Year Three
Annual Report
September 2006

Russell J. Hemley, Director
Ho-kwang Mao, Associate Director
Stephen A. Gramsch, Coordinator
Carnegie/DOE Alliance Center (CDAC):
A CENTER OF EXCELLENCE FOR HIGH PRESSURE
SCIENCE AND TECHNOLOGY

YEAR THREE ANNUAL REPORT

1. Overview
   1.1 Mission of CDAC 3
   1.2 Highlights from Year 3 4
   1.3 Year 3 Work Plan and Milestones 6

2. Scientific Progress
   2.1 High $P-T$ Phase Relations and Structures 10
   2.2 $P-V-T$ EOS Measurements 19
   2.3 Phonons, Vibrational Thermodynamics and Elasticity 22
   2.4 Plasticity, Yield Strength and Deformation 26
   2.5 Electronic and Magnetic Structure and Dynamics 27
   2.6 High $P-T$ Chemistry 36

3. Education, Training, and Outreach
   3.1 CDAC Graduate Students and Post-doctoral Associates 40
   3.2 CDAC Collaborators 43
   3.3 Undergraduate Student Participation 47
   3.4 DC Area High School Outreach 49
   3.5 Synergy of 21st Century High-Pressure Science and Technology Workshop 50
   3.6 Visitors to CDAC 56
   3.7 High Pressure Seminars 58

4. Technology Development
   4.1 High $P-T$ Experimental Techniques 60
   4.2 Facilities at Brookhaven, LANSCE, and Carnegie 64
   4.3 Commissioning and Activities at HPCAT 66

5. Interactions with NNSA/DP National Laboratories
   5.1 Overview 67
   5.2 Academic Alliance and Laboratory Collaborations 69

6. Management and Oversight
   6.1 CDAC Organization and Staff 71
   6.2 CDAC Oversight 73
   6.3 Second Year Review 74

7. Plans for Year 4 and Beyond
   7.1 Scientific and Educational Focus 75
   7.2 Implementation of CDAC Phase II 75
   7.3 HPCAT Upgrade 76

Appendix I CDAC Publications and Presentations for Year 3 81
Appendix II CDAC Synchrotron Users/Experiments (APS and NSLS) for Year 3 99
References 112
1. OVERVIEW

1.1 Mission of CDAC

High $P$-$T$ materials research is critical to the mission of the National Nuclear Security Administration in science-based stockpile stewardship\(^1\). The program encompasses a broad range of problems and materials – $d$- 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 these materials in crystalline, liquid, and amorphous phases and examination of phase transitions, equations of state, phonon dynamics, elasticity and plasticity, electronic and magnetic structures, and chemical reactions are essential. Moreover, addressing these problems requires the training of the next generation of scientists. The proper training of these students requires in turn their access to state-of-the-art facilities that may not be available to research groups in the NNSA Labs or in conventional academia. The Carnegie/DOE Alliance Center – CDAC – was created to support this NNSA mission.

Now completing its third year, CDAC continues to address these important needs of the NNSA in scientific research and training. The success of the past year has allowed us to grow and bring a broader range of universities into the alliance. CDAC is managed by Russell J. Hemley (Director), Ho-kwang Mao (Associate Director), and Stephen Gramsch (Coordinator). CDAC consists of six formal partners together with Carnegie (the CDAC Academic Partners): Princeton University (Tom Duffy), University of Chicago (Dion Heinz), University of Illinois (Dana Dlott), University of Alabama - Birmingham (Yogesh Vohra), University of California - Berkeley (Hans-Rudolf Wenk), and California Institute of Technology (Brent Fultz). Starting with Year 4, four new academic partners have joined CDAC: New Mexico State University (Kanani Lee), Florida International University (Surendra Saxena), Texas Tech University (Yanzhang Ma), University of Nevada - Reno (Dhanesh Chandra), and Arizona State University (Jeffrey Yarger). Scientists at the National Labs (the CDAC Laboratory Partners) obtain beam time and technical training, and access to ongoing high $P$-$T$ technique development at HPCAT, the dedicated high-pressure synchrotron x-ray facility at the Advanced Photon Source (APS). Laboratory scientists also take advantage of facilities at Carnegie (including NSLS). There is active cooperation with the Lujan Center in the development of high $P$-$T$ neutron scattering. Finally, CDAC has an extensive list of collaborators from some 145 institutions around the world.

![Figure 1. Aerial photograph of the Carnegie Institution campus in Washington, D.C. where the Geophysical Laboratory is located.](image)
CDAC is developing the next generation of high-pressure techniques and conducting systematic measurements of a full range of physical and chemical phenomena under extreme conditions. HPCAT, the dedicated high-pressure synchrotron x-ray facility at the Advanced Photon Source (APS) at Argonne National Laboratory is led by Ho-kwang Mao (Director) and Guoyin Shen (Project Manager). HPCAT has been developed for high pressure physics, chemistry and materials science, and is a centerpiece of the CDAC scientific program, providing technical developments and critical spectroscopic and diffraction tools. Construction of the two insertion device beamlines has been completed, and the microdiffraction station has been open to general users for nearly three years. Commissioning activities in the areas of x-ray absorption and emission, and resonant and non-resonant inelastic x-ray scattering have taken place, with this station accepting proposals from general users for approximately two years. At this point, well over 281 different users (i.e., from National Labs and academia) have conducted experiments at the facility in these two completed experimental hutches to date. Commissioning activities have been nearly completed on the two bending magnet beamlines, and these two stations will be accepting general users in the first run of 2007. The goal of four independently operating experimental hutches, a cornerstone of the initial HPCAT concept, has now been realized. High-pressure neutron facilities at LANSCE, LANL, synchrotron infrared spectroscopy at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL), and specialized high-pressure facilities at Carnegie complement this effort. At Carnegie, there are important new developments in high P-T spectroscopy of molecular systems, high P-T cell designs, and CVD diamond growth. Experiments in high-pressure geoscience and planetary science provide valuable insight into problems in stewardship science and provide an important training ground for students and other researchers for future work in the NNSA Laboratory complex. There are also close interactions with theorists at Center institutions, the National Laboratories, and throughout academia.

CDAC formally began operations on May 1, 2003 with the first funding year ending January 31, 2004. This report covers activities from the CDAC Academic Partners, Laboratory Partners, and University Collaborators since July 2005. Research carried out by National Lab partners, but done outside of the CDAC facilities, is not included.

1.2 Highlights from Year 3

Outreach and Training

CDAC continues to make excellent progress in outreach and training, an important part of its mission. The following are highlights, in particular as it relates to students:

- Facilitated continual growth of users at HPCAT. To date, more than 281 users have conducted experimental work at the sector.
- Increased the number of CDAC collaborations/facility users. Some 411 outside collaborators from over 145 institutions have worked with us on Stewardship Science-related projects.
- Science supported Ph.D. thesis work of 19 students at CDAC partner universities and Carnegie and encouraged career development.
- CDAC student, Wendy Mao began an Oppenheimer fellowship at LANL and Jung-fu Lin began a Lawrence Fellowship at LLNL.
- CDAC supported the Synergy of 21st Century High-Pressure Science and Technology Workshop at Argonne in May 2006, which featured 59 lectures from leading high pressure scientists from academia and the National Laboratories.
- Hosted numerous visitors to other CDAC facilities (e.g., Carnegie and NSLS) for training and technique development and established enhanced and expanded collaborations with high pressure programs at all NNSA Labs.
- Hosted undergraduate and high school interns at Carnegie and HPCAT. This past year, eight students were working on CDAC-related research projects.
Figure 2. Participants listen to a lecture at the 2006 Synergy of 21st Century High-Pressure Science and Technology Workshop held at the Advanced Photon Source.

Scientific Breakthroughs

Some 362 papers have been published since the start of the Center as a result of the support from the grant. This list includes papers describing work carried out by the CDAC Academic Partners, Carnegie research supported by the grant, and research carried out at HPCAT and CDAC facilities at NSLS. (The list 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 included articles published in the major high-impact journals.

- **High pressure inelastic scattering of H₂O reveals bonding changes and dissociation**: LLNL scientists carried out direct measurements of the electronic structure of water. Complementary measurements carried out by LANL and Carnegie reveal x-ray induced dissociation².

- **New findings in heavy rare earth metals at high pressure**: The Alabama-Birmingham group uncovered new trends in pressure-induced structural phase transformations in the heavy rare earth holmium³.

- **Tribological properties of metal sulfides**: X-ray studies of metal sulfides carried out at Texas Tech reveal new insight into their high-pressure tribological properties⁴.

- **Pressure induced phase transitions in PbTiO₃**: A team from Carnegie carried out theoretical calculations that predict colossal ferroelectricity in PbTiO₃ under pressure⁵, which is now being examined by in situ Raman and x-ray techniques ⁶.

- **Polymers and their composites**: Equations of state of a series of important polymers and composites were measured for the first time using light scattering techniques at LANL and Carnegie⁷⁹.

- **Effect of shear stress and strain on high P-T transformations of iron**: The shear stress and strain on the phase transition in iron was identified by the researchers at Texas Tech¹⁰.

- **Reflectivity of iron at high pressure**: Important advances in temperature calibration at high pressure with synchrotron IR reflectivity measurements on iron at high pressure collected by the Heinz group at the University of Chicago at the U2A beamline at NSLS¹¹.
- **Texture development at high pressure**: The Berkeley, Princeton, and Carnegie groups carried out systematic investigation of the texture development in MgSiO₃ perovskite\textsuperscript{12,13}.

- **Plastic behavior of post-perovskite**: Members of the Berkeley, Princeton, and Carnegie teams also reported new insights into the plastic behavior of post-perovskite deep in the Earth’s interior have been reported by CDAC collaborators from Berkeley, Princeton, and Carnegie\textsuperscript{14}.

- **Magnetic state of hcp iron-nickel**: Scientists from Caltech and Carnegie, together with the team at HPCAT, found that the high-pressure hcp phase of Fe-Ni remains non-magnetic, using synchrotron Mössbauer spectroscopy at low temperatures\textsuperscript{15}.

- **Novel transition metal nitrides**: A former CDAC summer undergraduate intern and a team from Carnegie, Université Pierre et Marie Curie, and Democritos National Simulation Center synthesized two new transition metal nitrides using laser heated diamond cell techniques\textsuperscript{16}.

- **Nitrides of platinum and iridium**: LLNL scientists used HPCAT to characterize new nitrides, showing that platinum and iridium nitrides contained pairs of single-bonded nitrogen atoms\textsuperscript{17}.

- **Combining synchrotron IR spectroscopy and dynamic compression**: Infrared radiation detectors were tested at U2A beamline to establish the feasibility of real-time infrared measurements during dynamic compression\textsuperscript{18}.

- **Metal-insular transitions**: Carnegie scientists and collaborators studied the antiferromagnetic Bi-based high-T\textsubscript{c} parent compound by Raman spectroscopy, x-ray diffraction, and resistivity techniques\textsuperscript{19}.

- **Morphology tuned ZnS nanobelts**: New insights into the behavior of wurtzite-type ZnS have been reported from LANL. The observed mechanisms could enable an understanding of the microscopic mechanisms at work in these materials, with the goal of synthesizing functional nanocomposites with excellent mechanical properties\textsuperscript{20}.

- **Interface dynamics at high pressure**: The Illinois group continues to develop an ultrafast nonlinear vibrational spectroscopic technique to understand the dynamics of interfaces under laser-generated shock waves, and in high static pressures produced in an anvil apparatus\textsuperscript{21}.

- **X-ray induced synthesis of 8H diamond**: LANL scientists collaborating with colleagues from Carnegie and the University of Arizona found that exposure of single crystal graphite to intense synchrotron x-ray radiation results in new polymorphism of carbon\textsuperscript{22}.

- **Large single crystal CVD diamond**: The Carnegie group has continued their work on CVD diamond synthesis for a broad range of applications including both static and dynamic compression in collaboration with teams at SNL and LANL\textsuperscript{23}.

- **High-pressure gigahertz-ultrasonic interferometry**: Advances in gigahertz interferometry at Carnegie provide an important complement to existing techniques for elasticity studies under pressure\textsuperscript{24}.

### 1.3 Work Plan and Milestones for Year 3

CDAC’s mission includes a comprehensive scientific program, education, training and outreach component, and technology development. Within the context of these sections, milestones have been set for each year of CDAC. Nearly all of the Year 3 goals were met, and we are on track for meeting – and in many cases have already met our expectations for Year 4. The Year 3 milestones from the original proposal are listed below in bold.

**Scientific Program**

1. We will fully exploit the laser-heating techniques for determination of the phase relations of high and low-Z materials over the broadest possible P-T range (>300 GPa and
>6000 K). The electron, phonon, structural, and molecular bonding transitions of hydrogen from the low-temperature molecular insulating solid to the high-temperature metallic fluid will be elucidated.

High P-T measurements on H₂ were extended using laser heating techniques. The pressure dependence of the H₂ band gap and low energy excitons in H₂ were directly determined using inelastic x-ray scattering. Studies by Carnegie and LLNL also led to improved determination of the phase diagram of H₂O, and constraints on superionic behavior. Bonding breakdown of H₂O under pressure was also identified with these techniques.

2. The liquid-vapor and liquid-liquid critical points and coexistence curves for carbon and metals will be explored at high-pressure and very high temperature (up to 10,000 K). This will by necessity also include direct determination of subsolidus phase transformations and melting relations.

The temperature range of laser heating techniques was extended to above 9000 K in studies of carbon. The equations of state of numerous materials were determined by x-ray diffraction. The equation of state (EOS) of BeH₂ was determined by Brillouin scattering. Complementary experiments were carried out by LLNL colleagues on Be.

3. In addition, combining laser heating techniques with radial x-ray diffraction will allow detailed measurements of the combined P-T dependence of yield strength and therefore direct information on rheological properties in a hitherto inaccessible domain.

Changes at high pressure with time (creep) and temperature (recrystallization) were documented. In-situ measurements of phase transformations in steels and Ti at high temperature were performed.

4. Investigations of solubility and phase relations of compounds and mixtures will continue, including incompatible metals that become alloys, and stable compounds that dissociate at ultrahigh pressure and temperature.

The discovery of new nitrides provided an excellent example of new compound and alloy formation under pressure. As discussed above, x-ray-induced and pressure-induced dissociation of H₂O was documented.

5. Real time SFG measurements will be obtained to reveal the chemistry of polymer binder energetic material interfaces.

SFG data on the surfaces of the energetic materials HMX and TATB have been obtained. In addition, new Brillouin and Raman scattering studies of various polymers and energetic materials were completed.

6. The determination of P-T-V EOS of standard materials (begun in Year 2) will be completed and incorporated into the EOS database at LLNL and LANL for hydrocode applications. Expansion of full investigations to other key materials will be integrated with dynamic compression studies and theoretical models (e.g., ASCI).

The equations of state for a series of polymeric materials were determined. As part of this effort, the computational group at Carnegie has computed the thermoelastic properties of Fe as functions of pressure and temperature. We are working with the laboratories to incorporate EOS data obtained in CDAC in laboratory simulations as part of NNSA milestones.

7. Ultrahigh-accuracy and -efficiency diffraction studies will be extended to the lanthanide series and integrated with electronic, magnetic and phonon studies to establish systematics in f-electron systems.

Advances in diffraction techniques had led to improved systematics for understanding the high-pressure behavior of these metals. Both LLNL and LANL are using HPCAT to obtain data crucial for improving our understanding of nuclear weapons performance.
Education and Training

1. Support for education and training of the proposed 14 graduate students will continue, as will the support for the two CDAC post-doctoral fellows.

In Year 3, 13 graduate students and two postdoctoral associates were directly supported by funding allocated to the six academic partners. One graduate student supported by LANL and two graduate students supported by LLNL carried out thesis research on CDAC-related topics. In addition, the four new CDAC academic partners have recruited six graduate students and one postdoctoral associate into their groups. As described in Section 3.1, this part of the CDAC education and outreach effort has been extremely productive. At Carnegie, developments in neutron diffraction to be implemented at LANSCE and eventually the Spallation Neutron Source (SNS) are the focus of one postdoctoral fellow working closely with a research scientist. These appointments are more thoroughly discussed in Section 3.1.

2. The summer school/workshop program will be continued.

In Year 3, the Synergy of 21st Century High Pressure Science and Technology meeting held at the APS was sponsored in part by CDAC (travel support for student attendees) and also served as a venue for the gathering of CDAC students, postdoctoral associates, academic partners and laboratory
partners. The emphasis of this meeting on cutting-edge science complemented the themes outlined in the CDAC Summer School held during Year 2, which focused on core theory and techniques in high pressure science. CDAC will continue to support student attendance at similar meetings. A second CDAC Summer School is anticipated for the summer of 2007, to be coupled with an advisory committee meeting at which time the future of the CDAC educational program will be discussed.

3. A workshop/retreat to plan for the educational program for CDAC beyond year three will be held, following reviews by the Advisory Committee.

With the inception of Phase II of the CDAC program in January 2006 following recommendation by the CDAC Advisory Committee, the support of graduate students in the Center has been continued with an increased number of students. Input from the advisory committee therefore will be sought in 2007 (during Year 5) as to the best way for the CDAC educational and outreach program to move forward.

**Technique Development**

1. The sample sizes in DACs above 100 GPa will be improved from the current limit of $10^{-4}$ mm$^3$ to 1 mm$^3$, thus enabling neutron diffraction in the megabar range.

The Carnegie synthesis of large single crystal CVD diamond has produced diamond single crystals greater than 10 carats$^{23}$; this development is allowing samples of the sizes mentioned above to be compressed toward the megabar range. Although we have not yet broken the megabar neutron diffraction barrier, we have pressurized very large single crystals for neutron diffraction$^{39}$. A high pressure test bed for the SNS has been set up at LANSCE.

2. Electron and phonon band structures and transport measurements will be developed at simultaneous high P-T.

We continued to make progress on extending single crystal diffraction to higher pressure. Neutron diffraction measurements have been conducted above 30 GPa$^{39}$ and the combination of large anvil and Kirkpatrick-Baez focusing should make 50 GPa studies possible in Year 4.

3. We will also explore pulsed laser heating experiments and time resolved measurements of IR reflectivity and electrical conductivity, as well as x-ray diffraction.

There was important progress in each of these areas. As mentioned above, in situ high P-T x-ray diffraction with laser-heating has been extended to above to above 9000 K$^{40}$. Pulsed heating/Raman spectroscopy was developed$^{41}$. SNL and Carnegie have tested time-resolved synchrotron IR spectroscopy. The Carnegie group has developed new electrical methods using FIB technology.

4. New classes of DACs will be developed for comprehensive studies with multiple x-ray, neutron, optical, electrical, and magnetic probes over an extensive P-T range.

Several new DACs were developed for integration of multiple probes and for reaching higher P-T conditions. P-V-T calibrations using both optical and x-ray methods were extended at Carnegie$^{73}$ and through a LLNL/Carnegie collaborations$^{42}$.

5. Developments launched in Year 2 will be completed including the new opportunities in combined static and dynamic compression.

Considerable progress was made in the use of high P-T x-ray diffraction techniques with resistive heating for amorphous phases$^{43}$. Techniques for obtaining quantitative texture information from single diffraction images, without imposing sample symmetry were extended$^{44}$. Building on the success of the laser-shock molecular interface studies mentioned above$^{30}$, high-pressure, grazing incidence cells for use with SFG measurements are being constructed and tested.
2. SCIENTIFIC PROGRESS

Year 3 of the CDAC program has led to many results in all areas of emphasis. The following sections discuss selected experimental studies supported fully or in part by CDAC and made possible by the Center. Following earlier Annual Reports, the topics are divided into the following six categories:

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

Studies at high $P$-$T$ conditions made possible by advances at HPCAT are expanding the range of materials investigated within CDAC. Many of these studies are a direct result of improvements in laser heating and resistive heating techniques\(^{45}\), as well as in situ high $P$-$T$ Raman measurements with laser heating\(^{46}\). Several key results for phase relations and structures are representative of an increased effort toward advanced materials with special properties.

**Phase Relations of $H_2O$ under Extreme Conditions** – Furthering our understanding of $H_2O$ and other hydrogen-bonded systems impacts a broad range of problems, including detonation, aging, geophysics, life sciences, environment, and technology development. Last year, a Carnegie team used in situ high $P$-$T$ Raman spectroscopy and synchrotron x-ray diffraction, to observe a triple point on the melting curve of $H_2O$ at approximately 35 GPa and 1040 K. The melting temperature of $H_2O$ increases significantly above the triple point\(^{28}\). Similar results obtained using high $P$-$T$ Raman scattering and theoretical calculations were reported by CDAC collaborators from LLNL\(^{47,48}\). Previous synchrotron IR evidence for a low temperature transition found in ice VIII\(^{49}\) were confirmed by diffraction studies carried out at HPCAT that showed a structural transition near 14 GPa\(^{50}\).

CDAC postdoctoral fellow Sergei Tkachev, Alexander Goncharov, and Russell J. Hemley (Carnegie) are studying the protonic diffusion in ice VII using Raman spectroscopy at high pressures and temperatures. The samples of $H_2O$ and $D_2O$ are loaded in the same cavity in the diamond anvil cell (DAC) using a double gasket technique. A preliminary study to 15 GPa and 573 K show a very small diffusion coefficient. Higher pressure studies approaching the $P$-$T$ region of theoretically-predicted superionic phase of water are in progress.

**Dissociation of $H_2O$ and Formation of a High-Pressure O$_2$-H$_2$ Alloy** – Wendy Mao, a former CDAC graduate student now at LANL, together with Ho-kwang Mao, Jian Shu, Russell J. Hemley (Carnegie), Yue Meng, Michael Hu, Paul Chow (HPCAT), Peter Eng (University of Chicago) and Yong Q. Cai (National Synchrotron Radiation Research Center, Taiwan) carried out complementary measurements of $H_2O$ at higher pressures. A remarkable combined pressure and x-ray irradiation induced transformation in $H_2O$ was discovered. Mao and colleagues from Carnegie, HPCAT, and the University of Chicago cleaved $H_2O$ molecules, formed O-O and H-H bonds, and converted the O and H framework in ice VII into a new molecular alloy of O$_2$ and H$_2$. X-ray diffraction, x-ray Raman scattering and optical Raman spectroscopy demonstrated that this new crystalline solid differs from previously known phases (Fig 4). It displays surprising kinetic stability with respect to pressure, temperature, and further x-ray and laser exposure, thus opening new possibilities for studying molecular interactions in the fundamental O$_2$-H$_2$ system\(^{2}\). Carnegie summer high school student Alexander Levedahl (St. Anselm's Abbey School) carried out follow-up up studies of the high $P$-$T$ stability of the molecular alloy.
Hydrogen under Extreme Conditions – There has been continued progress in the study of hydrogen under extreme conditions. Laser-heating/Raman scattering methods developed in CDAC collaborations have been extended, allowing the measurement of hot bands of the vibron at LLNL and further measured at Carnegie in hydrogen and other systems. These important measurements constrain the intramolecular potential under extreme conditions. The effect of temperature on the pressure-dependent vibron coupling in resistively heating vibron measurements was examined. High school student Andrew Kung (Winston Churchill HS, Potomac, MD) assisted in 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. Led by CDAC research scientist Chang-Sheng Zha, the work has led to improvements in resistive heating of compressed H$_2$ that will be used in advancing the methods to higher pressures and temperatures. The experimental results have also been complemented by recent first-principles simulations carried out in CDAC.

Effect of Shear Stress on High P-T Transformations of Iron – Iron is one of the most abundant materials in our globe and dominates the Earth’s core. Thus the structural properties and the physics are important and critical for its application, as well as understanding the interior of the Earth. For the first time, Yanzhang Ma and the Texas Tech group explored the effect of shear stress and strain on the phase transition in iron from the bcc to the hcp phase using synchrotron x-ray diffraction measurements in a rotational DAC. Figure 5 (left) shows that the design of the cell allows rotation of the anvil on the piston side of piston-cylinder high-pressure apparatus. With the applied load firmly supporting the anvils, the rotation of the diamond anvil produces shear stress and strain on the sample and leads to strong plastic deformation. This, along with the fact that diamond is transparent to a wide range of frequencies, makes it possible to fully explore the properties of materials under high pressure and large shear. The group successfully utilized the rotational DAC in in situ x-ray diffraction measurements to study the effect of shear on the phase transformation, the lattice disorder, and transformation-induced plasticity of materials.
Ma’s group has found that the initial transition is observed to take place at the reduced pressure of 10.8 GPa under pressure and shear operation, while a complete phase transformation was observed at 15.4 GPa. The rotation of an anvil causes limited pressure elevation and makes pressure symmetric in the sample chamber before the phase transition. It does, however, cause a significant pressure increase at the center of the sample and brings about a large pressure gradient during the phase transformation. The resistance to the phase interface motion is enhanced due to strain hardening during the pressure and shear operations on iron and this further increases the transition pressure. The work of macroscopic shear stress and the work of the pressure and shear stress at the defect tips account for the pressure reduction of the iron phase transition.

**Figure 5.** Left, schematic diagram of the rotational diamond anvil cell, showing the anvils, the sample chamber, and the alignment of x-ray beam for the in situ x-ray diffraction measurements. Right, x-ray diffraction patterns after the second compression operation and rotation of 180° at different positions along the diameter of the sample plate in comparison with pressure distribution at similar positions. The values marked on the diffraction patterns indicate the distance from the center, where the diffraction pattern was taken. The “-” and “+” signs respectively indicate the distances to the left and right side of sample center.

**High Pressure X-ray Diffraction of Metal Sulfides** – Metal dichalcogenides are excellent solid lubricants due to their graphitic structure and weak inter-layer bonding, which combine to facilitate shear when the direction of sliding is parallel to the planes. One of the typical metal dichalcogenides is tungsten disulfide (WS₂), which can be either dispersed into liquid lubricants, like graphite, to reduce the friction and wear between moving surfaces; or used as a solid lubricant by itself. WS₂ is an intrinsic solid lubricant and it functions effectively as a lubricant in air and inert gases as well as in high vacuum over a large temperature range. In the solid, the molecular units line up to form a hexagonal crystal structure in which the adjacent molecules along [001] direction interact through weak van der Waals forces (Fig. 6, left). The unit cell includes two adjacent layers and thus has hexagonal symmetry with a 2H arrangement. As part of the Ph.D. thesis project of **Emre Selvi**, the Texas Tech group, which also includes **Yanzhang Ma**, **Resul Aksoy**, **Atila Ertas**, and **Allen White** carried out high pressure synchrotron x-ray diffraction experiments to investigate the properties of WS₂ to 26 GPa at room temperature. By fitting the P-V data to its EOS parameters, the bulk modulus was determined. The c-axis of the hexagonal structure is found to be much more compressible than the a-axis⁴ (Fig. 6, right).
Figure 6. Left, the crystal structure of WS₂. The solid circles represent tungsten atoms, and the open circles represent sulfur atoms. Right, the ratio of the axial reduction with pressure for WS₂.

Another disulfide, MoS₂, has a crystal structure and applications similar to those of WS₂. As part of his Ph.D. thesis project at Texas Tech, Resul Aksoy and his advisor and coauthors, Yanzhang Ma, Emre Selvi, Ming C. Chyu, Atila Ertas, and Allen White investigated the high-pressure behavior of MoS₂, by synchrotron x-ray diffraction, to nearly 40 GPa at room temperature. The ratio of the compressibilities of the c-axis to the a-axis is approximately 3 at lower pressures (below 10 GPa). The ratio gradually decreases with increasing pressure with an apparent, phase transformation at high pressure and low temperature (Fig. 7)⁵⁵.

Elemental Structures – In high-pressure physics, Olga Degtyareva (former CDAC research scientist, now at the University of Edinburgh) and a group from Carnegie studied elemental sulfur, selenium, tellurium, and arsenic and found many high-pressure phases crystallized in novel chain or incommensurate structures⁵⁶. Chalcogenic elements that are not superconductors at ambient pressure all become superconducting when compressed into body-centered orthorhombic (bco) and α-Po structures. Superconducting bco phase has an incommensurate structure, and the modulations decrease under pressure in the α-Po structure. The study clarified the problem of high-pressure sulfur structure and established the relationship between novel, high-pressure, crystal structures and superconductivity of the Group VI elements.

Study of Ti21βS to 70 GPa – Ti21βS is a Ti alloy of importance to NNSA programs. High-pressure experiments were performed on Ti21βS, which forms nanometer-sized particles at high pressure, by Nenad Velisavljevic, Neal Chesnut, and Liliana Sanchez at LANL. X-ray diffraction data were collected to above 70 GPa. In the second experiment, it was possible to again
identify the Ti21βS bcc phase. Additional diffraction peaks were observed, however and it was possible to assign these to the hcp phase. The Ti21βS phase is therefore a mixture of bcc and hcp phases. The c/a ratio of this phase decreases from 1.60 at ambient conditions to 1.57 at 36 GPa, and then as pressure is increased to 44 GPa, the c/a ratio jumps back up to a value 1.61 and remains in this range up to the highest pressure. The change in c/a ratio at 40 GPa is interpreted in terms of a change in electronic structure, leading to stiffening of the lattice in one direction. Separate equations of state were fit for the bcc phase (Fig. 8) and the hcp phase of Ti21βS. In this pressure range (40 GPa), no structural phase change was observed. However, as the pressure is further increased, the peak intensities corresponding to the Ti21βS hcp phase start to decrease at and above ~58 GPa.

**High-Pressure Behavior of Quantum Dots** – Kirill Zhuravlev, a postdoctoral associate working on Robert Sander's group at LANL, has been comparing the high-pressure behavior of nanometer-sized PbSe quantum dots with the bulk material. With increasing pressure, bulk PbSe transforms from the NaCl structure into a new, apparently orthorhombic phase, consistent with the behavior of PbSe quantum dots. The high-pressure behavior of PbSe quantum dots is found to also depend on the size of the dots. Between 13.6 and 15.5 GPa, PbSe quantum dots 12 nm in diameter transform to yet another high pressure, lower-symmetry phase (Fig. 9). Sharp volume discontinuities and hysteresis upon decompression of the PbSe samples indicate some intriguing behavior in the quantum dot phase. These aspects of the high-pressure behavior of this material are currently under investigation.

**High-Pressure X-ray Diffraction of Giant Dielectric Constant Materials** – CaCu₃Ti₄O₁₂ (CCTO) was recently found to exhibit an unusual dielectric performance, such that its dielectric constant can reach up to 10⁵ at room temperature, while remaining independent of frequency and temperature in the DC range to 10⁶ Hz, and from 100 to 600 K. Potential technical applications are anticipated in the electronic and medical technology industries, thus it is imperative to investigate the origin of such a giant dielectric constant. After intensive studies since the discovery of this effect in CCTO, many believe that it is due to an extrinsic mechanism such as the microstructure of ceramic or single crystal samples rather than intrinsic properties of the CCTO crystal. CCTO exhibits remarkably strong nonlinear...
current-voltage characteristics due to an intrinsic electrostatic barrier at the grain boundaries. Hence, it has been suggested that the giant dielectric constant could be caused by the creation of barrier layer capacitance, primarily at the twin boundaries or the interface between grains and grain boundaries or between sample and electrodes.

In collaboration with Jianjun Liu of the University of Nebraska at Omaha, Yanzhang Ma led the Texas Tech group in measuring the high-pressure x-ray diffraction of CCTO under both hydrostatic and uniaxial compression. The cubic structure of CCTO is stable up to 57 GPa, but it was observed that CCTO has an unusual compression behavior under hydrostatic pressure. Specifically, the volume reduction is less than that under uniaxial compression below 25 GPa; above 25 GPa the volume reduction starts to approach and finally reach the same value as that under the uniaxial compression at about 30 GPa (Fig. 10, left). These remarkable phenomena are explained using a model in which the samples are composed of grains that have shells stiffer than the cores (Fig. 10, right)

Figure 10. Left, volume reduction under hydrostatic and uniaxial compression. Open circles, uniaxial compression; solid line, fitted results; solid square, hydrostatic compression. Error bar indicates the uncertainties in volume reduction. Inset (a), difference between volume reduction under at constant pressure for hydrostatic and uniaxial compression. Inset (b), difference between hydrostatic and uniaxial pressure needed to induce an equivalent volume reduction. In the insets, the horizontal dot-dash lines are reference lines showing no change. The vertical dot-dash line marks the midpoint of the volume change from its maximum to 0. The solid curves and the dotted lines are merely guides to the eye. Right, difference in work done on compressing CCTO under the same pressure with hydrostatic and uniaxial conditions.

Pressure Induced Phase Transitions in PbTiO₃ – Lead titanate PbTiO₃, one of the simplest ferroelectrics with the perovskite structure and the end member of a series of technologically important relaxor ferroelectrics, has been extensively studied by theoretical and experimental methods. In addition, PbTiO₃ has not only played an important role in understanding the origins of ferroelectricity in perovskite-structured compounds but also in understanding the properties of relaxor ferroelectrics. Motivated by the need to understand the behavior of PbTiO₃ at high pressure and low temperature, Muhetaer Ahart, in collaboration with others at Carnegie, has used x-ray diffraction and Raman spectroscopy to investigate single crystals of the material under hydrostatic pressure and from 20 K to room temperature.

High pressure, low temperature (high-energy-high-resolution) x-ray diffraction was carried out at sector 11-ID-C of the APS. Figure 11 shows the pressure dependence of the positions of the [100] and [001] Bragg peaks between 5 and 15 GPa at 10 K. The results are consistent with the predictions from first principles calculations. Monoclinic phases were also found in other relaxor ferroelectric solid solutions at ambient pressure. This result shows that the large strain piezoelectricity in solid solutions of PbTiO₃ arises from the behavior of the parent material itself, while the other components tune the transition pressure.
Raman bands of PbTiO$_3$ show dramatic changes around 20 GPa at 20 K. Most importantly the number of higher frequency bands is doubled, indicating a zone boundary instability in PbTiO$_3$. Based on the experimental results and recent theoretical calculations, a good candidate for the symmetry of PT above 20 GPa would be rhombohedral. In this nonpolar structure the distortion from the cubic structure is due to antiphase rotations of the oxygen octahedral around the [111] direction, which result from the condensation of zone-boundary modes (R25), thus doubling the unit cell. Splitting of the A$_1$ and E modes above 20 GPa at 20 K is related to the zone boundary instability-induced phase transition.

**New Properties of Dense Oxides and Silicates** – Following the synthesis of the post-perovskite phase in MgSiO$_3$, former CDAC graduate student Wendy Mao (LANL) and colleagues from Carnegie, ANL, and the University of Chicago sought to address the question of whether Fe can play a major role in this phase as the core-mantle boundary (CMB) represents the region where the silicate mantle is in contact with the liquid, Fe-rich outer core. They conducted a number of DAC synchrotron x-ray experiments at the very challenging ultrahigh P-Ts of the CMB that demonstrate that this phase can incorporate a considerable amount of the Fe which leads to large increases in density relative to MgSiO$_3$ post-perovskite$^{58, 59}$. The vast reservoirs of liquid Fe and Fe-poor silicates at the CMB provide favorable chemical-physical conditions for the formation of Fe-rich post-perovskite silicate which may hold the key to understanding the geophysical and geochemical properties of the CMB (Fig. 12).

The group has subsequently reported a major new finding in high-pressure geophysics. The work focuses on iron-rich post-perovskites and the ultralow-velocity zones. The boundary layer between the crystalline silicate lower mantle and the liquid iron core contains regions with ultralow seismic velocities. Such low compressional and shear wave velocities and high Poisson’s ratio are also observed experimentally in a post-perovskite silicate phase containing up to 40 mol% FeSiO$_3$ endmember. The iron-rich post-perovskite silicate is stable at the P-T and chemical environment of the CMB and can be formed by core-mantle reaction. Mantle dynamics may lead to further accumulation of this material into the ultralow-velocity patches that are observable by seismology$^{60}$.

**Figure 11.** Pressure dependence of Bragg peak position [100] and [001] (left) and lattice parameter (right) in a single crystal of PbTiO$_3$. The [111] Bragg peak shows obvious splitting at 14 GPa at 10 K. This is consistent with the monoclinic distortion predicted theoretically$^5$.

**Figure 12.** Left: schematic diagram of the reaction boundary between a Fe-poor mantle and Fe-rich core and the accumulation of Fe-rich post-perovskite in ULVZ. Right: X-ray diffraction pattern for Fs40 post-perovskite at 138 GPa ($\lambda=0.3344 \, \text{Å}$).
Using nuclear resonant inelastic x-ray scattering coupled with EOS measurements the team was able to determine aggregate sound velocities for a post-perovskite composed of 40% of the Fe endmember, i.e. (Mg$_{0.6}$Fe$_{0.4}$)SiO$_3$. The determined compressional and shear wave velocities indicate that post-perovskite with Fe can reproduce the dramatic depression in seismic velocities in ultralow velocity zones (ULVZ)—i.e. thin 5-40 km thick patches of depressed compressional and shear wave velocities (decreases of ~10 and ~30% relative respectively to PREM) observed just above the CMB—providing an alternative explanation for the origin of ULVZ. Although further studies of post-perovskite as a function of temperature and Fe concentration are still needed, these results provide an exciting new direction into the dominating role Fe-rich post-perovskite may play at the CMB.

**High-Pressure Perovskites** – CDAC graduate student Claire Runge (Princeton) carried out a detailed study of MgGeO$_3$ perovskite to determine how its properties compare with those of the MgSiO$_3$ post-perovskite phase. Minerals adopting the perovskite structure are the dominant phases in the Earth’s lower mantle. The perovskite structure also is adopted by a wide range of inorganic compounds, many of which have technological applications as ferroelectrics and superconductors. Germanates have been used extensively as low-pressure analogs for silicates as they undergo similar phase transition sequences at lower pressures.

Using synchrotron x-ray diffraction and the laser-heated DAC the EOS of MgGeO$_3$ perovskite was determined between 25-66 GPa (Fig. 13). The EOS and structural parameters were also calculated using density functional theory. Comparison with previous work on the post-perovskite phase allowed the Princeton group to determine that the density increased by 2.0(0.7)% across the transition. The bulk sound velocity change across the transition is small and is likely to be negative (-0.5(1.6)% from experiment and -1.2% from theory). These results are similar to previous findings for the (Mg,Fe)SiO$_3$ system. Germanate and silicate perovskites also show similar trends in axial compressibilities although germanates show more anisotropy than silicates. As one example of its application as an analog material, deformation studies on MgGeO$_3$ post-perovskite have been used to infer slip systems relevant to understanding deformation and seismic anisotropy in the deep mantle. The results obtained by the group provide support for the concept that germanates may be suitable analogs for the mechanical behavior of silicates at high pressures.

![Figure 13. Comparison of experimental pressure-volume measurements for MgGeO$_3$ perovskite and post-perovskite phases. Solid circles, perovskite data (this study); open circles, post perovskite data. Solid and dashed curves are fits using 3rd order Birch-Murnaghan EOS for the perovskite and post-perovskite data, respectively.](image)

**Carnegie** Postdoctoral Fellow Pierre Beck, along with Alexander Goncharov and Russell J. Hemley is currently studying a San Carlos olivine under high P-T conditions using Raman spectroscopy. In these studies, the sample is pressed in an Ir ribbon, which serves as a laser absorber, and Ar serves as both pressure medium and thermal insulator, while the temperature achieved upon heating by a YLF laser are measured through radiometry. Spectra acquired at 9 and 13 GPa to 2000 K show the expected softening and broadening of the observed Raman active modes. For temperatures above 1800 K the transition to the $\beta$-phase is observed. The absence of any $\gamma$-phase
rules out the presence of a significantly high thermal pressure (<2 GPa). The phase transition appears to be reversible upon cooling.

**High Pressure X-ray Diffraction of ThSiO$_4$ and HfSiO$_4$ – Kimberly Tait**, a graduate student of **Robert Downs** at the **University of Arizona** working at **LANL** has carried out a series of high-pressure studies of zircon (ZrSiO$_4$), hafnon (HfSiO$_4$), and thorite (ThSiO$_4$). These three minerals that crystallize in the space group $I4_1/amd$ and all occur naturally in the earth’s crust during the later stages of magmatic activity. Minerals with the zircon-type structure show wide chemical stability and are among several crystalline phases under consideration for the immobilization and disposal of high-actinide radioactive wastes$^{61}$. Natural samples of these minerals tend to be partly metamict due to the presence of these radioactive elements in their structures and have compositional substitutions among the cations, which tend to make them poor candidates for x-ray diffraction studies. Previous shock experiments$^{64,65}$ and DAC experiments$^{66-68}$ show that zircon undergoes a phase transition at high pressures and temperatures. The high-pressure phase is a scheelite-type structure ($I4_1/a$) named reidite$^{69}$ to which zircon transforms at 20 GPa$^{68}$. Although several x-ray diffraction and Raman spectroscopy experiments have been performed on zircon, there was no information about the high pressure phases of thorite and hafnon, nor was there any systematic study of their equations of state. ThSiO$_4$ has a polymorph, huttonite (monoclinic $P2_1/n$); the low-density, high-symmetry thorite transforms to huttonite (lower-symmetry, higher density) at $\sim$1200°C$^{70}$. This is contrary to the general expectation based on a comparison to lanthanide orthophosphates-the low temperature polymorphs have a monzonite (monoclinic) structure and the high-temperature polymorphs have the zircon (tetragonal) structure$^{71}$. No such high temperature studies had been documented in the literature for hafnon. Besides the anomalous phase transformations for ThSiO$_4$, the molar volume of thorite is higher than that of huttonite, which would suggest that huttonite should be more stable at higher pressure.

Tait used a hafnon sample that was grown in a platinum crucible from a Li$_2$MoO$_4$ melt which was about 5% by weight HfO$_2$·SiO$_2$$^{72}$. A new sol-gel hydrothermal synthetic technique has also been developed and will be used in future work on thorite. This synthesis technique has been perfected over a considerable amount of time and there is no unreacted ThO$_2$ in the final sample. Data were collected to 48 GPa at the HPCAT 16-ID-B beamline, using approximately 5 GPa pressure steps to determine the bulk modulus and characterize the high pressure phases of hafnon. At approximately 27 GPa hafnon undergoes a phase transition to the previously undetermined scheelite-type structure ($I4_1/a$), which was predicted due to the zircon-reidite phase transition, but no further phase transitions were observed. Tait studied thorite, which is radioactive and had to be loaded at **LANL** and shipped via the requirements of the APS. The sample was well crystalline but at 12 GPa the sample peaks became weak and appeared to become amorphous, which might be due to a chemical reaction with the pressure medium, or due to perhaps particle size effects arising from the synthesis conditions. Further high pressure Raman work is being carried out in coordination with the **University of Arizona**.

**Melting and Phase Relations in the Fe-FeO System – The Heinz group at the University of Chicago** has collected extensive data on the melting and phase relations in the Fe-FeO system from 18 to 136 GPa spanning bulk compositions from 5 to 90 weight % FeO. They have shown that the system is not a solid solution as some had predicted$^{73}$ up to at least the core – mantle boundary. This is an important result; since the melting temperature of FeO at the Earth’s core mantle boundary is significantly greater than the melting temperature of pure Fe$^{73,74}$, a complete solid solution would be incompatible with the energy requirements of the geodynamo. The eutectic temperature was bound in this system using the same method used in the Fe-Fe$_3$S system. The eutectic temperature rises rapidly closely following the melting curve of pure Fe up to 96 GPa, and thus there is not a significant melting point depression with respect to pure Fe. The nature of studying binary phase diagrams with x-ray diffraction naturally allows the simultaneous determination of the end-members. Thus this group has very precise densities of the co-existing phases that will allow a calculation of the maximum allowable oxygen content of the outer core,
allow an EOS calibration of FeO, and provide information on the iron-wüstite buffer at high pressures and temperatures.

### 2.2 P-V-T EOS Measurements

The P-V-T EOS is one of the most basic pieces of information needed for predicting material behavior and validating codes that are crucial to stockpile stewardship science. A broad range of techniques at CDAC are used and further refined for these experiments. These methods include x-ray and neutron diffraction studies of crystalline and non-crystalline materials, including polymers, as well as sound velocity measurements using high-pressure Brillouin scattering and ultrasonic techniques. These experiments complement dynamic compression studies. The EOS of low-Z materials,\textsuperscript{75-78} provide a critical baseline required for understanding the kinetics, thermal transport, and other important properties of detonation and other chemical processes\textsuperscript{30, 75, 76, 78}. Combined density functional theory molecular dynamics and path-integral Monte Carlo simulations have shown that many-body effects are extremely important in describing the observed phenomena even in these apparently simple systems\textsuperscript{79, 80}.

**Megabar Diffraction of Be** – Beryllium is an important material in nuclear science and technology. CDAC made possible beam time for LLNL scientists to carry out angle-dispersive x-ray diffraction studies of simple materials. Led by Will Evans and Choong-shik Yoo, the group includes graduate students Zsolt Jenei and Amy Lazicki, who have studied the high-pressure behavior and EOS of beryllium, an important material for the nuclear power industry and a broad range of advanced technologies such as aerospace, alloys, x-ray windows. Be is an anomalous metal because of its unusual physical properties, but it is also one of the simplest metals with only four electrons per atom. Thus studies of Be are also of basic scientific interest as a model system for developing predictive theoretical models. The group has studied the crystal structure and determined the EOS of Be up to pressures approaching 200 GPa, an important technical achievement made possible by the facilities available at HPCAT.

**Low-Z Compounds** – CDAC supports facilities used by students working with other groups in the SSAAP program. University of California – Davis graduate student Amy Lazicki, along with a group from UC-Davis, HPCAT, and LLNL, found a remarkable stability of the N$^3$ ion in Li$_3$N to a sixfold volume reduction\textsuperscript{81}. A new (γ) phase is discovered above 40(±5) GPa, with an 8% volume collapse and a band gap quadrupling at the transition determined by synchrotron x-ray diffraction and inelastic x-ray scattering. γ-Li$_3$N ($Fm\overline{3}m$, Li$_3$Bi-like structure) remains stable up to 200 GPa, and calculations do not predict metallization until 8 TPa. The work has been done in collaboration with the theoreticians Warren Pickett and Richard Scalettar; the group has also studied phase transitions in Li$_2$O.

**Sung Keun Lee** (formerly of Carnegie, now at Seoul National University) and colleagues from the University of Chicago (Peter Eng and Matthew Newville), HPCAT (Michael Hu and Yue Meng), and Carnegie (Jinfu Shu and Ho-kwang Mao) studied the near K-edge structures of boron and oxygen of v-B$_2$O$_3$ glass to 22.5 GPa, revealing pressure-induced bonding changes. Direct \textit{in situ} measurements show a continuous transformation from tri-coordinated to tetra-coordinated boron beginning at 4-7 GPa, forming dense tetrahedral v-B$_2$O$_3$. After decompression from high pressure the bonding reverts back to tri-coordinated boron but with the data suggesting a permanent densification\textsuperscript{82}.

**Polymers** – Polymers and their composites play important roles in DOE and DOD munitions applications, including in high explosives (as binders), structural materials, and armor. However, many currently employed material models used in modeling and describing their behavior are overly simplified, and are not constructed based on polymer physics and associated molecular level insights. The goal of this work is to provide improved experimental input into these models for a variety of polymeric materials. The complexity of polymers, including their multiphase structure, possible presence of filler materials, and rate and temperature dependent behavior, requires the application of multiple experimental techniques to fully capture their behavior, particularly under high P-T...
conditions, including dynamic loading scenarios. Dana Dattlebaum and colleagues at LANL are employing multiple approaches to the construction of EOS functions for these materials, including piston-cylinder measurements, Brillouin scattering, x-ray diffraction, vibrational spectroscopy, plate impact experiments, and positron annihilation lifetime spectroscopy.

This group has completed measurements on poly(tetrafluoroethylene) (PTFE) at HPCAT, measuring x-ray diffraction as a function of pressure. PTFE has at least four known phases near ambient temperature and pressure. The dynamic mechanical behavior of PTFE is highly influenced by the crystalline phase transitions. They have collected high fidelity diffraction patterns to confirm the known phase behavior of PTFE, and extracted pressure-volume relationships to 10 GPa. In doing so (and with the aid of Raman spectroscopy results), they have also discovered a new phase “V” at pressures > 5 GPa in PTFE (Fig. 14). They have extended their measurements to examine the phase behavior in the related fluoropolymers poly(chloro-trifluoroethylene) (PCTFE), poly(chloro-trifluoroethylene-co-vinylidene fluoride) (Kel-F 800), and poly(tetrafluoroethylene-co-hexafluoropropylene-co-vinylidene fluoride) (THV 500). So far (to 14 GPa), despite similar molecular structures, the crystalline domains associated with these polymers do not appear to undergo any crystalline phase transitions. These findings will ultimately be linked to the mechanical properties of these polymers, particularly in comparison to the behavior of PTFE. The brightness of the source at APS resulting in high quality diffraction patterns may allow us to eventually extract P-V data from the presumed triclinic (helical) structure.

Certain polymer materials of interest do not contain any crystalline content. In order to acquire EOS data on these materials, the group has pursued piston-cylinder pressure-volume measurements, optical microscopy (giving stiffened compression curves), and impulse stimulated light scattering. In collaboration with Muhetaer Ahart and Russell Hemley at Carnegie, Dattlebaum’s group at LANL have recently initiated Brillouin scattering measurements on three amorphous, and low crystalline content polymers: a crosslinked poly(dimethylsiloxane) material (Sylgard® 184), a polyethylene terpolymer, and a polyester-urethane co-polymer. The sound speeds for these three distinct polymer systems have been measured from ambient pressure to approximately 12 GPa in DACs using Brillouin scattering (Fig. 15). These results appear to be the first comprehensive Brillouin scattering results on polymers at high pressure. With the exception of Sylgard® 184, both transverse and longitudinal acoustic modes were observed for at slightly elevated pressures and above for all the polymers. For these materials, P-V isotherms were constructed from the Brillouin-scattering data and fit to a range of empirical/semi-empirical EOS. From this analysis the isothermal bulk modulus and its pressure derivative were obtained. Besides the EOS, mechanical properties were also analyzed in relation to the second order elastic constants and Poisson’s ratios.

Finally, the group initiated new experiments on the high explosive material tri-amino-trinitrobenzene (TATB). They are working to extend the known isothermal compression curve for TATB using high pressure powder diffraction at HPCAT and anticipate that this work will continue into the next year.
Figure 15. Left: representative Brillouin spectra at various pressures (in GPa) of Sylgard® 184. The longitudinal modes are seen on either side of the intense Rayleigh line. Right: pressure dependence of the longitudinal (L mode) and transverse (T-mode) sound velocities for polymers measured in this study.

**EOS of Gelatin** – Gelatin is one of the most versatile hydrocolloids, and has a wide variety of uses, including as a model of human tissues. At Carnegie, a team led by Muhetaer Ahart is using Brillouin scattering techniques to obtain the EOS of gelatin. The Brillouin scattering experiments are carried out from ambient pressure to 12 GPa from 0 to 100 °C. Figure 16 (left) shows a typical Brillouin spectrum at 3.23 GPa at 25 °C. The Rayleigh scattering line (elastic scattering) at the zero frequency as well as the Brillouin scattering lines (inelastic scattering) at around 6 GHz for transverse acoustic mode and at around 14 GHz for longitudinal acoustic mode are observed. The sound velocity at any given pressure is a direct measure of the pressure, and so accurate P-V data are possible (Fig. 16, right).

Figure 16. Left: a representative Brillouin spectrum of gelatin at 3.23 GPa. The strong line at zero frequency is the Rayleigh scattering line, L- and T-mode represent the longitudinal and transverse acoustic modes, respectively. Right: Pressure dependence of density of gelatin. The open circles represent the experimentally obtained density and the solid line represents the Vinet EOS fit. ($K_0 = 7.6$ GPa and $K_0' = 13.98$).

**Binary Iron-Light Element Systems at High Pressure** – Dion Heinz and his group at the University of Chicago have studied binary iron-light element systems at high pressure, in particular the Fe-Fe₃S and Fe-FeO systems. A manuscript on the thermal EOS of Fe₃S was published this year and a manuscript detailing melting in the Fe-Fe₃S system has been submitted. The group determined the eutectic temperature in the Fe-Fe₃S system up to 60 GPa and placed a lower bound at 80 GPa. Comparison with their Fe-Fe₃S melting data with the melting curve of pure Fe indicates that the melting point depression of Fe, due to sulfur alloying in the
melt, amounts to 600-800 K over the pressure range of this study (30 to 80 GPa). The Heinz group’s melting point depression of 600-800 K is identical to that calculated by ab initio methods, for a Fe-S-O melt at 330 GPa, the pressure of the inner core / outer core boundary. Most estimates of pure Fe melting at this pressure are in the range 5300-6700 K, applying a ~700 K melting point depression to this range implies a minimum inner core / outer core boundary temperature of 4600-6000 K.

The Chicago group has also studied stoichiometric FeS (troilite) up to 80 GPa with the laser heated DAC and x-ray diffraction. Troilite undergoes a series of phase transitions with increasing pressure and temperature that may be important for interpretation of future Martian seismic data. They have determined the P-T boundary of the FeS (IV) and FeS (V) polymorphs, data at higher pressures indicate another possible phase transition and they are currently working on the structure.

**Reflectivity of Iron at High Pressure** – The Heinz group at the University of Chicago has also collected some reflectivity data for iron at high pressure at NSLS beamline U2A. One of the biggest sources of error for temperature measurement using the spectroradiometric method is the sample emissivity (both magnitude and wavelength dependence). Reflectivity measurements were made on an iron foil and powder up to 50 GPa at ambient temperature in an attempt to estimate the spectral emissivity of iron. Some of this data looks good, but a complete analysis has been difficult due to an unexpected non-linear relation between beam current and intensity. The group is still trying to figure out the best way to account for this. Even though it has been difficult to determine the absolute magnitude of the reflectivity it is apparent that the slope of the reflectivity decreases with pressure indicating that the grey body approximation becomes a better approximation at higher pressures and ambient temperature.

**Accurate P-T Calibration** – Pressure determination is central to all high-pressure experiments. The commonly used ruby fluorescence pressure scale has high intrinsic precision (±0.5% in pressure under hydrostatic conditions above 20 GPa) but uncertain accuracy (±5%) because it is a secondary scale calibrated by less precise (±5%) primary standards deduced from high-temperature shock-wave data on metals. Efforts are being made among the high-pressure community to develop pressure scales at high temperature. The Carnegie and Princeton groups are extending such calibrations to >1000 K with the integrated Brillouin and x-ray method. Yingwei Fei and colleagues continue to extend x-ray calibration to high P-T conditions. Additional studies have been carried out in collaboration between LLNL and Carnegie.

### 2.3 Phonons, Vibrational Thermodynamics, and Elasticity

The study of phonon dynamics in highly compressed materials is crucial for understanding thermodynamic properties, elasticity, and phase transition mechanisms. To this end, measurements of the elastic tensor provide information on elastic wave propagation, mechanical stability, interatomic interactions, material strength, and phase transition mechanisms. HPCAT and LANL have provided capabilities, to advance the state of the art in phonon experiments. Gigahertz ultrasonic interferometry and Brillouin spectroscopy serve as additional important tools for elucidating fundamental elastic properties of materials.

**Effects of Vacancies on the Phonons in FeAl at High Pressure** – Brent Fultz's group at Caltech began research on FeAl. The most interesting results were obtained from very recent high pressure measurements on samples of FeAl that were quenched from different high temperatures to preserve a vacancy concentration as high as 3%. Compared to the control sample, the sample with excess vacancies was known to have a broadening and stiffening of the phonon partial DOS of 57Fe. (This was consistent with prior work with inelastic neutron scattering.) This effect of vacancies becomes significantly larger at higher pressures (Fig. 17). The trend is clearly a systematic one, as are the stiffenings of the phonons in each material with increasing pressure. The vacancies in FeAl alter characteristic interatomic forces, changing the anharmonicity, expressed as a larger Grüneisen parameter. Further interpretations of the results are underway using a lattice
The dynamics inversion method, where the interatomic forces are tuned to match the measured scattering or phonon partial DOS curves (Fig. 17). The goal is to identify which force constants undergo the largest stiffening in the presence of vacancies.

New neutron inelastic scattering experiments on FeAl were performed with the LRMECS chopper spectrometer at the Intense Pulsed Neutron Source at Argonne National Laboratory. These measurements were superior to the group’s previous measurements because they used a new furnace for in-situ measurements that had a much lower background, and produced higher-quality data than previous work with the PHAROS instrument at LANL. The group plans to modify the present furnace to reach temperatures of 700°C or so, and try the measurements once again on LRMECS in the Fall of 2006. Density functional computations on FeAl were begun in conjunction with the PHONON software package of K. Parlinski. Computations for different volumes of the cubic unit cell show phonon stiffening consistent with the experimental results on the material without vacancies. This work will continue in Year 4.

Cluster Expansions of Phonon DOS – To date, alloy free energies, phase diagrams and equations of state have been successfully interpreted in terms of the thermodynamics of local atom configurations. Cluster expansion hierarchy can be performed systematically, and it is often found that most of the configurational thermodynamics depends on the statistical numbers of pairs of atoms of the different chemical species in an alloy. An open question is how successful will be this cluster expansion method in accounting for the phonon entropy.

The Fultz group at Caltech has also explored the effects of local order on the $^{57}$Fe partial density of states (pDOS) in alloys and thin films of FeCr using inelastic nuclear resonant scattering (INRXS) at HPCAT. A cluster expansion of the alloy pDOSs was used to determine the basis and structure that most accurately represents the thin film multilayer results published previously by Ruckert, Keune, Sturhahn, et al. The alloys used in this cluster expansion were shown to be suitable by fitting to thin film multilayers. The thin film multilayer pDOSs constructed using pair clusters of first- and second-nearest-neighbors were found to be very similar to the pDOSs from the thin-film results. The contribution to the $^{57}$Fe pDOSs from each of the terms in the cluster expansion was determined, showing the effects of local order on the pDOSs explicitly. Evidence of strong magnetoelastic effects was seen in the energy range of 20-25 meV, consistent with dispersion curves in the literature. A manuscript is in preparation for Physical Review B and the work is part of the Ph.D. thesis of CDAC student Matthew S. Lucas.

Elastic Tensor of Alunite – In a collaboration between Tom Duffy’s group at Princeton, CDAC-affiliated postdoctoral associate Sergio Speziale (Berkeley), and Juraj Majzlan (Freiburg), determined the single-crystal elastic constants of alunite ($\text{KAl}_3(\text{SO}_4)_2(\text{OH})_6$) by Brillouin spectroscopy. Alunite and related Fe-Al sulfates attract attention because they are associated with acid mine drainage, a widely recognized environmental problem. There is also increasing interest in sulfates as important components of planetary surfaces, for example on Europa or Mars. Characterization of the elastic properties of hydrous sulfates is an important step in constraining the
Overall thermodynamics of these phases. Brillouin experiments were performed to give elastic constants (in GPa) \( C_{11} = 181.9 \pm 0.3, C_{33} = 66.8 \pm 0.8, C_{44} = 42.8 \pm 0.2, C_{12} = 48.2 \pm 0.5, C_{13} = 27.1 \pm 1.0, C_{14} = 5.4 \pm 0.5 \). The Voigt-Reuss-Hill average of bulk and shear moduli are 62.6 and 49.4 GPa, respectively. The Poisson ratio and the elastic Debye temperature are 0.19 and 654 K, respectively. The high value of the ratio \( C_{11}/C_{33} = 2.7 \) and the large discrepancy between the elastic and heat capacity Debye temperature are characteristic of the anisotropic structure of alunite.

**Elastic Properties of Hydrous Materials** – Hydrous minerals in subduction zones are potential agents for transporting water to the deep Earth. Properties of these minerals, especially elastic moduli, are needed to model seismic wave speeds in subduction zones and hence place constraints on cycling of \( \text{H}_2\text{O} \) through subduction zones. Zoisite is a metamorphic mineral of the epidote group containing 2 wt % water. It is likely to be one of the important phases in subduction zone environments. In this study, the single-crystal elastic constants of zoisite \( \text{Ca}_2\text{Al}_3\text{Si}_3\text{O}_{12}(\text{OH}) \) were determined by CDAC graduate student Zhu Mao (Princeton) using Brillouin scattering at ambient conditions. Brillouin spectra were recorded in 37 directions for three separate crystal planes. The density of the sample and the orientation of each plane were determined by single-crystal diffraction using energy dispersive techniques at X17C of the NSLS. The complete elastic tensor was then obtained by an inversion of the acoustic velocity and orientation data. The Voigt-Reuss-Hill averages of the aggregate bulk modulus, shear modulus and Poisson’s ratio were determined. These results resolve discrepancies in previous static compression studies and provide the first determination of the shear modulus of zoisite.

**Elastic Properties of Oxide Spinels** – In collaboration with Hans Reichmann (GeoForschungsZentrum Potsdam), Steve Jacobsen (formerly of Carnegie, now at Northwestern University) used GHz-ultrasonic interferometry to probe the high-pressure elastic properties of dense oxide spinels with general formula \( \text{AB}_2\text{O}_4 \). Because of their abundance in the Earth and ubiquity in materials science as magnetic and superconducting materials, spinel-structured phases are among the most well-studied materials both theoretically and experimentally. Well over 100 natural and synthetic phases adopt this structure. However, the single-crystal elastic constants of many spinels, especially those containing transition metal elements, are unknown because they are optically opaque to light-scattering techniques. The complete elastic tensor of magnetite \( (\text{Fe}_3\text{O}_4) \) and the zinc-aluminate spinel \( (\text{ZnAl}_2\text{O}_4, \text{gahnite}) \) has been determined to 10 GPa using GHz-ultrasonic interferometry. In addition, sound velocities and elastic constants have been determined for the silicate spinel \( \gamma-(\text{MgFe})_2\text{SiO}_4 \) (ringwoodite), thought to be the dominant phase in the transition zone region of Earth’s mantle (410-660 km depth). Trends indicate that spinels containing transition metals on both the \( \text{A} \) and \( \text{B} \) sites of \( \text{AB}_2\text{O}_4 \) follow different elasticity systematics than those without any, or only one transition metal (Fig. 18).

**Figure 18.** Plot of Birch’s Law for spinel-structured phases. GHz-ultrasonic interferometry has been used to determine the bulk sound velocity \( (V\phi) \) of several dark or opaque spinel phases including \( \gamma-(\text{MgFe})_2\text{SiO}_4 \) (ringwoodite), gahnite, magnetite, and fanklinite. Trends indicate that those spinels with transition metals on both the \( \text{A} \) and \( \text{B} \) sites of \( \text{AB}_2\text{O}_4 \) follow a trend 5-times more negative than those without any or only one transition metal.

For this work at Carnegie, Jacobsen set up the only GHz-ultrasonic interferometry laboratory in the US. This novel acoustic technique is being used to probe the elastic properties of microscopic samples at high-pressures in the DAC. The instrument measures compressional and
shear-wave travel times through parallel-polished platelets as thin as 20-30 µm thickness. By operating at 0.5 to 3 GHz, travel times down to 10-15 nanoseconds can be measured interferometrically with a precision of a few tens of picoseconds. The technique is ideally suited for determining the single-crystal elastic constants of opaque materials not suitable for light-scattering methods. Short acoustic wavelengths (5-10 µm at 1-2 GHz) allow very small high-pressure samples to be studied24. Jacobsen moved to Northwestern University as an Assistant Professor in September 2006, where he will continue to collaborate with CDAC projects.

Texture Development at High Pressure – The core of the Berkeley contribution to CDAC is to study the influence of non-hydrostatic stress on crystals and polycrystals, particularly at high and ultrahigh pressure and temperature, and to investigate the effects on anisotropic physical properties. Anisotropy in polycrystals is largely determined by preferred orientation (texture), which evolves during deformation and is modified during recrystallization and phase transformations. To this end Rudy Wenk’s group has been developing synchrotron diffraction techniques, particularly those involving the DAC in the radial geometry and multianvil systems. The group has also been active in applying time-of-flight neutron diffraction techniques to texture problems. The experimental data are in the form of 2D diffraction images and 1D diffraction spectra. New methods, based on the Rietveld procedure, have been developed to extract quantitative information about texture and stress. Overall, the group has used a variety of experimental user facilities in this work, including synchrotron x-ray facilities12, 44, 98-102.

Some of the research has involved improving experimental techniques (e.g. DAC gasket technology, neutron furnaces) and data processing. A breakthrough has been the capability of obtaining quantitative texture information from single diffraction images, without imposing sample symmetry. Also the group was able to document strain distribution in the DAC. Gasket technology was greatly improved by changing from a boron-epoxy gasket that produced high background to a small boron-epoxy ring, surrounded by kapton.

Graduate student Lowell Miyagi (Berkeley) has carried out systematic investigations of texture development in MgSiO3 perovskite, and has found that the material displays different texture types depending on synthesis conditions and starting material. So far he has been able to document a 100 texture (transforming from ringwoodite), a 012 texture (transforming from olivine) and a 001 texture (transforming from enstatite). Furthermore the texture changes with time (at constant pressure) and also during heating (recrystallization). Recently a strong texture has been observed in Ge-post-perovskite and Si-post-perovskite. The 110 texture is compatible with [001] pencil glide which makes sense since [001] is the direction of the octahedral chains in the structure. Recently group members had the opportunity to perform experiments with the D-DIA apparatus at APS and produced a strong (010) texture, distinctly different from the (100) texture observed in the Si and Ge post-perovskites. D-DIA experiments on analogs (including CaGeO3 perovskite) provide an excellent complement to diamond anvil experiments14, 103.

Graduate student Jenny Pehl (Berkeley) has used these neutron diffraction techniques to reveal the fact that textures that develop during deformation have profound implications for seismic anisotropy in the earth. She has been able to use information about microscopic mechanisms gained from DAC experiments to simulate macroscopic anisotropy development in the lower mantle and found that perovskite texture alone can explain the observed seismic anisotropy near the CMB. Texture changes during phase transformations further confirmed a strong variant selection in many systems (Fe, Zr, Ti and most dramatically in quartz). This is attributed to intercrystalline stresses that develop, in quartz perhaps associated with mechanical Dauphine twinning that may become a useful paleopiezometer for tectonic as well as shock stresses. An exciting new area of research has been the in situ observation of stress distributions during straining with the high resolution engineering neutron diffractometers ENGIN-X and SMARTS104.
2.4 Plasticity, Yield Strength, and Deformation

Understanding the behavior of key materials at high plastic strain ($\varepsilon_{P} > 100\%$), and high strain rates (up to $10^{5}$) is crucial for science-based stockpile stewardship. The texture provides data for interpreting active deformation mechanisms, and phase transformations induced by pressure and temperature produce systematic changes in texture patterns. The new work in CDAC builds on the semi-empirical modeling techniques developed to extract elasticity information from the x-ray and neutron diffraction studies on textured polycrystals$^{105-110}$. The focus of much of this work is the influence of non-hydrostatic stress on crystals and polycrystals, particularly at high and ultrahigh pressure, and to investigate the effects on anisotropic physical properties. The anisotropy in polycrystals is largely determined by preferred orientation (texture) and how texture evolves during deformation and is modified during recrystallization and phase transformations. Experimental data have been applied to extract quantitative information about texture and stress.

**Plastic Behavior of Post-Perovskite Deep in the Earth’s Interior** – Sebastien Merkel and colleagues from Berkeley, Princeton, and Carnegie reported direct measurements of the plastic behavior of post-perovskite deep in the Earth’s interior. Under the pressures of the CMB (2900 km below the surface), the main constituent of the deep mantle, silicate perovskite, undergoes a phase transition to a post-perovskite phase whose mechanical properties remain unknown. Merkel’s team monitored the development of lattice preferred orientation in an analogue of silicate post-perovskite plastically deformed above 100 GPa. The experiments were carried out inside a diamond anvil pressure cell and the measurements performed using x-ray diffraction at HPCAT (Fig. 19). From these measurements, it was discovered that (100) and (110) slip dominate the plastic deformation of post-perovskite. The CMB is a critical region for the Earth’s dynamics and seismologists have long documented anisotropy at these depths. Seismic anisotropy is the expression of deformation and dynamics and with the measurement capabilities developed as a result of this research, it can now be interpreted. Moreover, the application of this experimental technique is not limited to geophysics and it can now be extended to improve our understanding of the plastic behavior of a whole array of materials under extreme conditions of pressure, stress, and temperature$^{14}$.

![Figure 19. Contribution of silicate post-perovskite to seismic anisotropy in D″ after 20% deformation in shear. Left: crystal structure of CaIrO$_3$-type silicate post-perovskite. Upper right: anisotropy of compressional (Vp) and shear (Vs) wave velocities determined from texture analysis of x-ray diffraction data. Lower right: model derived from diffraction data depicting the participation of MgSiO$_3$ post-perovskite in lower mantle and D″ dynamics, leading to anisotropy in sound velocities. The model predicts simple shear parallel to the CMB.](image-url)
**Synergy Between Static and Dynamic Compression and Theory** – Combined shock and dynamic experiments provide the opportunity for advances in understanding ultrahigh P-T rheological behavior. SiC is an example of a material whose strength, elastic, and optical properties have attracted strong interest from both shock-wave and static compression communities\textsuperscript{111-113}. The fabrication of large single crystal CVD diamond at Carnegie has led to an LDRD project at SNL to study the elastic-plastic response of diamond on dynamic compression. Related studies of interfaces and cracks under pressure were investigated in Year 3 with the picosecond vibrational SFG technique in Dana Dlott's lab at Illinois.

### 2.5 Electronic and Magnetic Structure and Dynamics

Understanding the complex interplay of electronic and magnetic structure is fundamental to many problems associated with stockpile stewardship science.

**Bonding and Electronic Structure of H$_2$O** – A LLNL group, consisting of Choong-shik Yoo, Will Evans, Hyunchae Cynn, Magnus Lipp, and graduate students Amy Lazicki and Zsolt Jenei have carried out inelastic x-ray scattering (x-ray Raman) spectroscopy of high-pressure phases of water, in collaboration with Paul Chow and Michael Hu at HPCAT. These studies are aimed at addressing controversies regarding the high-pressure properties of water and build on techniques also used by the Carnegie team at HPCAT\textsuperscript{2, 114}. The technique provides data that is equivalent to x-ray absorption, but utilizes a hard x-ray to avoid absorption by diamond. These new and challenging measurements rely on optimized experimental systems and the brilliance of a 3rd generation synchrotron source. For this research program, specialized cells have been designed and built, as shown in Fig. 20 (top). Although the studies are currently at a preliminary stage, the group has measured x-ray Raman spectra of water (H$_2$O) in phases VI and VII, (Fig. 20, bottom). Using modeling techniques developed by collaborators Uwe Bergmann (Lawrence Berkeley National Laboratory) and Anders Nilsson (Stanford Synchrotron Radiation Laboratory), these spectra can be used to test and validate different models of the local structure and bonding of water molecules. The work is currently being extended to higher P-T conditions, as discussed in Section 2.1.

**Absence of Magnetism in hcp Iron-Nickel at 11 K** – The Fultz group at Caltech has led nuclear forward scattering experiments to test explanations as to why zero HMF is observed in hcp Fe, whereas \textit{ab initio} calculations show that hcp Fe should be antiferromagnetic (Fig. 21). Together with Michael Y. Hu (HPCAT), Paul Chow (HPCAT), Ronald E. Cohen (Carnegie), and Maddury Somayazulu (Carnegie), the Fultz group at Caltech has completed work that was central to the Ph.D. thesis of CDAC student Alexander Papandrew.

Synchrotron Mössbauer spectroscopy (SMS) was performed on an hcp-phase alloy of composition Fe$_{92}$Ni$_{8}$ compressed to 21 GPa in a DAC and cooled to 11 K. The SMS spectrum showed no hyperfine magnetic field. Density functional theoretical calculations predict antiferromagnetism in both hcp Fe and hcp Fe-Ni. For hcp Fe, these calculations predict no hyperfine magnetic field, consistent with previous experimental observations. For hcp

![Figure 20. Top, X-ray Raman cell and schematic. Left, image of cell, with large aperture for collecting inelastically scattered photons. Right: schematic diagram of x-ray Raman system. Bottom: x-ray Raman spectra of H$_2$O in two of its room temperature, high pressure phases.](image-url)
Fe-Ni, however, substantial hyperfine magnetic fields are calculated, but these were not observed in the present work. There are two possibilities that can explain this negative result. First, small but significant errors in the generalized gradient approximation density functional may lead to an erroneous prediction of magnetic order, or of erroneous hyperfine magnetic fields in antiferromagnetic hcp Fe-Ni. Alternately, the presence of quantum fluctuations with periods much shorter than the lifetime of the nuclear excited state would prohibit the detection of moments by the SMS technique. A manuscript describing this work is being published in Physical Review Letters\textsuperscript{15}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure21.png}
\caption{Left: Michael Hu (HPCAT), Rebecca Stevens (Caltech), and Alexander Papandrew (Caltech) working at HPCAT. Right: SMS spectra from Fe\textsubscript{92}Ni\textsubscript{8} at various temperatures and pressures. The numerical scale applies only to the topmost curve, and is provided as a reference. Solid lines are theoretical fits to the data. At 0 GPa and 296 K, the sample is bcc; at 21 GPa it is hcp\textsuperscript{15}.}
\end{figure}

\textbf{Rare Earth Metals} – Another example of CDAC support of other groups is \textit{University of California – Davis} graduate student Brian Maddox’s collaboration with a group from LLNL and HPCAT. They reported resonant inelastic x-ray scattering (RIXS) and x-ray emission spectroscopy (XES) results on Gd metal to 113 GPa which suggest Kondo-like aspects in the delocalization of 4f electrons. In RIXS, they measured the 3d - 2p\textsubscript{L\textalpha} emission after resonant excitation through the Gd L\textsubscript{III} edge. The XES experiment consists of measuring the nonresonant 4d - 2p L\textgamma\textl emission after excitation with high-energy x rays. Analysis of the RIXS data reveals a prolonged and continuous delocalization with volume throughout the entire pressure range, so that the volume-collapse transition at 59 GPa is only part of the phenomenon. Moreover, the L\textgamma x-ray emission spectroscopy spectra indicate no apparent change in the bare 4f moment across the collapse, suggesting that Kondo screening is responsible for the expected Pauli-like behavior in magnetic susceptibility\textsuperscript{115}.

\textbf{Novel Transition Metal Nitrides} – Former CDAC summer undergraduate intern Andrea F. Young together with Eugene Gregoryanz (former CDAC Scientist, now at the \textit{University of Edinburgh}), Chrystele Sanloup (\textit{Université Pierre et Marie Curie}), Sandro Scandolo (Democritos National Simulation Center in Trieste), and Russell J. Hemley and Ho-kwang Mao (Carnegie) discovered and characterized two new transition metal nitrides, IrN\textsubscript{2} and OsN\textsubscript{2}, using laser-heated diamond-anvil cell techniques. Synchrotron x-ray diffraction was used to determine the structures of novel nitrides and the equations of state for both the parent metals as well as the newly synthesized materials. These new compounds have bulk moduli comparable with those of traditional superhard materials. For IrN\textsubscript{2}, the measured bulk modulus (K\textsubscript{0} = 428 GPa) is just below that of diamond (K\textsubscript{0} = 440 GPa). \textit{Ab initio} calculations indicate that both compounds have a metal:nitrogen stoichiometry of 1:2 and that nitrogen intercalates in the lattice of the parent metal in the form of singly bonded N-N units\textsuperscript{16}.

The work extended previous work at CDAC on HfN, ZrN, NbN\textsuperscript{116, 117}, and PtN\textsubscript{2}\textsuperscript{117}. For NbN, T\textsubscript{c} was found to weakly depend on pressure in the regime from 4 to 42 GPa. Band structure calculations were performed in an effort to understand this interesting behavior. X-ray diffraction data from HPCAT show that the nitrides do not exhibit any structural phase transformations up to 52 GPa. The hardness of these nitrides was measured in cooperation with Yusheng Zhao’s group at LANL. Materials with high hardness are of prime importance for wear-resistant and protective
coatings. This work on nitrides complements studies carried out by LLNL scientists at HPCAT, described below.

A Carnegie team led by Xiao-Jia Chen performed pressure effects on the superconducting transition temperature \( T_c \) and the electronic stiffness of niobium nitride\(^{118}\). \( T_c \) was found to increase initially with pressure and then saturate up to 42 GPa (Fig. 22). Combining phonon and structural information on the samples obtained from the same single crystal, a nonmonotonic pressure dependence of the electronic stiffness was derived, which rises moderately at low pressure while dropping slightly at high pressure. The theory of Gaspari and Gyorffy\(^{119}\) was found to reproduce the observed low-pressure results qualitatively but fails to predict the high-pressure data. The observed pressure effect on \( T_c \) is attributed to the pressure-induced interplay of the electronic stiffness and phonon frequencies.

![Figure 22. Left: Dependence of the superconducting transition temperature \( T_c \) with pressure in a niobium nitride single crystal. The error bars give the transition onset uncertainty. The solid curve is a fit to the experimental data. Right: Pressure dependence of the normalized electronic stiffness in niobium nitride up to 30 GPa.](image)

**Electronic Spin Transition of in (Mg,Fe)O** – Pressure-induced electronic spin-pairing transitions of iron in (Mg,Fe)O (magnesiowüstite) have been examined theoretically for half a century. Since magnesiowüstite is considered to constitute a considerable volume fraction of the lower mantle (~20%) and is probably iron-rich compared with silicate perovskite, an understanding of the electronic spin-pairing transition of (Mg,Fe)O is crucial to modeling deep-Earth geodynamics and geochemistry; however, experimental difficulties have hampered the observation of the electronic spin transition in mantle minerals under high pressures for decades. Recent developments in the X-ray Emission Spectroscopy (XES) and Nuclear Forward Scattering (NFS) at 16-IDD of the HPCAT, Advanced Photon Source (APS) are ideally suited to understand the spin states of iron in magnesiowüstite in the lower mantle pressures. Jung-Fu Lin (LLNL) and colleagues have recently observed at HPCAT an electronic transition of iron in magnesiowüstite with synchrotron Mössbauer and x-ray emission spectroscopies under high pressures\(^{120, 121}\). Synchrotron Mössbauer studies show that the quadrupole splitting disappears and the isomer shift drops significantly across the spin-pairing transition of iron in (Mg\(_{0.75},\text{Fe}_{0.25}\))O between 52 and 70 GPa\(^{121}\), whereas the presence of the satellite peak (K\(_\beta^1\)) in the x-ray emission spectra below 55 GPa is characteristic of the magnetic state of iron and the absence of the satellite peak above 67 GPa indicates the collapse of the magnetization (Fig. 23)\(^{120}\). Based upon *in situ* x-ray emission spectroscopy and x-ray diffraction to pressures of the lowermost mantle, this group found that an observed high-spin to low-spin transition of iron in magnesiowüstite results in an abnormal compressional behavior between the high-spin and the low-spin states\(^{120}\).

The temperature effect is important for addressing the spin transition and its effects in the lower mantle, as the Earth’s lower mantle. Although experimental studies on the spin transition are mostly limited to high pressure and room temperature due to the technical difficulties, recent theoretical predictions show that the spin transition of ferrous iron in magnesiowüstite would occur...
continuously over an extended pressure range (a spin crossover) under the $P-T$ conditions of the lower mantle, since the changes in other physical properties of magnesiowüstite are continuous across the spin crossover. Future developments in the high $P-T$ XES and NFS techniques at HPCAT will help better understanding of the spin transitions in these materials.

Figure 23. Left: representative synchrotron Mössbauer spectra of (a) $(\text{Mg}_{0.75}\text{Fe}_{0.25})\text{O}$ and (b) $(\text{Mg}_{0.75}\text{Fe}_{0.25})\text{O}$ with stainless steel (SS) as a function of pressure at room temperature (2). Black line: modeled spectrum. Right: x-ray emission spectra of $(\text{Mg}_{0.75}\text{Fe}_{0.25})\text{O}$ under high pressures and 300 K[116]. Insert, the integrated area intensity of the satellite peak as a function of pressure. The intensity of the satellite peak decreases significantly across the spin transition at ~55 GPa.

**IR Detector Testing for Dynamic Compression Measurements** – One of the many important goals of the CDAC scientific program is to work toward merging the gap between the static and dynamic compression communities. A key aspect of this work was explored during Year 3 of CDAC as Dan Dolan from Sandia and collaborators R. Hacking and K. Moy from Bechtel Nevada tested several infrared radiation detectors at the CDAC-supported U2A beamline at NSLS to establish the feasibility of real-time infrared measurements during dynamic compression events. Technical challenges include demonstrating that the synchrotron produces sufficient light during the time duration of a dynamic compression experiment, typically ~1000 ns. Also, detectors fast enough to follow the pulsed synchrotron output are necessary. In this experiment, light from the visible-ultraviolet ring was passed through a FTIR spectrometer, and then focused onto the detectors after suitable beam conditioning. The detector output from a InGaAs photodiode is shown in Fig. 24. The well-resolved pulses suggest that real-time infrared reflectance measurements of dynamic shock compression events are feasible on the U2A beamline. Signals from HgCdTe and HgCdZnTe detectors suffered from high background, but with operation in the single pulse mode, measurements are possible.
Superconductivity at High Pressure – Stanford University student Tanja Cuk, a student of Zhi-Xun Shen, working at CDAC facilities with Viktor Struzhkin at Carnegie investigated the high pressure behavior of Bi-based high-\(T_c\) superconductors, including pressure-induced insulator-metal transitions in AF Bi materials on studies of new classes of superconducting compounds. These high-\(T_c\) superconductors, oxides, nitrides, hydrogen compounds, borides, and carbides are potentially important for fundamental science and for application as high-temperature/high-critical parameter superconductors. For example, Struzhkin’s group also completed a study of possible superconductivity in Na under pressure. The experiments performed thus far (to 100 GPa) do not show signs of superconductivity from Na down to 5 K, work done with a high school intern, Jacob Cohen (Yeshiva of Greater Washington). Carnegie colleagues Ronald Cohen and Zhigang Wu are performing theoretical calculations (results shown in Fig. 25) on superconductivity in sodium. Raman studies were also carried out for Os (osmium) to 60 GPa ad 10-300 K to understand non-adiabatic contributions to electron-phonon coupling in collaboration with colleagues Yuri Ponomov and Alexander Goncharov.
Isotope Effect in High-Temperature Superconductors

– The isotope effect is an important experimental probe in revealing the underlying pairing mechanism of superconductivity. Early measurements of the isotope effect on the superconducting transition temperature $T_c$ provided key experimental evidence for the phonon-mediated pairing and supported strongly the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity in conventional materials. When high-temperature superconductivity was discovered in copper oxides, the oxygen isotope exponents, defined by $\alpha = -d\ln T_c / d\ln M$ with $M$ being the isotopic mass, were promptly measured. Experiments have revealed a much richer and more complex situation. The Carnegie group, led by Viktor Struzhkin and Xiao-Jia Chen, has now developed a phonon-mediated $d$-wave BCS-like model in order to explain the elaborate oxygen isotope effect$^{19}$. The model accounts for the magnitude of the isotope exponent as functions of the doping level as well as the variation between different cuprate superconductors. The doping dependence of $\alpha$ in YBa$_2$Cu$_3$O$_{7-\delta}$ resembles that of $d\ln T_c / dP$, signaling a nice correlation between the isotope and pressure effects, as shown in Fig. 26. Based on the measurements of both $T_c$ and Raman shift of the $B_{1g}$ phonon mode, it was also predicted that the pressure dependence of $\alpha$ for the optimally doped YBa$_2$Cu$_3$O$_{7-\delta}$ would be similar to that of the pressure coefficient of $T_c$. A unified picture for the isotope effect in cuprates is then given at ambient condition and under pressure, and supported with good agreement between theory and experiments.

Figure 25. Calculated $T_c(P)$ in sodium$^{122}$. Sodium has much lower $T_c$ than lithium in the fcc phase, although it has the same predicted trend to increase dramatically with increasing pressure. Above 120 GPa there is a theoretically predicted phase transition in sodium.

Figure 26. Left: Oxygen isotope exponent $\alpha$ vs the superconducting transition temperature $T_c$ in YBa$_2$Cu$_3$O$_{7-\delta}$. Theory: solid line (lower and upper curves for the underdoped and overdoped sides, respectively); experiment: open diamond, solid circle, solid squares, and open up triangles are the experimental data points taken from different groups. A maximum in $\alpha$ around $T_c \sim 50$ K is believed to be associated with the chain oxygen ordering. Right: Pressure dependence of both the oxygen isotope exponent $\alpha$ and pressure coefficient of $T_c$, $d\ln T_c / dP$, in the optimally doped YBa$_2$Cu$_3$O$_{7-\delta}$$^{19}$.
The Carnegie group has also reported measurements of the oxygen isotope effect in other cuprates. Optimally doped single crystals of Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4+\delta}$ (n=1,2,3) have an isotope exponent that decreases with increasing the number of CuO$_2$ layers in a manner inversely correlating with $T_c$ in this homologous family. This behavior contrasts with the general belief that the isotope effect can be negligible for the optimally doped cuprates. These results highlight the important role played by phonons and interlayer coupling in high-temperature superconductivity. The mercury-based cuprate superconductor HgBa$_2$Ca$_{n-1}$Cu$_n$O$_{2n+2+\delta}$ has a higher $T_c$ both at ambient conditions and under pressure than any member of this homologous series, and the $T_c$ strongly depends on the number of CuO$_2$ layers per unit cell. The Carnegie group used a phonon-mediated $d$-wave BCS-like model to investigate the pressure effects. Fig. 27 shows the calculated $T_c$ as a function of pressure up to 50 GPa for the optimally doped HgBa$_2$Ca$_{n-1}$Cu$_n$O$_{2n+2+\delta}$ (n=1,2,3), respectively. Pressure is increased, $T_c$ increases initially until passing a saturation at critical pressure, and at higher pressures $T_c$ slightly decreases. The theoretical results are in very good agreement with those experimentally obtained early at Carnegie in collaboration with University of Houston group led by Paul Chu. This is the first application of the phonon-mediated $d$-wave BCS model to the pressure effect in cuprate superconductors. The significant $T_c$ increase under pressure points to the possibility of enhancing $T_c$ at ambient condition in compressed structures obtained through the preparation of epitaxial films deposited on substrates having smaller lattice parameters than those of the optimally doped Hg-based compounds.

**Figure 27.** Pressure dependence of the superconducting transition temperature $T_c$ in the optimally doped HgBa$_2$Ca$_{n-1}$Cu$_n$O$_{2n+2+\delta}$ (n=1,2,3). Symbols represent experimental data and curves are the theoretical results.

**Insulator Metal Transitions** – The metal-insulator transition in the Bi-based high-$T_c$ parent compound was also studied by Viktor Struzhkin (Carnegie) and his collaborators. Phonon and magnon scattering suggest a metal-insulator transition around 25 GPa, whereas resistivity studies indicate an onset of a sluggish insulator to metal transition below 2-5 GPa. Since standard resistivity measurements in a DAC are hampered by huge contact resistance, the focused ion beam facility at Stanford has been used to prepare good contacts to their samples. The lower pressure range is being tested by graduate student Tanja Cuk (Stanford). Also underway are x-ray, Raman, and IR studies of the simple hydrides (silane – SiH$_4$) and germane (GeH$_4$), in a systematic search for possible insulator-metal transitions and novel superconductivity. Preliminary results obtained by a Carnegie team lead by Xiao-Jia Chen indicate metallization above 30 GPa on the basis of synchrotron IR measurements at U2A (Fig. 28). In addition, the crystal structure was refined by Olga Degtyareva (former CDAC research scientist, now at the University of Edinburgh), based on powder x-ray diffraction data collected at CDAC. Measurements of transport properties are in progress. Resistivity studies in Bi$_{57}$FeO$_3$ across the spin-crossover transition have shown that samples become nearly metallic above 55 GPa. A theoretical description of the transition would imply both magnetic collapse and Mott-type behavior at comparable pressures. It appears that this transition may be instrumental in providing strong coupling in this material between magnetic and...
electric polarization through the elastic lattice interactions. Further experiments are underway to test this hypothesis.

**Figure 28.** Transmission photographs of silane SiH₄ in a DAC under pressure. Grains of ruby are used for pressure determination. G and S represent the gasket and sample, respectively. Images are taken at 20.1 GPa (transmitted light) and 31.6 GPa (reflected light), showing the dramatic changes in optical properties.

It has been suggested that the maximum magnitude of colossal magnetoresistance occurs in mixed-valent manganites with a tolerance factor \( t = 0.96 \). However, at \( t \sim 0.96 \) most manganites have relatively low values of the metal-insulator transition temperature at \( \sim 60–150 \) K. The Carnegie group recently found that a 50 Å La₀.₉Sr₀.₁MnO₃ thin film with \( t = 0.96 \) grown on a \(<100>\) SrTiO₃ substrate has a metal-insulator transition above room temperature, which represents a doubling of the transition temperature compared with its value in the bulk material. It was shown that this spectacular increase is a result of the epitaxially compressive strain-induced reduction of the Jahn-Teller distortion

X-ray emission spectra of compressed Ge below the Ge K edge were measured at Sector 16 the Carnegie, NSLS, and HPCAT teams. The spectra show that the width of the valence band does not show any pressure dependence in the semiconducting diamond-type structure of Ge below 10 GPa. On the other hand, in the metallic β-Sn phase above 10 GPa, the valence band width increases under compression. Density functional calculations show increasing valence band width under compression both in the semiconducting phase (contrary to experiment) and in the metallic β-Sn phase of Ge (in agreement with observed pressure-induced broadening). The pressure-independent valence band width in the semiconducting phase of Ge appears to require theoretical advances beyond standard DFT or GW approximations

**Multiferroic Materials** – Synchrotron Mössbauer and x-ray emission measurements, combined with x-ray diffraction, have also been completed on a variety of other potentially useful iron-containing materials, including GdFe₃(BO₃)₄, yttrium iron garnet (Y₃Fe₅O₁₂) and Bi₅₇FeO₃. Measurements on GdFe₃(BO₃)₄ showed that the spin-crossover in the paramagnetic state could be clearly observed and that this transition has a profound influence on the other properties of the material, such as the optical gap and the anomaly in the P-V relation. In particular, the quadrupole splitting at the transition is a sensitive indicator of the low-spin state. In Y₃Fe₅O₁₂ varying the pressure through the electronic transition to above 55 GPa, optical measurements of the band gap indicate an irreversible electronic transition. Interestingly, the recovered material is amorphous. Further studies by NFS and XES techniques are required to understand the magnetic properties at the transition. Resistivity studies in Bi⁵⁷FeO₃ across the spin crossover transition in pressure were complemented by synchrotron Mössbauer measurements of the effect of temperature on the transition. The results are compatible with a simple energy-activation model for the two-phase mixture (low-spin and high-spin phases) at the transition.

**Structural Trends in Heavy Rare Earth Metals** – Pressure-induced structural phase transformations in heavy rare earth holmium have been studied by Yogesh Vohra’s group at Alabama–Birmingham via energy dispersive x-ray diffraction to 62 GPa at ambient temperature. The complete sequence of hcp->Sm-type->dhp->fcc->dfcc (hR24) is observed for the first time with transitions at 10, 19, 54, and 58 GPa, respectively. The fcc phase is not observed as a pure phase in holmium under pressure. Figure 29 shows the structural sequence observed in energy dispersive x-ray diffraction studies on holmium. As with many other rare earths, the regions of stability of the several phases are observed to overlap, and significant hysteresis is observed. The measured volume
compression for holmium is $V/V_0 = 0.526$ at 62 GPa. The heavy rare earth metal terbium was studied at HPCAT at 16-ID-B beamline using angle dispersive x-ray diffraction to pressures up to 160 GPa. These angle dispersive data are of extremely high quality and are currently being refined to identify various low symmetry structures that are common to rare earth metals after f-delocalization at high pressures.

Reduced Radiative Conductivity of $(\text{Mg,Fe})\text{O}$ at High Pressure – The flow of heat in Earth’s deep interior plays an important role in the dynamics, structure, and evolution of the planet. Heat from the very hot core can flow outward by convection, radiation, and conduction. The relative amount of heat flow from these mechanisms is currently under debate. Experiments performed at Carnegie in facilities supported by CDAC show that the radiative component of thermal conductivity in $(\text{Mg,Fe})\text{O}$ is reduced upon reaching the low-spin state. The team consisting of Alexander Goncharov, Viktor Struzhkin, and Steven Jacobsen (formerly of Carnegie, now at Northwestern University) subjected single crystals of $(\text{Mg,Fe})\text{O}$ to pressures exceeding 60 GPa and measured optical spectra in a wide spectral range. In contrast to prevailing notions, they observed enhanced absorption of the sample in the mid- and near infrared spectral range, indicating that the sample is effectively blocking much of the light compared with low pressure conditions. The notion of reduced radiative heat transfer in low-spin phases challenges existing theories on superplume stability in the lower mantle, which appears to require high thermal conductivities in order to mitigate huge temperature gradients calculated for the case of constant thermal conductivity. This work, which was published in *Science*\textsuperscript{129}, also gives a new insight into the interpretation of the optical spectra of this important transition metal-containing oxide\textsuperscript{129}. 

**Figure 29.** Observed pure phases in Ho up to 62 GPa. Reflections from the copper pressure marker are indexed with an asterisk, oxide peaks are marked ‘o’, and gasket peaks are denoted ‘g’. Emission lines are truncated for clarity of presentation. The fcc phase is observed in conjunction with the dhcp phase just before the transition to distorted fcc, but never as a pure phase. The relevant pressure step was only 3.7 GPa, placing strict limits on the range of stability for the phase. The final member of the rare earth sequence, distorted fcc, is fit to a 24 atom unit cell in space group 166, denoted hR24.
2.6 High P-T Chemistry

Work in the area of high pressure-high temperature chemistry spans a wide range of endeavor, from investigating novel phase transformations to the high-pressure, high temperature synthesis of new materials, and developing advanced analytical capabilities for evaluating chemical reactions in the bulk and at interfaces, all at extreme conditions.

Nitrides of Platinum and Iridium – Synthesis of superhard materials under P-T conditions is one of the fundamental problems in materials science. Noble metals do not easily form compounds with other elements, but this can be changed under pressure. Alexander Goncharov (Carnegie) and collaborators at LLNL found that platinum and iridium nitrides synthesized under conditions of 50 GPa and 2500 K contain pairs of single-bonded nitrogen atoms. Contrary to initial assumptions, the stoichiometry of the compounds is MeN₂ (Me=Pt,Ir) and they form pyrite–like structures, as determined from x-ray diffraction, Raman spectroscopy, x-ray photoemission spectroscopy and first principles theoretical calculations. The materials possess an extremely high bulk modulus (350-400 GPa), are recoverable to ambient conditions, and appear to have high hardness¹⁷ (Fig. 31). The work builds on previous studies carried out in CDAC by Eugene Gregoryanz (currently at the University of Edinburgh) and colleagues at Carnegie and HPCAT¹¹⁷. This research is also complemented by x-ray diffraction and computational studies, described above¹⁶.

Morphology Tuned Wurtzite-Type ZnS Nanobelts – LANL’s Zhongwu Wang and colleagues reported new insights into the behavior of wurtzite-type ZnS with respect to structural stability, phase transformation and fracture. Wurtzite-type ZnS nanobelts have a metal-dominated surface morphology, which has the lowest surface energy (Fig. 32). Such a particular low-energy surface structure greatly expands the structural stability of wurtzite to 6.8 GPa from an unstable phase at ambient conditions, and further results in an in-situ fracture upon the explosive transformation from wurtzite to sphalerite. The group combined in-situ synchrotron x-ray diffraction
and TEM characterization, and observed the broken particle size to be ~10 nm. This study provides a better understanding of the morphology-tuned mechanisms that differ from those existing in bulk and three-dimensional nanoparticle counterparts. The result provides information important for designing the optimum path for synthesis of the multi-functional nanoforms with enhanced optical and electronic properties for technological application. There has been some evidence for the role of nanoparticles in earthquakes mechanisms as well as the useful symbiosis between the strong mechanical properties of nano-building blocks within a mixture of brittle nanobelts and soft protein in several kinds of biocomposites, such as bone and nacre. The observed mechanisms could enable an understanding of the microscopic mechanisms at work in these materials, with the goal of synthesizing functional nanocomposites with excellent mechanical properties.

**Hydrocarbon Synthesis at High Pressure** – A Carnegie-LLNL project supported by CDAC in Year 1 showed that methane can be abiogenically produced, at the pressures and temperatures of Earth’s mantle, from carbonate minerals. A Bassett hydrothermal diamond anvil cell (HDAC) coupled with a temperature controller designed and constructed at Geophysical Laboratory, and provided by CDAC to the group of Henry Scott at Indiana University – South Bend, is being used for ongoing hydrocarbon synthesis experiments. This apparatus can be used for in situ measurements of samples between ambient pressure and 10 GPa (~300 km in depth) and up to 800°C. The current experiments are expanding the P-T-X range to determine if additional hydrocarbons (i.e., heavier than methane) can indeed form at conditions relevant to Earth’s mantle. In addition to Raman spectroscopy and x-ray diffraction, the synchrotron infrared spectroscopy at beamline U2A of the National Synchrotron Light Source is now being used as an analytical technique. New techniques will investigate the role of \( f\text{O}_2 \) by buffering the DAC measurements.

**Pressure-Induced Transformations in Complex Alkali Hydrides** – Complex alkali metal based hydrides such as LiAlH\(_4\), LiNH\(_2\), and others are particularly attractive due to their high theoretical H\(_2\) content (e.g. LiAlH\(_4\) has 10.5 wt% H\(_2\)) for on-board hydrogen storage in vehicular applications. However, the parameters of hydrogen desorption/adsorption (decomposition temperature, pressure, kinetics, reversibility, etc.) of these complex hydrides have to be improved before they find widespread practical use. It is now well established that ball milling these complex hydrides can lead to a lowering of the hydrogen desorption temperature and enhanced kinetics (in the presence of catalysts). At this time, the underlying mechanisms which improve the dehydriding properties due to ball milling are still not clear. In mechano-chemical milling, the hydride materials crushed between the hardened steel balls may experience dynamic pressures up to 6 GPa. Therefore, in addition to particle size reduction, pressure-induced transformations may also occur in the hydrides. In addition, theoretical predictions have shown the possibility of significant densification (~20% decrease in molar volume) in the predicted high pressure phase. Recently, the group at University of Nevada-Reno, consisting of Dhanesh Chandra and Raja Chellappa collaborated with Carnegie scientists Steve Gramsch, Russell Hemley, Jung-Fu Lin and Yang Song to investigate the effects of pressure on LiAlH\(_4\) by in-situ Raman spectroscopy. If such dense high

![ZnS nanobelts](image)
pressure phases can be quenched to lower pressures, this may lead to a class of materials that are both gravimetrically as well as volumetrically efficient for hydrogen storage.

The pressure-induced effects on the Al-H bonding in LiAlH₄ are in contrast to the temperature effects reported by earlier workers in a Raman study of NaAlH₄. The Al-H stretching modes even in the melt indicate a strong Al-H bond and thus suggest that improvements in hydrogen desorption due to catalyst addition can be explained in terms of a weakening of this bond. It was suggested in this group’s previous study that the inclusion of a high pressure process (such as ball milling) can help in such bond weakening. Now in Year 4 of the program, the group at Nevada-Reno is a CDAC academic partner, and this work will continue with a study of the high pressure behavior of various complex hydrides such as LiNH₂, LiBH₄, and others to systematically investigate the effect of pressure on the bonding characteristics and phase transformations in these compounds.

**Interface Dynamics at High Pressure** – At Illinois, Dana Dlott’s research group is developing an ultrafast nonlinear vibrational spectroscopic technique termed broadband multiplex vibrational sum-frequency generation spectroscopy (SFG) to understand the dynamics of interfaces subjected to high dynamic pressures produced using laser-generated shock waves, and high static pressures produced in IR-transmitting anvil apparatus. In the second-generation SFG spectrometer, a femtosecond broad band infrared (IR) pulse and a narrow band picosecond visible pulse are combined at the sample surface or at an interface to give a spectrum that selectively probes molecular vibrations at interfaces. The group has now studied self-assembled monolayers (SAMs), energetic materials and fuel-cell electrodes. Molecular monolayers have been a continuing area of study, and now the group is moving toward studies of the surfaces and interfaces of energetic materials, on fuel cell electrodes, and is developing a diamond anvil apparatus that is optimized for nonlinear coherent spectroscopies.

At Illinois, Hackjin Kim has carried out studies of energetic material surfaces and interfaces with a preliminary study on PBX9501, which is a composite consisting of HMX crystals and estane binder (Fig. 33). This work has been extended by postdoctoral associate Eric Surber and graduate student Aaron Lozano. In previous work, it was noted that HMX surfaces gave spectra with a good degree of variability, leading to the discovery that all HMX crystals studied, which are in the (insensitive) β-HMX form, have tiny bits of (sensitive) δ-HMX scattered over their surfaces. The δ-HMX had not been observed by any previous techniques, because methods such as electron microscopy that can see the tiny crystals cannot distinguish their crystal form and methods such as x-ray diffraction have not been able to see the tiny crystals. As a result of this work on the HMX and now RDX surfaces, it now appears that there is a tremendous variability of surface structures depending on how and where the crystals were manufactured.

The group has also been developing the capability to study small molecules on active electrodes relevant to fuel cells, in collaboration with analytical chemist Andrzej Wieckowski. These are nanotextured electrodes under a thin layer of aqueous electrolyte. The immediate goal here is to understand the surface science of CO on Pt-based electrodes. CO is a poison in electrochemistry and it is a product that results from the decomposition of many useful fuels such as methanol and formic acid. Ultimately, the long-term objective will be to extend this expertise to study electroadsorbed CO with static and dynamic shock compression. The motivation for the static experiments is a better fundamental understanding of electrochemistry, since there are

![Figure 33. Schematic of the interface between the face of an HMX crystal and an estane binder. SFG spectra see only the one-half of the HMX molecule at the crystal surface plus the molecular groups at the estane surface.](image-url)
no high-pressure spectroscopy experiments known at this point. The motivation for the shock compression experiments stems from earlier measurements of SAMs. The SAMs were very interesting, but the long-chain molecules have a complicated response. CO should have a much simpler response that can be better understood, and CO produces a giant SFG signal. This work is leading up to using shock compression as the ultimate probe of shock front structure.

**Nitrogen at High Pressure** – A team consisting of Eugene Gregoryanz (University of Edinburgh), Alexander Goncharov, Maddury Somayazulu, Razvan Caracas, Russell Hemley, Ho-kwang Mao (Carnegie), and Chrystele Sanloup (Université Pierre et Marie Curie), continued study of nitrogen under extreme conditions. By combining x-ray synchrotron diffraction and different heating techniques the group has characterized phase transformations and structures of nitrogen compressed up to 170 GPa and heated above 2500 K. The x-ray diffraction data show that the familiar molecular phase $\varepsilon$-N$_2$ undergoes two successive structural changes to the complex molecular phase $\zeta$ (at 62 GPa) and the newly discovered $\kappa$ (at 110 GPa). The latter becomes semiconducting and amorphous upon further compression, and if subjected to very high temperatures ($>2000$ K), the material transforms to the nonmolecular cubic gauche phase, at pressures above 135 GPa.

**Group 14 Hydrides at High Pressure** – Among molecular crystals, solid hydrogen carries a particular status due to the quantum nature of the H$_2$ molecule and its fundamental interest. Metallic hydrogen has been predicted to be a superconductor with high transition temperatures in monatomic structures due to correlated fluctuations between electrons and holes in the band-overlap state. As discussed above, dense solid hydrogen has so far defied all attempts at metallization. Recently, Neil Ashcroft$^{125}$ suggested that the dense group IVa hydrides should undergo a transition to a metallic and superconducting state at pressures considerably lower than may be necessary for hydrogen since it has already undergone a chemical precompression. High-pressure studies are therefore an emerging challenge in order to throw important insight on the process of metallization and high-temperature superconductivity in such a hydrogen-rich material. The Carnegie group, led by Xiao-Jia Chen, has performed various measurements including x-ray diffraction and Raman and infrared spectroscopy, on compressed silane SiH$_4$ up to 67 GPa. The pressure-induced insulator-metal transition has been found near 30 GPa, as described in detail in Section 2.5.

**X-ray Induced Synthesis of 8H Diamond** – Carbon is one of the most abundant interstellar materials, while x-ray radiation pervades the universe. A group of LANL scientists including Zhongwu Wang, Yusheng Zhao, Qing Xue, and Ren-Guan Duan, along with Robert T. Downs from the University of Arizona, and Razvan Caracas, Chang-Sheng Zha, and Russell J. Hemley from Carnegie have shown that exposure of single crystal graphite to intense synchrotron x-ray radiation results in new polymorphic phase of carbon$^{22}$. Characterization by Raman spectroscopy, electron and x-ray diffraction demonstrates that the 8H diamond based on $sp^3$-bonding readily forms in these experiments. 8H diamond has a hexagonal unit cell [P6$_3$/mmc (#194)] with 16 carbon atoms in the unit cell and can be described as 75% cubic diamond (3C) and 25% lonsdaleite (2H), as illustrated in Fig. 34. The appreciable stability of 8H diamond is confirmed by first-principles calculations. A higher measured density relative to cubic diamond and lonsdaleite is found, and is ascribed to compressive stresses at nanoparticle surfaces. The formation of 8H diamond by x-ray irradiation has implications for the formation of planets and interstellar dust, and adds a new dimension to the polymorphism of carbon$^{22}$. First-principles theoretical results show that the formation of the 8H phase should be favored at high pressures (Fig. 35).
Figure 34. Crystallographic configurations of one unit cell of 8H diamond. Left: difference between cubic diamond (3C) with the sphalerite structure and lonsdaleite (2H) with the wurtzite structure; middle: one unit cell of 8H diamond that includes 75% 3C diamond and 25% 2H diamond (marked by the dotted lines); right: atomic arrangement of (001) and (010) facets of 8H diamond22.

Figure 35. First-principles calculations of 8H compared with 3C and 2H diamond. Variation of the total energy with volume for the three polymorphs 2H, 8H and 3C computed in the local density approximation of density functional theory. The volume is in bohr\(^3\) (1bohr = 0.529177 Å) and the energy in hartrees (1Ha = 27.2116 eV). The inset shows cross-sections through the valence electron density. The charge distribution in 8H combines features from both the 2H and 3C polymorphs22.

3. EDUCATION, TRAINING, AND OUTREACH

3.1 CDAC Graduate Students and Post-doctoral Associates

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 stockpile stewardship science. In Year 3 of the CDAC initiative, our ten academic partners supported a total of 19 graduate students and three postdoctoral associates.

Princeton: Claire Runge (MA, 2006)
Zhu Mao

Caltech: Alex Papandrew (Ph.D., 2006)
Matt Lucas
Joanna L. Dodd
Justin Purewall

Chicago: Chris Seagle

Berkeley: Jenny Pehl (Ph.D., 2006)
Lowell Miyagi

Alabama: Nicholas C. Cunningham
Joel D. Griffith (M.S., 2006; continuing study for Ph.D.)
Nenad Velisavljevic (Ph.D., 2006)
Illinois: Wentao Huang (Postdoctoral)  
Aaron Lozano  
Eric Surber (Postdoctoral)  

Arizona State: Erin Oelker  
Janelle Jenkins  

New Mexico: Stefanie Japel (Postdoctoral)  

Texas Tech: Resul Aksoy  
Emre Selvi  

FL International: Srinivas Kulkarni  
Nishad Phatak  

Figure 36. Caltech graduate student Matt Lucas at work on the x-ray spectroscopy beamline 16-I-D at HPCAT.  

In addition, three graduate students supported by the National Labs, Kimberly Tait (LANL, University of Arizona), Zsolt Jenei (LLNL, University of Stockholm), and Amy Laziecki (LLNL, University of California, Davis), are working directly with the high-pressure groups. Postdoctoral associate Kirill Zhuravlev (Washington State University) is also working with the high pressure group at LANL.  

Texas Tech also supported four undergraduate students: Alysa Daniel, Michael Foss, Kelly Keply, and Stephanie Monk. This group was also assisted by Qiliang Cui, a professor from Jilin University (China).  

At this point, five graduate students have received their Ph.D. degrees with CDAC support. Three of them, James Patterson, (University of Illinois, 2004), Wendy Mao (University of Chicago, 2005) and Nenad Velisavljevic (University of Alabama-Birmingham, 2006), have continued working in the area of stewardship science. Patterson is now at the Institute of Shock Physics, Washington State University, headed by Yogendra Gupta, Mao is at Los Alamos National Laboratory working in the LANSCE division and Velisavljevic is at Los Alamos National Laboratory working in the group of Neal Chesnut and Yusheng Zhao.  

CDAC graduate students continue their work on a wide variety of problems in experimental high pressure research relevant to stockpile stewardship science, spanning the fields of materials science, physics, chemistry and high-pressure mineral physics and geophysics. In addition, the Carnegie Institution has a well-established post-doctoral program, and a competitive predoctoral program as well as internships for college undergraduates and high school students. The close integration of computational theory within CDAC provides an environment in which graduate students in this area become intimately familiar with advanced experimental techniques and results, in addition to receiving exposure to state-of-the-art computational methods (e.g., Refs.133-135).
Publications and presentations involving CDAC-supported students and post-doctoral associates in Year 3 are listed below.

Publications


Huang, W., J. E. Patterson, A. S. Lagutchev and D. D. Dlott, Shock compression spectroscopy with high time and space resolution, *AIP Confer. Proc.*, in press.


Presentations


Mao, Z., F. Jiang and T. S. Duffy, Single-crystal elasticity of zoisite Ca$_2$Al$_3$Si$_3$O$_{12}$(OH) by Brillouin scattering, COMPRES Annual Meeting (Mohonk, NY, June, 2005).
Velisavljevic, N., Simultaneous electrical and x-ray diffraction studies on f-electron metals at high pressures using designer diamond anvils, Second Annual SSAAP Symposium (Las Vegas, NV, August 23-24, 2005).

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 current group of CDAC collaborators includes 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**
C. J. Benmore
J. A. Cowan
W. Sturhahn
J. Urquidi
J. Zhao

**Arizona State University**
K. Leinenweber
J. Yarger

**Auburn University**
Y. C. Chen
J. Dong
T. Tzeng

**Bayerisches Geoinstitut, Bayreuth**
Tiziana Boffa Ballaran
L. S. Dubrovinsky
D. J. Frost
Anastasia P. Kantor
I. Y. Kantor
Catherine A. McCammon

**Brookhaven National Laboratory**
G. L. Carr
C. C. Kao
Lisa Miller

**Bulgarian Academy of Sciences**
I. K. Bonev
I. Mitov
Dania Paneva
Rossitsa D. Vassileva

**California Institute of Technology**
O. Delaire
S. Kung
H. Su

**California State University at Channel Islands**
Tabitha Swan-Wood

**Case Western Reserve University**
J. Van Orman

**Carleton College**
Frances R. Reid

**Chinese University of Hong Kong**
H. Q. Lin

**CLCR Rutherford Appleton University**
W. G. Marshall

**Cleveland State University**
J. Vitali

**Colby College**
Elizabeth Littlefield
Lawrence Berkeley National Laboratory
J. F. Banfield
B. Gilbert
LENS, Florence
M. Santoro
Max Planck Institut für Chemie, Mainz
R. Boehler
D. A. Dzivenko
M. I. Eremets
Max Planck Institut für Festkörperforschung, Stuttgart
G. Gu
H. U. Habermeier
C. T. Lin
K. Syassen
C. Ulrich
H. Zhang
Moscow State University
B. N. Feygelson
Nagoya University
T. Okuchi
National Cheng-Kung University, Taiwan
J. Kung
National Institute for Materials Science, Japan
S. Nakano
T. Sekine
National Institute of Standards and Technology
S. Prosandeev
National Research Council, Ottawa
D. J. Klug
J. S. Tse
National Synchrotron Radiation Research Center, Taiwan
Y. Q. Cai
C. C. Chen
C. T. Chen
P. Chow
E. P. Huang
H. Ishii
I. P. Jarringe
C. Kendziora
Naval Research Laboratory
S. J. Charles
J. E. Butler
New Jersey Institute of Technology
J. P. Carlo
C. Cui
Y. Qin
T. Tyson
Z. Zhong
New Mexico State University
B. Kiefer
Northern Illinois University
D. E. Brown
M. R. Frank
Northwestern University
K. Brister
S. Jacobsen
Nuclear Research Center-Negev, Israel
I. Halevy
Oak Ridge National Laboratory
M. Guthrie
C. A. Tulk
Physikalisches Institut, Germany
K. J. Choi
G. Guenthrodt
Purdue University
P. C. Doerschuk
Rensselaer Polytechnic Institute
A. Sharma
E. B. Watson
Russian Academy of Sciences, Moscow
A. G. Gavriliuk
Rutgers University
Martha Greenblatt
M. V. Lobanov
Royal Institution, London
P. McMillan
E. Soignard
St. John Fisher College
Kristina M. Lantzky
School of Physics & Astronomy, Tel Aviv, Israel
A. Milner
M. P. Pasternak
Scripps Oceanographic Institute
I. Gan
I. Gertsman
J. E. Johnson
T. Lin
Seoul National University, Korea
S. K. Lee
Soliel, France
R. Fourme
Steacie Institute for Molecular Science, Canada
S. Patchkovskii
Stanford University
G. E. Brown
Tanja Cuk
SUNY-Stony Brook
J. Chen
Jennifer Kung
B. Li
L. Li
C. Martin
J. B. Parise
L. Wang
D. J. Weidner
Technological Institute for Superhard and Novel Carbon Materials, Russia
N. R. Serebryanaya
3.3 Undergraduate Student Participation

A number of university undergraduate students participating in the highly successful Carnegie Summer Intern Program 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 are provided with an introduction to scientific research, and within the structure of CDAC, are learning about the important problems in the field of high-pressure research. During the summers of 2005-2006, the following students participated in this program.

2005:

Edward Banigan, Georgetown University
*Equations of State of MgAl₂O₄ Spinel*

Elizabeth Littlefield, Colby College
*Effects of Water on the Behavior of MgSiO₃ Clinopyroxene at High Pressure*

Lisandra Rosario, Universidad Metropolitana (Puerto Rico)
*Solid Solutions in the Hematite-Alumina System*
Isaac Tamblyn, Dalhousie University (Canada)
Molecular Dynamics Simulations of H2-He Mixtures

Catherine Tarabrella, West Virginia University
Crystal Structures of CsI and CsCl at High Pressures

Figure 37. 2005 Carnegie summer intern Elizabeth Littlefield (Colby College) at the U2A infrared beamline at the National Synchrotron Light Source. Elizabeth worked with Steve Jacobsen (now at Northwestern University).

2006:

Cheng Chin, Columbia University
Optical Emission Spectroscopy of Simulated Microwave Plasma Enhanced CVD Diamond Growing Process

Benjamin Haugen, University of Colorado
Optical Absorption Spectra of Iron-Bearing Magnesium Silicate Perovskite at Lower Mantle Pressures

Seth Jacobsen, Cornell University
A Genetic Algorithm for Predicting High-Pressure Phases of Water Ice

Frances Reid, Carleton College
High-Pressure Synchrotron Infrared Studies of OH in Silicate Perovskite

Robert Thomas, University of Maryland
Platinum Group Element Partitioning in the Iron-Sulfur-Ruthenium System

Figure 38. Summer interns working on CDAC projects as part of the 2006 Carnegie Summer Intern Program. Top row (l-r): Frances Reed (Carleton College), Benjamin Haugen (University of Colorado), and Seth Jacobsen (Cornell University). Bottom row (l-r): Cheng Chin (Columbia University) and Robert Thomas (University of Maryland).
Former CDAC summer undergraduate intern Andrea F. Young was the first author on two papers in 2006. The first, published in Physical Review Letters, was on the discovery of new metal nitrides. This work was done in collaboration with former CDAC Scientist Eugene Gregoryanz (currently at the University of Edinburgh), Crystele Sanloup (Université Pierre et Marie Curie), Sandro Scandolo (Democritos National Simulation Center in Trieste), Russell J. Hemley, and Ho-kwang Mao (Carnegie)\textsuperscript{16}. The second paper was on a theoretical study of PtN\textsubscript{2} and appeared in Physical Review B\textsuperscript{136}. He carried out the latter work during a 2005 internship summer in Trieste at the Democritos National Simulation Center. He has finished studies at Columbia University will be starting graduate school in physics.

### 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. In 2005, two students from Washington, DC and one student from New York worked on various projects with Carnegie scientists. In 2006, Jacob Cohen returned to work with Viktor Struzhkin to work on the quantum effects of a phase transition. Alexander Levedahl and CDAC lab manager/research scientist Maddury Somayazulu the preparation and characterization of a hydrogen clathrate hydrates. Andrew Kung worked with CDAC lab manager/research scientist Chang-Sheng Zha on the development of resistive heating methods for hydrogen at high pressure. Kung measured the frequency of the H\textsubscript{2} vibron at 20 GPa, from 300 to 500 K. All three students are continuing their work at Carnegie over the course of the 2006-2007 school year. 2005 high school student Cheng Chin returned to Carnegie as a summer intern and continued his work with Chih-Shiue Yan.
2005:

Cheng Chin, Forest Hill High School, New York (Columbia University, fall of 2005)  
Optimizing Parameters for CVD Diamond Synthesis

Daniel Cohen, Yeshiva of Greater Washington, Washington, DC  
Quantum Effects on a Phase Transition

Jacob Cohen, Yeshiva of Greater Washington, Washington, DC  
Superconductivity in Compressed Sodium; Exchange Correlation Functionals for PbTiO3

2006:

Jacob Cohen, Yeshiva of Greater Washington, Washington, DC  
Quantum Effects on a Phase Transition

Andrew Kung, Winston Churchill High School, Potomac, MD  
Development of Resistive Heating Methods for Hydrogen at High Pressure

Alexander Levedahl, St. Anselm’s Abbey School, Washington, DC  
Preparation and Characterization of a Hydrogen Clathrate Hydrate

3.5 Synergy of 21st Century High-Pressure Science and Technology Workshop

A workshop was convened to explore the synergy of 21st century high-pressure science and technology. It was held from April 29 to May 1, 2006 at the APS. The workshop jointly sponsored by CDAC, COMPRES, and HPCAT. The meeting featured an extensive array of forward-looking presentations along with ample opportunities for discussions among the 112 scientists and 20 graduate students and postdoctoral researchers in attendance. The attendees represented the fields of physics, chemistry, materials science, biology, and earth and planetary sciences, from both academic institutions and the National Labs around the country.

The aims of the Workshop were to review the status of US high-pressure research and to identify future grand challenges in the following nine thrust areas:

- Integrated high pressure science
- Dense condensed-matter physics
- Chemical bonding under compression
- High-pressure materials research
- High-pressure petrology and mineralogy
- Deep Earth geochemistry
- Mission to the Earth’s core
- High pressure seismology and elasticity
- Biological and organic systems under pressure
Fifty-nine talks were given by experts from a wide variety of disciplines within the field of high pressure research. The talks reviewed the surge of high pressure discoveries in recent years as well as the technological advances in the development of new high-pressure instrumentation and analytical probes, and raised scientific and technological issues concerning the upcoming challenges for high pressure research in the 21st century. The group discussed the great scientific potential in establishing a next-generation “synergetic consortium” that would integrate state-of-the-art high-pressure techniques, facilities, and probes, and make them readily accessible to multidisciplinary high-pressure scientists. The consortium would enable high-pressure specialists and non-specialists alike to focus on specific scientific goals which were previously hindered due to technical limitations.

In the three-day workshop, presentations focused on the synergy and interdisciplinary nature of the multiple subfields of high-pressure science and technology. On the first day, an introductory session explored the chemical and physical fundamentals of matter at high densities. These presentations set the stage for an extensive group of talks that demonstrated how both static and dynamic experiments, particularly in combination with each other, along with condensed-matter theory, can provide a means to unravel the phenomena governing the behavior of matter under extreme conditions. The second day started with an overview of recent progress in seismology and geodynamics and then identified questions to be answered and the role that high pressure mineral physics can play in sorting out some of the pressing questions in these fields. Answers to some of these problems were pursued during talks in the later sessions on high-pressure mineral sciences, in which new results, developments, and technologies were presented. The day ended with two talks outlining current work in the area of biological and organic systems under high pressure. On the third day, recent developments in the studies of Earth’s deep interior were discussed from both experimental and theoretical viewpoints. The need for a synergetic consortium was further emphasized in these presentations, for example, to lead the development of a new generation of “designer” samples and anvils, integrated studies with various probing techniques, cooperation between theory and experiment, and coordinated educational efforts among different research groups. Besides the in-depth discussions in the APS conference room, two facility tours of the APS were provided during the workshop.

The participant reception to the program was overwhelmingly positive, with many compliments on the outstanding quality of the talks and discussions. The workshop will result in a publication of a series of visionary papers in the Proceedings of the National Academy of Sciences, designed to illustrate the synergetic nature of the interdisciplinary field of high pressure research.

Students – Workshop students came from universities throughout the United States as well as from the National Laboratories. A detailed list of students and postdoctoral researchers and their home institutions is given below:
Figure 43. Students and lecturers of the 2006 Workshop on Synergy of the 21st Century High-Pressure Science and Technology, held at the Argonne National Laboratory

Lecturers – Lectures were given in 11 sessions throughout the workshop. The following lists are divided by session and give the lecturers, their institutions, and the titles of the lecture(s) they presented. Lecturers supported by CDAC funds (staff, partners, post-docs, etc) are designated by an asterisk (*).

SESSION 1: Integrated High Pressure Science

Ho-kwang Mao* (Carnegie), Synergy in high-pressure research
Roald Hoffman (Cornell University), The chemical imagination at work in very tight places
Chi-Chang Kao (Brookhaven), *Electronic structure of materials under high pressure*
David J. Stevenson (Caltech), *Planetary high pressure physics inside and outside our solar system*

![Image](image1.png)

*Figure 44. Left to right: Roald Hoffman (Cornell University) and David Stevenson (Caltech) presenting talks in the first session.*

**SESSION 2: Dense Condensed-Matter Physics I**

Russell J. Hemley* (Carnegie), *Current problems in high-pressure science*
Brent Fultz* (Caltech), *Phonon thermodynamics in materials under extreme conditions*
Dana Dlott* (University of Illinois), *Interfaces at high pressure*
Alexander Goncharov* (Carnegie), *Optical spectroscopy under extreme conditions*
Viktor V. Struzhkin* (Carnegie), *Magnetism and superconductivity at high pressures*

**SESSION 3: Dense Condensed-Matter Physics II**

Yogendra Gupta (Washington State University), *Understanding condensed matter at extreme conditions: how to integrate dynamic and static compression methods*
Yogesh Vohra* (University of Alabama – Birmingham), *Grand challenges in f-electron metals research at high pressures and low temperatures using designer diamond anvils*
Malcolm F. Nicol (UNLV), *On some not-so-sharp phase transitions*
Stan Tozer, (National Magnetic Laboratory), *Spectroscopies to aid in the B P/T exploration of condensed matter physics*
Wolfgang Sturhahn (Argonne), *Inelastic x-ray and nuclear resonant scattering*
Ji Feng (Cornell University), *Metallization of structural distortion under high pressure*

![Image](image2.png)

*Figure 45. Left to right: Malcolm F. Nicol (University of Nevada – Las Vegas) and Yogendra Gupta (Washington State University) presenting talks in the third session.*

**SESSION 4: Chemical Bonding under Compression**

Raymond Jeanloz (Berkeley), *Gigabar pressures and kilovolt chemistry*
Choong-Shik Yoo (LLNL), *Electronic structure of materials under high pressure*
Nancy Ross (Virginia Tech), *Electron density of materials at high pressure*
Jeffrey L. Yarger* (Arizona State University), *Structural transformations in liquids and*
glasses under extreme conditions

Yusheng Zhao (LANL), Neutron’s prospects on the future hydrogen economy

Martin Kunz (Advanced Light Source), Experimental opportunities at the high-pressure beamline 12.2.2 of the ALS

SESSION 5: High Pressure Seismology and Elasticity

Adam M. Dziewonski (Harvard University), Seismic tomography and mineral physics: questions to be answered

Donald V. Hemberger (Caltech), Review of lower mantle seismic complexity

Barbara Romanowicz (Berkeley), Towards direct seismic waveform inversion for thermal and compositional 3D structure of the mantle: what we need from mineral physics

David A. Yuen (University of Minnesota), The role of high pressure mineral physics in geodynamics

Donald Weidner (SUNY – Stony Brook), Measuring stress at high pressure

SESSION 6: Mission to the Earth’s Core

Bruce A. Buffett (University of Chicago), Evolution and dynamics of the Earth’s core: current questions and new opportunities

Wendy L. Mao (LANL), Elasticity of Fe-rich silicate post-perovskite

Jie Li (University of Illinois), Thermal expansion of iron-rich alloys and the light element composition of the core

Dion L. Heinz* (University of Chicago), Experimental studies of core materials at core conditions

Guoyin Shen* (HPCAT), Experimental studies of phase diagram of iron

SESSION 7: High Pressure Mineral Sciences I

Juhn G. Liou (Stanford University), Orogenic UHP garnet peridotite: a new window for mantle petrochemical processes

William A. Bassett and Kenji Miebe (Cornell University), Hydrothermal DAC, the value of visual observations

Ross Angel (Virginia Tech), Determining intersite cation partitioning at high pressure
J. Michael Brown (University of Washington), Whither mineral physics?
Yingwei Fei* (Carnegie), Challenges in studying the chemistry of deep interior of the Earth
Thomas S. Duffy* (Princeton University), Elastic properties of hydrous minerals and implications for seismic studies of the upper mantle

SESSION 8: High Pressure Mineral Sciences II

Jay Bass (University of Illinois), Some recent advances in velocity measurements at high pressures and implications for the Earth
Baosheng Li (SUNY – Stony Brook), Characteristics of thermal and chemical heterogeneities in the lower mantle
Hans-Rudolf Wenk* (Berkeley), Deformation experiments at ultrahigh pressure: where we are and where we should be going
Robert C. Liebermann (SUNY – Stony Brook), Ultrasonic measurements of sound velocities in minerals under mantle pressure and temperature conditions in conjunction with synchrotron x-radiation
Yanbing Wang (University of Chicago), High P-T structural refinement of CaSiO3 (±Al2O3) perovskite
Jennifer M. Jackson* (Carnegie), Physical properties of minerals and melts under high-pressure

SESSION 9: Biological and Organic Systems under Pressure

Keith Brister (Northwestern University), Opportunities at ultra low high pressures
Anurag Sharma (Rensselaer Polytechnic Institute), Organic synthesis and biology at high pressures

SESSION 10: Deep Earth Geochemistry, Petrology and Mineralogy I

Ronald E. Cohen* (Carnegie), Theory of iron at high pressure and temperature
Renata M. Wentzcovitch (University of Minnesota), Dissociation of MgSiO3 in the cores of the giants and in terrestrial exoplanets
John B. Parise (SUNY – Stony Brook), The way frameworks respond to pressure
Anne M. Hofmeister (Washington University), High pressure thermal conductivity
Joseph Smyth (University of Chicago), Effects of hydration on physical properties of mantle minerals
Sang-Iheon Shim (MIT), Phase transition in the Earth’s mantle
Abby Kavner (UCLA), Experimental high pressure mineral physics in 3-Di
Steven D. Jacobsen* (Carnegie), Identifying hydration in the mantle transition zone: emerging constraints from mineral physics and seismology

SESSION 11: Deep Earth Geochemistry, Petrology and Mineralogy II

Harry W. Green (UC – Riverside), Shearing instabilities at high pressure, application to deep earthquakes, and progress toward experiments in-situ
Shun-Ichiro Karato (Yale University), Deep mantle melting and geochemical tests of the transition-zone water-filter model
Jiuha Chen (SUNY – Stony Brook), Melts density study at high pressures using x-ray absorption and diffraction enhanced imaging
Larrisa Dobrzhinetskaya (UC – Riverside), A look inside of diamond-growing fluid: observations from natural samples and experiments
William B. Durham (LLNL), High-pressure rheology: challenges and opportunities
3.6 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.

<table>
<thead>
<tr>
<th>Visitors</th>
<th>Affiliation</th>
<th>Project</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jennifer Ciezak</td>
<td>NIST; Aberdeen Army Laboratory</td>
<td>Energetic materials</td>
<td>September 8, 2005-ongoing</td>
</tr>
<tr>
<td>N. Nath</td>
<td>Physics Dept., Indian Institute Of Technology, Kanpur</td>
<td>Interlayer exchange coupling in Fe/Nb multilayers</td>
<td>September 29, 2005</td>
</tr>
<tr>
<td>M. D. Fuller</td>
<td>Fuller &amp; Associates</td>
<td>Diamond analysis</td>
<td>October 3, 2005</td>
</tr>
<tr>
<td>Lore Kiefert</td>
<td>American Gem Trade Association</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Y. Zhao</td>
<td>Lawrence Livermore National Laboratory</td>
<td>Clathrates Hydrates: Science and Technology</td>
<td>October 14, 2005</td>
</tr>
<tr>
<td>Valentina Degtyareva</td>
<td>Institute for Solid State Physics, Chernogolovka</td>
<td>High pressure crystallography</td>
<td>October 17, 2005 – December 20, 2005</td>
</tr>
<tr>
<td>S. N. Tkachev</td>
<td>Hawaiii Institute of Geophysics and Planetology</td>
<td>Compressibility of Hydrated and Anhydrous Sodium Silicate-based Liquids and Glasses, as Analogues for Natural Silicate Melts, by Brillouin Scattering Spectroscopy</td>
<td>October 31, 2005</td>
</tr>
<tr>
<td>R. Clark</td>
<td>Morgan Crucible</td>
<td>Diamond analysis</td>
<td>November 3, 2005</td>
</tr>
<tr>
<td>E. Surber</td>
<td>University of Illinois Urbana-Champaign</td>
<td>Diamond cell work</td>
<td>November 7-14, 2005</td>
</tr>
<tr>
<td>J. Butler</td>
<td>Naval Research Lab. Smithsonian Institution</td>
<td>Diamond analysis</td>
<td>November 8, 2005</td>
</tr>
<tr>
<td>J. Post</td>
<td>Naval Research Lab.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q. Peng</td>
<td>University of Connecticut</td>
<td>Localization of plastic shear events in glassy materials</td>
<td>November 17, 2005</td>
</tr>
<tr>
<td>J. Feldman</td>
<td>Naval Research Lab. George Mason University</td>
<td>Hydrogen</td>
<td>November 17, 2005</td>
</tr>
<tr>
<td>E. V. Tisper</td>
<td>Naval Research Lab.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nathalie Bolfan-Casanova</td>
<td>Laboratoire Magmas et Volcans</td>
<td>Water in the Earth’s mantle</td>
<td>December 12-13, 2005</td>
</tr>
<tr>
<td>D. Andrault</td>
<td>Institut de hysique du Globe du Paris</td>
<td>Mineral properties at high pressure and temperature</td>
<td>December 13, 2005</td>
</tr>
<tr>
<td>Wendy L. Mao</td>
<td>LANL</td>
<td>Hydrogen storage and D$^o$ collaboration projects</td>
<td>December 27, 2005-January 8, 2006</td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Topic</td>
<td>Date</td>
</tr>
<tr>
<td>--------------</td>
<td>----------------------------------</td>
<td>----------------------------------------------------------------------</td>
<td>------------------</td>
</tr>
<tr>
<td>Michelle</td>
<td>University of California – Los</td>
<td>Investigating the mechanical properties of self-organized nanomaterials and new ultra-incompressible superhard materials</td>
<td>January 4-11, 2006</td>
</tr>
<tr>
<td>Weinberger</td>
<td>Angeles</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Min Ouyang</td>
<td>University of Maryland – College</td>
<td>Nanospintronics: quantum mechanics, nanomaterial synthesis and device discovery</td>
<td>January 5, 2006</td>
</tr>
<tr>
<td>College Park</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K. Delaney</td>
<td>University of Illinois, Urbana-Champaign</td>
<td>Simulating the behavior of hydrogen fluid at high pressure</td>
<td>January 12, 2006</td>
</tr>
<tr>
<td>R. Clark</td>
<td>Morgan Crucible</td>
<td>Diamond analysis</td>
<td>January 12, 2006</td>
</tr>
<tr>
<td>T. Autrey</td>
<td>Pacific Northwest National Library</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Chellappa</td>
<td>University of Nevada – Reno</td>
<td>Raman work on aluminum hydrides</td>
<td>February 8-24, 2006</td>
</tr>
<tr>
<td>Tanja Cuk</td>
<td>Stanford University</td>
<td>Hi Tc superconductors under pressure transport properties</td>
<td>February 6-April 24, 2006</td>
</tr>
<tr>
<td>R. Hamburg</td>
<td>University of Illinois</td>
<td>Diamond analysis</td>
<td>February 21, 2006</td>
</tr>
<tr>
<td>R. Spirto</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Boone</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Walters</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K. Esler</td>
<td>Talk on quantum Monte Carlo methods for simulating matter under extreme conditions</td>
<td>February 23, 2006</td>
<td></td>
</tr>
<tr>
<td>J. Lucek</td>
<td>Diamond Innovations</td>
<td>Diamond analysis</td>
<td>February 27, 2006</td>
</tr>
<tr>
<td>Wren Montgomery</td>
<td>University of California – Berkeley</td>
<td>Talk on high-pressure prebiotic chemistry</td>
<td>February 27, 2006</td>
</tr>
<tr>
<td>Liping Huang</td>
<td>University of Michigan</td>
<td>Talk on demystifying the behaviors of network-forming systems under extreme conditions</td>
<td>February 28, 2006</td>
</tr>
<tr>
<td>Yufei Meng</td>
<td>Sun Yat-sen University</td>
<td>Talk on defects and coloration mechanism of brown diamond</td>
<td>March 7-14, 2006</td>
</tr>
<tr>
<td>D. Lakshtanov</td>
<td>University of Illinois Urbana-Champaign</td>
<td>Gas loading</td>
<td>March 9, 2006</td>
</tr>
<tr>
<td>M. Newton</td>
<td>University of Warwick Naval</td>
<td>Diamond analysis</td>
<td>March 10, 2006</td>
</tr>
<tr>
<td>J. Butler</td>
<td>Research Lab.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Reiclin</td>
<td>National Science Foundation</td>
<td>Diamond analysis</td>
<td>March 10, 2006</td>
</tr>
<tr>
<td>Kristina</td>
<td>University of Nevada – Las Vegas</td>
<td>Lab visit after APS meeting</td>
<td>March 17, 2006</td>
</tr>
<tr>
<td>Lipinska-Kalita</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Patricia Kalita</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C. L. Gobin</td>
<td>C. L. Gobin</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wendy Mao</td>
<td>LANL</td>
<td>Hydrogen storage and D collaboration projects</td>
<td>April 5, 2006</td>
</tr>
<tr>
<td>L. Bildsten</td>
<td>University of California – Santa</td>
<td>Physics of white dwarfs</td>
<td>April 17, 2006</td>
</tr>
<tr>
<td>J. Palfreman</td>
<td>Palfreman Film Group</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Nugent</td>
<td>Chicago Tribune</td>
<td>Interview with R. J. Hemley</td>
<td>May 4, 2006</td>
</tr>
<tr>
<td>D. Dlott</td>
<td>University of Illinois Urbana-Champaign</td>
<td>Talk on vibrational spectroscopy with high time and space resolution</td>
<td>May 8, 2006</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Speaker</td>
<td>Affiliation</td>
<td>Topic</td>
<td>Date</td>
</tr>
<tr>
<td>-------------------------</td>
<td>------------------------------------------------------</td>
<td>----------------------------------------------------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>J. Hwang</td>
<td>Taiwan University</td>
<td>Diamond analysis</td>
<td>May 9-11, 2006</td>
</tr>
<tr>
<td>C. Chu</td>
<td>University of Chicago</td>
<td>Pulsed laser system</td>
<td>May 25, 2006</td>
</tr>
<tr>
<td>T. Baofang</td>
<td>Rensselaer Polytechnic Institute</td>
<td>Talk on following biofuels to the extreme</td>
<td>May 26, 2006</td>
</tr>
<tr>
<td>J. Chang</td>
<td>University of Arizona</td>
<td>Talk on hydrogen storage in clathrate</td>
<td>May 31-June 2, 2006</td>
</tr>
<tr>
<td>W. Holder</td>
<td>Wesleyan University</td>
<td>Tour of the Geophysical Laboratory</td>
<td>June 16, 2006</td>
</tr>
<tr>
<td>Y. Ma</td>
<td>Texas Tech University</td>
<td>Laser heating</td>
<td>July 7-24, 2006</td>
</tr>
<tr>
<td>A. C. Kollias</td>
<td>University of California – Berkeley</td>
<td>Extending accuracy of QMC from total energies to observables and small differences of energies</td>
<td>August 1, 2006</td>
</tr>
<tr>
<td>I. Khodakovsky</td>
<td>University of Dubna</td>
<td>Library research</td>
<td>August 14, 2006</td>
</tr>
<tr>
<td>A. Prisco</td>
<td>GI Corporation</td>
<td>Diamond analysis</td>
<td>August 14, 2006</td>
</tr>
<tr>
<td>R. Gat</td>
<td>GI Corporation</td>
<td>Diamond analysis</td>
<td>August 15, 2006</td>
</tr>
<tr>
<td>C. Hill</td>
<td>Penn State Electro-Optics Center</td>
<td>Diamond analysis</td>
<td>August 29, 2006</td>
</tr>
<tr>
<td>C. Tulk</td>
<td>Oak Ridge National Laboratory</td>
<td>SNAP update</td>
<td>September 12, 2006</td>
</tr>
<tr>
<td>S. Chae</td>
<td>University of Uppsala</td>
<td>Gas loading ammonia</td>
<td>September 21-22, 2006</td>
</tr>
<tr>
<td>J. Molaison</td>
<td>HPCAT</td>
<td>Helium gas loading</td>
<td>September 26-27, 2006</td>
</tr>
<tr>
<td>A. Martinez</td>
<td>Opticut, Inc.</td>
<td>Diamond cutting</td>
<td>September 29-October 2, 2006</td>
</tr>
<tr>
<td>Svetlana Kharlamov</td>
<td>Argonne National Laboratory</td>
<td>Sample preparation in DAC for synchrotron experiments</td>
<td>October 2-October 4, 2006</td>
</tr>
<tr>
<td>W. Sturhahn</td>
<td>Argonne National Laboratory</td>
<td>Talk on sound velocities of iron-bearing Earth materials under extreme conditions</td>
<td>October 9-October 10, 2006</td>
</tr>
</tbody>
</table>

### 3.7 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.

<table>
<thead>
<tr>
<th>Speaker</th>
<th>Affiliation</th>
<th>Topic</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>N. Nath</td>
<td>Physics Dept., Indian Institute Of Technology, Kanpur</td>
<td>Interlayer exchange coupling in Fe/Nb multilayers</td>
<td>September 29, 2005</td>
</tr>
<tr>
<td>Y. Zhao</td>
<td>LANL</td>
<td>Superhard materials</td>
<td>October 14, 2005</td>
</tr>
<tr>
<td>L. Shi</td>
<td>George Mason University</td>
<td>Superconductivity of alkali metals under high pressure and revisions of Harrison's tight-binding theory</td>
<td>October 20, 2005</td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Topic</td>
<td>Date</td>
</tr>
<tr>
<td>-----------------------</td>
<td>------------------------------------</td>
<td>----------------------------------------------------------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>S. N. Tkachev</td>
<td>Hawaii Institute of Geophysics and Planetology</td>
<td>Compressibility of hydrated and anhydrous sodium silicate-based liquids and glasses, as analogues for natural silicate melts, by Brillouin scattering spectroscopy</td>
<td>October 31, 2005</td>
</tr>
<tr>
<td>E. Surber</td>
<td>University of Illinois Urbana-Champaign</td>
<td>Surfaces and interfaces of high explosives probed by nonlinear spectroscopy</td>
<td>November 8, 2005</td>
</tr>
<tr>
<td>Q. Peng</td>
<td>University of Connecticut</td>
<td>Localization of plastic shear events in glassy materials</td>
<td>November 17, 2005</td>
</tr>
<tr>
<td>Sara Seager</td>
<td>Carnegie</td>
<td>Interiors of low-mass exoplanets</td>
<td>December 1, 2005</td>
</tr>
<tr>
<td>M. Ouyang</td>
<td>University of Maryland – College Park</td>
<td>Nanospintronics: quantum mechanics, nanomaterial synthesis and device discovery</td>
<td>January 5, 2006</td>
</tr>
<tr>
<td>Michelle Weinberger</td>
<td>UCLA</td>
<td>Investigating the mechanical properties of self-organized nanomaterials and new ultra-incompressible superhard materials</td>
<td>January 10, 2006</td>
</tr>
<tr>
<td>Kris Delaney</td>
<td>University of Illinois Urbana-Champaign</td>
<td>Simulating the behavior of hydrogen fluid at high pressure</td>
<td>January 12, 2006</td>
</tr>
<tr>
<td>Jennifer Jackson</td>
<td>Carnegie</td>
<td>Melting investigations of iron at high-pressure using synchrotron Mossbauer spectroscopy</td>
<td>January 27, 2006</td>
</tr>
<tr>
<td>T. Autrey</td>
<td>Pacific Northwest National Library</td>
<td>Mechanistic studies of molecular hydrogen formation from borane ammonia complexes</td>
<td>February 2, 2006</td>
</tr>
<tr>
<td>S. Tkachev</td>
<td>Carnegie</td>
<td>Brillouin spectroscopy studies of hydrated and anhydrous sodium</td>
<td>February 22, 2006</td>
</tr>
<tr>
<td>K. Esler</td>
<td>University of Illinois</td>
<td>Quantum Monte Carlo methods for simulating matter under extreme conditions</td>
<td>February 23, 2006</td>
</tr>
<tr>
<td>P. Beck</td>
<td>Carnegie</td>
<td>Martian and chondritic meteorites impact record</td>
<td>February 24, 2006</td>
</tr>
<tr>
<td>Wren Montgomery</td>
<td>University of California – Berkeley</td>
<td>High-pressure prebiotic chemistry</td>
<td>February 27, 2006</td>
</tr>
<tr>
<td>Liping Huang</td>
<td>University of Michigan</td>
<td>Demystifying the behaviors of network-forming systems under extreme conditions</td>
<td>February 28, 2006</td>
</tr>
<tr>
<td>Angele Ricolleau</td>
<td>Inst. Phys du Globe</td>
<td>Subduction of the oceanic crust in the Earth's lower mantle; a petrological study</td>
<td>March 8, 2006</td>
</tr>
<tr>
<td>Yufei Meng</td>
<td>Sun Yat-sen University</td>
<td>Defects and coloration mechanism of brown diamond</td>
<td>March 10, 2006</td>
</tr>
<tr>
<td>M. Newton</td>
<td>University of Warwick</td>
<td>Studies of defects in diamond</td>
<td>March 10, 2006</td>
</tr>
<tr>
<td>C. Glass</td>
<td>ETH, Zurich</td>
<td>USPEX - Predicting crystal structures of new phases</td>
<td>March 23, 2006</td>
</tr>
<tr>
<td>S. Vance</td>
<td>University of Washington</td>
<td>Physical chemistry, fluid dynamics, and the search for life in extraterrestrial oceans</td>
<td>March 24, 2006</td>
</tr>
<tr>
<td>J. Xu</td>
<td>Carnegie</td>
<td>Moissanite anvils and anvil pressure cells used in neutron diffraction</td>
<td>March 31, 2006</td>
</tr>
</tbody>
</table>
4. TECHNOLOGY DEVELOPMENT

4.1 High P-T Experimental Techniques

Heating and Spectroscopic Methods – An important part of the CDAC mission has been the advancement of high-temperature/high pressure techniques by bringing together the technical strengths from academic and the National Labs (both NNSA and other DOE Labs). Indeed, the many advances in dynamic ultrahigh-pressure techniques such as laser driven shocks produced from intense laser sources\textsuperscript{137, 138}, gas-guns\textsuperscript{139}, and magnetic compression methods\textsuperscript{140} and continued refinements of DAC techniques at the NNSA Labs form a natural complement to activities within CDAC\textsuperscript{141, 142}. Advances made in high-temperature methods at ultrahigh pressure are providing new links to dynamic compression experiments. The Nd-YLF double-sided laser method\textsuperscript{143, 144} has been extended to include CO\textsubscript{2} laser heating as well as simultaneous Raman spectroscopy\textsuperscript{45, 145}, and this technique has become routine in a number of laboratories, among them the groups of Choong-shik Yoo and Joe Zaug/Jonathan Crowhurst at LLNL, and the CDAC group at Carnegie.

Laser heating in the DAC has been further developed by Alexander Goncharov (Carnegie) to allow in situ Raman studies to higher temperatures. Various coupler materials and configurations were tested, that allow performing several runs in simple molecular materials (H\textsubscript{2} and N\textsubscript{2}) to approximately 1000 K and 60 GPa. Also different thermal insulations are being tested. This work is in progress. In addition, a pulsed Raman apparatus has been constructed at Carnegie\textsuperscript{17}. The latter provides a substantial suppression of the thermal radiation, so experiments to higher temperatures will be feasible. A pulsed heating technique with 10 ns pulsed YAG laser is being developed. This technique allows reaching high temperatures in a short period of time, so the experiments can be performed in a time domain, reducing the risk of chemical reactivity. This development is also in progress. Data from nuclear resonant inelastic scattering measurements show that the Planck function and the temperature as measured by NRIXS are good agreement up to at least 1700 K\textsuperscript{146}, indicating that spectroradiometric determination of the temperature is reliable. Meanwhile, resistively-heated DACs, which provide a temperature accuracy of ±5 K, have been extended to above 1000 K at megabar $P$, even for hydrogen\textsuperscript{147}. The state of the art in this technique is undergoing a period of rapid change at Carnegie as well under the leadership of CDAC research scientists Maddury Somayazulu and Chang-Sheng Zha, who are leading the development of new cell designs for use in a variety of x-ray and optical spectroscopy experiments. Available sample
volumes continue to increase with improvements in gasketing methods now in use at a number of CDAC nodes.\textsuperscript{148, 149}

Rotational DAC (RDAC) studies were discussed in Section 2.1. Since the RDAC possesses the advantages a DAC — flexible, compact, and light-weight — along with the unique function of generating shear stress and strain, it may well be expected that the rotational diamond anvil to become one of the most powerful methods in the exploration of materials under pressure and shear. The technology can be extensively utilized to explore the effect of shear stress, pressure and temperature of a variety of materials.

Non-linear optical methods developed at Illinois, including the recent breakthrough in the use of vibrational sum-frequency generation (SFG) to probe molecules at interfaces, are undergoing continuous development and are being applied to high-pressure problems. Now in its second generation, the technique can now be applied to investigate the structure, chemistry and aging properties of molecules at interfaces and crack propagation relevant to stockpile stewardship. Much of this work will set the stage for new advances in high-pressure materials science, including the use of free-electron lasers and combined static/laser shock methods.

At Carnegie, Brillouin spectroscopy has been an important technique for measuring subtle structural effects at high pressure. During Year 3, the spectrometer was completely upgraded under the direction of Muhetaer Ahart, the most important new feature being an acoustic modulator and double shutters at the entrance to the scattering pass, which make it possible to reduce the elastically scattered (Rayleigh) light, and which now allows the use of the Rayleigh light to control the stabilization system. The control units, photon-counting system, and all the piezo-devices have been upgraded or replaced, so now the detected signal can be obtained from the control unit directly. Since the installation of these upgrades, the acquisition time for Brillouin spectra has decreased by an order of magnitude (e.g., tens of minutes to a few minutes). These improvements should bring the technique firmly into the array of capabilities available to the CDAC membership.

\textbf{CVD Diamond} – The most important breakthroughs in the area of technology development have been in the area of epitaxial CVD diamond growth, where the Carnegie group has continued to perfect processes for the fabrication of single crystal diamond by the microwave plasma CVD process. The primary effort during the past year has been on increasing growth rates, which now are consistently 50-200 \(\mu\)m/hr, based on the quality of the diamond produced. Now the Carnegie group can routinely produce 10-carat, half-inch thick single-crystal diamonds of varying quality (Fig. 31). An important factor in the success of the CVD process was the close collaboration with a group from LANL early on in the CDAC program.\textsuperscript{150} As grown, the material has high fracture toughness and upon high temperature/high pressure annealing (a process also developed and perfected at Carnegie) its hardness can increase dramatically, reaching values some 50% higher than conventional diamond.\textsuperscript{150} During the first year of our program CDAC graduate student Wendy Mao, now at LANSCE/LANL, showed that the new diamond can be used to generate multimegabar pressures.\textsuperscript{151} Additional studies of the strength and annealing effects were also carried out this year by undergraduate summer intern Cheng Chin, who applied novel spectroscopic methods that had been pioneered in the Carnegie labs.\textsuperscript{152} The team has also made colorless single-crystal diamonds, transparent from the ultraviolet to infrared wavelengths with their CVD process.\textsuperscript{153, 154}

Yogesh Vohra’s group at the University of Alabama-Birmingham continues to develop complementary designer anvil technology as part of CDAC. An isotopically enriched \textsuperscript{13}C homoeptaxial diamond layer of 6±1 microns thickness was grown on top of a brilliant cut diamond anvil by a microwave plasma chemical vapor deposition process for application as a pressure sensor. Figure 49 shows the isotopically enriched \textsuperscript{13}C beveled diamond anvil employed in high pressure experiments to 156 GPa. This isotopically enriched diamond tip was then used in conjunction with a natural isotopic abundance diamond anvil to generate high pressure on the sample. This group provided a calibration for the \textsuperscript{13}C Raman mode of this extremely thin epitaxial layer to 156 GPa using ruby fluorescence and the EOS of copper as secondary pressure standards. The nonlinear calibration of the \textsuperscript{13}C Raman mode pressure sensor is compared with similar calibrations of \textsuperscript{12}C.
Raman edge and a good agreement is obtained. The Raman signal from the $^{13}$C epitaxial layer remained a distinct singlet to 156 GPa and pressure calibration is independent of sample mechanical strength or the diamond anvil geometry. The use of an even thinner layer would allow calibration further into the ultra high pressure regime where use of other optical sensors has proven to be difficult.

**High-Pressure Magnetic and Electronic Measurements** – At Carnegie, Viktor Struzhkin has pioneered both high-pressure Kβ x-ray fluorescence and high-pressure Mössbauer spectroscopy, which complement magnetic susceptibility measurements. Measurements of Kβ x-ray fluorescence in Fe$_3$O$_4$ (magnetite) to 80 GPa, show clear evidence of spin collapse at 60 GPa, compatible with available Mössbauer data. Further improvements in nuclear inelastic resonant x-ray scattering allow measurements of the phonon density of states (Fe) or the partial phonon density of states (FeO) over a broad pressure range up to 150 GPa, including diluted systems. Similar measurements could give information on the valence band behavior in other correlated transition metal oxides.

**Struzhkin** is also exploring the possibilities of combining laser heating, external heating, and low-temperature cryostat techniques at Sectors 3 and 16 at APS (Argonne) to extend the $P$-$T$ range currently available for synchrotron Mössbauer techniques. The group is able to reach 200 GPa at 300 K, 2500 K at 90 GPa, using DAC technique. Low-temperature measurements have been conducted down to 10-20 K on the Bi$^{57}$FeO$_3$ single crystal sample in He pressure medium through the spin-crossover transition.

Measurements of electrical resistance in a sample at high pressure are still very challenging, despite the progress made over the past several years. The Carnegie group is developing the technique to make good quality ohmic contacts to a sample in DAC using the focused ion beam (FIB) instrument at the Stanford Nanofabrication Facility (in collaboration with Professor Zhi-Xun Shen and graduate student Tanja Cuk of Stanford University). Nanofabrication techniques will allow better control over sample preparation and also will make possible much smaller samples suitable for multimegabar transport measurements. We also established a collaboration with the FIB facility at the University of Maryland, close to our Washington, DC campus (Fig. 50).
Figure 50. Preparation of diamond anvils for electrical resistivity measurements. Top: Focused Ion Beam deposition of the electrodes on the diamond anvils (University of Maryland). Bottom: Sample of a Bi-based high temperature superconductor on top of diamond anvil in contact with electrodes. Bottom left: sample before application of pressure. Bottom right: Sample in Ar pressure medium at 40 GPa.

At Carnegie, the Struzhkin group also combined optical spin resonance techniques, including time resolved Faraday rotation spectroscopy (TFRF), with DAC methods to investigate semiconductor quantum dots. These materials (QDs) are attractive candidates for scalable solid state implementations of quantum information processing based on their electron spin states. The detailed spin properties of QDs will strongly depend on the quantum confinement effect. For example, confined carriers in QDs are relatively decoupled from their dissipative environment as compared with systems of higher dimensionality, such as quantum well, which are expected to inhibit spin relaxation processes and result in extended spin coherence times. In addition, the electronic and excitonic Lande g-factors of QDs showed strong dependence on their sizes. Such quantum confinement effects can be directly engineered by the reduction in inter-atomic lattice constants through the application of hydrostatic pressure. The group has carried out measurements to explore the effect of high pressure on spin coherence dynamics on CdSe QDs, building up

Figure 51. Top: TRFR spectrum of 6.8nm CdSe QDs at 1.0GPa (open circles). The oscillatory behavior can be well described by the exponentially decaying Larmor precession of electron and exciton spins (red curve). Bottom: pressure dependence of electronic and excitonic g-factors of 4nm CdSe QDs revealing a sudden increase of g-factors at high pressure.
towards investigations of new types of semiconductor quantum structures and some preliminary results were shown in Fig. 51. The mechanism of such a spin-pressure dependence is currently under investigation. The results of this research will not only be of great fundamental interest, enabling tuning spin properties to be closely correlated with structural changes, but they may also have direct implication of QD-based device applications by revealing the stability of spin properties under extreme conditions.

4.2 Facilities at Brookhaven, LANSCE, and Carnegie

High-pressure IR measurements are becoming an increasingly important part of the CDAC research effort, and one of the techniques with which CDAC is growing the high-pressure material science community. The Carnegie group developed the field of high-pressure synchrotron IR micro-spectroscopy, which takes advantage of the enormous flux advantage of synchrotron radiation at long wavelengths relative to conventional broad band sources, to address geophysical problems. Now, however, the recently upgraded U2A beamline at the NSLS, which is also managed and operated by this group with support from CDAC funds, features a custom-built long working distance IR microscope for diffraction-limited high P-T studies, and an optical/Raman grating spectrometer system with Ar, Kr, and Ti-sapphire lasers. Under CDAC, NNSA Labs have become 20% members of the U2A PRT. As needs arise, experiments can be carried out at beamline X17C and the newly created beamline X17B3 for high P-T diffraction. These diffraction facilities were previously managed by Carnegie under the NSF COMPRES consortium, but are now managed by the CARS group at Chicago. Both monochromatic and polychromatic diffraction can be performed with equipment that includes single-crystal and powder diffractometers, along with ruby luminescence systems for pressure measurement. The close working relationship between the CARS group at Chicago and the HPCAT group at Carnegie ensures that the facilities at X17 can be used at short notice. Both the x-ray and IR facilities are supported by a common sample preparation lab, and together they allow state-of-the-art diffraction and IR/Raman/optical spectroscopy to be performed on-site on the same samples.

**Figure 52. Optical layout of the Synchrotron Infrared U2A beamline. Inset: U2A beamline optical hutch.**

**High P-T Neutron Scattering** – Neutron-based probes have several unique advantages for the study of materials, particularly those of importance for stockpile stewardship, and are complementary to synchrotron x-ray and laser optical probes. A key part of the CDAC program from the beginning has been to support the development of high-pressure neutron scattering at LANSCE. Since that time, Rudy Wenk's group at Berkeley has been working to develop standard procedures for direct image analysis of synchrotron diffraction data with the Rietveld method. At
LANL, the group initially investigated texture changes taking place during phase transformations of hexagonal metals\textsuperscript{34, 35, 164}. A significant portion of the thesis work of CDAC graduate student Jenny Pehl was concerned with advancing the methods of quantitative data analysis\textsuperscript{44}, which she did in collaboration with LANSCE staff members Sven Vogel and Darrick Williams. Current CDAC graduate student Lowell Miyagi is continuing this work, and is addressing phase transformations under applied as well as residual stress. The $\alpha$–$\beta$ quartz transformation was originally used as a model system, with the results extended to other systems such as but also applying it to metals such as iron\textsuperscript{33}, and important Earth materials such as magnesiowustite\textsuperscript{165}, and silicate perovskites\textsuperscript{98}. This research will continue in Year 4\textsuperscript{166-168}. New CDAC academic partner Kanani Lee from New Mexico State University is currently utilizing the LANSCE facility to investigate the effects of pressure on rates of radioactive decay.

The Spallation Neutron Source (SNS) at ORNL, which will be completed in 2007, will be the world’s most powerful neutron source, and CDAC is poised to take advantage of the facility’s capabilities. The Carnegie group and scientists at Stony Brook (led by John Parise) and ORNL (led by Christopher Tulk), are involved in the planning and construction of the dedicated high-pressure instrument (SNAP), which is one of the second set of instruments to be approved and funded. The project’s goal is to create new classes of instrumentation to utilize the extraordinary neutron flux of the SNS, develop state-of-the-art high-pressure devices for the facility, and advance the pressure range of neutron studies beyond present limits (tens of GPa) and improve sample size by orders of magnitude. The project is in Year 3 of its five-year plan, and the project is on schedule. At the third annual SNAP meeting held in April 2006 at the SNS, CDAC was represented by Carnegie’s Jian Xu, who presented the latest progress in neutron diffraction pressure cell development. CDAC academic partner Brent Fultz (Caltech) is also the PI on the ARCS spectrometer, which is also in the first group of instruments to be brought on line at the SNS.

The Carnegie labs are continuing to upgrade existing facilities for use by the broader high pressure community. Upgraded spectroscopic facilities include improved capabilities for laser heating (Fig. 55) as well as those for Raman, IR and Brillouin measurements, all made possible through the CDAC grant. Support facilities such as the gas loading and diamond cell preparation

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure53.png}
\caption{Layout for SNAP, the high-pressure instrument and beamline being created at the Spallation Neutron Source. There is close collaboration with the high-pressure program at the Lujan Center at LANSCE, where tests of components are taking place.}
\end{figure}
labs, have also undergone minor renovations over the last year under the CDAC grant. Additional developments were made in the Carnegie GHz ultrasonics laboratory (Fig. 54) and the CVD anvil facility, where a laser cutting and shaping system (Bettonville) has been installed. These improvements were supported by other grants and by Carnegie funds.

Figure 54. GHz-ultrasonic interferometer at Carnegie. Pictured clockwise from lower left are: 18-GHz mainframe sampling oscilloscope, 2-GHz RF generator, 6-GHz RF generator with internal pulse modulator, external pulse modulator (top), optical microscope for buffer-rod alignment, with diamond cell beneath objective, connected to the oscilloscope channel set. GHz-ultrasonic interferometry has been made possible through high-speed RF and microwave technologies developed during the telecom boom.

Figure 55. Facilities at Carnegie Top left: Maddury Somayazulu in the gas loading laboratory; top right: Jinfu Shu in the sample preparation laboratory; bottom left: Alexander Goncharov in the laser heating laboratory; bottom right: former CDAC predoctoral associate Shih-Shiue Ho (now at Case Western University) in the CVD diamond facility.

4.3 Commissioning Activities at HPCAT

A significant portion of the CDAC budget has gone to obtaining a 30 percent share of member beam time at HPCAT, where commissioning activities are now nearing completion (Fig. 56). Insertion device beamlines ID-B (monochromatic powder diffraction) and ID-D (spectroscopy) have been operating in general user mode for nearly three years, and now the bending magnet beamlines have started accepting general user proposals through the APS system. Both BM-B and BM-D will focus on white beam diffraction, and both will have single crystal diffraction capabilities, in addition to serving as routine powder diffraction instruments. Stations BM-B, BM-D and ID-D are currently capable of handling cryostats for low-temperature work down to liquid helium temperatures, and station ID-B will soon have this capability as well. Laser heating is operating routinely in ID-B for high pressure diffraction measurements, and the long-term plan is to have laser heating available for x-ray spectroscopy experiments in ID-D as well. Online ruby/Raman systems are now being
installed on the bending magnet beamlines, and will soon be available on the ID beamlines as well. Now that there will be four simultaneously operating experimental stations at the HPCAT facility, a series of “Technical Briefs” detailing the capabilities of each of the stations are currently being prepared and will be posted on the CDAC web site so that the CDAC community will have access to updated information on each of the beamlines. This will help the research groups make optimal choices of the beamlines for their research projects. Reviews of the use of synchrotron facilities to study materials under extreme conditions, show the dramatic progress that has been made in this area of research over the past few years169, 170.

![Facilities at HPCAT](image)

**Figure 56.** Facilities at HPCAT. Top left: 16ID-D; top right: 16ID-B; bottom left: Raman system; bottom right: laser heating system.

**Peter Liermann**, the beamline scientist at HPCAT who is leading the efforts at station BM-D, has commissioned the beamline as a white beam station but will add monochromaters for operating in large energy ranges in the near future. During commissioning on BM-D, a 5µm x 5 µm focal spot at the sample position has been routinely achieved. This group has carried out a number of studies at low temperatures (using a flow type liquid He cryostat) and plans to develop resistively heated diamond cell capabilities in the near future. The BM-D station has an on-line Raman system capable of measuring ruby luminescence, Raman and spectroradiometry without moving the sample. To accommodate the single crystal Laue techniques being developed, an on-line CCD is being integrated into the experimental setup. This will therefore be the only station that is capable of doing both white beam and monochromatic diffraction in powders and single crystals at extreme pressures and temperatures.

5. INTERACTIONS WITH NNSA/DP LABORATORIES

5.1 Overview

One of the goals of CDAC is to provide access to the state-of-the-art facilities maintained by the groups of our academic partners, including synchrotron beamlines and the CDAC high-pressure
labs. CDAC members are encouraged to meet at the regularly scheduled HPCAT meetings at APS. There are also frequent visits to National Labs, university nodes, or Carnegie for planning and coordination of efforts, integration of results, integration with ASC, and other stockpile stewardship programs. In all cases, travel support for graduate students has been provided from the core CDAC budget. The CDAC Summer School of Year 2, and the SSAAP Symposium in Year 1 (Albuquerque) and Year 2 (Las Vegas) SSAAP Symposium and Synergy of 21st Century High-Pressure Science and Technology Workshop (Section 3.5) of Year 3 discussed in Section 3.5 were highly successful ventures from the CDAC perspective, in that they in have all provided a forum in which possible research collaborations between graduate students from academic groups and NNSA Lab personnel were explored.

- **Experiments performed at HPCAT.** The integrated HPCAT facility has all four of its experimental stations operating in general user mode, providing an excellent forum for people with many different areas of expertise to interact and initiate new research directions. Records of visits by NNSA Labs, CDAC academic partners, CDAC collaborators, and other users are listed below in Appendix II.

- **Technique development and training at Carnegie.** During Year 3, a total of 42 different scientists came to Carnegie for periods of one day to several weeks, for training, sample preparation or to perform specific measurements in the high-pressure laboratories. Continuous technique development brings numerous people to Carnegie and serves as a focus for interactions among new and experienced researchers. This has been enhanced by the additional office and lab space provided by the Institution.

- **Visits to other facilities.** The Carnegie synchrotron IR beamline (U2A) continues to be useful platform for interactions. Users from a variety of disciplines within the structure of CDAC have used the facility in the past year; lists of users at U2A are reported in Appendix II. The first SNAP workshop took place at LANL in April 2004. The second was held at the Spallation Neutron Source (SNS) in June 2005, and the latest was held at the SNS in April 2006. The meetings were attended by a number of CDAC academic partners, laboratory partners and collaborators. A number of new collaboration possibilities were also discussed.

- **Annual meetings and summer schools.** The SSAAP annual meetings (March 2004, Albuquerque and August 2005, Las Vegas) have both been very well-attended and were highly productive as forums where CDAC partners, students, post-doctoral fellows, and staff were able to discuss research directions and initiate collaborative efforts. The 2005 CDAC Summer School and 2006 Synergy of 21st Century High-Pressure Science and Technology Workshop both brought a many graduate students together with CDAC partners and collaborators to discuss current directions in high pressure research of interest to stockpile stewardship science.

- **Experiments performed at NNSA/DP facilities.** Proposed experiments at unique facilities in the NNSA/DP Labs will provide opportunities for scientific exchange in addition to training of students. The most notable example is the extensive use of LANSCE (Lujan Center) by CDAC students, postdoctoral fellows, and staff for high-pressure neutron scattering. An exciting initiative that emerged last year is the implementation of the new CVD diamond technology at Z and possible combined static/dynamic compression experiments there. CVD initiative with SNL began in Year 1 and continued into Year 2 with the award of an LDRD to the SNL for this work. In addition, planning began in Year 3 for laser shock experiments to be carried out at the APS (diffraction diagnostics) and U2A (infrared diagnostics). Currently, the projects are in the feasibility study stage, but work continues in an effort to bring the shock compression and static compression communities closer together, as stated in the CDAC mission.

The CDAC website, located at [http://www.cdac.gl.ciw.edu](http://www.cdac.gl.ciw.edu), serves as a primary source of information to the CDAC community and the public (Fig. 57). Featuring an array of scientific and technical developments, meeting announcements and links, beam time updates, the site serves as a “window to the world” of high-pressure research not only at CDAC, but throughout the US and
CDAC beam time is allocated based on the membership shares of each of the contributing members. At this point, all four experimental stations are fully commissioned and are accepting users through the General User Proposal program at the APS as well as from the member partners. 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%), University of Nevada-Las Vegas (25%). At this point, that means approximately 30-35 shifts per beamline in a typical run period (about 200 shifts total) will go to CDAC academic partners and their students, along with National Laboratory partners. During Year 3, 37 proposals were submitted for beam time through CDAC (26 from National Lab scientists and 11 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. In the future, it will most likely become necessary to award beam time to those proposals not awarded GUP time on a competitive basis. This will have the undesirable effect that good proposals will be denied around the world. Lists of all of the CDAC partners, scientists, and collaborators, as well as records of all applicable publications and abstracts can also be found on the CDAC website and are updated regularly. Several times a month, a new research highlight is posted on the website, detailing information on new papers or research breakthroughs that have been supported by CDAC. Technical notes on high pressure techniques, briefs on HPCAT and U2A experiments, and leading references in the high pressure field are also being prepared for the broader high pressure community.

5.2 Academic Alliance and Laboratory Collaborations

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 implementation of CDAC Phase II, 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 its ability to steer future developments at the facility.

Figure 57. Screen shot of the CDAC website, http://cdac.gl.ciw.edu
beam time, but that has not happened as yet. Having three experimental stations with diffraction capabilities will help keep beam time for the CDAC community quite available.

**LLNL** – The history of collaborations between Carnegie and members of the LLNL PAT Directorate H-Division, currently headed by Robert Cauble has continued. Within CDAC, the partnership through HPCAT has been expanded to include each of the groups within the division, as indicated by the support of group leaders Giulia Galli (now at University of California – Davis), Neil C. Holmes, Andy K. McMahan, John A. Moriarty, Choong-Shik Yoo, and David A. Young. Graduate students Amy Lazicki (UC-Davis) and Zsolt Janei (University of Stockholm) have also been involved with CDAC-related projects through HPCAT. There are specific individuals representing a variety of Directorates with special interests in various CDAC science projects including Jagan Akella, William Durham (now at MIT), William Evans, and Joe Zaug. People working on collaborations within CDAC or have interacted closely with CDAC scientists include Bruce Baer, Sorin Bastea, Larry Boercker, Stanimir Bonev (now at Dalhousie University), Brian Bonner, Ricky Chau, Jonathan Crowhurst, Hyunchae Cynn, Dan Farber, Larry Fried, Valentin Iota-Herbei, Jung-Fu-Lin (former Carnegie postdoctoral fellow and CDAC research scientist), Magnus Lipp, Riad Manaal, Andy McMahan, Jeff Nguyen, Tadashi Ogitsu, Jae-Hyun Park, Robert Rudd, and Eric Schwegler. CDAC is also actively involved in an initiative to develop new in situ x-ray probes in shock wave experiments; this effort involves G. W. (Rip) Collins, Damien Hicks, Jon Eggert, and Peter Cellers.

**LANL** – The unique neutron facilities at the Lujan Center of LANSCE will be combined with expertise and instrumentation developments of the alliance members in order to develop high-pressure neutron diffraction and scattering capabilities for stockpile stewardship, Lujan Center director Alan Hurd, and scientists Yusheng Zhao, Zhongwu Wang, Robert P. Currier, Luke L. Daemen, Konstantin Lokshin, Junhua Luo, Donald D. Hickmott, Wendy L. Mao, Robert McQueeney, and Robert von Dreele are participating in projects supported by CDAC. In particular, Rudy Wenk’s group at Berkeley has been instrumental in developing texture analysis capabilities at HIPPO. In addition to neutron scattering, Yusheng Zhao’s group has been collaborating with CDAC in characterizing the new CVD diamond material developed at Carnegie. Other LANL collaborators and contacts include William Anderson, Robert Hixson, Rachel Hixon, David Moore, and David Schiferl. Brent Fultz has collaborated for several years with scientists at the Lujan Center and MST, and Dana Dlott interacts regularly with David Moore and David Funk. Other LANL scientists involved in ongoing collaborations with CDAC include Robert Sander, Dana Dattlebaum, Neal Chesnut, Joanna Casson, Lilliana Sanchez, Aaron Koskelo, Luc Daemen, Konstantin Lokshin, Christian Pantea, Jiang Qian, Zhongwu Wang, Didier Saumon, University of Arizona graduate student Kimberly Tait and postdoctoral associate Kirill Zhuravlev.

**SNL** – There have been new initiatives proposed between the Carnegie group and George Samara’s group on piezoelectrics. At Carnegie, Ron Cohen and Muhetaer Ahart are collaborating with the SNL group on theory and experiments, respectively. Experiments carried out in Marcus Knudson’s group, including the isentropic compression experiments on the Z accelerator, provide a powerful complement to Carnegie’s DAC studies. The new diamond initiative with Daniel Dolan mentioned above has led to an LDRD grant at SNL and diamond substrates supplied to Carnegie for CVD diamond. The laser shock compression feasibility work carried out at BNL and mentioned above is providing another opportunity for interaction between the Lab and other parts of the CDAC community. Others investigating collaborative projects with CDAC personnel include Lalit Chabildas, Mike Furnish, and Tracy Vogler.

**Other Labs** – There are also collaborators at other national facilities and centers. We interact closely with HiPSec at the University of Las Vegas – Reno, which is directed by Malcolm Nicol. HiPSec is also a NNSA-supported member of HPCAT. The in situ x-ray shock wave initiative at HPCAT involves Yogendra Gupta at the Washington State University Institute of Shock Physics. Groups directed by J. Robertson (ORNL), Christopher Tulk (ONRL), Gene Ice
In addition to his work at LANSCE, Brent Fultz serves on the PAC for IPNS and is the PI for the ARCS spectrometer, to be one of the first five instruments at the SNS. As mentioned above, Russell J. Hemley and Ho-kwang Mao are co-PIs of the high-pressure instrument at the SNS (SNAP), which is in the second set of five beamlines to be built at the facility. CDAC provides a forum for interactions between NNSA/DP scientists and the wider academic community. Dudley R. Herschbach (Harvard University and Senior Fellow at Carnegie) is an active member of the CDAC community, as is Joe Feldman (formerly at the Naval Research Laboratory). Luca Lutterotti (Trento, Italy) and Siegfried Matthies (Dresden) continue to visit Berkeley to further develop the Rietveld texture code for quantitative analysis, and particularly refining it to study the elastic behavior of textured materials.\textsuperscript{163, 171, 172}

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 three years, the following former post-doctoral 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.

- Olga Degtyareva (University of Edinburgh; from Carnegie)
- Mark Frank (Northern Illinois University; from Carnegie)
- Eugene Gregoryanz (University of Edinburgh; from Carnegie)
- Jennifer Jackson (California Institute of Technology; from Carnegie)
- Steve Jacobsen (Northwestern University; from Carnegie)
- Boris Kieffer (New Mexico State; from Princeton)
- Jie Li (University of Illinois; 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 (Renssalaear 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

In this section, the management and oversight of CDAC, including the organizational structure and managerial activities of the past year, are reviewed.

6.1 CDAC Organization and Staff

The Center is 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. 58. 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, National Lab 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.
At Carnegie the CDAC staff consists of 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
- Premyslaw Dera  
  Crystallography
- Yingwei Fei  
  Geochemistry and Petrology
- Joe Feldman  
  Senior Visiting Fellow
- Alexander Goncharov  
  Optical Spectroscopy
- Dudley Herschbach  
  Senior Visiting Fellow
- Burkhard Militzer  
  Computational Theory
- Viktor Struzhkin  
  Electronic and Magnetic Properties

Joe Feldman, from the Naval Research Laboratory, came to Carnegie in January of 2006 as a Senior Visiting Fellow. He is collaborating with CDAC researchers on theoretical studies of the properties of hydrogen at high pressures and temperatures.

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

- Olga Degtyareva  
  Research Scientist (now at the University of Edinburgh)
- Stephen Gramsch  
  CDAC Coordinator/Research Scientist
- Morgan Phillips  
  Administrative Assistant
- Maddury Somayazulu  
  Lab Manager/Research Scientist
- Chang-Sheng Zha  
  Lab Manager/Research Scientist

In January of 2006, Olga Degtyareva took a position at the Centre for Science at Extreme Conditions at the University of Edinburgh, Scotland, joining former CDAC Research Scientist Eugene Gregoryanz. Chang-Sheng Zha joined CDAC as a Lab Manager/Research Scientist in April of 2006 and has been assisting Maddury Somayazulu with training CDAC visitors in state-of-the-art high pressure methods.

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

- Szczesny Krasnicki  
  (CVD diamond growth)
- Jinfu Shu  
  (sample preparation and powder diffraction)
• Jian Xu (neutron diffraction/cell development)
• Chih-shiue Yan (CVD diamond growth)

High-pressure facilities at NSLS are staffed by beamline scientists who support the CDAC effort. They are:

• Quanzhong Guo (X17B)
• Jingzhu Hu (X17C)
• Zhenxian Liu (U2A, salary partially supported by CDAC)

A number of predoctoral and postdoctoral associates at Carnegie supported by the Institution, other grants, or outside fellowships worked on CDAC tasks during Year 3. Their contributions also include training CDAC students and visitors in high-pressure experimental techniques:

• Muhetaer Ahart (Aihaiti)
• Pierre Beck
• Jinyang Chen (now at Shanghai University)
• Xiao-Jia Chen
• Jennifer Ciezak
• Yang Ding
• Shih-Shian Ho (now at Case Western University)
• Steven Jacobsen (now at Northwestern University)
• Jennifer Jackson
• Tim Jenkins
• Joseph Lai
• Yufei Meng
• Sergey Tkachev

At the end of 2005, Jinyang Chen returned to the School of Environmental and Chemical Engineering at Shanghai University, and Pierre Beck and Sergey Tkachev came to Carnegie from the ENS Lyon and the Hawaii Institute of Geophysics and Planetology, respectively, to begin work as Research Associates. Joseph Lai joined the CVD group from Florida State University. Shih-Shian Ho is now a doctoral student at Case Western University. In August 2006, Steven Jacobsen took a faculty position in the Department of Geological Sciences at Northwestern University. Jennifer Jackson will be starting as an assistant professor in Mineral Physics at the California Institute of Technology in November 2006.

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)
• Jon H. Egger (LLNL)
• Daniel Farber (LLNL)
• David Funk (LANL)
• Marcus Knudson (SNL)
• David Schiferl (LANL)
• Choong-shik Yoo (LLNL)
• 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 Hurd (LANL)
- Chi-chang Kao (Brookhaven)
- Christian Mailhiot (LLNL)
- George A. Samara (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 has renewed their commitment to serving through Year 4 of the CDAC program.

The 2005 Advisory Committee meeting was held on May 31, 2005 at HPCAT, in conjunction with the first CDAC Summer School. Six members of the Advisory Committee were present, along with Thomas Duffy and Dana Dlott (CDAC Academic Partners from Princeton University and University of Illinois, respectively) and Guoyin Shen from University of Chicago/GSECARS (now the HPCAT Project Manager). An overview of the activities from Year 2 was presented by Russell Hemley. Ho-kwang Mao presented a report on the scientific and technological developments that have occurred at HPCAT, and Stephen Gramsch presented a report on CDAC education and outreach. Discussions took place throughout and after the presentations. The advisory committee also considered the merits of the proposed expansion of CDAC to include four more academic partners, as well as an increased share of the HPCAT beam time. The reaction to the committee’s report to NNSA/SSAAP was extremely favorable, and at the beginning of Year 4, Phase II of the CDAC program was initiated.

### 6.3 Second Year Review

On September 22, 2005, the Year 2 CDAC Review was held at the Advanced Photon Source, Argonne National Laboratory. A morning session of presentations outlining the mission and scientific and technical scope of the CDAC effort was followed by a tour of the APS and HPCAT facilities and a poster viewing session. In the afternoon, presentations by a representative from each of the National Labs discussed ongoing and planned collaborations, and presentations by each of the academic partners provided an overview of scientific progress made during the year at their institutions.

**Review Presentations:**

- Russell J. Hemley (Overview)
- Ho-kwang Mao (HPCAT Scientific Overview)
- Guoyin Shen (HPCAT Technical Overview)
- Stephen Gramsch (Education, Training and Outreach)
- Choong-shik Yoo (LLNL)
- Dana Dattlebaum (LANL)
- Jianzhong Zhang (LANL)
- Daniel Dolan (SNL)
- Brent Fultz (Caltech)
- Dana Dlott (Illinois)
- Tom Duffy (Princeton)
- Dion Heinz (Chicago)
- Yogesh Vohra (Alabama-Birmingham)
- Hans-Rudolf Wenk (UC-Berkeley)
7. PLANS FOR YEAR 4 AND BEYOND

7.1 Scientific and Educational Focus

As we move forward into Year 4 of the CDAC program, we have made an effort to focus on key materials with special properties at high pressure and temperature, and will continue to extend the results we have reported on here. Support of graduate students will continue to be a primary goal of the program, and will expand to include a total of 20 students in the whole of the Center in Years 4 and 5. We will also continue our education and outreach efforts to sponsor student travel (not just for those in CDAC, but also for our collaborators and other students with an interest in the field), to meetings of direct interest to the high pressure materials science community. For example, CDAC will cosponsor SMEC2007, held in Miami, by supporting student travel and organizing the scientific meeting (more information on SMEC2007 can be found on the internet at http://www.cesmec.fiu.edu). We also plan to hold another version of our summer school during the upcoming program year. Finally, we will continue to support beamline operations and upgrades at HPCAT (see upgrade proposal submitted to DOE-BES in Section 7.3 below) with the goal of keeping this facility available to our academic and laboratory partners.

7.2 Implementation of CDAC Phase II

With the implementation of Phase II of the CDAC program in January 2006, we have been working to achieve the goals set out in the proposal which was enthusiastically endorsed by the CDAC Advisory Committee at its meeting in May 2005. The proposal included requests for the following:

- **Extension to a Five Year Cycle** – The initial grant period for CDAC is now five years, and will end in January 2008. This extension has given us additional flexibility in planning the expansion of our partner groups and preparing for the future of our Center.

- **Increase in the number of partners** – In addition to our original partner group, we have added groups from Texas Tech University (Yanzhang Ma), New Mexico State University (Kanani Lee), Arizona State University (Jeff Yarger), Florida International University (Surendra Saxena), and University of Nevada-Reno (Dhanesh Chandra). Each of these academic partners has recruited students to work on CDAC-related projects and is training these students. Many of these students have taken already taken advantage of our beam time allocation program. Due to differences in the costs of supporting students at these universities (tuition, stipends, and cost of living), this growth in the number of CDAC students is now accomplished with variable size awards. At New Mexico State University, Lee’s group has nearly finished building a new DAC laboratory, including four Syntek symmetric DACs, two preparation microscopes, a microdrill press, a micro-EDM and a Raman system. Ma’s group at Texas Tech is working in many areas, including exploring the effect of shear stress and strain on the phase transition in iron from the bcc to the hcp phase using synchrotron x-ray diffraction measurements in a rotational DAC, carrying out high pressure synchrotron x-ray diffraction experiments to investigate the properties of WS2 to 26 GPa at room temperature, and investigating the high-pressure behavior of MoS2, by synchrotron x-ray diffraction, to nearly 40 GPa at room temperature. At Arizona State University, the Yarger group has started preliminary work to characterize correlations between pressure-induced amorphization and polyamorphism in glassy systems as well as the enhanced glass-forming ability of materials at high pressure. Chandra and the group at the University of
Nevada – Reno plans to conduct a systematic study of the pressure-induced phase transformations in alkali metal complex hydrides. The compounds chosen for study include LiNH$_2$, LiBH$_4$, and NaBH$_4$. The high pressure Raman spectroscopy studies will be performed at Carnegie. Synchrotron x-ray powder diffraction studies will be performed at Advanced Light Source high pressure beamline as well as at HPCAT, APS. The high pressure Raman spectroscopy data on LiNH$_2$ has already been collected up to 25 GPa and the data analysis is ongoing. A high pressure sample preparation laboratory will be set up at Reno and DAC, EDM for gasket preparation, and other equipment will be acquired during the course of the year. Saxena’s group at Florida International University has been involved in the high pressure research community for a number of years. With their affiliation with CDAC, their work on hydrides and novel carbide and nitride systems will receive additional emphasis. The Saxena group also is working on high $P$-$T$ calibration scales for the DAC, as well as methods for measuring the strength of materials using high pressure techniques.

- **Enlarge the CDAC share at HPCAT** – Beam time at HPCAT has become extremely competitive with the growth in the field (see section 7.3.3 below). As of January 2006, the CDAC membership in HPCAT has now gone to 30%. We have divided this allocation equally between the National Lab and CDAC Academic groups. As we have now moved operations at HPCAT to four simultaneously operating hutch (three diffraction, one spectroscopy), the availability of beam time for all CDAC partner groups has grown significantly, and nearly all requests for beam time can be accommodated.

- **Additional CDAC support scientists** – The success of pioneering studies and student and collaborator trainings at state-of-the-art facilities strongly depends upon on-site expert help and support. We have added a research scientist at Carnegie to help with increased efforts in the areas of student/visitor training and technique development. CDAC research scientists will also continue to assist CDAC users at HPCAT and NSLS.

- **Instrumentation development** – We have continued our work on high $P$-$T$ cells for neutron diffraction at LANSCE and SNAP, and on improving designs for resistively heated DACs. We are also now prepared to support feasibility studies and experimental collaboration at NSLS and HPCAT in the area of laser shock compression measurements coupled with synchrotron IR and x-ray diagnostics at these facilities.

- **Infrastructure at Carnegie facilities** – The infrared spectroscopy beamline U2A at the NSLS, also supported in part by the NSF, is now fully supported for CDAC users. A number of CDAC students, postdoctoral associates, academic partners and laboratory partners have taken advantage of this highly productive and cutting-edge facility, including members of the CDAC shock compression community. In addition, a state-of-the-art videoconferencing facility for the Carnegie campus is in the planning stages. This capability will enhance communication between all nodes in the CDAC community.

### 7.3 HPCAT Upgrade

Designed in 1998, HPCAT has pioneered the new-generation, high-pressure, synchrotron facility in which multiple techniques are integrated at a single sector for the advancement of multidisciplinary high-pressure research. The HPCAT program has been exceedingly successful in terms of scientific impact, technological advances, and user community development. To advance HPCAT for the second decade, the upgrade proposed the addition of four novel high-pressure synchrotron techniques that have recently become feasible and practical, as well as overall improvements of x-ray optics components in order to fully utilize the high brilliance source anticipated from the APS upgrade.

For the high-pressure x-ray microprobe, the present spatial resolution limit of 3-5 µm will be improved by an order of magnitude to 200-300 nm. This upgrade is very timely for emerging high-pressure nanoscience. It may also enable the next breakthrough of maximum static pressure beyond the present record of 300-500 GPa. For the high-pressure inelastic x-ray scattering program, we
propose to add analyzers and detectors with 100 meV energy resolution, which will greatly expand the present program of 1 eV resolution and open a large new research area for in-depth study of electronic energy levels at high pressures. For high-pressure x-ray diffraction, we will add a high-resolution diffractometer to improve the d-spacing resolution by an order of magnitude greater than the present state of the art. This upgrade will enable discoveries of numerous intricate, subtle structural changes accompanying important electronic, magnetic and phonon transitions. For the high-pressure laser-heating system, we will implement an innovative rotating optical system to allow laser heating and x-ray diffraction through different paths. As a result, the long-awaited study of high P-T deformation and rheological experiments will become possible.

We will upgrade the 16ID x-ray optics train for higher brilliance. High-pressure x-ray studies are often brilliance-limited. Higher brilliance enables new, more powerful experiments, or leads to higher efficiency for existing techniques. We have thoroughly investigated and identified the key components that need to be strengthened, improved, or replaced for robust operation with maximum brilliance. 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 (by one to two orders of magnitude) due to the source upgrades: first, a local enhancement at 16ID by adding the second undulator in the next couple of years, and then a facility-wide upgrade of the APS storage ring and lattice in the next decade. The unmatched brilliance, matching optics, and novel integrated techniques at HPCAT will provide the superior tools for the U.S. research community to lead the next level of development of high-pressure energy science in the foreseeable future.

Most of the existing HPCAT x-ray optics components were designed eight years ago based on a single undulator. They need to be upgraded for the anticipated higher power and brilliance and for maximizing its capabilities. The proposed upgrade of high heat load components adopts recent APS designs, which exceed the requirements of double undulator operation and will also make the components likely survivable to the future APS upgrade project after 2014. The proposed Kohzu double crystal monochromometer is well proven in many APS sectors and other facilities and will enhance capabilities for tighter focus, maintaining precise positional and energy stability, and will greatly increase the efficiency in challenging x-ray spectroscopy experiments. The proposed replacement of silicon by large diamond crystals in the branching double crystal monochrometer is based on the proven performance of water-cooled diamond crystal under high heat load, and should provide much improved efficiency. Improved beamline optics and increased brilliance provide unique opportunities for new techniques dedicated for high pressure research: high resolution inelastic x-ray scattering, high resolution x-ray diffraction, and sub-micron probes. These techniques have been developed for samples at ambient conditions, but previously limited for high pressure research due to insufficient flux and efficiency. The design of the novel rotation laser heating technique is based on decades of experience, and is an extension of the existing laser heating system at HPCAT for rheology and elasticity studies at high P-T.

### 7.3.1 HPCAT Overview

High Pressure Collaborative Access Team (HPCAT) was established by the U.S. high-pressure community to advance cutting-edge, multidisciplinary, high-pressure science and technology using synchrotron radiation (SR) at Sector 16 of the APS. HPCAT institution members, including Carnegie (the managing member), LLNL, University of Nevada at Las Vegas, University of Hawai’i, and CDAC, raised the initial 5-year (1999-2004), $15.45M, HPCAT construction/commission funds from federal and private sources. The current 5-year (2004-2009) HPCAT operation funds ($10.7M total) are supported jointly by DOE-NNSA ($6.9M) and DOE-BES ($3.8M grant to CIW, DE-FG02-99ER45775). This ~$2.1 M annual operation budget covers the personnel cost of HPCAT on-site team and operation expenses including costs for the beamline upkeep, user support, and a modest amount for instrumentation maintenance and improvement.

The HPCAT facility has established four operating beamlines in nine hutches. Two beamlines are split in energy space from the insertion device (16ID) line, while the other two are
divided into two fans from the bending magnet (16BM) line. Through collaboration with other APS sectors and other facilities, an array of novel x-ray diffraction and spectroscopic techniques has been integrated with high pressure-temperature instrumentation at HPCAT. With a multidisciplinary approach and multi-institution collaborations, the high-pressure program at the HPCAT has been enabling myriad scientific breakthroughs in high-pressure physics, chemistry, materials, and Earth and planetary sciences as shown by the quality and quantity of its publications.

With a string of successes beyond our initial expectations, we are now facing three new challenges. First, increasing demand of beam time at this highly desirable facility has generated an acute beam time shortage in the user community. Secondly, new synchrotrons abroad (e.g., DIAMOND at RAL) and newly upgraded high-pressure beamlines (e.g., at ESRF and SPring-8) have followed the HPCAT approach, but started with superior undulator source brilliance, and thus have an advantage over HPCAT. Thirdly, through the seven-year HPCAT experience, we have identified key components that need improvements and developed innovative ideas that could lead the next-level breakthroughs in high-pressure synchrotron instrumentation, but our routine operation budget does not contain sufficient funds for substantial improvements and new instrumentation. These three challenges can all be met by the proposed HPCAT upgrade.

Specifically key optical components will be upgraded to eliminate the heat-load problem and improve the beam intensity, image quality, and stability on the samples by 5-10 times (with the present source brilliance) to bring it on par with the newest beamlines abroad. With the anticipated second undulator at Sector 16 and the overall APS upgrade in the horizon, the source brilliance of HPCAT will be unmatched in the next decade. We will optimize the integrated hardware and software operation system and effectively double the useful user beam time. We will implement a submicron x-ray probe, 100 meV-resolution inelastic x-ray spectrometer, high-resolution x-ray diffractometer, and rotation laser-heating system, thus enabling next generation advancement in high-pressure research.

### 7.3.2 Second Undulator at HPCAT and the APS Ring Upgrade

The current insertion device at HPCAT is a standard APS type-A, 2.5-m undulator. The 5-m long straight section of each sector has sufficient room for two undulators. To maintain competitiveness and greatly improve efficiency, in the short term, APS has been upgrading the undulators to different designs and adding a second undulator to sectors based on need. Most high-pressure x-ray spectroscopy techniques are intensity-limited, and the increase in intensity can be translated directly into more efficient use of beam time, and will enable new experiments which have been impractical due to the lack of intensity. Furthermore, the two-undulator system will allow independent control of undulator parameters for two concurrently operating ID beamlines, thus nearly doubling our usable ID beam time.

In the long term (in a decade), APS is planning new storage ring lattice and whole facility upgrade. Several options are being seriously considered as we prepare for this upgrade. Foremost amongst these is the energy-recovery LINAC (ERL) which may offer a revolutionary upgrade path that brings fourth-generation capabilities to the APS while preserving all that we have today and involving less user disruption than would a storage ring lattice upgrade. Having the second undulator together with the new APS innovative developments in the accelerator lattice and insertion devices, we anticipate an increase in x-ray radiation brilliance by more than an order of magnitude at HPCAT. The present HPCAT high heat load optics upgrade will also prepare us for the anticipated high brilliance.

### 7.3.3 Progress Report

The HPCAT user program has been in operation since 2003. During that time, ~80% of the available user beam time (~200 days per calendar year) has been allocated to member users and to the APS general user proposals (GUPs) through a Web-based proposal system. The APS Beamtime Allocation Committee allocates the available time to the highest rated proposals by the Proposal-Review-Panels (PRPs). HPCAT allocates the remaining 75%, based on member user’s requests and
the need of instrumentation and technique commissioning and instrument setup/alignment. A total of 396 experiments have been performed since 2003 at HPCAT by over 350 scientists and students. Number of “person-visits” has reached 772 so far (Fig. 60). The experimental program is oversubscribed by a large number of highly rated beam time proposals submitted by talented scientists who publish successfully in top-rated journals and involve large numbers of students in their research.

**Oversubscription** – The HPCAT sector has become heavily oversubscribed, which is illustrated by the GUP program at HPCAT. The oversubscription factor is defined to be the ratio of the number of shifts requested by GUP users to the number of shifts awarded (i.e., number available) to GUP users. The average oversubscription rate is 6.5 (if only counting first choice, it is 3.7) (Fig. 59). The oversubscription rate was temporarily relieved in the summer of 2006 due to the opening of 16BM-B and 16BM-D to general users, but it is expect to rise again very soon. Given the fact that we generally receive highly rated beam time proposals, this factor is too high above the warning line (~2) and eventually discourage users from submitting new proposals. The proposed HPCAT upgrade will greatly enhance the efficiency of beam time usage (by a factor of 10) and hence significantly increase available beam time. We do not anticipate a significant drop of the oversubscription rate, because the upgrade will also enhance the capabilities of existing techniques and introduce new capabilities, thus generating new science to be explored. The remaining challenge has been to balance the desire to give beam time to as many highly rated proposals as possible while providing sufficient beam time to each experiment to accomplish the intended goals.

**Publications** – At the time of this upgrade, research at HPCAT has resulted in 164 publications, and the number is growing at an accelerated rate. All of these publications appeared in published journal articles or book sections. Twenty-one percent (21%) of these publications (35) appeared in “high profile journals” (*Science, Nature, Proceedings of the National Academy Science, Physical Review Letters*). In addition, five Ph.D. dissertations and two Master’s thesis were based in part on research conducted at HPCAT. APS maintains a publication database that includes all peer-reviewed publications from each APS sector. In 2005, HPCAT has the second largest number (next to GSECARS which is five years ahead of HPCAT, but HPCAT has higher number of high-profile papers) of publications (61) in the database of any of the non-protein crystallography sectors at the APS. In 2006 up to August, HPCAT has surpassed GSECARS publications in both quality and quantity. Most publications resulting from work at HPCAT include one or more HPCAT beamline scientists as co-authors.

![Figure 59. Left: numbers of “person-visits” since 2003. Right: Oversubscription rate, the ratio of the number of shifts requested by GUP users to the number of shifts awarded, in the HPCAT user program. The HPCAT as the first choice is shown in red, with all choices in blue.](image-url)
Outreach and Community Development – Efforts are being made to ensure the HPCAT facility is responsive to the needs of the HPCAT members and the scientific community, and that the community is made aware of the capabilities of the facility. Some examples of the outreach efforts that we have undertaken include:

High Pressure Committee (HPC) Meeting – The committee consists of all HPCAT member groups and a number of other leading groups in the U.S. The HPC meets regularly (3-4 times a year), reviews the progress of HPCAT, and provides advices on the developments.

CDAC is a community outreach program promoting high-pressure “energy science”, and distributes all CDAC beam time (which is 30% of the total HPCAT member beam time) to high-pressure researchers at three national laboratories and 143 universities. General users who work on “energy science” (defined in the most liberal term as in the 2003 BESAC Report), therefore, has two channels to access HPCAT beam time: GUP and CDAC.

Workshop on Rheology and Elasticity at Ultrahigh Pressure and Temperature – HPCAT co-organized the COMPRES-sponsored workshop held on Oct 21-23, 2005 at APS. Experts in DAC design, large volume high-pressure apparatus, and data analysis discussed the current state of ultra-high pressure deformation studies and future developments.

Workshop on Synergy of 21st Century High-Pressure Science and Technology – The workshop was held April 29 through May 1, 2006 at the APS, which was organized by HPCAT and co-sponsored by CDAC and COMPRES. The meeting featured an extensive array of forward-looking presentations along with ample opportunities for discussions among the 112 scientists and 20 graduate students and postdoctoral researchers in attendance from the fields of physics, chemistry, materials science, biology, and earth and planetary sciences, from both academic institutions and the National Labs around the country.

Argonne Neutron and X-ray Summer School – HPCAT has participated in this two week school since 2004. Students perform hands-on experiments using the micro-diffraction equipments at HPCAT beamlines.

High Pressure Special Interest Group – HPCAT organizes a special interest group on high pressure techniques and applications at the APS. This group meets monthly.

7.3.4 HPCAT Facility Upgrade Project

Supplementary Material Available

For a complete description 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 3*

A. CDAC Publications


---

* We list publications and presentations for 2005-2006, including all work supported fully or in part by CDAC. This list therefore includes work carried out at HPCAT by all of its members and users during this period.


Duffy, T., Synchrotron facilities and the study of deep planetary interiors, Reports on Progress in Physics, 68, 1811-1859 (2005).


Hemley, R. J., V. V. Struzhkin and R. E. Cohen, Measuring high-pressure electronic and magnetic properties, in *Treatise on Geophysics* (Elsevier, in press).


Kumar, R. S., A. L. Cornelius and M. Nicol, Structure of nanocrystalline ZnO up to 85 GPa, *Synthetic Metals*, in press.


B. CDAC Presentations


Ahart, M., R. E. Cohen and R. J. Hemley, High-pressure Raman scattering and x-ray diffraction study of relaxor ferroelectric \(0.96\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3-0.04\text{PbTiO}_3\), *Bull. Am. Phys. Soc. (APS March Meeting)* (Los Angeles, CA, March 21-25, 2005).


Chellappa, R., High pressure Raman spectroscopy studies on pentaerythritol, neopentylglycol, and \(\text{LiAlH}_4\), *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).


Cohen, R. E., Low symmetry ground state in PMN: Random fields via unit-cell twinning, or multiscale disorder in relaxors, Fundamental Physics of Ferroelectrics 2005 (Williamsburg, VA, February 6-9, 2005).


Cohen, R. E., Computation of thermal, elastic, and magnetic properties at high pressure, Frontiers in High Pressure Research (Kibbutz Ein-Gudd, Dead Sea, Israel, March 2-7, 2006).

Cohen, R. E., Theory of iron at high pressure and temperature (invited), Workshop on Synergy of 21st Century High-Pressure Science and Technology (Argonne, IL, April 29-May 1, 2006).


Cohen, R. E. and X. Sha, Thermoelasticity of iron from first-principles (invited), ASC Road Show (Lawrence Livermore National Laboratory, Livermore CA, May 16, 2005).


Degtyareva, O., R. Caracas, E. Gregoryanz, M. Somayazulu, R. E. Cohen, H. K. Mao and R. J. Hemley, Charge-density wave in the incommensurate phase of metallic sulfur at megabar pressure, IUCr Meeting (Florence, Italy, August, 2005).

Degtyareva, O., E. Gregoryanz and R. J. Hemley, Phase diagrams and complex crystal structures of selected elements, Third Meeting of the Study of Matter at Extreme Conditions (SMEC) (Miami, FL, April 17-21, 2005).


Dlott, D. D., Nanotechnology energetic material dynamics studied with nanometer spatial resolution and picosecond temporal resolution (invited, plenary talk), *Sixth International Symposium on Special Topics in Chemical Propulsion* (Santiago, Chile, March, 2005).

Dlott, D. D., The new wave in shock waves (invited), *Department of Physics, University of Southern California* (Los Angeles, CA, April, 2005).

Dlott, D. D., Vibrational energy in molecules and molecular nanostructures (invited), *Department of Physics, University of Southern California* (Los Angeles, CA, April, 2005).


Dlott, D. D., Vibrational energy in molecules and molecular nanostructures (invited), *University of Maryland, Department of Chemistry* (Baltimore, MD, October, 2005).


Dlott, D. D., Vibrational energy in molecules and molecular nanostructures (invited), *University of Michigan, Department of Chemistry* (Ann Arbor, MI, November, 2005).


Dlott, D. D., Vibrational energy in molecules and molecular nanostructures (invited), *Michigan State University, Department of Chemistry* (East Lansing, MI, November, 2005).

Dlott, D. D., Interfaces at high pressure (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).


Dlott, D. D., Vibrational energy in molecules and molecular nanostructures, *Auburn University* (Auburn, IL, April, 2006).


Duffy, T. S., Elastic properties of mantle minerals at high pressures (invited), *Geological Society of America Annual Meeting* (Salt Lake City, UT, October 17, 2005).

Duffy, T. S., Elastic properties of hydrous minerals and implications for seismic studies of the upper mantle (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).


Duffy, T. S., Recent advances in deep Earth studies (invited), *Department of Geophysical Sciences, University of Chicago* (Chicago, IL, February 24, 2006).


Evans, W. J., High pressure beryllium: Static and elastic properties, *Joint 20th AIRAPT - 43rd EHPRG International Conference on High Pressure Science and Technology* (Karlsruhe, Germany, June 27-July 1, 2005).


Fultz, B., The DANSE project (invited), *Neutron Science Software Initiative Workshop NeSSI-3* (Santa Fe, NM, April 29, 2005).

Fultz, B., Neutron scattering and the entropy of materials (invited), *University of New Orleans Chemistry Department Colloquium* (New Orleans, LA, May 6, 2005).


Fultz, B., Phonon thermodynamics in materials under extreme conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).

Fultz, B., Mössbauer diffractionmetry (invited), *Fourth Nassau Mössbauer Symposium* (Garden City, NY, January 14, 2006).

Fultz, B., Dynamic data-driven data applications systems for the domain of neutron scattering research (invited), *Workshop at the National Science Foundation Headquarters* (Washington, DC, January 19, 2006).

Fultz, B., Inelastic neutron scattering and entropy (invited), *Indiana University Department of Physics Colloquium* (Bloomington, IN, May 30, 2006).


Goncharov, A., Optical spectroscopy under extreme conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).


Goncharov, A. F., J. C. Crowhurst, J. K. Dewhurst and A. Sharma, Cubic boron nitride under high pressures and temperatures, *Joint 20th AIPART - 43rd EHPRG International Conference on High Pressure Science and Technology* (Karlsruhe, Germany, June 27-July 1, 2005).


Heinz, D., Experimental studies of core minerals at core conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).


Hemley, R. J., Synchrotron studies of materials at extreme conditions (invited), (Orlando, FL, 2005).

Hemley, R. J., New materials chemistry under pressure (invited), *Howard University Department of Chemistry* (Washington, DC, February 11, 2005).


Hemley, R. J., Materials under pressure: new findings and phenomena (invited), *Finish Physical Society* (Helsinki, Finland, March 16, 2005).


Hemley, R. J., Compressing materials from simple to complex: New findings and phenomena (invited), *Joint 20th AIPART - 43rd EHPRG International Conference on High Pressure Science and Technology* (Karlsruhe, Germany, June 27-July 1, 2005).


Hemley, R. J., Diamond windows on new chemistry (invited), *Wesleyan University* (Middletown, CT, September 30, 2005).

Hemley, R. J., New findings in materials under pressure (invited), *Massachusetts Institute of Technology* (Cambridge, MA, February 6, 2006).

Hemley, R. J., Overview of new developments and future prospects in high-pressure research (invited), *Frontiers in High Pressure Research* (Kibbutz Ein-Gued, Dead Sea, Israel, March 2-7, 2006).

Hemley, R. J., New findings in materials under pressure (invited), *Dalhousie University* (Halifax, Nova Scotia, Canada, March 23, 2006).

Hemley, R. J., Emerging diamond technology and the science of extreme conditions (invited), *ICOPS* (Traverse City, Michigan, June 4-8, 2006).

Hemley, R. J., Current problems in high-pressure science (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
Hemley, R. J., New findings in molecular systems under pressure (invited), ACS National Meeting (San Francisco, CA, September 10-14, 2006).

Hemley, R. J., New findings in materials under pressure (invited), University of Virginia, Chemistry Department (Charlottesville, VA, October 20, 2006).

Hemley, R. J., New findings in materials under pressure (invited), 53rd Midwest Solid State Conference (Kansas City, Missouri, October 6-8, 2006).

Hemley, R. J., New findings in materials under pressure (invited), Fall 2006 Joint Meeting of the Texas sections of the American Physical Society, American Association of Physics Teachers, Zone-13 of the Society of Physics Students, Forum on Industrial and Applied Physics, National Society of Hispanic Physicists, and National Society of Black Physicists (Arlington, TX, October 5-7, 2006).

Hemley, R. J., New studies of low-Z systems under pressure, Sixth International Conference on Cryocrystals and Quantum Crystals (Kharkov, Ukraine, September 3-7, 2006).


Hemley, R. J., C. S. Yan and S. S. Ho, Prospects of large single crystal CVD diamond, 1st International Industrial Diamond Conference (Barcelona, Spain, October 20-21, 2005).


Jackson, J. M., Physical properties of minerals and melts under high-pressure (invited), Workshop on Synergy of 21st Century High-Pressure Science and Technology (Argonne, IL, April 29-May 1, 2006).


Jacobsen, S. D., Identifying hydration in Earth's interior (invited), 21st Century Center of Excellence Program, Tohoku University (Sendai, Japan, July 22, 2005).

Jacobsen, S. D., High-pressure crystal chemistry and hydrogen storage in the Earth's mantle (invited), Northwestern University, Department of Geological Science (Evanston, IL, April 15, 2005).

Jacobsen, S. D., High-pressure crystal chemistry and hydrogen storage in the Earth's mantle (invited), Princeton University, Department of Geosciences (Princeton, NJ, April 7, 2005).


Jacobsen, S. D., Bridging experimental and observational geophysics for identifying hydration in the Earth's interior, Bayerisches Geoinstitut (Bayreuth, Germany, October 17, 2005).

Jacobsen, S. D., Identifying hydration in the Earth's interior, Tohoku University, Graduate School of Science (Sendai, Japan, July 22, 2005).

Jacobsen, S. D., Identifying hydration in the mantle transition zone: Emerging constraints from mineral physics and seismology (invited), Workshop on Synergy of 21st Century High-Pressure Science and Technology (Argonne, IL, April 29-May 1, 2006).

Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, Yale University, Department of Geology and Geophysics (New Haven, CT, January 20, 2006).

Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, Northwestern University, Department of Geological Sciences (Evanston, IL, February 13, 2006).

Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, Virginia Polytechnic Institute and State University, Department of Geological Sciences (Blacksburg, VA, February 23, 2006).

Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, University of Minnesota, Department of Geology and Geophysics (Minneapolis, MN, March 2, 2006).

Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, University of Illinois Chicago, Department of Earth and Environmental Science (Chicago, IL, September 7, 2006).


Jenkins, T., R. J. Hemley, H. K. Mao, W. Mao, V. V. Struzhkin, B. Militzer and J. Leao, Examination of hydrogen clathrates vibrational spectra by inelastic neutron scattering *American Conference on Neutron Scattering* (St. Charles, IL, June 18-22, 2006).


Lee, K., Pressure and chemistry-dependent electron capture radioactive decay, *Ludwig Maximilians University* (Munich, Germany, June 30, 2006).

Lee, K., Pressure and chemistry-dependent electron capture radioactive decay, *Bayerisches Geoinstitut* (Beyreuth, Germany, July 6, 2006).


Ma, Y., High pressure research at Texas Tech University (plenary presentation), *Chinese High Pressure Conference* (Jilin, China, August 1, 2006).

Ma, Y., Application of synchrotron x-ray in high pressure (invited), *Southwest Jiatong University* (Chengdu, China, July 23, 2006).


Mao, H. K., Synergy of high-pressure research (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).


Mao, H. K., High-pressure synergetic consortium - A new approach to high-pressure research at national facilities (invited), *Future Frontiers in High-Pressure Science with ERL X-Ray Beams Workshop* (Cornell University, Ithaca, NY, June 5-6, 2006).

Mao, H. K., High-pressure - A new dimention in physics, chemistry, materials science, geoscience, and biology (plenary talk), *Academia Sinica's Biannual Meeting* (Taipei, Taiwan, July 1-5, 2006).

Mao, H. K., New diamond science and technology for the 21st century (invited), *Taipei International Meeting Center* (Taipei, Taiwan, July 7, 2006).
Mao, H. K., The formation of elasticity, rheology, and dynamics of iron-rich silicate in core-mantle boundary layer (keynote talk), *19th General Meeting of the International Mineralogical Association* (Kobe, Japan, July 23-28, 2006).

Mao, H. K., Core-mantle interaction - The formation, elasticity, rheology, and dynamics of iron-rich silicate in core-mantle boundary layer (invited), *Fifth International Conference on Synchrotron Radiation in Materials Science (SRMS-5)* (Chicago, IL, July 31, 2006).


Miao, S., M. Kocher, B. Fultz, P. Rez, Y. Ozawa, R. Yazami and C. C. Ahn, Local electronic structure of layered Li$_{1.33}$Ni$_{0.33}$Mn$_{0.33}$Co$_{0.33}$O$_2$, *Electrochemical Society Fall Meeting* (Los Angeles, CA, October 18, 2005).


Militzer, B., Path integral simulations of hydrogen-helium mixtures in planet interiors (invited), *SMEC* (Maimi, FL, April, 2005).


Qiu, W., Calibration of an isotopically enriched carbon-13 layer pressure sensor to 156 GPA in a diamond anvil cell, Second Annual SSAAP Symposium (Las Vegas, NV, August 23-24, 2005).


Shen, G., Experimental studies of phase diagram of iron (invited), Workshop on Synergy of 21st Century High-Pressure Science and Technology (Argonne, IL, April 29-May 1, 2006).


Struzhkin, V. V., Applications of NRIXS and NFS techniques at high pressures (invited), Workshop on Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation (Argonne National Laboratory, Argonne, IL, February 12-13, 2005).

Struzhkin, V. V., X-ray emission spectroscopy, Frontiers in High Pressure Research (Kibbutz Ein-Gued, Dead Sea, Israel, March 2-7, 2006).

Struzhkin, V. V., Magnetism and superconductivity at high pressures (invited), Workshop on Synergy of 21st Century High-Pressure Science and Technology (Argonne, IL, April 29-May 1, 2006).

Struzhkin, V. V., Optimizing hydrogen clathrates for hydrogen storage, Sixth International Conference on Cryocrystals and Quantum Crystals (Kharkov, Ukraine, September 3-7, 2006).


Velisavljevic, N., Simultaneous electrical and x-ray diffraction studies on f-electron metals at high pressures using designer diamond anvils, Second Annual SSAAP Symposium (Las Vegas, NV, August 23-24, 2005).

Vohra, Y., Grand challenges in f-electron metals research at high pressures and low temperatures using designer anvil cells (invited), Workshop on Synergy of 21st Century High-Pressure Science and Technology (Argonne, IL, April 29-May 1, 2006).

Vohra, Y., Basic science and applications of vapor grown diamonds of high pressure research (invited), Gordon Conference on Research at High Pressure (Biddeford, ME, June 25-30, 2006).


Wenk, H. R., Texture information from radial DAC experiments and relevance for deep earth geophysics, illustrated with examples, COMPres Workshop on Rheology and Elasticity Studies at Ultra-High Pressures and Temperatures (Argonne, IL, October 21-23, 2005).

Wenk, H. R., Deformation experiments at ultrahigh pressure: Where we are and where we should be going (invited), Workshop on Synergy of 21st Century High-Pressure Science and Technology (Argonne, IL, April 29-May 1, 2006).


Xu, J., Progress on moissanite anvil cells in neutron diffraction studies (invited), *The 2nd SNAP Symposium* (Spallation Neutron Source, Oak Ridge National Laboratory, Oakridge, TN, July 17-20, 2005).

Xu, J., Application of high-pressure research - in Biosciences (invited), *The 15th Annual Conference on Life and Food Sciences* (Harbin Institute of Technology, Harbin, China, August 15, 2005).

Xu, J., Progress on moissanite anvil cells in neutron diffraction studies (invited), *High-Pressure Science and Technology - 2005* (Beijing Synchrotron Research Facility, Institute of High Pressure Physics, Chinese Academy of Sciences, Beijing, China, September 6, 2005).


Yan, C. S., New developments in fabrication of large single crystal diamond by chemical vapor deposition, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).


Yarger, J., Structural transformations in liquids and glasses under extreme conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).

Yarger, J., High-pressure and spin enhanced neutron scattering (invited), *Argonne National Laboratory, Intense Pulsed Neutron Source* (Argonne, IL, April, 2006).

Yarger, J., High-pressure quenched glasses (invited), *Arizona State University, Chemistry & Biochemistry Symposium* (Tempe, AZ, October, 2006).


APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for Year 3

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.

<table>
<thead>
<tr>
<th>User Name</th>
<th>Affiliations</th>
<th>Project</th>
<th>Dates</th>
</tr>
</thead>
<tbody>
<tr>
<td>M. Lucas</td>
<td>California Institute of Technology</td>
<td>16-ID-D NFS Raman spectroscopy</td>
<td>July 23-25, 2005</td>
</tr>
<tr>
<td>A. Papandrew</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. F. Lin</td>
<td>LLNL</td>
<td>Raman spectroscopy</td>
<td>July 25, 2005</td>
</tr>
<tr>
<td>I. S. Lynbutin</td>
<td>ICRAS</td>
<td>FeD – magnetic crystals</td>
<td>July 26-August 2, 2005</td>
</tr>
<tr>
<td>V. Struzhkin</td>
<td>Carnegie</td>
<td>Raman spectroscopy</td>
<td>July 27-29, 2005</td>
</tr>
<tr>
<td>G. Amulele</td>
<td>University of Hawaii</td>
<td>EOS: Olivine, SiC, boron carbide Raman spectroscopy</td>
<td>July 28-31, 2005</td>
</tr>
<tr>
<td>S. Mariappan</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Goncharov</td>
<td>Carnegie</td>
<td>XRD: Water Laser Heating</td>
<td>August 1-5, 2005</td>
</tr>
<tr>
<td>P. Liermann</td>
<td>Carnegie</td>
<td>Raman spectroscopy</td>
<td>August 5-7, 2005</td>
</tr>
<tr>
<td>S. Merkel</td>
<td>University of California – Berkeley</td>
<td>Radial diffraction: Silicate post perovskite</td>
<td>August 5-7, 2005</td>
</tr>
<tr>
<td>A. Kubo</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>L. Miyagi</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Merkel</td>
<td>University of California – Berkeley</td>
<td>Raman spectroscopy</td>
<td>August 6-8, 2006</td>
</tr>
<tr>
<td>T. Duffy</td>
<td>California – Berkeley Princeton</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Mitchell</td>
<td>ANL-MSD</td>
<td>Manganate perovskites: XRD</td>
<td>August 9-10, 2005</td>
</tr>
<tr>
<td>J. Hill</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Olga Degtyareva</td>
<td>Carnegie</td>
<td>XRD,Na,S,AS Raman spectroscopy</td>
<td>August 9-12, 2005</td>
</tr>
<tr>
<td>B. Maddox</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td>XRD</td>
<td>August 10-15, 2005</td>
</tr>
<tr>
<td>J. F. Lin</td>
<td>LLNL</td>
<td>Raman spectroscopy</td>
<td>August 13, 2005</td>
</tr>
<tr>
<td>J. Santillan</td>
<td>MIT</td>
<td>XRD</td>
<td>August 12-15, 2005</td>
</tr>
<tr>
<td>S. Landin</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D. Shim</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Lazicki</td>
<td>LLNL</td>
<td>XRD and laser heating Be</td>
<td>August 16-18, 2005</td>
</tr>
<tr>
<td>W. Evans</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H. Cynn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z. Jenei</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Jennifer Jackson</td>
<td>ANL</td>
<td>(Mg,Fe)SiO$_3$ perovskite: XRD</td>
<td>August 18, 2005</td>
</tr>
<tr>
<td>J. Lang</td>
<td>ANL</td>
<td>Neutron x-ray summer school experiments</td>
<td>August 20, 2005</td>
</tr>
<tr>
<td>B. Olsen</td>
<td>University of California – Berkeley</td>
<td>Neutron School</td>
<td>August 19-20, 2005</td>
</tr>
<tr>
<td>----------------------------</td>
<td>-------------------------------------</td>
<td>----------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>G. Sauteiede</td>
<td>University of Delaware</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N. Suwarromaml</td>
<td>NOIT</td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Kim</td>
<td>University of Mexico</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Ziemann</td>
<td>University of Notre Dame</td>
<td></td>
<td></td>
</tr>
<tr>
<td>L. Debeer-Schmitt</td>
<td>University of Alabama – Birmingham</td>
<td></td>
<td></td>
</tr>
<tr>
<td>N. Cunningham</td>
<td>Princeton</td>
<td></td>
<td></td>
</tr>
<tr>
<td>G. Lau</td>
<td>West Virginia University</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P. Filson</td>
<td>State University of New York, Stony Brook</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Koo</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Cemils</td>
<td>University of Nevada – Las Vegas</td>
<td>Heavy fermion materials: XRD</td>
<td>August 22-25, 2005</td>
</tr>
<tr>
<td>H. Brooks</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Kumar</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C. Pareda</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E. Sokol</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Orwig</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Jacobsen</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Bennett</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. McClure</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Pravica</td>
<td>University of Nevada – Las Vegas</td>
<td>XRD</td>
<td>August 23-25, 2005</td>
</tr>
<tr>
<td>H. P. Lierman</td>
<td>Carnegie</td>
<td>X-ray Raman spectroscopy</td>
<td></td>
</tr>
<tr>
<td>G. Shen</td>
<td>Carnegie</td>
<td>Commissioning and testing of single crystal and powder x-ray diffraction techniques on 16BM-B</td>
<td>October 3, 2005</td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td>Silicate post-perovskite: XRD</td>
<td>October 11-14, 2005</td>
</tr>
<tr>
<td>H. Liu</td>
<td>HPCAT</td>
<td>Raman spectroscopy</td>
<td>October 12, 2005</td>
</tr>
<tr>
<td>J. F. Lin</td>
<td>LLNL</td>
<td>X-ray Raman spectroscopy</td>
<td>October 13, 2005</td>
</tr>
<tr>
<td>V. Iota</td>
<td>LLNL</td>
<td>XRD - Iodine 12 and Gallium Phosphide</td>
<td>October 14-17, 2005</td>
</tr>
<tr>
<td>H. Cynn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Liu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z. Jenei</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H. Giefers</td>
<td>University of Nevada – Las Vegas</td>
<td>XRD</td>
<td>October 20-22, 2005</td>
</tr>
<tr>
<td>C. Gobin</td>
<td>University of Nevada – Las Vegas</td>
<td>XRD</td>
<td>October 20-21, 2005</td>
</tr>
<tr>
<td>C. D. Martin</td>
<td>State University of New York, Stony Brook</td>
<td>Perovskite ot post-perovskite transition in NaMgF6: XRD</td>
<td>October 23-24, 2005</td>
</tr>
<tr>
<td>Tanja Cuk</td>
<td>Stanford University</td>
<td>Cuprate superconductors: XRD</td>
<td>October 26, 2005</td>
</tr>
<tr>
<td>V. Struzhkin</td>
<td>Carnegie</td>
<td>XRD</td>
<td>October 26, 2005</td>
</tr>
<tr>
<td>A. Goncharov</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P. Liermann</td>
<td>HPCAT</td>
<td>Commissioning of BM-D</td>
<td>October 26, 2005</td>
</tr>
<tr>
<td>G. Shen</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Crowhurst</td>
<td>LLNL</td>
<td>Noble metal nitrides: XRD</td>
<td>October 27, 2005</td>
</tr>
<tr>
<td>Name(s)</td>
<td>Institution</td>
<td>Method</td>
<td>Date</td>
</tr>
<tr>
<td>-------------------------</td>
<td>------------------------------------</td>
<td>---------------------------------</td>
<td>---------------------------</td>
</tr>
<tr>
<td>R. Kumar</td>
<td>University of Nevada – Las Vegas</td>
<td>XRD</td>
<td>October 28, 2005</td>
</tr>
<tr>
<td>Patricia Kalita</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Jaconsen</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C. Jensen</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D. Antonion</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Pravica</td>
<td>University of Nevada – Las Vegas</td>
<td>X-ray Raman spectroscopy</td>
<td>October 28-30, 2005</td>
</tr>
<tr>
<td>A. Bennett</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. McClure</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Feng</td>
<td>LLNL</td>
<td>X-ray Raman spectroscopy</td>
<td>October 28- November 11, 2005</td>
</tr>
<tr>
<td>C. S. Yoo</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. F. Lin</td>
<td>LLNL</td>
<td>X-ray Raman spectroscopy</td>
<td>October 29, 2005</td>
</tr>
<tr>
<td>X. Qin</td>
<td>University of Hawaii</td>
<td>XRD studies</td>
<td>November 1-7, 2005</td>
</tr>
<tr>
<td>G. Amulele</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Balogh</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td>Silicate post-perovskite: XRD</td>
<td>November 6-11, 2005</td>
</tr>
<tr>
<td>W. Luo</td>
<td>JHU</td>
<td>Amorphous alloys</td>
<td>November 10-11, 2005</td>
</tr>
<tr>
<td>H. Sheng</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>X. Chen</td>
<td>Carnegie</td>
<td>High Pressure Structural Study of Silane and Germane</td>
<td>November 12, 2005</td>
</tr>
<tr>
<td>C. Jin</td>
<td>Chinese Academy of Science</td>
<td>X-ray Raman spectroscopy</td>
<td>November 15-18, 2005</td>
</tr>
<tr>
<td>D. Dattelbaum</td>
<td>LANL</td>
<td>Polymers XRD</td>
<td>November 16-19, 2005</td>
</tr>
<tr>
<td>L. Sanchez</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Pravica</td>
<td>University of Nevada – Las Vegas</td>
<td>Iron: NRIXS</td>
<td>November 16-18, 2005</td>
</tr>
<tr>
<td>R. Sander</td>
<td>LANL</td>
<td>Quantum Dots: XRD</td>
<td>November 16-19, 2005</td>
</tr>
<tr>
<td>K. Zhuravlev</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Pietryga</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H. Cynn</td>
<td>LLNL</td>
<td>Synchrotron Mössbauer spectroscopy</td>
<td>November 17-21, 2005</td>
</tr>
<tr>
<td>J. Z. Jiang</td>
<td>Zhe Jiang University</td>
<td>The atomic structure of Ti elemental metallic glass</td>
<td>November 20, 2005</td>
</tr>
<tr>
<td>V. Struzhkin</td>
<td>Carnegie</td>
<td>NFS</td>
<td>November 23-28, 2005</td>
</tr>
<tr>
<td>Olga Degtyareva</td>
<td>Carnegie</td>
<td>XRD on elements</td>
<td>November 22-27, 2005</td>
</tr>
<tr>
<td>Valentina Degtyareva</td>
<td>Carnegie</td>
<td>XRD on alloys</td>
<td>November 22-27, 2005</td>
</tr>
<tr>
<td>S. Kharlamova</td>
<td>XFD/APS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Somayazulu</td>
<td>Carnegie</td>
<td>XRD on S/Se/As</td>
<td>November 22-24, 2005</td>
</tr>
<tr>
<td>A. Gavriliuk</td>
<td>Carnegie</td>
<td>NFS</td>
<td>November 23-28, 2005</td>
</tr>
<tr>
<td>J. McClure</td>
<td>University of Nevada – Las Vegas</td>
<td>BM-D commissioning experiments</td>
<td>November 28-December 9, 2005</td>
</tr>
<tr>
<td>O. Tschauerer</td>
<td>University of Nevada – Las Vegas</td>
<td>X-ray Raman spectroscopy</td>
<td>December 2-3, 2005</td>
</tr>
<tr>
<td>M. Pravica</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Kumar</td>
<td>Florida International University</td>
<td>High pressure study of iron oxide: XRD</td>
<td>December 7-9, 2005</td>
</tr>
</tbody>
</table>

103
<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Title</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>W. Evans</td>
<td>LLNL</td>
<td>Low-Z materials: XRD</td>
<td>December 8-13, 2005</td>
</tr>
<tr>
<td>M. Lipp</td>
<td>LLNL</td>
<td>Eu and EuN</td>
<td>December 10, 2005</td>
</tr>
<tr>
<td>G. Lee</td>
<td>University of Nevada – Las Vegas</td>
<td>X-ray emission spectroscopy</td>
<td>December 13, 2005</td>
</tr>
<tr>
<td>H. Cynn</td>
<td>University of Nevada – Las Vegas</td>
<td>X-ray emission spectroscopy of (Fe,Mg)SiO3 at high pressure</td>
<td>December 16, 2005</td>
</tr>
<tr>
<td>Z. Jenei</td>
<td>University of Nevada – Las Vegas</td>
<td>Comissioning experiminetns in BM-D</td>
<td>December 16-19, 2005</td>
</tr>
<tr>
<td>O. Tschauner</td>
<td>University of Hawaii</td>
<td>C3N4, superhard materials: NFS</td>
<td>December 19-20, 2005</td>
</tr>
<tr>
<td>W. Mao</td>
<td>LANL</td>
<td>X-ray emission spectroscopy of (Fe,Mg)SiO3 at high pressure</td>
<td>December 16-19, 2005</td>
</tr>
<tr>
<td>M. Jacobsen</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>C. S. Yoo</td>
<td>Cornell University</td>
<td>Resistive heating experiment</td>
<td>December 14, 2005</td>
</tr>
<tr>
<td>B. Maddox</td>
<td>University of Nevada – Las Vegas</td>
<td>Resistive heating experiment</td>
<td>December 14, 2005</td>
</tr>
<tr>
<td>P. Zinin</td>
<td>University of Hawaii</td>
<td>C3N4, superhard materials: NFS</td>
<td>December 19-20, 2005</td>
</tr>
<tr>
<td>J. Balogh</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>L. Ming</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>M. Pravica</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>Z. Quine</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>E. Romano</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>D. Hartnett</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>B. Yulga</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>H. Giefers</td>
<td>University of Nevada – Las Vegas</td>
<td>EOS studies on PETN XRD in BM-D</td>
<td>December 19-21, 2005</td>
</tr>
<tr>
<td>H. P. Liermann</td>
<td>HPCAT</td>
<td>Commissioning of BM-D</td>
<td>January 31, 2006</td>
</tr>
<tr>
<td>J. F. Lin</td>
<td>LLNL</td>
<td>Electronic spin transition of iron in magnesiowustite – (Mg,Fe)O at high pressures and high temperature</td>
<td>February 6, 2006</td>
</tr>
<tr>
<td>S. Merkel</td>
<td>University of California – Berkeley</td>
<td>High pressure deformation of MgSiO3 post-perovskite</td>
<td>February 7, 2006</td>
</tr>
<tr>
<td>L. Miyagi</td>
<td>University of California – Berkeley</td>
<td>High pressure deformation of MgSiO3 post-perovskite</td>
<td>February 7, 2006</td>
</tr>
<tr>
<td>S. Speziale</td>
<td>University of California – Berkeley</td>
<td>High pressure deformation of MgSiO3 post-perovskite</td>
<td>February 7, 2006</td>
</tr>
<tr>
<td>A. Kubo</td>
<td>University of California – Berkeley</td>
<td>High pressure deformation of MgSiO3 post-perovskite</td>
<td>February 7, 2006</td>
</tr>
<tr>
<td>X. Hong</td>
<td>University of Chicago</td>
<td>X-ray diffraction and absorption of amorphous GeO2 under pressure</td>
<td>February 9-10, 2006</td>
</tr>
<tr>
<td>R. Kumar</td>
<td>University of Nevada – Las Vegas</td>
<td>High pressure nuclear inelastic scattering experiments on Fe-Si alloys at ambient and low temperatures</td>
<td>February 10, 2006</td>
</tr>
<tr>
<td>P. Chow</td>
<td>University of Nevada – Las Vegas</td>
<td>High pressure nuclear inelastic scattering experiments on Fe-Si alloys at ambient and low temperatures</td>
<td>February 10, 2006</td>
</tr>
<tr>
<td>G. Chesnut</td>
<td>LANL</td>
<td>High pressure XRD of metals and Polymers; Teflon, titanium and its alloy, copper, tungsten</td>
<td>February 12, 2006</td>
</tr>
<tr>
<td>D. Dattlebaum</td>
<td>LANL</td>
<td>High pressure XRD of metals and Polymers; Teflon, titanium and its alloy, copper, tungsten</td>
<td>February 12, 2006</td>
</tr>
<tr>
<td>L. Sanchez</td>
<td>LANL</td>
<td>High pressure XRD of metals and Polymers; Teflon, titanium and its alloy, copper, tungsten</td>
<td>February 12, 2006</td>
</tr>
<tr>
<td>L. Ehm</td>
<td>State University of New York, Stony Brook</td>
<td>Structure of liquid Iodine at high pressure and temperature</td>
<td>February 12-14, 2006</td>
</tr>
<tr>
<td>N. Cunningham</td>
<td>University of Alabama – Birmingham</td>
<td>Multimegabar Structural transformations in Heavy Rare Earth Metal Terbium</td>
<td>February 15-17, 2006</td>
</tr>
<tr>
<td>A. Stemshorn</td>
<td>University of Alabama – Birmingham</td>
<td>Multimegabar Structural transformations in Heavy Rare Earth Metal Terbium</td>
<td>February 15-17, 2006</td>
</tr>
<tr>
<td>W. Qiui</td>
<td>University of Alabama – Birmingham</td>
<td>Multimegabar Structural transformations in Heavy Rare Earth Metal Terbium</td>
<td>February 15-17, 2006</td>
</tr>
<tr>
<td>H. Giefers</td>
<td>University of Nevada – Las Vegas</td>
<td>Phonon density of states in Fe-Sn and Fe-Dy compounds under high pressure</td>
<td>February 15-19, 2006</td>
</tr>
<tr>
<td>M. Pravica</td>
<td>University of Nevada – Las Vegas</td>
<td>Phonon density of states in Fe-Sn and Fe-Dy compounds under high pressure</td>
<td>February 15-19, 2006</td>
</tr>
<tr>
<td>S. Gramsch</td>
<td>Carnegie</td>
<td>High pressure EOS of FeAlO3</td>
<td>February 19, 2006</td>
</tr>
<tr>
<td>R. Chellappa</td>
<td>University of Nevada – Reno</td>
<td>High pressure synchrotron diffraction studies on LiAlH4</td>
<td>February 19-20, 2006</td>
</tr>
<tr>
<td>W. M. Chien</td>
<td>University of Nevada – Reno</td>
<td>High pressure synchrotron diffraction studies on LiAlH4</td>
<td>February 19-20, 2006</td>
</tr>
<tr>
<td>J. Jackson</td>
<td>ANL</td>
<td>Synchrotron Mössbauer spectroscopy of mantle minerals at high pressure</td>
<td>February 22, 2006</td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Title</td>
<td>Date</td>
</tr>
<tr>
<td>-----------------------</td>
<td>------------------------</td>
<td>----------------------------------------------------------------------</td>
<td>---------------------</td>
</tr>
<tr>
<td>Wendy Mao</td>
<td>Carnegie</td>
<td>High-pressure/temperature study of Fe-Mg silicate in post-perovskite phase</td>
<td>February 22, 2006</td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Jennifer Jackson</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Crowhurst</td>
<td>LLNL</td>
<td>Determination of the high-pressure melting curve of iron and the structure of liquid iron using angle-dispersive x-ray diffraction</td>
<td>February 24, 2006</td>
</tr>
<tr>
<td>A. Goncharov</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Brown</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Lucas</td>
<td>California Institute of Technology</td>
<td>FeAl vacancy effects in vibrational entropy by inelastic nuclear resonant x-ray scattering</td>
<td>February 26, 2006</td>
</tr>
<tr>
<td>I. Halevy</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kimberly Tait</td>
<td>LANL</td>
<td>High P-T phase relationships of first row transition metal monosulfides</td>
<td>February 26, 2006</td>
</tr>
<tr>
<td>Wendy Mao</td>
<td>LANL</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H. K. Mao</td>
<td>Carnegie</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td></td>
<td></td>
</tr>
<tr>
<td>X-ray diffraction studies of (Mg, Fe)SiO₃ post perovskite at high pressure and high temperatures</td>
<td>February 26-27, 2006</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H. P. Liermann</td>
<td>Florida Institutional University</td>
<td>Compression of high-pressure standards (MO) at high-pressure and temperature in resistive heated DAC</td>
<td>March 5, 2006</td>
</tr>
<tr>
<td>S. V. Raju</td>
<td>Florida Institutional University</td>
<td>Compresson of high-pressure standards (Mo) at high pressure and temperature in resistively heated DA</td>
<td>March 9-11, 2006</td>
</tr>
<tr>
<td>S. Kulkarni</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Dinnebin</td>
<td>MPI Solid State Research</td>
<td>High Pressure XRPD</td>
<td>March 10, 2006</td>
</tr>
<tr>
<td>H. Liu</td>
<td>HPCAT</td>
<td>Mechanisms responsible for pressure induced phase transitions in ZnO</td>
<td>March 11, 2006</td>
</tr>
<tr>
<td>B. Hinrichsen</td>
<td>Max Planck Institut für Festkörperforschung</td>
<td>Mechanism responsible for pressure induced phase transition in ZnO and other binary and ternary oxides</td>
<td>March 11-13, 2006</td>
</tr>
<tr>
<td>R. Dinnebier</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K. Sugimoto</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. McClure</td>
<td>University of Nevada – Las Vegas</td>
<td>Testing of Laue and EDX approach to SXD experiments at high pressure</td>
<td>March 15, 2006</td>
</tr>
<tr>
<td>C. S. Yoo</td>
<td>LLNL</td>
<td>Studies of structural transition in low-Z compounds</td>
<td>March 15, 2006</td>
</tr>
<tr>
<td>H. Cynn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Lipp</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>W. Evans</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. P. Perrillat</td>
<td>University of Illinois – Urbana Champaign</td>
<td>X-ray Raman spectroscopy</td>
<td>March 15-24, 2006</td>
</tr>
<tr>
<td>D. Lakhtanov</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P. Dera</td>
<td>Carnegie</td>
<td>Testing of Laue and EDX approach to SXD experiments at high pressure</td>
<td>March 15-19, 2006</td>
</tr>
<tr>
<td>S. Sinogeikin</td>
<td>HPCAT</td>
<td>Raman spectroscopy</td>
<td>March 21, 2006</td>
</tr>
<tr>
<td>H. K. Mao</td>
<td>Carnegie</td>
<td>X-Ray diffraction of H₂O at high pressures</td>
<td>March 25, 2006</td>
</tr>
<tr>
<td>J. Shu</td>
<td>LANL</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wendy Mao</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Jennifer Jackson</td>
<td>Carnegie</td>
<td>X-ray diffraction on mantle minerals at high-pressure</td>
<td>March 25-26, 2006</td>
</tr>
<tr>
<td>Jennifer Ciezak</td>
<td>Carnegie</td>
<td>High Pressure Crystallographic Analysis of Sodium Azide: Raman spectroscopy</td>
<td>March 29-31, 2006</td>
</tr>
<tr>
<td>H. K. Mao</td>
<td>Carnegie</td>
<td>X-ray Raman spectroscopy</td>
<td>March 30-31, 2006</td>
</tr>
<tr>
<td>C. Gobin</td>
<td>University of Nevada – Las Vegas</td>
<td>16ID-B XRD</td>
<td>March 30-31, 2006</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Project Description</td>
<td>Date</td>
</tr>
<tr>
<td>------------</td>
<td>------------------------------</td>
<td>-------------------------------------------------------------------------------------</td>
<td>-----------------------</td>
</tr>
<tr>
<td>J. McClure</td>
<td>University of Nevada – Las Vegas</td>
<td>Powder diffraction studies on low-Z and high-Z oxides</td>
<td>March 31-April 2, 2006</td>
</tr>
<tr>
<td>O. Tschauner</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Bommanavar</td>
<td>HPCAT</td>
<td>NFS studies of gamma Fe$_2$O$_3$ nanoparticles under high pressure; Raman spectroscopy</td>
<td>April 1-2, 2006</td>
</tr>
<tr>
<td>B. Yulga</td>
<td>University of Nevada – Las Vegas</td>
<td>16-ID-B XRD</td>
<td>April 2-3, 2006</td>
</tr>
<tr>
<td>Z. Quine</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Pravica</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Kumar</td>
<td>University of Nevada – Las Vegas</td>
<td>Low temperature x-ray diffraction studies on CeCu$_2$Si$_2$, Ag, Au and Pt under pressure</td>
<td>April 5, 2006</td>
</tr>
<tr>
<td>C. S. Yoo</td>
<td>LLNL</td>
<td>Powder diffraction in 16-ID-B Raman spectroscopy</td>
<td>April 5-6, 2006</td>
</tr>
<tr>
<td>H. Cynn</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>W. Evans</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Lipp</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V. Struzhkin</td>
<td>Carnegie</td>
<td>Effect of broadening of spin-crossover tuned by pressure in transition metal oxides; Raman spectroscopy</td>
<td>April 5-10, 2006</td>
</tr>
<tr>
<td>A. Goncharov</td>
<td>Carnegie</td>
<td>16-ID-B, XRD</td>
<td>April 10, 2006</td>
</tr>
<tr>
<td>Kimberly Tait</td>
<td>LANL</td>
<td>Compressive yield strength measurements of novel metals in the DAC</td>
<td>April 11, 2006</td>
</tr>
<tr>
<td>P. Liermann</td>
<td>Carnegie</td>
<td>Pressure-induced spin transition in iron nitrides</td>
<td>April 12, 2006</td>
</tr>
<tr>
<td>Yue Meng</td>
<td>Carnegie</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td>Silicate post-perovskite: XRD</td>
<td>April 13, 2006</td>
</tr>
<tr>
<td>A. Lazicki</td>
<td>LLNL</td>
<td>High pressure magnetic properties of light rare-earths using XES</td>
<td>April 14, 2006</td>
</tr>
<tr>
<td>B. Maddox</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H. Giefers</td>
<td>University of Nevada – Las Vegas</td>
<td>16IDB XRD</td>
<td>April 14-16, 2006</td>
</tr>
<tr>
<td>C. Gobin</td>
<td>University of Nevada – Las Vegas</td>
<td>16IDB, XRD; Raman spectroscopy</td>
<td>April 14-17, 2006</td>
</tr>
<tr>
<td>R. Kumar</td>
<td>University of Nevada – Las Vegas</td>
<td>High pressure x-ray diffraction studies of Telluride and hydride compounds</td>
<td>April 17, 2006</td>
</tr>
<tr>
<td>Patricia Kalita</td>
<td>University of Nevada – Las Vegas</td>
<td>High pressure studies of Ba$_2$Se$_3$ and Sb$_2$Se$_3$; Raman spectroscopy</td>
<td>April 15-17, 2006</td>
</tr>
<tr>
<td>M. Jacobsen</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. McClure</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Maddox</td>
<td>LLNL</td>
<td>Resonant x-ray inelastic scattering in compressed rare earths</td>
<td>April 18, 2006</td>
</tr>
<tr>
<td>A. Lazicki</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P. Dera</td>
<td>Carnegie</td>
<td>Test of a new approach to high pressure white beam Single-crystal diffraction and ESAFS with rare-earth Metal organic crystals</td>
<td>April 19-22, 2006</td>
</tr>
<tr>
<td>Lauren Barkoski</td>
<td>George Washington University</td>
<td>BMD</td>
<td>April 19-22, 2006</td>
</tr>
<tr>
<td>Kimberly Tait</td>
<td>LANL</td>
<td>Compression behavior of Hafnon and Sulfides at high pressure and temperature in a resistive heated DAC. Compression measurements of Thorite at ambient temperature in DAC</td>
<td>April 22-24, 2006</td>
</tr>
<tr>
<td>A. Bommanavar</td>
<td>HPCAT</td>
<td>Raman spectroscopy</td>
<td>May 29, 2006</td>
</tr>
<tr>
<td>M. Hu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N. Velisavljevic</td>
<td>LANL</td>
<td>High pressure x-ray diffraction of metals and polymers</td>
<td>June 1-3, 2006</td>
</tr>
<tr>
<td>Dana Dattlebaum</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Sinogeikin</td>
<td>HPCAT</td>
<td>Raman spectroscopy</td>
<td>June 3, 2006</td>
</tr>
<tr>
<td>H. K. Mao</td>
<td>Carnegie</td>
<td>Raman spectroscopy</td>
<td>June 3, 2006</td>
</tr>
<tr>
<td>Wendy Mao</td>
<td>LANL</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Sinogeikin</td>
<td>HPCAT</td>
<td>Raman spectroscopy</td>
<td>June 7-9, 2006</td>
</tr>
<tr>
<td>V. Prakapenko</td>
<td>GSECARS</td>
<td>High-temperature studies</td>
<td>June 7-9, 2006</td>
</tr>
<tr>
<td>A. Kuznetsov</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Name(s)</td>
<td>Institution/Location</td>
<td>Project Title</td>
<td>Date</td>
</tr>
<tr>
<td>-------------------------</td>
<td>-----------------------------------------------</td>
<td>-------------------------------------------------------------------------------</td>
<td>-----------------------</td>
</tr>
<tr>
<td>L. Gao</td>
<td>University of Illinois – Urbana-Champaign</td>
<td>High pressure effect on orbital ordering in transition metal oxides; Raman spectroscopy</td>
<td>June 9-13, 2006</td>
</tr>
<tr>
<td>J. Wang</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C. Bin</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Parsons</td>
<td>University of Edinburgh</td>
<td>Sample lab and ruby, organic project</td>
<td>June 2006</td>
</tr>
<tr>
<td>S. Moggach</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Y. Ding</td>
<td>HPCAT ANL</td>
<td>High pressure effect on orbital ordering in transition metal oxides</td>
<td>June 9-11, 2006</td>
</tr>
<tr>
<td>Y. Ren</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>M. Lucas</td>
<td>California Institute of Technology</td>
<td>Fe-Ni alloys: XRD</td>
<td>June 14-19, 2006</td>
</tr>
<tr>
<td>B. Olson</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Larson</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Hirschauer</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Walters</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z. Quine</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Goncharov</td>
<td>Carnegie</td>
<td>Study of the EOS and structure of low-Z materials</td>
<td>June 16-20, 2006</td>
</tr>
<tr>
<td>H. Giefers</td>
<td>University of Nevada – Las Vegas</td>
<td>Commissioning in BM-B</td>
<td>June 16-19, 2006</td>
</tr>
<tr>
<td>J. Liu</td>
<td>Chinese Academy of Sciences – HPCAT</td>
<td>High pressure induced phase transitions for rare earth compounds</td>
<td>June 17-18, 2006</td>
</tr>
<tr>
<td>Y. Li</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H. Liu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Merkel</td>
<td>University of California – Berkeley</td>
<td>Simultaneous high-pressure and temperature investigation of memory effects in the phase transitions of iron</td>
<td>June 21, 2006</td>
</tr>
<tr>
<td>M. Ahart</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Kumar</td>
<td>UNLV</td>
<td>Heavy fermion materials: XRD</td>
<td>June 21-24, 2006</td>
</tr>
<tr>
<td>Y. Li</td>
<td>ESRF</td>
<td>XRD</td>
<td>June 25, 2006</td>
</tr>
<tr>
<td>C. D. Martin</td>
<td>State University of New York, Stony Brook</td>
<td>NaMgF$_3$ at high pressure: XRD</td>
<td>June 23-24, 2006</td>
</tr>
<tr>
<td>H. K. Mao</td>
<td>Carnegie</td>
<td>X-ray diffraction of deuterated H$_2$ at high pressure ID-B; Raman spectroscopy</td>
<td>June 24-30, 2006</td>
</tr>
<tr>
<td>J. Shu</td>
<td>LANL</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wendy Mao</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>V. Struzhkin</td>
<td>Carnegie</td>
<td>XRD</td>
<td>June 26-30, 2006</td>
</tr>
<tr>
<td>L. Jing</td>
<td>ESRF</td>
<td>XRD</td>
<td>June 26, 2006</td>
</tr>
<tr>
<td>P. Dera</td>
<td>Carnegie</td>
<td>Tests of oscillation Laue analysis approach to structure solution from white beam diffraction BM-D</td>
<td>June 28-July 5, 2006</td>
</tr>
<tr>
<td>Lauren Borkowski</td>
<td>University of Nevada – Las Vegas – UNIPD</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Lavina</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Yulga</td>
<td>University of Nevada – Las Vegas</td>
<td>Single crystal diffraction of epsilon oxygen and nitrogen under high pressure BM-B/D</td>
<td>July 1-2, 2006</td>
</tr>
<tr>
<td>E. Romano</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>K. Zhuravlev</td>
<td>LANL</td>
<td>Quantum dots under pressure: XRD</td>
<td>July 1-3, 2006</td>
</tr>
<tr>
<td>N. Cunningham</td>
<td>University of Alabama – Birmingham</td>
<td>High pressure x-ray diffraction of metals ID-B/BM-B</td>
<td>July 3-7, 2006</td>
</tr>
<tr>
<td>W. Qiu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N. Velisavljevic</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Pietryga</td>
<td>LANL</td>
<td>XRD</td>
<td>July 1-3, 2006</td>
</tr>
<tr>
<td>Kimberly Tait</td>
<td></td>
<td>High P-T phase relationships of first Row transition metal monosulfides ID-B, DAC XRD</td>
<td>July 5-7, 2006</td>
</tr>
<tr>
<td>H. Giefers</td>
<td>University of Nevada – Las Vegas</td>
<td>X-ray emission spectroscopy</td>
<td>July 5-10, 2006</td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Topic</td>
<td>Date</td>
</tr>
<tr>
<td>----------------------</td>
<td>------------------------------------</td>
<td>-----------------------------------------------------------------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>H. Scott S. Huggins</td>
<td>Indiana University – South Bend</td>
<td>High pressure EOS of Fe₃P (ID-B)</td>
<td>July 7-9, 2006</td>
</tr>
<tr>
<td>L. George S. Vennila</td>
<td>FIU</td>
<td>High pressure and temperature study of MAX hydrides and perovskite XRD in BM-D</td>
<td>July 7-10, 2006</td>
</tr>
<tr>
<td>Jennifer Jackson</td>
<td>Carnegie</td>
<td>Raman spectroscopy</td>
<td>July 10, 2006</td>
</tr>
<tr>
<td>M. Jacobsen J. Baker E. Baxter J. Keen</td>
<td>University of Nevada – Las Vegas</td>
<td>High pressure characterization of Bi₂Se₃, Sb₂Te₃, and solid solution 50/50 Bi₂Te₃/Sb₂Te₃ ID-B</td>
<td>July 13-14, 2006</td>
</tr>
<tr>
<td>Patricia Kalita</td>
<td>University of Nevada – Las Vegas</td>
<td>ID-B and Raman spectroscopy</td>
<td>July 12-14, 2006</td>
</tr>
<tr>
<td>J. McClure</td>
<td>University of Nevada – Las Vegas</td>
<td>ID-B and Raman spectroscopy</td>
<td>July 15-18, 2006</td>
</tr>
<tr>
<td>H. Giefer</td>
<td>University of Nevada – Las Vegas</td>
<td>ID-B and Raman spectroscopy</td>
<td>July 15-17, 2006</td>
</tr>
<tr>
<td>Lee S. Keun</td>
<td>Seoul National University</td>
<td>Raman spectroscopy</td>
<td>July 17, 2006</td>
</tr>
<tr>
<td>P. Dera</td>
<td>Carnegie</td>
<td>Single crystal diffraction commissioning in BM-B</td>
<td>July 19-22, 2006</td>
</tr>
<tr>
<td>P. Shafe B. Huberti L. Fiorenino</td>
<td>UNLV</td>
<td>Visitors</td>
<td>July 17, 2006</td>
</tr>
<tr>
<td>V. Iota</td>
<td>LLNL</td>
<td>Bonding changes in compressed molecular solids</td>
<td>July 19, 2006</td>
</tr>
<tr>
<td>W. Evans</td>
<td>LLNL</td>
<td>Ambient and high-temperature crystal structures, phase transitions and equations of state of materials at high pressures by EDXD</td>
<td>July 19-23, 2006</td>
</tr>
<tr>
<td>O. Tschauner</td>
<td>UNLV</td>
<td>XRD in BM-B</td>
<td>July 19-20, 2006</td>
</tr>
<tr>
<td>C. Gobin</td>
<td>UNLV</td>
<td>XRD in BM-B</td>
<td>July 18-20, 2006</td>
</tr>
<tr>
<td>W. Xiao</td>
<td>Chinese Academy of Sciences</td>
<td>Raman system and ID-B</td>
<td>July 21, 2006</td>
</tr>
<tr>
<td>Wendy Mao</td>
<td>LANL</td>
<td>High P-T study of Fe-Mg silicate in post-perovskite phase; Raman spectroscopy</td>
<td>July 23, 2006</td>
</tr>
<tr>
<td>Lauren Borkowski</td>
<td>University of Nevada – Las Vegas</td>
<td>Single crystal diffraction commissioning in BM-D</td>
<td>July 26-29, 2006</td>
</tr>
<tr>
<td>M. Lipp B. Baer</td>
<td>LLNL</td>
<td>f-metal behavior at high pressures and high temperatures using DAC</td>
<td>July 26-31, 2006</td>
</tr>
<tr>
<td>J. McClure P. Dera</td>
<td>University of Nevada – Las Vegas</td>
<td>OLA diffraction study of Cr₂O₃</td>
<td>July 26-31, 2006</td>
</tr>
<tr>
<td>C. S. Yoo</td>
<td>LLNL</td>
<td>f-metal behavior at high pressures and high temperatures using DAC</td>
<td>July 25-31, 2006</td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td>Commissioning in BM-D</td>
<td>July 26-31, 2006</td>
</tr>
<tr>
<td>J. Liu</td>
<td>Chinese Academy of Sciences</td>
<td>XRD</td>
<td>July 21-27, 2006</td>
</tr>
<tr>
<td>W. Xiao</td>
<td>GIG</td>
<td>ID-B diffraction</td>
<td>July 23-26, 2006</td>
</tr>
<tr>
<td>X. Li</td>
<td>Chinese Academy of Sciences</td>
<td>High-pressure behavior of some rare earth sesquioxides</td>
<td>July 29-30, 2006</td>
</tr>
<tr>
<td>B. Yulga</td>
<td>University of Nevada – Las Vegas</td>
<td>Angular-dispersive x-ray studies of organic materials</td>
<td>August 3, 2006</td>
</tr>
</tbody>
</table>
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).

<table>
<thead>
<tr>
<th>User Name</th>
<th>Affiliations</th>
<th>Project</th>
<th>Dates</th>
</tr>
</thead>
<tbody>
<tr>
<td>B. Chen</td>
<td>University of California – Berkeley</td>
<td>High pressure XRD and IR study of polytypically disordered nano-ZnS</td>
<td>August 1-4, 2005</td>
</tr>
<tr>
<td>G. Lager</td>
<td>University of Louisville</td>
<td>High-pressure infrared studies of hydrogarnet and OH-topaz</td>
<td>August 10-13, 2005</td>
</tr>
<tr>
<td>J. Bass, J. Wang, C. Sanchez-Valley</td>
<td>University of Illinois – Urbana-Champaign</td>
<td>Quantitative analysis of hydrogen content of high pressure phases and its effect on elastic properties</td>
<td>August 15-22, 2005</td>
</tr>
<tr>
<td>T. Zhou</td>
<td>New Jersey Institute of Technology</td>
<td>Infrared and Raman spectroscopic studies of FeS under high pressure</td>
<td>August 25-27, 2005</td>
</tr>
<tr>
<td>H. Long</td>
<td>SUNY – Stony Brook</td>
<td>Investigation on cell assemblies for mantle rheology</td>
<td>August 29, 2005</td>
</tr>
<tr>
<td>Z. Liu</td>
<td>Carnegie</td>
<td>Beamline development</td>
<td>September 1-27, 2005</td>
</tr>
<tr>
<td>L. Wang</td>
<td>SUNY – Stony Brook</td>
<td>IR studies of olivine</td>
<td>September 28-29, 2005</td>
</tr>
<tr>
<td>M. Pravica, O. Tschauner, M. Nicol, B. Yulga, C. Gobin</td>
<td>University of Nevada – Las Vegas</td>
<td>Infrared spectroscopy on energetic materials at high pressure and on shock synthesized glasses properties</td>
<td>October 5-9, 2005</td>
</tr>
<tr>
<td>N. Hyatt, J. Hriljac, M. Colligan</td>
<td>University of Sheffield, University of Birmingham</td>
<td>High-pressure Raman and infrared studies of layered perovskites</td>
<td>October 11-15, 2005</td>
</tr>
<tr>
<td>Wren Montgomery</td>
<td>University of California – Berkeley</td>
<td>Synchrotron FTIR studies of cyanuric acid</td>
<td>November 6, 2005</td>
</tr>
<tr>
<td>H. Jung</td>
<td>University of California – Riverside</td>
<td>Effect of pressure on slip system of olivine</td>
<td>November 7, 2005</td>
</tr>
<tr>
<td>J. Zhang</td>
<td>University of California – Riverside</td>
<td>Synchrotron IR studies of water in eclogite</td>
<td>November 8, 2005</td>
</tr>
<tr>
<td>S. Jacobsen, Z. Liu</td>
<td>Carnegie</td>
<td>A synchrotron-IR study of OH in silicate perovskite</td>
<td>November 10-11, 2005</td>
</tr>
<tr>
<td>C. Melendres, F. Hahn</td>
<td>Université de Poitiers</td>
<td>In-situ synchrotron far infrared spectroscopy at microelectrodes</td>
<td>November 14-22, 2005</td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Topic</td>
<td>Date</td>
</tr>
<tr>
<td>-----------------------</td>
<td>----------------------------------</td>
<td>----------------------------------------------------------------------</td>
<td>--------------------</td>
</tr>
<tr>
<td>J. Smedley</td>
<td>Brookhaven</td>
<td>Characterization of impurities in diamond</td>
<td>January 10, 2006</td>
</tr>
<tr>
<td>P. Allen</td>
<td>SUNY – Stony Brook</td>
<td>Light absorption by Fe impurities in MgO at high pressure</td>
<td>January 16-20, 2006</td>
</tr>
<tr>
<td>T. Sun</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Yu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Tse</td>
<td>University of Saskatchewan</td>
<td>High-pressure infrared study of a lubricant additive – ZDDP</td>
<td>January 27-29, 2006</td>
</tr>
<tr>
<td>Y. Song</td>
<td>University of Western Ontario</td>
<td></td>
<td></td>
</tr>
<tr>
<td>G. Lager</td>
<td>University of Louisville</td>
<td>Affect of x- and z-site substitutions on the high-pressure behavior of hydrogarnet</td>
<td>January 30-Feb. 3 2006 February 9, 2006</td>
</tr>
<tr>
<td>Z. Liu</td>
<td>Carnegie</td>
<td></td>
<td></td>
</tr>
<tr>
<td>X. Chen</td>
<td>Carnegie</td>
<td>High-pressure optical spectroscopy of hydrogen-based electron materials</td>
<td>February 10-12, 2006</td>
</tr>
<tr>
<td>A. Goncharov</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Jennifer Ciezak</td>
<td>Carnegie</td>
<td>High-pressure vibrational characterization of energetic materials</td>
<td>February 14-16, 2006</td>
</tr>
<tr>
<td>T. Jenkins</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D. Dolan</td>
<td>Sandia</td>
<td>Characterizing the emissivity of materials under dynamic compression</td>
<td>February 17-18, 2006</td>
</tr>
<tr>
<td>M. Madlener</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R. Hacking</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P. Allen</td>
<td>SUNY – Stony Brook</td>
<td>Light absorption by Fe impurities in MgO at high pressure</td>
<td>February 27-March 2, 2006</td>
</tr>
<tr>
<td>T. Sun</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Yu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heather Watson</td>
<td>Carnegie</td>
<td>Synchrotron-IR measurement of OH in Al-bearing silicate perovskite</td>
<td>March 3-6, 2006</td>
</tr>
<tr>
<td>M. Pravica</td>
<td>University of Nevada – Las Vegas</td>
<td>Infrared spectroscopy on energetic materials at high pressure and on shock synthesized glasses properties</td>
<td>March 9-12, 2006</td>
</tr>
<tr>
<td>M. Nicol</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Yulga</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C. Gobin</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Zhou</td>
<td>New Jersey Institute of Technology</td>
<td>Infrared and Raman spectroscopic studies of FeS under high pressure</td>
<td>March 13-17, 2006</td>
</tr>
<tr>
<td>Z. Qin</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q. Cui</td>
<td>Jilin University</td>
<td>High-pressure infrared studies on Se, Te, AlN and C3N4</td>
<td>March 18-19, 2006</td>
</tr>
<tr>
<td>C. Seagle</td>
<td>University of Chicago</td>
<td>The spectral emissivity and conductivity of iron from reflectance measurements at high pressure</td>
<td>March 28-31, 2006</td>
</tr>
<tr>
<td>D. Heinz</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Tyson</td>
<td>New Jersey Institute of Technology</td>
<td>High-pressure Raman scattering measurements on manganites</td>
<td>April 5-7, 2006</td>
</tr>
<tr>
<td>P. Gao</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Smedley</td>
<td>Brookhaven</td>
<td>Characterization of impurities in diamond</td>
<td>April 14, 2006</td>
</tr>
<tr>
<td>T. Zhou</td>
<td>New Jersey Institute of Technology</td>
<td>Infrared and Raman spectroscopic studies of FeS under high pressure</td>
<td>April 24-28, 2006</td>
</tr>
<tr>
<td>Z. Qin</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gianluca Iezzi</td>
<td>Università di Chieti</td>
<td>The high-pressure behavior of amphiboles</td>
<td>May 26-29, 2006</td>
</tr>
<tr>
<td>G. D. Ventura</td>
<td>Università di Roma</td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Tyson</td>
<td>New Jersey Institute of Technology</td>
<td>Exploring strain effects in manganite films with infrared spectroscopy</td>
<td>June 1-5, 2006</td>
</tr>
<tr>
<td>P. Gao</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>G. Lager</td>
<td>University of Louisville</td>
<td>Affect of x- and z-site substitutions on the high-pressure behavior of hydrogarnet</td>
<td>June 6-9, 2006</td>
</tr>
<tr>
<td>J. Smedley</td>
<td>Brookhaven</td>
<td>Characterization of impurities in diamond</td>
<td>June 14-15, 2006</td>
</tr>
<tr>
<td>O. Tschauner</td>
<td>University of Nevada – Las Vegas</td>
<td>Infrared spectroscopy on energetic materials at high pressure</td>
<td>July 12-15, 2006</td>
</tr>
<tr>
<td>B. Yulga</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C. Gobin</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A. Gordon</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Jacobsen</td>
<td>Carnegie</td>
<td>Synchrotron-IR measurement of OH in Al-bearing silicate perovskite</td>
<td>July 17-20, 2006</td>
</tr>
<tr>
<td>Heather Watson</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Frances Reid</td>
<td>Carleton College</td>
<td></td>
<td></td>
</tr>
<tr>
<td>User Name</td>
<td>Affiliations</td>
<td>Project</td>
<td>Dates</td>
</tr>
<tr>
<td>------------</td>
<td>----------------------------------</td>
<td>------------------------------------------------------------------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>J. Hu</td>
<td>University of Chicago</td>
<td></td>
<td>August 3-9, 2005</td>
</tr>
<tr>
<td>B. Li</td>
<td>SUNY – Stony Brook</td>
<td>Elastic wave velocity of mantle silicates</td>
<td>August 6-8, 2005</td>
</tr>
<tr>
<td>Y. Ma</td>
<td>Texas Tech University</td>
<td>High pressure study of tetragonal boron B-192</td>
<td>August 11-21, 2005</td>
</tr>
<tr>
<td>R. Aksoy</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E. Selvi</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Lundin</td>
<td>Massachusetts Institute of</td>
<td>Crystal structure and crystal chemistry of perovskite-structured</td>
<td>August 25-29, 2005</td>
</tr>
<tr>
<td>J. Santillan</td>
<td>Technology</td>
<td>materials at high pressures</td>
<td></td>
</tr>
<tr>
<td>D. Shim</td>
<td>Massachusetts Institute of</td>
<td>4-Laue mono</td>
<td>August 30-September 10, 2005</td>
</tr>
<tr>
<td>S. Lundin</td>
<td>Technology</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Santillan</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Rekhi</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Q. Guo</td>
<td>Geolab</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Zhu Mao</td>
<td>Princeton University</td>
<td></td>
<td>September 10-1  2005</td>
</tr>
<tr>
<td>F. Jiang</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B. Chen</td>
<td>University of California –</td>
<td></td>
<td>September 14-18, 2005</td>
</tr>
<tr>
<td>M. Finnegan</td>
<td>Berkeley</td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Shu</td>
<td>Carnegie</td>
<td>Study of micro-minerals in eclogite and peridotite of ultrahigh pressure metamorphic belt in Donghai, Jiangsu Province, China</td>
<td>September 21-24, 2005</td>
</tr>
</tbody>
</table>

C. X17 (NSLS)

This facility is not supported by CDAC, but provides additional x-ray diffraction capabilities that supplement those available at HPCAT. The X17 facility consists of X17C, the superconductor wiggler beamline, the first dedicated high-pressure x-ray beamline in the world, and X17B, a dedicated beamline for variable temperature (cryogenic to laser heating) diffraction. These beamlines are supported by the National Science Foundation through the EAR COMPRES consortium and are managed by Carnegie. CDAC Academic and National Lab Partner experiments that do not require HPCAT facilities are given beam time on X17 through the Carnegie PRT allocation if they are not awarded beam time through the NSLS General User Proposal program. User support is provided by beamline scientists Jingzhu Hu (X17B) and Quanzhong Guo (X17C).
<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Topic</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Y. Ma J. Sandhu</td>
<td>Texas Tech University</td>
<td>Laser heating</td>
<td>September 24-28, 2005</td>
</tr>
<tr>
<td>F. Zhang</td>
<td>Florida International University</td>
<td>Structural investigation of defect pyrochlores at high pressures</td>
<td>September 28-October 1, 2005</td>
</tr>
<tr>
<td>J. Xu</td>
<td>Carnegie</td>
<td>Structure of single-crystal wüstite (FeO) under high pressures</td>
<td>October 4-7, 2005</td>
</tr>
<tr>
<td>J. Chen</td>
<td>SUNY – Stony Brook</td>
<td>Liquid phase transition at high pressure and high temperature</td>
<td>October 9-14, 2005</td>
</tr>
<tr>
<td>W. Qiu J. Griffith N. Cunningham</td>
<td>University of Alabama – Birmingham</td>
<td>Crystal structure and compressibility of transition metal nanoparticles under high pressures and high temperatures</td>
<td>October 10-15, 2005</td>
</tr>
<tr>
<td>B. Chen</td>
<td>University of California – Berkeley</td>
<td>High pressure XRD and IR study of polytypically disordered nano-ZnS</td>
<td>October 26-November 1, 2005</td>
</tr>
<tr>
<td>S. Sen S. Gaudio</td>
<td>University of California – Davis</td>
<td>Structure of single-crystal wüstite (FeO) under high pressures</td>
<td>November 7-11, 2005</td>
</tr>
<tr>
<td>T. Duffy</td>
<td>Princeton University</td>
<td>EOS and phase transitions in mantle minerals</td>
<td>November 10-15, 2005</td>
</tr>
<tr>
<td>H. Rong J. Shu</td>
<td>Institute of Geology, CAGS (China) Carnegie</td>
<td>X-ray and infrared studies of inclusions in diamond from chromite of harzburgite, ophiolite, Tibet, China</td>
<td>November 11-20, 2005</td>
</tr>
<tr>
<td>F. Zhang</td>
<td>University of Michigan</td>
<td>Structural investigation of defect pyrochlores at high pressures</td>
<td>March 7-9, 2006</td>
</tr>
<tr>
<td>T. Duffy Zhu Mao F. Zhang</td>
<td>Princeton University Physics Institute of CAS</td>
<td>Pressure induced structure evolution of novel strongly correlated perovskite system Ca$_{1-x}$Sr$_x$MoO$_3$ (M=Cr,Fe,Mn)</td>
<td>March 9-11, 2006</td>
</tr>
<tr>
<td>C. Jin</td>
<td>Jilin University</td>
<td>Phase transitions and properties study of earth’s upper mantle mineral under high pressure and high temperature</td>
<td>March 11-16, 2006</td>
</tr>
<tr>
<td>Y. Ma</td>
<td>Texas Tech University</td>
<td>High pressure study of tetragonal boron B-192</td>
<td>March 17-20, 2006</td>
</tr>
<tr>
<td>Michelle Weinberger Abby Kavner</td>
<td>University of California – Los Angeles</td>
<td>Strength measurements of new ultrahard materials by radial diffraction</td>
<td>March 29-April 3, 2006</td>
</tr>
<tr>
<td>Q. Guo</td>
<td>University of Chicago</td>
<td>X-ray and laser system setup</td>
<td>April 3-30, 2006</td>
</tr>
<tr>
<td>I. Halevy J. Dodd</td>
<td>California Institute of Technology</td>
<td>High pressure properties of hydrogen-amorphized RCo$_x$Hx</td>
<td>April 4-8, 2006</td>
</tr>
<tr>
<td>H. Rong J. Shu</td>
<td>Institute of Geology CAGS, (China) Carnegie</td>
<td>Study of micro-minerals in eclogite and peridotite of ultrahigh pressure metamorphic belt in Donghai, Jiangsu Province, China</td>
<td>April 8-17, 2006</td>
</tr>
<tr>
<td>G. Hulber V. Cestone D. Kies D. Dominguez</td>
<td>Naval Research Laboratory</td>
<td>In situ EDXRD of the structural changes in PdDx for x&gt;0.90</td>
<td>April 20-28, 2006</td>
</tr>
<tr>
<td>Name</td>
<td>Institution</td>
<td>Project Description</td>
<td>Date</td>
</tr>
<tr>
<td>-----------------------</td>
<td>------------------------------------</td>
<td>-------------------------------------------------------------------------------------</td>
<td>--------------------</td>
</tr>
<tr>
<td>J. Chen</td>
<td>SUNY – Stony Brook</td>
<td>Liquid phase transition at high pressure and high temperature</td>
<td>May 2-8, 2006</td>
</tr>
<tr>
<td>T. Yu</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>L. Ehm</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Michelle Weinberger</td>
<td>California Institute of Technology</td>
<td>Strength measurements of new ultrahard materials by radial diffraction</td>
<td>May 5-7, 2006</td>
</tr>
<tr>
<td>I. Halevy</td>
<td>California Institute of Technology</td>
<td>Large vacancy concentrations in iron-aluminum alloys, crystallographic and thermodynamic properties under high pressure</td>
<td>May 31-June 5, 2006</td>
</tr>
<tr>
<td>J. Dodd</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T. Duffy</td>
<td>Princeton University</td>
<td>EOS and laser heating</td>
<td>June 5-10, 2006</td>
</tr>
<tr>
<td>Zhu Mao</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F. Zhang</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I. Halevy</td>
<td>California Institute of Technology</td>
<td>High pressure effect on crystallographic properties of vanadium alloying</td>
<td>June 7-12, 2006</td>
</tr>
<tr>
<td>M. Lucas</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J. Hu</td>
<td>University of Chicago</td>
<td></td>
<td>July 14-16, 2006</td>
</tr>
<tr>
<td>S. Jacobsen</td>
<td>Carnegie</td>
<td>Perovskite</td>
<td>July 17-18, 2006</td>
</tr>
<tr>
<td>F. Reid</td>
<td>Carleton College</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S. Sandeep</td>
<td>NSLS</td>
<td>In (OH)₂</td>
<td>July 20-24, 2006</td>
</tr>
<tr>
<td>J. Wang</td>
<td>National Cheng Kung University</td>
<td>H₂BO₃</td>
<td>July 26-31, 2006</td>
</tr>
<tr>
<td>C. Bin</td>
<td>University of California – Berkeley</td>
<td>The compressibility, surface energy, and phase stability of nano-titania</td>
<td>August 1-7, 2006</td>
</tr>
<tr>
<td>M. Kruger</td>
<td>University of Missouri</td>
<td></td>
<td></td>
</tr>
<tr>
<td>V. Dharmaraj</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F. Zhang</td>
<td>University of Michigan</td>
<td>Structural investigation of defect pyrochlores at high pressures</td>
<td>August 2-7, 2006</td>
</tr>
<tr>
<td>J. Xu</td>
<td>Carnegie</td>
<td>Structure of single-crystal wüstite (FeO) under high pressures</td>
<td>August 10-16, 2006</td>
</tr>
<tr>
<td>Q. Guo</td>
<td>University of Chicago</td>
<td>Optical table and laser system re-setup</td>
<td>August 10-September 10, 2006</td>
</tr>
<tr>
<td>D. Klug</td>
<td>NRCC, Saskatchewan</td>
<td>High-pressure low-temperature studies of novel clathrate hydrates</td>
<td>August 16-18, 2006</td>
</tr>
<tr>
<td>J. Tsei</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E. Selvi</td>
<td>Texas Tech University</td>
<td>High-pressure x-ray diffraction study of the giant dielectric constant material</td>
<td>August 18-25, 2006</td>
</tr>
<tr>
<td>R. Aksoy</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
References
41. Seagle, C. T. and D. Heinz, to be published.
76. Xu, J., H. K. Mao and R. J. Hemley, to be published.
80. Militzer, B., Quantum monte carlo simulation of high pressure materials, *Contributed talk, meeting of the American Geophysical Union* (San Francisco, CA, December, 2004).


122. Wu, Z., to be published.


