa J. Fallas	Carnegie University of Nevada – Reno	High pressure studies on hydrogen and energy storage materials	April 4-10, 2008
Y. Ma E. Selvi	Texas Tech University	High *P-T* x-ray diffraction of $PbMoO_4$	April 5-8, 2008
N. Velisavljevic	LLNL	High pressure inelastic x-ray scattering on Zr metal	April 5-10, 2008

J. Shu	Carnegie	High-pressure study of $FeCr_2O_4$	April 9-11, 2008
L. Miyagi	University of California – Berkeley	Texture development in perovskite, relevant to deformation conditions in the Earth	April 9-12, 2008
Kimberly Tait H. P. Liermann R. Downs	Royal Ontario Museum HPCAT University of Arizona	Single crystal high-pressure diffraction of hafnon	April 10-13, 2008
V. Iota M. Lipp	LLNL	XES of lanthanide in a DAC	April 10-15, 2008
M. Ahart	Carnegie	Phase transition of PMN-PT	April 11-15, 2008
T. Duffy Zhu Mao Susannah Dorfman Lisha Xie	Princeton University	Continuing study of the high-pressure phases of oxide garnet	April 12-15, 2008
W. Yang	HPCAT	EXAFS scan	April 16-19, 2008
T. Yamanaka J. Shu	Carnegie	Study on Ice-VII, chromite and $PbTiO_3$	April 19-22, 2008
K. Litasov	Carnegie	Melting vs. decarbonation of magnesite under lower mantle conditions	April 20-22, 2008
W. Yang	HPCAT	Liquid structure of Cs under pressure in DAC	April 21-24, 2008
Kristina Lipinska-Kalita Patricia Kalita D. Kurzydlovski	University of Nevada – Las Vegas Warsaw University	Study of ion-conductive ceramics	April 22-23, 2008
M. Somayazulu	Carnegie	EOS of B_4C	April 22-23, 2008
Olga Shebanova	HPCAT	Alkali metal-transition metal alloys	April 23-24, 2008
F. Peng	HPSynC	Radial-diffraction	June 1-13, 2008
O. Tschauner	University of Nevada – Las Vegas	Compton scanning on amorphous gadolinite	July 11-14, 2008
H. Cynn	LLNL	High temperature diffraction	June 13-17, 2008
C. Zeng L. Wang	HPSynC	Phase transitions in crystalline and amorphous phases of CeAl	June 14-16, 2008
Jie Li Y. Xiao L. Gao B. Chen	University of Illinois	Electronic structure of iron in $(Mg,Fe)SiO_3$ perovskite and post-perovskite up to Mbar pressure	June 14-17, 2008
M. Ahart	Carnegie	Pressure induced phase transition in PMN-PT II	June 14-17, 2008
M. Somayazulu P. Lazer	Carnegie Uppsala University	B_4C	June 16-19, 2008
J. Z. Jiang	Zhejiang University	Phase transition in metallic glasses CeAl	June 18-20, 2008
Elizabeth Tanis J. Howard Samantha Combs	University of Nevada – Las Vegas	NRIXS on alpha-Fe solid solution, NFS on Al silicate and Fe_3P	June 18-21, 2008
P. E. Janolin	Carnegie	Compression and phase transition in nano - $PbTiO_3$	June 19-20, 2008

J. H. Klepis Z. Jenei	LLNL	Plastic deformation of transition metals using a high resolution x-ray diffraction under uniaxial compression and investigation on EOS of vanadium at high temperature (~150 and ~300 oC)	June 20-24, 2008
M. Pravica S. Tkachev	UNLV	Hydrocarbons at high pressure	June 20-24, 2008
Lyci George V. Drozd	Florida International University	High-pressure study of $Mg(AlH_4)_2$, $Mg(BH_4)_2$, Mg_2FeH_6	June 21-22, 2008
M. Winterrose I. Halevy Lisa Mauger J. Munoz H. Tan J. Raney	California Institute of Technology	Pressure-induced magnetic transitions and invar behavior in $L1_2$ alloys	June 21-27, 2008
Amy Lazicki	Carnegie	XRD of LiB at high pressure, and Li at high *P-T*	June 22-23, 2008
L. C. Ming X. R. Liu P. Zinin	University of Hawai'i	High *P-T* synthesis of diamond from amorphous BC; high-pressure phases of C_3N_4	June 23-26, 2008
L. Wang	HPSynC	Powder diffraction of Y_2O_3	June 25-26, 2008
W. Yang	HPSynC	Fe site occupation study on $(Mg_{1-x},Fe_x)SiO_3$ perovskite structure	June 26-27, 2008
M. Lang	University of Michigan	Material modifications under high pressure	June 26-27, 2008
Q. Mei G. Shen	HPCAT	Wavelength change and beamline issue resolution	June 26-27, 2008
W. Yang Y. Xiao	HPSynC HPCAT	Nuclear forward scattering study of ^{57}Fe in $(Mg_{1-x},Fe_x)SiO_3$ perovskite	June 27-29, 2008
L. Stevens D. Robins	LANL	High-pressure XRD study of Hf, ,3'-diamino-4,4'-azoxyfurazan	June 27-28, 2008
F. Peng	HPSynC	Radial diffraction	June 27-29, 2008
Z. Qiaoshi	Zhejiang University	Mechanism of phase transitions in metallic glasses	June 27-29, 2008
W. Yang	HPSynC	Fe site occupation study on $(Mg_{1-x},Fe_x)SiO_3$ perovskite structure	June 29-July 1, 2008
Y. Xiao	HPCAT	Nuclear forward scattering study of prussian blue	June 29-July 1, 2008
O. Tschauner O. Grubor-Urosevic S. Tkachev	University of Nevada – Las Vegas	Single crystal white beam diffraction	June 30-July, 3
Melike Abliz	HPSynC	High pressure x-ray diffraction experiment on Nb_3Se_4 and Nb_3S_4	July 1-3, 2008
S. Tkachev B. Yulga E. Romano	University of Nevada – Las Vegas	X-ray diffraction studies of hydrocarbons at high pressure	July 1-3, 2008
W. Yang	HPSynC	Adjustment of the large K-B mirror and beamline optimization of 16BMD station	July 7-8, 2008
T. Yamanaka	Carnegie	Single crystal diffraction studies of $FeCr_2O_4$ and $PbTiO_3$ using diamond anvil	July 8-11, 2008
H. Cynn	LLNL	Grain boundary mapping in DAC	July 9-14, 2008
H. P. Liermann	HPCAT	Radial diffraction on TaC at simultaneous high *P-T* in the resistive heated DAC	July 11-13, 2008

H. Cynn M. Lipp B. Baer Chantel Aracne W. Evans	LLNL	f-metal behavior at high temperatures and high pressures using external heating	July 11-14, 2008
M. Lipp	LLNL	X-ray Raman spectroscopy of sodium azide in a DAC	July 11-18, 2008
F. Pang	HPSynC	The research on TiN stress and elasticity under high pressure	July 13-14, 2008
L. Wang	HPSynC	High-pressure x-ray diffraction studies of Y_2O_3	July 14-15, 2008
W. Yang	HPCAT	Development of x-ray absorption method	July 14-24, 2008
W. Yang	HPCAT	Microdiffraction of Ge under pressure in a DAC	July 16-17, 2008
E. Gregoryanz	University of Edinburgh	High-pressure structures of lithium	July 16-18, 2008
D. Ikuta	HPCAT	Application of crystal structure analysis to rock thin section	July 17-18, 2008
C. Zeng	HPSynC	The phase transition in metallic glass CeAl	July 18-19, 2008
O. Tschauner	University of Nevada – Las Vegas	Single crystal diffraction on energetic materials	July 18-20, 2008
M. Pravica S. Tkachev A. Johnson W. Pravica	University of Nevada – Las Vegas	X-ray Raman experiments on nitrogen-containing compounds at high pressures	July 18-20, 2008
S. Maglio	University of Nevada – Las Vegas	An *in situ* study of basalt stability and phase boundaries	July 19-21, 2008
M. Pravica	University of Nevada – Las Vegas	Studies of single crystalline cyclopentane at high pressure	July 20-22, 2008
R. Kumar	University of Nevada – Las Vegas	X-ray Raman scattering studies on B4C , alkali borides and ammonia borane at high pressures	July 20-24, 2008
O. Tschauner O. Grubor-Urosevic S. Tkachev Allison Savage	University of Nevada – Las Vegas University of Iowa	Single crystal diffraction of $(Na,Ca)_2Nb_2O_6(OH,F)$, $Mg_2Al(SiAl)O_5(OH)_4$, PETN, RDX, TATB	July 21-24, 2008
Kanani Lee	New Mexico State University	High-pressure investigation of transition-metal compounds	July 23-25, 2008
S. Gramsch	Carnegie	X-ray Raman spectrum of B_6O	July 24-26, 2008
H. P. Liermann	HPCAT	Single crystal development	July 24-31, 2008
G. Chesnut D. Lovato	LANL	High-pressure x-ray diffraction of metals (lacthanides and actinides)	July 25-26, 2008
M. Lerche	HPSynC	Structural phase transition in the hydrogen storage material $Mg(BH_4)_2$	July 25-26, 2008
Q. Mei G. Shen	HPCAT	Structural changes of SiO_2 glass at high pressure	July 26-27, 2008
G. Chesnut	LANL	High-pressure x-ray diffraction of metals	July 26-28, 2008
H. K. Mao	Carnegie	Compression of electron gas in sodium	July 26-August 9, 2008
C. Zeng	HPSynC	The phase transition in metallic glass CeAl	July 27, 2008
W. Yang	HPCAT	Microdiffraction of metals under pressure in DAC	July 27-28, 2008

R. Kumar	UNLV	High-pressure x-ray diffraction studies on silicides and borides	July 30-August 1, 2008
Kimberly Tait	Royal Ontario Museum	Single crystal study of hafnon	July 31-August 5, 2008
Jennifer Ciezak	Army Research Laboratory/Carnegie	Single crystal study of N_2/H_2	July 5-8, 2008
H. K. Mao J. Shu Q. Zeng Y. Meng W. Mao	Carnegie HPSynC HPCAT Stanford University	$(Mg, Fe_{0.2})SiO_3$ and $(Mg, Fe_{0.3})SiO_3$ post-perovskite phase, >130 GPa, 2200 K	August 1-4, 2008
H. Liu	Harbin Institute of Technology	$Li_{1.5}Fe$ compression	August 1-4, 2008
W. Evans H. Cynn	LLNL	X-ray diffraction studies at high- *P-T* EOS of simple materials	August 2-4, 2008
W. evans H. Cynn Kerri Blobaum J. Jeffries	LLNL	Thermally-induced structural transitions in plutonium alloys	August 4-6, 2008
S. Maglio	University of Nevada – Las Vegas	Quantifying element mass transfer of REE-monazite at subduction zone conditions using the hydrothermal DAC and *in situ* x-ray fluorescence	August 4-6, 2008
Y. C. Tseng D. Haskel N. Souza Neto	Northwestern University Advanced Photon Source	Origin of suppressed ferromagnetism at low Si-doping in giant magnetocaloric materials $Gd_5(Si_xGe_{1-x})_4$	August 4-7, 2008
Svetlana Kharlamova	Carnegie	X-ray diffraction of NdFeAs compound at high pressures	August 6-7, 2008
P. E. Janolin	Carnegie	Pressure on ferroelectric nanopowders	August 7-8, 2008
Olga Shebanova	HPCAT	X-ray powder diffraction of CsPt in DAC	August 8, 2008
P. E. Janolin	Carnegie	X-ray powder diffraction of CsPt in DAC	August 8-9, 2008
L. Weng	HPSynC	Yield strength measurement of the ultrahard carbon phase	August 9-10, 2008
Amy Lazicki	Carnegie	Investigation of high-temperature bcc-fcc phase boundary of lithium	August 10-11, 2008
Q. Zeng	HPSynC	The high-pressure XRD study on CeAl and NiCoMnIn alloys	August 10-12, 2008
W. R. Scheidt M. Lerche	University of Notre Dame HPCAT	Pressure-induced phase change in the heme protein tetraphenylporphyrin	August 11-12, 2008

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. (Experiments denoted by an asterisk were carried out by the beamline scientist for the group).

User Name	Affiliations	Project	Dates
Y. Song Z. Dong D. Shakhvorostov	University of Western Ontario	Structural investigation of zeolites under high pressures by infrared microspectroscopy	July 3-5, 2007
Jennifer Ciezak	Carnegie/Army Research Lab	Energetic materials under extreme conditions: The low-temperature high-pressure IR spectra of RDX and PETN	July 11-12, 2007
W. Han	Brookhaven National Laboratory	FTIR spectroscopy of nano materials	July 13-15, 2007
T. Detrie N. Ross	Virginia Polytechnic and State University	Synchrotron spectroscopic study of prehnite at high pressure	July 16-20, 2007
J. Smedley	Brookhaven National Laboratory	Characterization of impurities in diamond	July 23, 2007
C. Holt S. Jacobsen Kimberly Adams A. Saal	Northwestern University Brown University	High-pressure synchrotron-infrared study of strong hydrogen bonding in pectolite and serandite	July 26-30, 2007
T. Tyson P. Gao	New Jersey Institute of Technology	Exploring strain effects in manganite films with infrared spectroscopy	August 1-5, 2007
C. S. Zha	Carnegie	High temperature infrared study for dense hydrogen	August 8-12, 2007
T. Zhou Z. Qin	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	August 14-16, 2007
D. Dolan M. Madlener M. Roderick R. Hickman J. Gluth R. Hacking	Sandia National Laboratory Bechtel Nevada	Characterizing the emissivity of materials under dynamic compression	August 23-31, 2007
J. Smedley	Brookhaven National Laboratory	Characterization of impurities in diamond	October 2, 2007
X. Chen	Carnegie	High-pressure optical spectroscopy of hydrogen-based materials	October 3-7, 2007
B. Yulga O. Tschauner S. Tkachev	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high pressure and temperature	October 10-12, 2007
W. Han	Brookhaven National Laboratory	FTIR spectroscopy of nano materials	Oct. 13-15, 2007
L. Wang	HPCAT	Effects of different solvent molecules on the compressibility of C_{60}	October 18-20, 2007
Jennifer Ciezak	Carnegie/Army Research Lab	Energetic materials under extreme conditions: The low-temperature high-pressure IR spectra of RDX and PETN	October 21-22, 2007
W. Panero D. Reaman Sabrina Huggins	Ohio State University	Solubility of two component systems at high *P-T*	October 23-26, 2007
Cathy Tarabrella	SUNY – Stony Brook	Vibrational properties of $MnPS_3$ under pressure	October 31-November 2, 2007

T. Tyson P. Gao	New Jersey Institute of Technology	Exploring strain effects in manganite films with infrared spectroscopy	November 5-9, 2007
Y. Song Z. Dong D. Shakhvorostov	University of Western Ontario	Structural investigation of zeolites under high pressures by infrared microspectroscopy	November 10-11, 2007
J. Chen T. Yu	SUNY – Stony Brook	IR spectroscopy of new high pressure phase of boron	November 15-16, 2007
C. Seagle W. Zhang	University of Chicago	Infrared optical properties of iron at high *P-T*	November 17-20, 2007
H. Liu	National Taiwan Normal University	Infrared studies of strongly correlated systems at high pressure	January 24-February 1, 2008
X. J. Chen	Carnegie	High-pressure optical spectroscopy of hydrogen-based materials	February 2-5, 2008
T. Tyson P. Gao	New Jersey Institute of Technology	High-pressure IR measurements on manganites	February 13-16, 2008
C. Seagle W. Zhang	University of Chicago	Infrared optical properties of iron at high pressure and temperature	February 18-22, 2008
Jennifer Ciezak	Carnegie Army Research Laboratory	Energetic materials under extreme conditions: The low-temperature high-pressure IR spectra of RDX and PETN	February 24-25, 2008
Jennifer Ciezak	Carnegie Army Research Laboratory	Compression of solid nitromethane to 50 GPa	February 28-March 1, 2008
B. Yulga S. Tkachev	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high pressure and temperature	March 3-7, 2008
W. Han S. Yu	Brookhaven National Lab Jilin University	High pressure study of water filled nanotubes	March 12-14, 2008
Wendy Panero D. Reaman Sabrina Huggins	Ohio State University	Solubility of two component systems at high-pressures and temperatures	March 18-20, 2008
L. Wang	HPCAT	Effects of different solvent molecular on the compressibility of C_{60}	March 27-28, 2008
J. Smedley	Brookhaven National Laboratory	Characterization of impurities in diamond	April 1, 2008
T. Zhou	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	April 3-8, 2007
D. Dolan M. Madlener J. Gluth R. Hickman	Sandia National Laboratory Bechtel Nevada	Characterizing the emissivity of materials under dynamic compression	April 9-11, 2008
A. Goncharov C. S. Zha	Carnegie	Infrared spectroscopy of hot dense hydrogen	April 16-18, 2008
B. Liu S. Yu	Jilin University	High pressure study of C_{60} nanomaterials	April 19-20, 2008
S. Yu B. Liu	Jilin University	Investigation of H_2O and organic substance storage in nanotubes by at pressure	April 21, 24-30, 2008
S. Yu	Jilin University	Investigation of H_2O and organic substance storage in nanotubes at high pressure	May 23-24, 2008
K. Otsuka	Yale University	*In situ* measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR	May 28-30, 2008
H. Liu	Harbin Institute of Technology	Infrared studies of strongly correlated systems at high pressure	June 2-8, 2008

T. Tyson P. Gao	New Jersey Institute of Technology	High-pressure IR measurements on manganites	June 9-12, 2008
Wendy Panero D. Reaman	Ohio State University	Solubility of two component systems at high-pressures and temperatures	June 18-21, 2008
B. Yulga S. Tkachev O. Tschauner E. Romano	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high *P-T*	July 9-13, 2008
B. Liu S. Yu	Jilin University	High pressure study of C_{60} nano materials	July 14-15, 2008
Michelle Weinberger Amy Lazicki	Carnegie	Infrared investigation of hydrogen storage materials	July 17-19, 2008
J. Smedley	Brookhaven National Lab	Characterization of impurities in diamond	July 21, 2008
Y. Song Z. Dong S. Xie	University of Western Ontario	Structural investigation of zeolites under high pressures by infrared microspectroscopy	July 24-27, 2008
C. Seagle W. Zhang	University of Chicago	Far IR reflectivity of iron at high pressure	July 28-31, 2008
C. S. Zha	Carnegie	High temperature infrared study dense hydrogen	August 1-3, 2008
H. Liu	Harbin Institute of Technology	Infrared studies of strongly correlated systems at high pressure	August 4-5, 2008
K. F. Mak M. Sfeir	Columbia University Brookhaven National Laboratory	Probing the electronic structure of graphene nanoribbons by infrared photoconductivity	August 8-9, 2008
Jennifer Ciezak	Carnegie/Army Research Laboratory	Energetic materials under extreme conditions: The low-temperature high-pressure IR spectra of RDX and PETN	August 11-12, 2008
Jennifer Ciezak Amy Lazicki	Carnegie/Army Research Laboratory Carnegie	Compression of solid nitromethane to 50 GPa	August 13-16, 2008
Kimberly Adams S. M. Thomas	Northwestern University	Ultraviolet to near-infrared reflectivity of solid and liquid methane with applications to icy satellite surface compositions	August 17-18, 2008

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