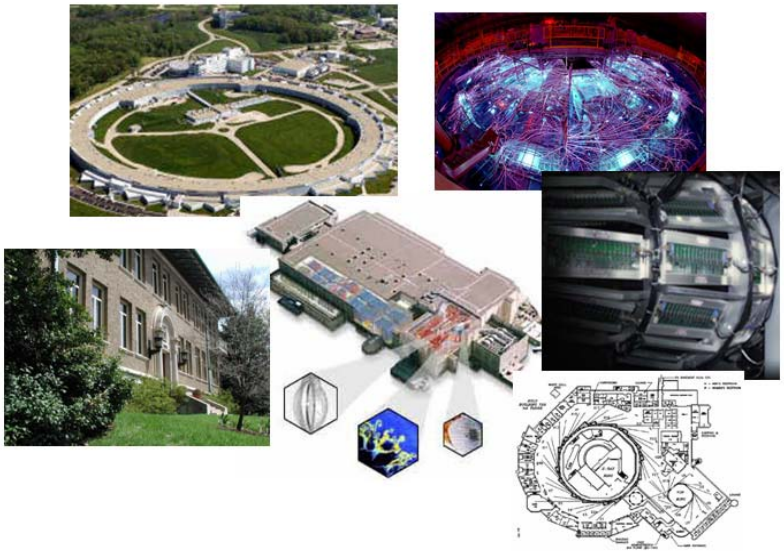
CDAC

CARNEGIE/DOE ALLIANCE CENTER

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

Year Two Annual Report

September 2005



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 TWO ANNUAL REPORT

1. OVERVIEW

1.1 Mission of CDAC

High *P-T* materials research is a burgeoning area in the physical sciences[1, 2], one that is critical to the NNSA's program in science-based stockpile stewardship[3]. This portfolio spans a broad range of materials and problems. The high *P-T* properties of a wide range of crystalline and non-crystalline solids, fluids, and composite materials need to be determined. These materials include *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 crystal and liquid structures, phase transitions, melting, equations of state, phonon dynamics, elasticity, plasticity, texture development, bonding, electronic, magnetic structures, and chemical reactions are essential. As important as these scientific problems are, their solutions also require the training of the next generation of scientists. The proper training of these students requires their access to state-of-the-art facilities that may not be available to research groups in their home environment. The Carnegie/DOE Alliance Center – CDAC – was created to solve these coupled problems.

Based at the Carnegie Institution, Washington, D.C., 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**). Scientists at the National Labs (the CDAC Laboratory Partners) benefit directly by obtaining beam time and technical training, and also through ongoing high *P-T* technique development at HPCAT, the dedicated high-pressure synchrotron x-ray facility at the Advanced Photon Source (APS), as well as at **Carnegie** (including NSLS) by CDAC personnel and affiliated **Carnegie** staff. There also continues to be strong cooperation with the Lujan Center in the development of high *P-T* neutron scattering. Finally, CDAC has an extensive list of collaborators, from some 127 institutions around the world. The need to enlarge CDAC stems from the unexpected success of our outreach program.

Figure 1. *Left: the front of the Abelson building at the* ***Carnegie Institution*** *in Washington DC. Right: the Research Building at the* ***Carnegie*** *campus.*

The mission of CDAC is to advance and perfect an extensive set of high *P-T* techniques and facilities, perform key studies on a broad range of materials in newly accessible *P-T* regimes, integrate and coordinate static, dynamic, and theoretical results for stewardship science applications, and to train a new generation of students, post-doctoral fellows, and other scientists in

the field. Building on **Carnegie's** history of pioneering the development of static high-pressure science and technology for geoscience applications, CDAC is pushing the scientific frontier forward in developing the next generation of high-*P* techniques and conducting systematic measurements of a full range of physical and chemical phenomena under extreme conditions.

HPCAT, the dedicated high-*P* 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 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 two 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 set to commence full general user operations in January 2006. At this point, well over 170 different users (*i.e.,* from National Labs and academia) have conducted experiments at the facility in these two completed experimental hutches to date. Construction is nearing completion and commissioning is underway on the two bending magnet beamlines, and the goal of four independently operating experimental hutches will be realized by mid-2006.

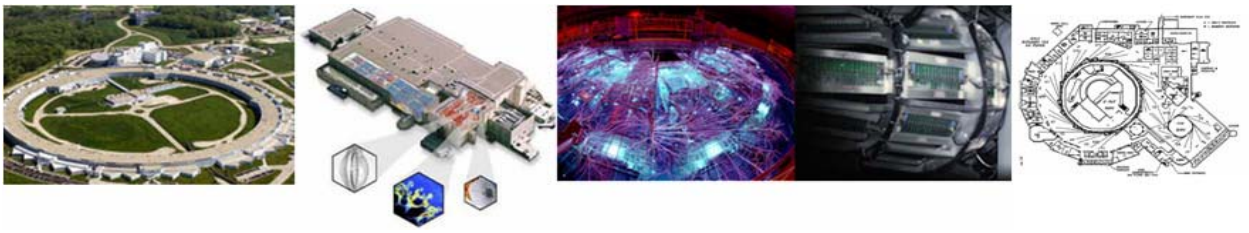


Figure 2. *Advanced Photon Source (APS), National Ignition Facility (**LLNL**), Z-machine (**SNL**), neutron beamline at LANSCE (**LANL**), and National Synchrotron Light System (**BNL**).*

HPCAT is complemented by high-pressure neutron facilities at LANSCE, synchrotron infrared spectroscopy at the National Synchrotron Light Source (NSLS) at **Brookhaven National Laboratory** (**BNL**), and specialized high-pressure facilities at **Carnegie**. Coordination with the research programs of leading high-pressure groups at Lawrence Livermore (**LLNL**), Los Alamos (**LANL**), and Sandia National Laboratories (**SNL**) have provided an unparalleled environment for addressing many important problems in stewardship science. There is also an extensive network of CDAC collaborators at universities throughout the country. Though the CDAC program is principally experimental, close interactions with theorists at Center institutions, the National Laboratories, and throughout academia augment the effort.

At **Carnegie**, important new developments in high *P-T* spectroscopy of molecular systems, high *P-T* cell designs, and CVD diamond growth have been ongoing. Our second year of operations has also seen advances in high-pressure neutron scattering at **LANL** as well as new collaborations in the area of superhard materials. Important projects underway among the academic partners include developments in phase diagrams, melting curves, and EOS of low-*Z* elements and compounds; synchrotron studies of nuclear resonant inelastic x-ray scattering of ordered and disordered iron alloys; radial x-ray diffraction studies of texture development in high-pressure phases; resonant and non-resonant inelastic x-ray scattering of *f*-metals under pressure; combined x-ray/transport measurements with new designer anvils; and sum-frequency generation for spectroscopy of interfaces under pressure. 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. All of these developments have set the stage for new advances in this growing area of materials science.

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

1.2 Highlights from Year Two

Outreach and Training

CDAC continues to make excellent progress in all areas of its mission, at a rate that exceeds expectations. The following are highlights in the area of outreach and training, in particular as it relates to students:

- Facilitated the significant growth of users at HPCAT. To date, more than 170 users have conducted experimental work at the sector.
- Increased the number of CDAC collaborations/facility users. Presently, some 280 outside collaborators from over 120 institutions are working with us on Stewardship Science-related projects.
- Presented 26 posters by CDAC affiliated scientists at the Second SSAAP Symposium in August 2005. Also, a number of posters were contributed by NNSA Lab scientists and their students and post-doctoral associates, as well as faculty, graduate students and post-doctoral associates of the CDAC Collaborators. This complements the 48 high-pressure materials science poster presentations at the 2004 SSAAP meeting.
- Supported Ph.D. thesis work of 14 students at CDAC partner universities and **Carnegie** and encouraged career development at NNSA Labs [*e.g.*, **Wendy Mao** completed her Ph.D. thesis in July 2005 and won an Oppenheimer fellowship at **LANL**].
- Supported research of post-doctoral fellows at CDAC institutions leading to hiring by NNSA Labs [*e.g.*, **Jung-fu Lin** won a Lawrence Fellowship at **LLNL**].
- Organized the first CDAC Summer School, Jun 1-3, 2005, where 33 students and post-docs learned about the state-of-the-art in high *P-T* materials science from world-leading experts in the field.
- Hosted numerous visitors to other CDAC facilities (*e.g.*, **Carnegie** and **NSLS**) for training and technique development.
- 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, seven students were working on CDAC-related research projects.

***Figure 3. Chi-Chang Kao** (NSLS) presenting his lecture on "Fundamentals of X-ray Spectroscopy" during the 2005 CDAC Summer School, Argonne National Laboratory*

Scientific Breakthroughs

The scientific productivity of CDAC has continued to grow. Some 260 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 such as *Physical Review Letters*, *Science*, *Nature*, and *Proceedings of the National Academy of Sciences*, many of which generated considerable interest in the public press world-wide.

- *Abiogenic generation of methane at high pressure*: This CDAC sponsored **Indiana University-South Bend**, **LLNL** and **Carnegie** collaboration established a new mechanism for generation of fuel resources, and was covered by over 50 newspapers and other media sources around the world[4].
- *Novel probes of molecular interfaces on shock compression*: This CDAC supported student project at the **University of Illinois** carried out by **James Patterson** demonstrated that sum frequency generation can be used to examine details of molecular interfaces[5].
- *Direct structural probes in pressure-induced transformations in glasses*: This combined x-ray and neutron study by **Argonne** and **Oak Ridge National Laboratories** as well as **Carnegie** and the **University of Wyoming** demonstrated that the structure of the archetypal network-forming glass GeO_2 undergoes a change in oxygen coordination of Ge from 4 to 5 to 6 between 6 and 15 GPa[6].
- *Sound velocity of hot dense iron*: In this *Science* paper, new techniques developed at CDAC and APS allowed the first direct measurements of the high *P-T* sound velocity of iron, work carried out by current Lawrence Fellow **Jung-Fu Lin**[7].
- *Mott transitions and magnetic collapse in simple oxides*: The Mott transition in compressed MnO and magnetic collapse in (Mg,Fe)O were identified by synchrotron x-ray diffraction and high-resolution x-ray emission spectroscopy at HPCAT[8, 9].
- *Structure and dynamics of novel hydrogen clathrate by neutron scattering*: This CDAC collaboration involving **LANL**, **Chicago**, **Rutgers**, and **Carnegie** and initiated by CDAC student and Oppenheimer Fellow **Wendy Mao** revealed an unusual order-disorder transition in a potentially important hydrogen storage material[10].
- *Ordering of hydrogen bonds in H_2O at high pressure and low temperature*: Inelastic x-ray scattering of near K-edge structure of oxygen reveals the change of hydrogen bonds at 250 MPa in liquid water and ices III, II, and IX from 300 to 4 K[11].
- *Phase diagram and hydrogen atom mobility in high P-T H_2O*: Combined optical, x-ray, and theoretical studies at **LLNL** and **Carnegie** reveal an unusual kink in melting curve of H_2O at 45 GPa and 1000 K[12] and a possible superionic phase[12-14].
- *Pressure-induced polymerization of formic acid*: This was discovered by a combination of optical spectroscopy, x-ray diffraction and theory at HPCAT, leading to a Chemistry and Materials Science Associate Directors Award from **LLNL**[15].
- *The discovery of a new phase of molecular oxygen*: Application of new techniques developed at CDAC has led to the identification of a new *P-T* phase and extended the phase diagram of oxygen[16].
- *Anomalous melting curve of Na at megabar pressures*: High *P-T* x-ray diffraction of Na at HPCAT reveals that the element melts below room temperature at high compression[17].
- *The discovery of ultrahard CVD diamond*: This **Carnegie/LANL** collaboration demonstrated that the single-crystal CVD can be made harder and/or tougher than any known crystalline material[18].

1.3 Work Plan and Milestones for Year Two

CDAC has a three-fold mission which includes a comprehensive scientific program, an education, training and outreach component and technological development goals. Within the context of these sections, milestones have been set for each year of CDAC. Nearly all of the Year 2 goals were met, and we are on track for meeting – and in many cases have already met – the milestones for Year Three. The Year Two milestones from the original proposal are listed below in bold.

Scientific Program

1. *Studies of simple molecular materials (e.g., H_2, H_2O, CH_4) will be extended to 2000 K and 200 GPa for detailed comparison with the shock-wave studies to establish, for example, the predicted superionic region of the high-T solids.*

The melting of H_2 was extended using laser heating techniques[19], complementing the earlier resistive heating methods[20]. Similar high *P-T* measurements were carried out on O_2 [16] and new phases and phase boundaries discovered. The determination of the phase diagram of H_2O provided constraints on superionic behavior[14]. The phase diagram was studied to above 100 GPa. The H_2 band gap and low energy excitons in H_2 were directly determined using inelastic x-ray scattering[21]. Bonding and transformations in H_2O[11], BN[22] and O_2[23, 24] were also identified with these techniques.

2. Measurements of phonons under pressure will be performed with the inelastic neutron spectrometer PHAROS at LANSCE and will serve as a reference point for higher P x-ray studies of phonons. FeAl, an alloy with substantial coherent inelastic scattering allowing detailed information to be obtained on specific vibrational modes will be studied.

Neutron measurements on FeAl reveal expected anharmonic behavior at high temperature[25]. Diffraction of fcc-disordered and $L1_2$ ordered Pt_3Fe alloys was measured[26]. Nuclear forward scattering (NFS) experiments were also conducted on related materials, as discussed below.

3. Ultrahigh-accuracy P-V-T EOS measurements of a series of standards (e.g., high-Z metals, rare gases, oxides, and hydrides) will be launched with the high-efficiency EOS determination mode. These measurements will also provide information on thermal effects on phase transformations, including melting.

The EOSs of numerous materials were determined by x-ray diffraction (*e.g.* Ref .27). The EOS of BeH_2 was determined by Brillouin scattering[28]. Complementary experiments were carried out by **LLNL** colleagues on Be[29]. The EOS of polymeric materials was also determined[30].

4. CDAC will extend rheological studies for benchmark solid materials with radial diffraction measurements to moderate temperatures in order to obtain first-order information about P-T effects on elasticity and strength. Information will also be obtained about high P-T deformation processes by comparing experimental texture data with polycrystal plasticity simulations.

Radial diffraction measurements of texture development and homogeneity of deformation in the DAC were carried out numerous materials. Unusual grain growth at the α-U phase transition in Pr metal was observed[31]. Changes at high pressure with time (creep) and temperature (recrystallization) were documented.[32, 33] *In-situ* measurements of phase transformations in steel[34], Zr[35] and Ti[36] at high temperature were performed. Diffraction of B_4C was measured at high pressure,[37, 38] and the behavior of SiC was examined using a variety of synchrotron techniques[39].

5. SFG experiments on the formation and structures of oxides and hydrides on metal surfaces studied in real time as a function of pressure and temperature, and test experiments with polymer binder energetic materials will begin.

Preliminary SFG data on the surfaces of the energetic materials HMX and TATB have also been obtained, complementing the laser shock results for hydrocarbon systems mentioned above[5].

6. CDAC will integrate the results with those obtained in the ASC program.

The main high pressure effort for the **Caltech** ASC Center has been the dynamic compression of Fe. As part of this effort, this group has computed the thermoelastic properties of Fe as functions of pressure and temperature.

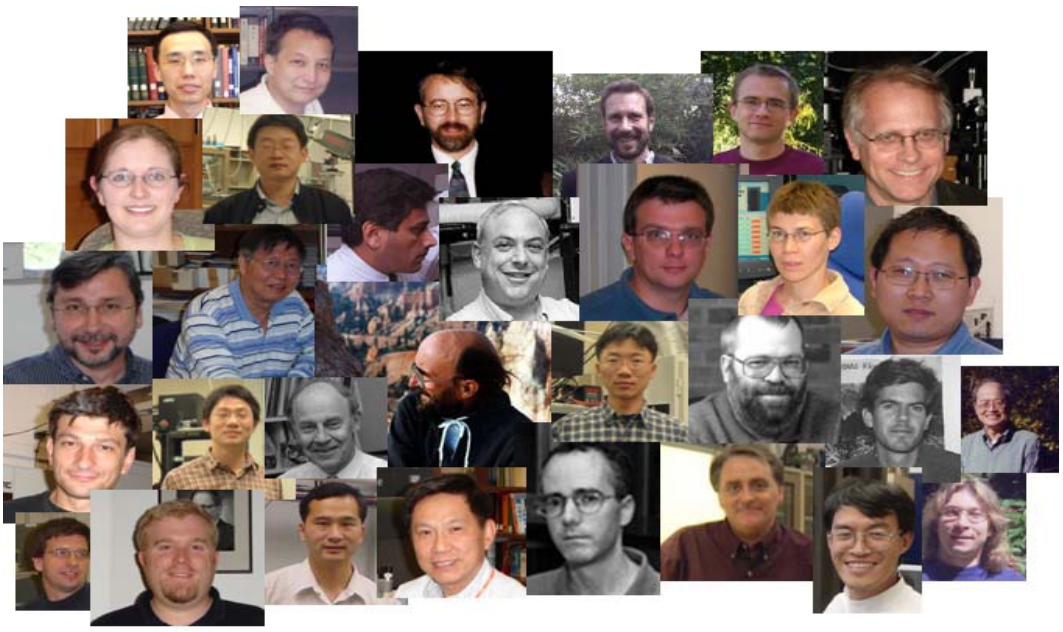


Figure 4. *Personnel from the seven academic institutions that comprise CDAC.*

<u>Education and Training</u>

1. The seven academic institutions of CDAC will expand the educational program to support an average of two graduate students each, or a total of fourteen in the Center.

In Year 2, 14 graduate students were directly supported by funding allocated to the six academic partners and **Carnegie**. One graduate student supported by **LANL** and one supported by **LLNL** carried out thesis research on CDAC-related topics. As described in Section 3.1, this part of the CDAC Education and Outreach effort has been extremely productive.

2. Two CDAC postdoctoral fellows will be recruited for Stewardship Science at LANSCE, HPCAT, and Carnegie.

At **Carnegie**, developments in neutron diffraction to be implemented at LANSCE and eventually SNAP are the focus of one postdoctoral fellow working closely with a research scientist. In addition, one of the **Carnegie** postdoctoral fellows, now stationed at HPCAT, is working on CDAC-related science and technique development. These appointments are more thoroughly discussed in Section 3.1.

3. A summer school/workshop will be organized to train graduate students and attract new ones into the field.

The CDAC Summer School was held June 1-3, 2005 at APS. 33 young scientists, many of them CDAC supported graduate students, took part in the school, which consisted of by 16 leading scientists from academia and the National Labs. Our outreach activities are discussed at greater length in Sections 3.5 and 3.8. The CDAC Summer School, the second SSAAP Symposium, and the Year Two Review have served as meetings for CDAC participants.

Technique Development

1. Accurate high-temperature studies in the DAC will be extended beyond 6,000 K. The sample size in DACs above 50 GPa will be enlarged from the current limit of 0.001 mm³ to 1 mm³.

In situ high *P-T* x-ray diffraction with laser-heating has been extended to above to above 7000 K[40]. Spectroscopic methods for *in-situ* high *P-T* studies began in Year 2 continued, including pioneering laser heating NRIXS measurements on Fe mentioned above[7]. The **Carnegie** synthesis of large single crystal CVD diamond has produced larger diamond anvils allowing high pressure samples in the above range.

2. Single-crystal neutron diffraction up to 50 GPa will be enabled at LANSCE.

We continued to make progress on extending single crystal diffraction to higher pressure. Neutron diffraction measurements have been conducted above 20 GPa[41] and the combination of large anvil and K-B focusing should make 50 GPa studies possible in Year Three.

3. A high-efficiency mode of EOS determination by x-ray diffraction will be developed. X-ray counting efficiency at HPCAT will be increased by 10 to 100 times above the present capability at APS.

P-V-T EOS determinations have become routine at HPCAT. The new Rietveld analysis procedures developed in the previous year were further refined[42, 43]. Notably, all of the milestones for HPCAT construction and commissioning were met and many were exceeded. These will be described in detail in Section 4.3.

4. Integration of the sound velocity determined with inelastic optical scattering (Brillouin) and inelastic x-ray scattering (phonon DOS) spectroscopy will performed to provide a highly accurate EOS and primary pressure scales to 1000 K at 100 GPa.

P-V-T calibrations using both optical and x-ray methods were extended at **Carnegie**[73] and through a **LLNL/Carnegie** collaborations[44].

5. Techniques for P-V-T EOS and structure determination of fluids and melts will be developed.

Considerable progress was made in the use of high *P-T* x-ray diffraction techniques with resistive heating for amorphous phases. Examples include measurements on liquid Na carried out as part of the high *P-T* melting experiments described above[17].

6. Radial diffraction capabilities for obtaining texture information will be developed and techniques for averaging powder neutron diffraction data to obtain structural information will be refined.

A recent breakthrough has been the development of techniques for obtaining quantitative texture information from single diffraction images, without imposing sample symmetry[43]. New DAC gasketing methods were also developed for these experiments[45].

7. New high-pressure grazing incidence cells for studies of interfaces under pressure with sum frequency generation (SFG) will be constructed and tested.

Builiding on the success of the laser-shock molecular interface studies mentioned above[5], high-pressure, grazing incidence cells for use with SFG measurements are being constructed and tested.

2. SCIENTIFIC PROGRESS

We now discuss in more detail selected experimental studies supported fully or in part by CDAC and made possible by the Center. Following the outline of the original proposal, we divide the

topics into the following six categories: 1. High *P-T* Phase Relations and Structures; 2. *P-V-T* Equation of State Measurements; 3. Phonons, Vibrational Thermodynamics and Elasticity; 4. Plasticity, Yield Strength and Deformation; 5. Electronic and Magnetic Structure and Dynamics; and 6. High *P-T* Chemistry.

2.1 High *P-T* Phase Relations and Structures

A larger number of *in-situ* x-ray diffraction measurements and structure refinements were carried out during the past year, principally at HPCAT. New submicron diffraction techniques should prove useful in fine-grained heterogeneous material of importance in stockpile stewardship. A new class of experiments using *in situ* laser heating is extending measurements to higher *P-T* conditions[46]. Resistive heating measurements have been complemented by *in situ* Raman measurements with laser heating[47]. New high-pressure x-ray and neutron diffraction techniques have been applied to study the anomalous pressure-induced structural changes in amorphous solids.

Phase Relations of H_2O under Extreme Conditions – The phase diagram and properties of H_2O at high pressure and temperature are essential for identifying and understanding numerous chemical reactions at extreme conditions, yet there has been comparatively little direct information on the behavior of H_2O above 300 K at tens of gigapascals. Measurements of the melting curve of H_2O at extreme conditions have been controversial for decades because of the different experimental techniques used in detecting melting in H_2O. Last year, the **Carnegie** team first used *in situ* Raman spectroscopy together with an externally-heated diamond cell to directly measure the melting curve of H_2O up to 22 GPa and 900 K using OH-stretching bands and translational modes of H_2O[48]. Using *in situ* high *P-T* Raman spectroscopy and synchrotron x-ray diffraction, the team observed 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 (Fig. 5)[14]. The discovery has been applied to understand the physics and chemistry of planetary interiors such as Neptune, Uranus, and Earth. Similar results obtained using high *P-T* Raman scattering and theoretical calculations were reported by CDAC collaborators from **LLNL**[13,12]. A combined experimental and theoretical study revealed a unique first-order thermodynamic transformation at low temperatures[49]. The synchrotron IR data was supplemented by direct structural studies carried out at HPCAT[50]. These measurements reveal a temperature independent transformation at 14 GPa.

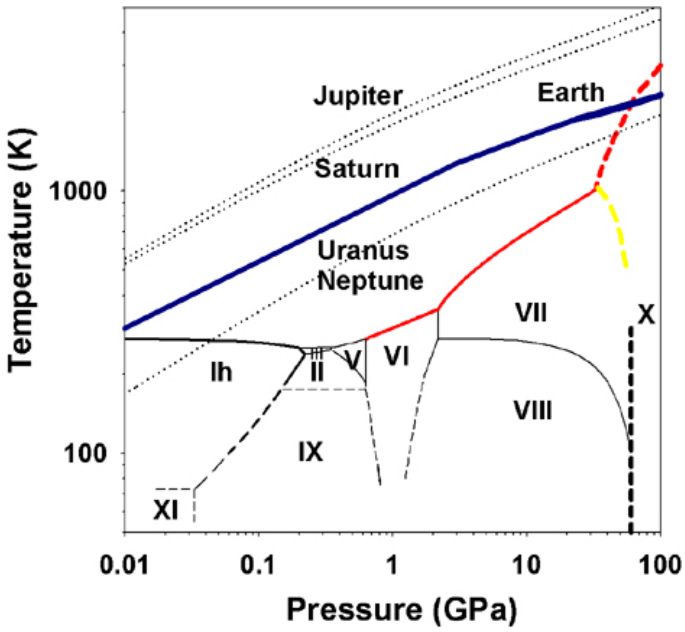


Figure 5. *Proposed new phase diagram of H_2O; dotted lines: isentropes in Jupiter, Saturn, Uranus, and Neptune respectively; blue solid line: geotherm[14].*

Novel Structures of Low-Z Elements – Recent developments in high-pressure methods and advances in x-ray crystallography have led to a new level of understanding of phase diagrams and structures of materials under pressure. Recently discovered phenomena such as complex phases of alkali metals, incommensurate host–guest structures, and incommensurately modulated structures have rendered obsolete the conventional wisdom about the range of structures possible in the elements. Novel behavior discovered in elemental sulfur last year[51] by the **Carnegie** group was

extended to its higher pressure superconducting phases[52]. The structure of the initial superconducting phase observed near 90 GPa was found to be incommensurate (Fig. 6).

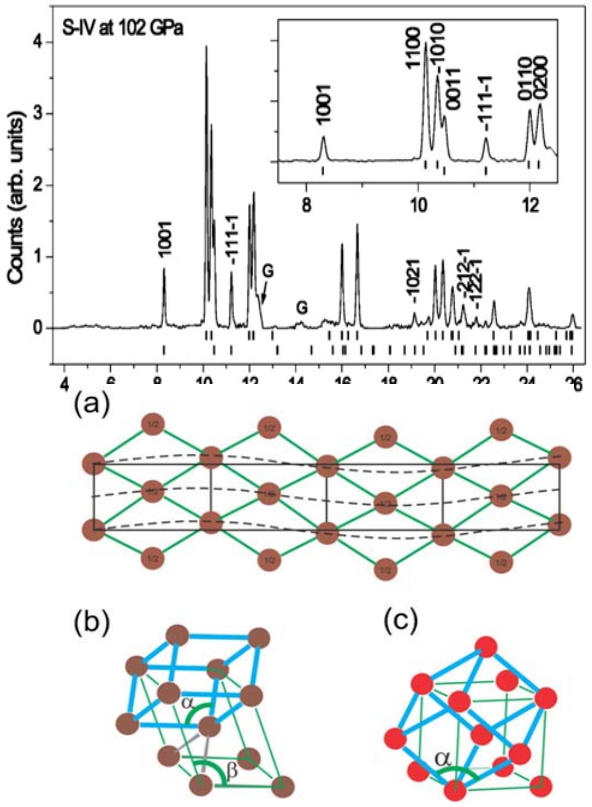


Figure 6. *Top: Diffraction profile of incommensurate S-IV at 102 GPa,. The upper and lower tick marks below the profile show the peak positions of the main and first-order satellite reflections, respectively. The inset shows the low-angle reflections. Some of the diffraction reflections are indexed with their hklm indices. Diffraction peaks from gasket are marked "G." Bottom: Structural relationship of the metallic phases in the group-VI elements. (a) The modulated bcm structure of Te-III and Se-IV four unit cell viewed down the a axis from. The six nearest-neighbor distances for each atom are shown. The modulation wave is indicated by the dashed lines. (b) Relationship between the average bcm structure thin lines and a primitive rhombohedral structure of b-Po thick lines. The monoclinic angle band the rhombohedral angle are shown. (c) Structural relation between the primitive rhombohedral structure thick lines and the body-centered cubic structure thin lines[52].*

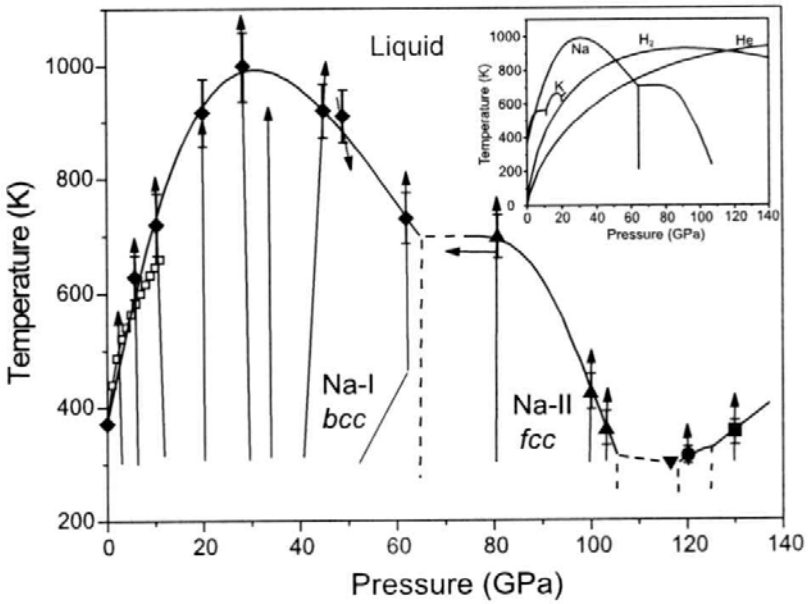


Figure 7. *The melting curve and phase diagram of Na to 130 GPa. The filled symbols correspond to the melting of different Na phases. The open squares are from previous work. Arrows show various P-T paths followed in the experiments. The inset shows the melting curve of Na in comparison with the melting curves of H_2, and He, and K[15].*

The transformation of molecular nitrogen to a single-bonded atomic nitrogen is of significant interest from a fundamental stand point and because it is among the most energetic non-nuclear material predicted. Working with the **Carnegie** group at HPCAT, scientists from the **Max Planck Institute für Chemie, Mainz** performed an x-ray diffraction of nitrogen at pressures up to 170 GPa. The major transformation of this diatomic phase into the single-bonded (polymeric) phase, recently determined to have the *cubic gauche* structure (*cg*-N), proceeds as a first-order transition with a volume change of 22%[53]. Additional measurements carried out by the **Carnegie** team revealed information on the transformation sequence prior to dissociation[54]. A related resistive heating Raman study of O_2 [16] has led to the discovery of a new high *P-T* phase and an entirely new phase diagram for this element. New phases of SO_2 under pressure were documented[55].

Detailed Raman measurements of ^{7}Li and ^{6}Li to 123 GPa at 180 K reveal new features that can be interpreted as resulting from a transformation toward a paired state[56]. Preliminary studies of the melting behavior of alkali metals were performed at HPCAT using resistive-heating/x-ray diffraction techniques. As discussed above, a group at **Carnegie** discovered remarkable behavior of Na under pressure. High-pressure high-temperature synchrotron diffraction measurements reveal a maximum on the melting curve of Na in the bcc phase at ~31 GPa and 1000 K and a steep decrease in melting temperature in its fcc phase (Fig. 7). The results extend the melting curve by an order of magnitude up to 130 GPa. Above 103 GPa, Na crystallizes in a sequence of phases with complex structures with unusually low melting temperatures, reaching 300 K at 118 GPa, and an increased melting temperature is observed with further increases in pressure[17]. The stability of Cu-Zn alloy phases at high pressure was examined and interpreted in terms of Hume-Rothery rules[57].

Dense Oxides and Fluorides – In an ongoing project at **Princeton**, **Tom Duffy**'s group is examining phase transitions, equations of state and structural properties of oxides, silicates, and germanates using x-ray diffraction at ultrahigh pressures of 50-200 GPa and 1000-3000 K. CDAC graduate student **Claire Runge** is studying high *P-T* perovskite phases of Cr_2O_3 and $MgGeO_3$. In the case of Cr_2O_3, high quality x-ray diffraction data suitable for structure refinements have been collected at HPCAT on the high-pressure phase from 37-75 GPa and at temperatures up to 1800 K. Similarly, $MgGeO_3$ perovskite has also been examined at HPCAT at 35-55 GPa and up to 1600 K. The goal of these projects is to understand the structural evolution of the perovskite phase as it approaches the post-perovskite ($CaIrO_3$-type) phase transition. Rietveld refinements of the post-perovskite phase give insights into the underlying structural mechanisms for the observed compressibility.

Recent zone-axis synchrotron x-ray diffraction experiments on single crystals reveal that $Fe_{1-x}O$ has a long-range defect-cluster order-disorder transition around 14 GPa, and existence of pressure-induced multiple phase transformations occur above 35 GPa (Fig. 8). These results indicate that $Fe_{1-x}O$ has very complex behaviors under compression, requiring a combination of many techniques to investigate the interactions of charge, spin, lattice, orbital moment, and defects in this system.[58] This research was conducted in partnership with **Carnegie**, **University of Arizona**, **ANL**, and **LANL**.

There has been considerable interest in the high-pressure behavior of metal dioxides. These materials exhibit extensive polymorphism at high pressures and a variety of transformation pathways leading to highly coordinated structures have been uncovered. Some high-pressure polymorphs in these systems have very high bulk moduli may qualify as strong or even superhard solids. High-pressure and high-temperature x-ray diffraction of SnO_2 demonstrates the existence of four phase transitions to 117 GPa (Fig. 9). The observed sequence of high-pressure phases for SnO_2 is rutile-type ($P4_2/mnm$) → $CaCl_2$-type ($Pnnm$) → pyrite-type ($Pa\bar{3}$) → ZrO_2 orthorhombic phase I ($Pbca$) → cotunnite-type ($Pnam$). The latter two phases were observed here for the first time in this system. The bulk moduli for the *Pbca* and *Pnam* phases of SnO_2 were determined by fitting *P-V* data to a second-order Birch-Murnaghan EOS. Rietveld refinements of powder diffraction patterns for both of these phases have also been successfully carried out. The group's static high-pressure results enabled them to provide an interpretation for previous shock compression data. The shock data show

evidence for two discontinuities along the Hugoniot curve, one above 47 GPa and another reaching completion around 115 GPa. The results indicate that the first transformation may be associated with the formation of the *Pbca* phase whereas the second transformation is consistent with the cotunnite-type phase.

Dion Heinz's group at the **University of Chicago** group, led by CDAC graduate student **Wendy Mao**,studied iron-containing orthopyroxenes and olivines at Earth core-mantle boundary conditions using a laser-heating DAC[59, 60]. These samples were studied *in-situ* at high *P-T* (>130 GPa and 1500-3000K) using x-ray synchrotron diffraction, nuclear resonant inelastic x-ray scattering, and x-ray emission spectroscopy. This group found that the post-perovskite phase can take up to 80% iron and exists in the low-spin (*i.e.* magnetic spin-paired) state. The discovery that the post-perovskite phase can accept a significant amount of Fe at *D*" conditions has profound implications on core-mantle interactions and may be a key to understanding the complex seismic signature observed in this region. The iron-rich phase is up to 20% denser than any known silicate at core-mantle boundary conditions. The high mean atomic number of the silicate greatly reduces the seismic velocity, and may provide a new explanation for ultra low velocity zones.

Rietveld refinement of monochromatic synchrotron x-ray powder diffraction data was used to study the evolution of octahedral tilting in the orthorhombic $NaMgF_3$ perovskite under pressure. Hydrostatic pressure conditions were ensured up to 16 GPa using He as a pressure medium. The tilting angles of MgF_6 octahedral framework were observed to increase with increasing pressure. The compression mechanism was observed to be dominated by the shortening of the octahedral Mg-F bond below 6 GPa, and then controlled by the increase of the octahedral tilting above 12 GPa.

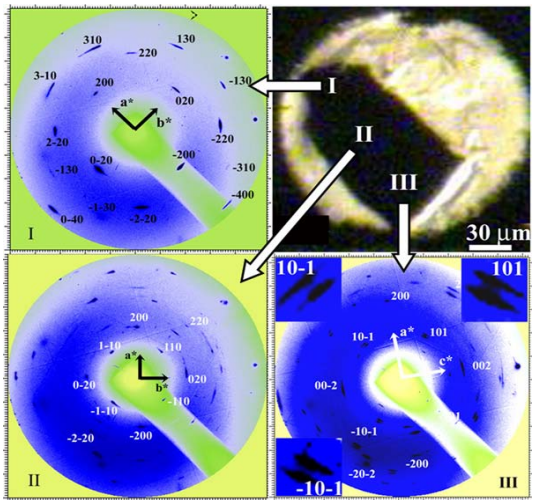


***Figure 8**. $Fe_{1-x}O$ single-crystal in a DAC at 35 GPa and the corresponding zone-axis diffraction patterns from locations **I, II,** and **III** of the sample. The indexing of each pattern is also shown. The insets in pattern **III** show details of the splittings of diffraction class 101[58].*

High-Pressure Melting and Melt Structures – The melting behavior of materials at high pressures is fundamental for materials science, as well as condensed matter physics and geophysics. CDAC graduate student Claire Runge (Princeton) has developed new synchrotron-based techniques for the determination of melting curves of metals at high pressures. By using a pair of sintered-diamond anvils in a large volume press, **Tom Duffy's** group was successful in carrying out high-resolution diffraction experiments that allowed recording of complete Debye-Scherer rings. They have used this method to measure the melting curve of silicon at pressures as high as 14 GPa with reversal experiments. In the coming year, this group will work on improving and extending this method to achieve higher pressures with increased precision. Angle-dispersive diffraction experiments in the multi-anvil press have considerable potential for studies including but not limited to phase transitions, crystal structure, and equations of state. The Princeton group also measured melting curves in the multi-anvil press by detection of the diffuse scattering from the melt using synchrotron x-rays. The group has extended the melting curve of Sn to 13 GPa, with this technique[61]. At the highest pressure, the measured melting curve lies about 20% below that suggested by

inferences from recent shock-wave experiments. Additional work is underway to extend this to still higher pressure with DACs.

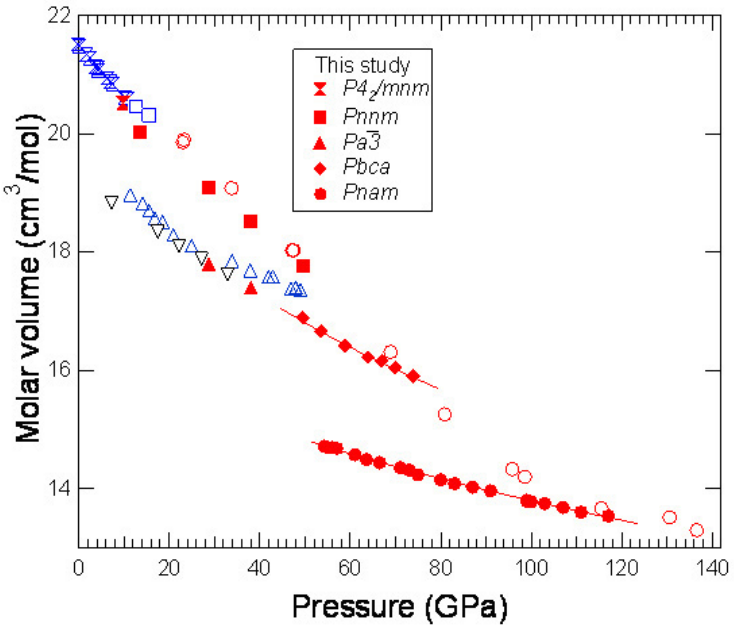


Figure 9. *P-V EOS of SnO_2 phases to 117 GPa. The open red circles represent shock compression data[234]. Solid lines are second-order Birch-Murnaghan equation fits to Pbca and Pnam phase data. Open symbols show previous static data[235, 236].*

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. New x-ray and neutron diffraction techniques have been developed to obtain highly accurate EOS data for a variety of materials. Measurement of sound velocity as a function of pressure and temperature by Brillouin spectroscopy provide information on the thermodynamic properties, in addition to giving the most accurate determinations of the EOS for fluid phases under static, very high-pressure conditions as described above[62,63]. Shock wave data have been, up to the present time, the primary experimental constraints on models of the giant planet interiors, and first-principles approaches carried out at **Carnegie** and **LLNL** are particularly valuable in this area of research, as a complement to shock wave technique. 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[64, 65].

Low-Z and Amorphous Materials – The EOS of various phases of Li[66], B[67], BN[22], and BeH_2 using different techniques have been determined. These provide a critical baseline required for understanding the kinetics, thermal transport, and other important properties of detonation and other chemical processes. A combination of techniques is being used for many materials, such as BeH_2 (Fig. 10) for which Brillouin scattering and x-ray diffraction are being applied[28, 66, 68 67 22]. Tests of volumetric methods for EOS studies of glasses and melts have also been performed. The use of Brillouin scattering for determination of the EOS of various polymers has begun in collaboration with **LANL** (**Dana Dattlebaum**) and the **Army Research Laboratory** (**Yolin Huang**). Direct volume method is currently applicable over the *P-T* range of resistively-heated DACs for determination of fluid densities with ±1% accuracy. CDAC is using this technique at HPCAT and extending it to higher temperature to determine the fluid *P-V-T* EOS of detonation products. Results can be used for validation of dynamic data and theoretical calculations.

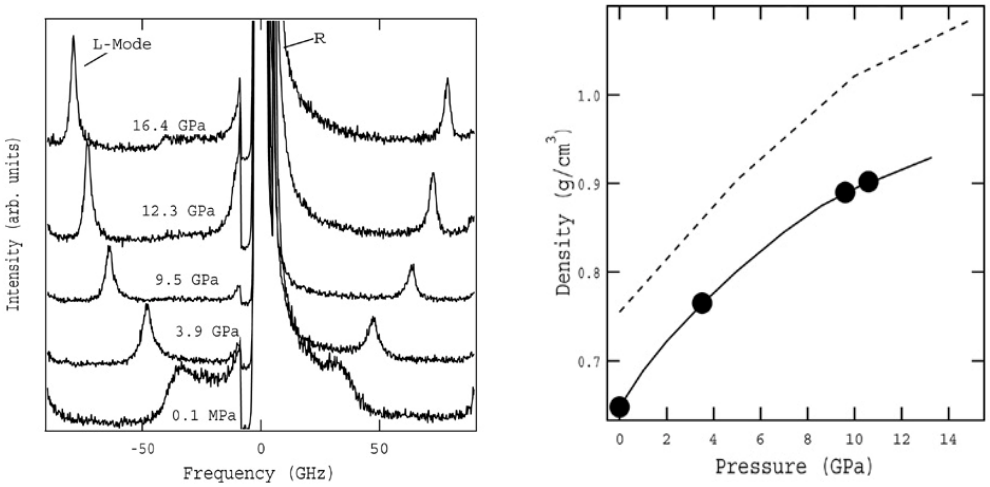


Figure 10. *Left: Brillouin spectra of vitreous BeH_2 at selected pressures. R indicates the Rayleigh scattering and the L-mode represents the Brillouin peaks of BeH_2. The broad Brillouin spectrum at ambient condition is due to multiple scattering between interfaces of amorphous grains. Right: Pressure-density EOS of BeH_2 at 300K. The symbols are the measured data and the solid line is the Vinet equation of state fit. The dashed line represents the theoretically calculated density of orthorhombic BeH_2 [68].*

It is now recognized that the post-perovskite phase occurs at high pressures in a wide range of silicate, germanate, and oxide compositions. Using the laser-heated DAC, **Tom Duffy's** group has investigated the physical properties of the post-perovskite phase synthesized from a natural pyroxene composition with Fe content (9 mol.%) close to that expected for the Earth's lower mantle. For post-perovskite, the measured EOS is consistent with theoretical calculations for the Fe-free end-member, suggesting compressibility is not strongly sensitive to iron content (Fig. 11). Their results also directly constrain the volume change associated with the perovskite – post-perovskite transition at ultrahigh pressures and that the bulk sound velocity is likely to *decrease* across the phase transition. Very recently, this group has carried out x-ray diffraction studies of the post-perovskite phase to 50-175 GPa in $MgSiO_3$ compositions containing 10 and 20 mol.% Al_2O_3. This data set will place some of the first experimental constraints on the effect of Al on the phase transition and physical properties of the high-pressure phase. In related work, the group has carried out an examination of the EOS, compressibility, and structural evolution (through Rietveld refinements) of the post-perovskite phase of $MgGeO_3$ from 7-200 GPa. The EOS and axial compressibilities provide a fundamental description of this material's structural response and this group's experimental data is examined in the context of theoretical calculations, elasticity systematics, and the behavior of the related perovskite-structured form.

Hematite is an end-member oxide containing ferric iron that has attracted much interest as a result of its structural and magnetic properties at high pressures and temperatures. A CDAC undergraduate student from **Princeton**, **John Vermylen,** has carried out the first study of the thermal EOS of hematite to 10.2 GPa and 1000 K using a multi-anvil apparatus and synchrotron x-ray diffraction at the GSECARS sector of APS (Fig. 12). The results are interpreted in terms of a Birch-Murnaghan-Debye model as well as a high- temperature finite strain EOS. The temperature derivative of the bulk modulus has been constrained for the first time, and the resulting value is found to be consistent with trends for other oxides and silicates. **Vermylen's** senior thesis on hematite received the 2005 Buddington Award for best thesis in the Geosciences Department.

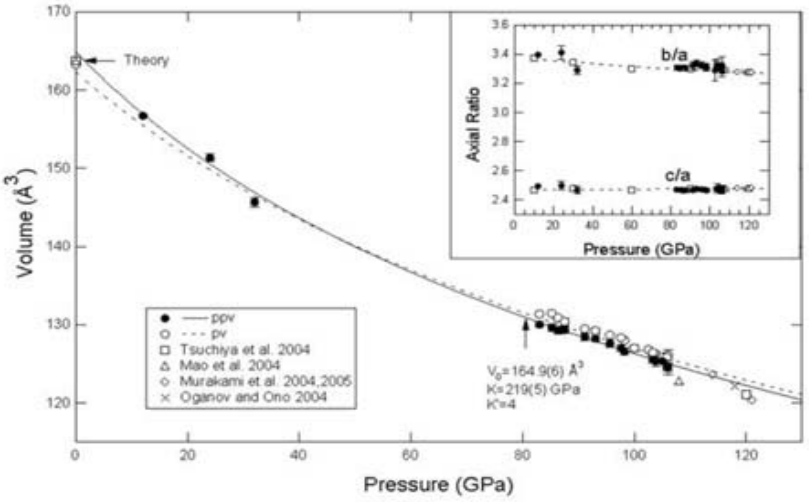


Figure 11. *The equation of state of perovskite and post-perovskite phases. The dashed curve is the experimentally determined equation of state for $MgSiO_3$ perovskite[237]. The solid curve shows a second-order Eulerian finite strain fit (K_0'=4.0) to the post-perovskite phase data. The theoretical zero-pressure volume for post-perovskite is from Ref.[238]. Inset - The pressure dependence of the axial ratios of the post-perovskite phase.*

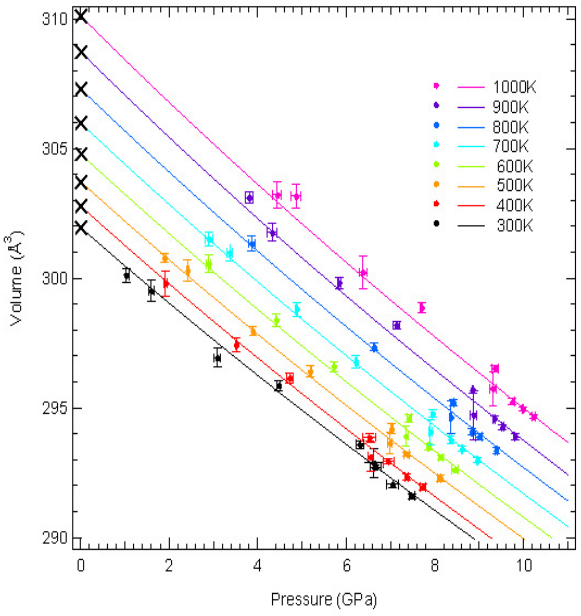


Figure 12. *P-V-T EOS of hematite. Crosses[239, 240] are ambient pressure, high-temperature data. Fits are obtained using a high-temperature finite strain equation.*

Dion Heinz's group at the **University of Chicago** has worked on the thermal EOS of Fe_3S to 80 GPa and 2500 K. **Christopher Seagle** was the main student who worked on this project. If one assumes that the temperature at the core-mantle boundary is 3500 K and that there is a 2% volume change upon melting (for both Fe and Fe_3S) then the density deficit that is observed between PREM and pure iron requires 13 wt% sulfur in Earth's core[69]

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[70, 71]. Efforts are being made among the high-pressure community to develop pressure scales at high temperature[72]. The **Carnegie** and **Princeton** groups are extending such calibrations to >1000 K with the integrated Brillouin and x-ray method. **Yingwei Fei** and colleagues[73] have extended x-ray calibration to high *P-T* conditions. Additional studies have been carried out in collaboration between **LLNL** and **Carnegie**[44].

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

Significant progress is being made in the study of phonon dynamics in highly compressed materials in order to understand thermodynamic properties, elasticity, and phase transition mechanisms, but has eluded high-pressure experimental investigation until very recently. The elastic tensor is important for understanding a range of properties of solids including elastic wave propagation, mechanical stability, interatomic interactions, material strength, and phase transition mechanisms.

Sound Velocity of Hot Dense Iron – As mentioned above, the first measurements of sound velocities of hexagonal close-packed iron (ε-Fe) at pressures up to 73 GPa and at temperatures up to 1700 K with nuclear inelastic x-ray scattering in a laser-heated DACs were reported by **Carnegie**, HPCAT, and others at APS (Fig. 13). The compressional-wave velocities (V_P) and shear-wave velocities (V_S) of ε-Fe decreased significantly with increasing temperature under moderately high pressures. V_P and V_S at high *P-T* conditions thus cannot be fitted to a linear relation, Birch's law, which has been used to extrapolate measured sound velocities to densities of iron in the Earth's interior. This result means that there are more light elements in Earth's core than have been inferred from linear extrapolation at room temperature[7].

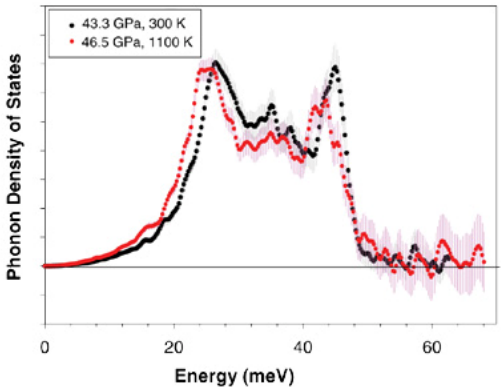


Figure 13. *DOS of ε-Fe at 43.3 (±2.2) GPa and 300 K (black curve) and 46.5 (±2.8) GPa and 1100 K (±100) (red curve). The spectral features of the DOS are shifted toward lower energies and the initial slope of the low-energy regime increases significantly at high temperature, indicating the softening of the lattice excitations. Debye sound velocities are derived from parabolic fitting of the DOS in the range of 3.5 to 14 meV*[7].

Lattice Strain Measurements – Radial diffraction allows collection of two-dimensional (ϕ and d-spacing) diffraction with a monochromatic x-ray beam and provides another mans to determine elastic properties. The radial x-ray technique is especially sensitive to the theoretically predicted pressure-induced elastic anomalies in metals[74,75]. A range of studies has been carried out on a variety of metals and brittle solids using DAC radial x-ray diffraction techniques. **Tom Duffy**'s group has examined shock-synthesized cubic silicon nitride[76], B_6O[77], and (Mg,Fe)O. New gasket designs by **Sebastien Merkel** (**Berkeley**) proved 100% dependable, had less background, and were easier to produce.

HPCAT has been an extraordinary resource for the researchers of the Dynamic Experimentation Division at **LANL**. The focus of these experiments has been two-fold. **Gary N. Chesnut** and colleagues have been studying a radial diffraction technique that allows an examination of the effects of deviatoric stress due to non-hydrostatic conditions. Radial diffraction, along with a custom-designed DAC, provides access to all stress angles, θ. θ is the angle between the reciprocal lattice vector of a diffracting plane and the compression axis. Fortunately, the stress-

strain conditions within the sample environment of a DAC are well defined[78]. By combining the existing theoretical work and the experimental results from HPCAT there is a wealth of information that can be attained. The elastic constants, which are currently unknown at pressure, for materials can be calculated for some structures. Another parameter that can be determined is the hydrostatic interplanar spacing, $d_p(hkl)$:

$$d_m(hkl) = d_p(hkl)[1 + (1- 3\cos^2\theta)Q(hkl)].$$

Here, $d_m(hkl)$ and $Q(hkl)$ are the measured d-spacing and a complicated function that depends on the properties of a particular material. By choosing the angle $\theta \approx 54.7$ degrees (the magic angle) the previous equation reduces to $d_m(hkl) = d_p(hkl)$. The effects of the deviatoric stresses at this angle have been removed from the measured d-spacing thus providing a hydrostatic result. This leads to more accurate equation of state parameters, as well as eliminating some of the controversy between various static experiments and dynamic experiments. This group is still in the process of analyzing the data, however they have thus far seen errors in pressure and volume on the order of a few percent in high symmetry structures. The low symmetry structures possess errors on at least the same order, if not greater. The issue of deviatoric stress is more of a concern for the low symmetry structures because a small deviation in the $d_m(hkl)$ can lead to a different structure determination[79].

The second focus of their experiment has been to study lanthanides such as Ce in order to better understand *f*-electron behavior. There are many outstanding debates in cerium literature that make it a prime candidate to test magic angle x-ray diffraction, and it exhibits a large volume collapses and an iso-structural phase transition. This research is leading them to a greater understanding of material properties at high pressure-temperature conditions by providing more information than can be attained by standard x-ray diffraction geometries and by providing more accurate EOS data.

Novel Oxide Materials – Studies of novel ferroelectric and piezoelectric materials at **Carnegie** have accelerated during the past year[80]. In these studies, there is growing interaction with **George Samara**'s group at **SNL**. High-pressure methods are used to obtain new insight into the origin of the unusual properties of these very important technological materials. New experiments have been carried out on lead based relaxor ferroelectric single crystals such as $PbZn_{1/3}Nb_{2/3}O_3$ (PZN)-$PbTiO_3$, $PbMg_{1/3}Nb_{2/3}O_3$ (PMN)-$PbTiO_3$ show giant piezoelectric properties[68, 81-83]. This experimental work involves a very strong and active collaboration with the computational condensed matter theory program directed by **Ronald Cohen**. The group has performed extensive linear response calculations on these materials. PMN is isotropic and cubic down to low temperatures according to experiments, but shows a much more distorted local structure. An end-member of a solid solution with $PbTiO_3$(PT), this material has a very large electromechanical coupling and the potential to revolutionize applications as diverse as naval sonar and hydrophones to medical ultrasonics and actuators. **Zhigang Wu** and **Cohen**[84] predicted an unexpected, new type of morphotropic phase transition with giant electromechanical coupling in pure $PbTiO_3$ at high pressures. Experiments are underway at **Carnegie** to test these predictions.

The elastic properties of garnet-structured materials are of interest because of their myriad technical applications, including high power laser amplifiers. **Tom Duffy's** group at **Princeton** investigated the elastic properties of a suite of garnets to 12 GPa by Brillouin scattering[85, 86], as well as CaO and even protein crystals[87, 88].CDAC graduate student from **Princeton**, **Zhu Mao**, used Brillouin scattering to measure the full elastic tensor of an orthorhombic Ca-Al hydrous silicate, zoisite, which is an important metamorphic mineral in subducting slabs[89]. Compared with the elastic moduli of the related mineral lawsonite, zoisite has a similar bulk modulus (125 GPa), but a 30% larger shear modulus (69 GPa) than lawsonite. The group has also carried out a study of the high-pressure elastic tensor of magnesium hydroxide (brucite). The elastic properties of brucite are fundamental to understanding the physics of strongly anisodesmic systems, hydrogen interactions at high pressure, and pressure-induced disorder. The six elastic tensor components were determined up to 14 GPa using Brillouin scattering. A compression curve constructed from their Brillouin data is in good agreement with previous x-ray diffraction data. The ratio of the linear compressibility

along the c and a axes decreased dramatically from 4.7 to 1.3 over the examined pressure range. Fitting aggregate elasticity data to a third-order finite strain EOS, the **Princeton** group obtained an adiabatic zero-pressure bulk modulus of 42.0 GPa with a pressure derivative of 7.3. For the aggregate shear modulus, they obtained a value of 34.7 GPa with a pressure derivative of 3.6. Brucite has a very large shear modulus pressure derivative (G'=3.6). The high-pressure elastic properties of the related aluminum hydroxide, diaspore, were also determined.

Entropy and the EOS – **Brent Fultz**'s group at **Caltech** continues to study the entropy of materials, particularly metallic alloys using inelastic neutron scattering or inelastic nuclear resonant x-ray scattering. The spectra are used to extract the phonon density of states, g(E), for example, and the thermodynamic partition function, Z, from which all thermodynamic information (free energy, entropy, etc.) can be derived. The change in phonon entropy of ordered and disordered alloys can be a substantial part of the entropy difference between the two phases. EOS measurements for a set of ordered and disordered alloys performed by synchrotron x-ray diffraction at **BNL** and at HPCAT show that the ordered alloy is initially more compressible, and more so as the atom size increases down the column of the periodic table containing Ni, Pd, Pt. These results are being compared to phonon observations from inelastic nuclear resonant scattering on ordered and disordered Pd_3Fe under pressure, and ordered and disordered alloys of Pt_3Fe at atmospheric pressure[90]. Related studies of the Fe-S, Fe-Ni, and Fe-C systems have been carried out by the **Carnegie** group[91].

In the course of her Ph.D. thesis research at **Caltech**, **Tabitha Swan-Wood** performed inelastic neutron scattering measurements on FeAl using the PHAROS instrument at LANSCE (**LANL**) and the LRMECS instrument (ANL)[25]. The high temperature measurements with PHAROS showed a most peculiar anharmonic behavior. The phonon frequencies remained essentially unchanged at elevated temperature, even though a large softening is expected from the anharmonicity of thermal expansion of the crystals against their bulk modulus. This anharmonic behavior may be caused by an elevated concentration of point defect in FeAl at high temperatures. This will be checked at HPCAT by high pressure inelastic nuclear resonant scattering on samples of FeAl with and without vacancies.

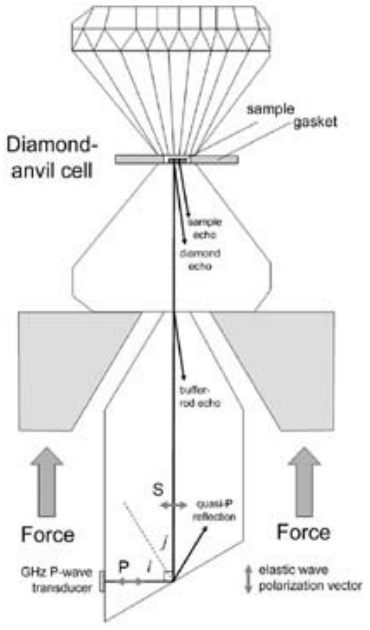


Figure 14. *GHz Ultrasonic interferometry DAC techniqe. Compressional and shear-wave travel times down to ~10 nanoseconds in duration can be measured on dense, opaque materials with a nominal accuracy of a few parts in a thousand. Compressional waves with 5-10 μm wavelengths are produced at a sputtered ZnO thin-film transducer. Purely-polarized shear waves are generated by P-to-S conversion upon reflection inside an acoustic buffer rod[92].*

GHz Ultrasonics – Ultrasonic interferometry is one of the most accurate standard methods for determining the elastic properties of materials at ambient and high pressures. Recent developments in the high-frequency acoustics laboratory by **Steven Jacobsen** at **Carnegie** have pushed ultrasonic interferometry into the 1-3 GHz range, making possible elastic properties measurements on samples as thin as 20-30 micrometers in the DAC (Fig. 14)[92-94]. GHz-measurements are now underway to accurately determine the shear moduli and single-crystal elastic constants of their CVD diamonds (Fig. 15) [92]. Although the current maximum pressure of GHz measurements is ~10 GPa, with the creation of larger CVD anvils, **Jacobsen** and colleagues are targeting the 50-100 GPa pressure range on single-crystal samples by Year 3. There are many important applications of the GHz-technique in studying the elastic properties of nuclear materials because opaque samples, which are difficult or impossible to study with optical methods, may readily studied using GHz-ultrasonic interferometry[95-97].

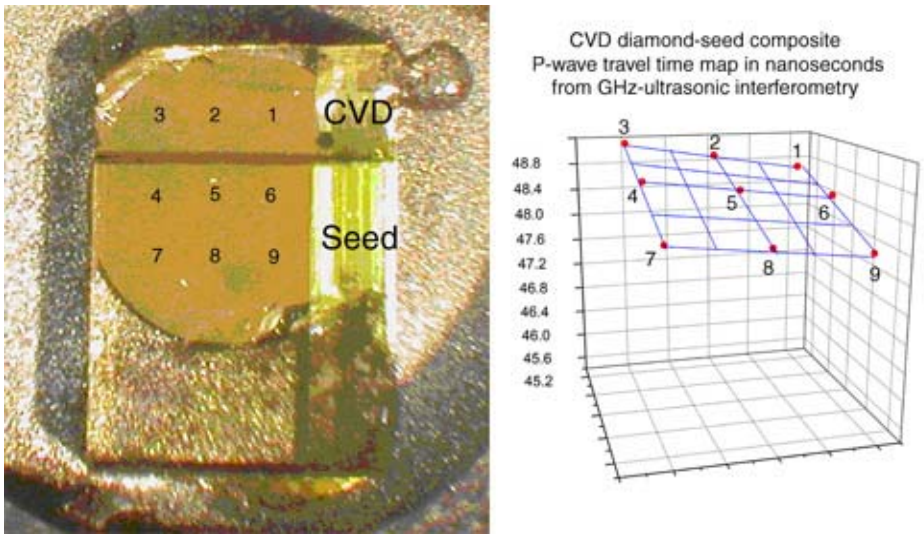


Figure 15. *CVD sample prepared for GHz-ultrasonic interferometry showing the location of [100] travel-time measurements in the CVD and seed diamonds (left). Map of the P-wave travel times (in nanoseconds) at right. From which C_{11} and C_{44} are determined with high accuracy. Other orientations have also been prepared in order to determine all the second-order elastic constants (C_{ij}) of the materials[92].*

Other Optical Measurements – Optimized optical properties of the window materials are essential for reliable VISAR measurements in shock-wave experiments[98-104]. CDAC is conducting new experiments to better characterize the properties of existing and potential VISAR window materials. The **Carnegie** group studied the optical and structural properties of Al_2O_3 the *in situ* investigation through the transformation to the Rh_2O_3-II structure[105]. Measurements of high *P-T* single-crystal elastic properties of Al_2O_3 carried out in Year Two and Three will answer questions that have arisen regarding shock data (including ruby line shifts) for this material[106], and will be extended to other brittle materials. Most recently, this group has begun to explore the potential for CVD diamond. Coordinated studies are being carried out at optical labs at **Carnegie**, **Princeton**, and **Chicago**. A collaboration between **LLNL** and **Carnegie** led to important new measurements of the optical and Raman spectra of Li to megabar pressure[56].

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 stewardship science. The texture provides data for interpreting active deformation mechanisms, and phase transformations induced by pressure and temperature

produce systematic changes in texture patterns. Studies of these phenomena at ultrahigh static pressure have become a reality as a result of CDAC. The Center is extending these measurements to ultrahigh *P-T* with laser-heated DACs at HPCAT and moderate pressure but high temperature at HIPPO[107].

For example, the *d*-spacings as a function of ϕ measured by radial diffraction reveal the strength, and the intensities of each reflection *(hkl)* as a function of ϕ give the texture, which can be monitored as a function of time at a given pressure. Semi-empirical modeling techniques have been developed to extract elasticity information from the x-ray and neutron diffraction studies described above on textured polycrystals[108-113]. **Rudy Wenk**'s group at **Berkeley** continues to refine plasticity simulations by using new methods, (*e.g.* Ref.[114]). Studies of high-pressure minerals by several groups within CDAC provide valuable insight into the behavior of materials important for stewardship science and serve as a test bed for direct studies of those materials at high pressure and temperature.

High Pressure Strength of Tungsten – The yield strength of polycrystalline W was investigated by the **Princeton** group using radial x-ray diffraction techniques under uniaxial compression up to 68.8 GPa. The ratio of yield strength to shear modulus is found to vary from 0.015-0.025 over the examined pressure range (Fig. 16). The static strength of tungsten is similar to that found along quasi-isentropic compression paths (1.6-2 GPa at stresses from 10-72 GPa), and is significantly smaller than the yield strength (ranging from 3.5 to 6.1 GPa at stress of 5-70 GPa) found in shock compression studies. These new results will lead to improved constitutive models for this transition metal which serves as a shock wave standard. Differences in strength between static and shock loading have direct applications in the determination of accurate static pressure scales (*i.e.,* ruby fluorescence) at high static pressures.

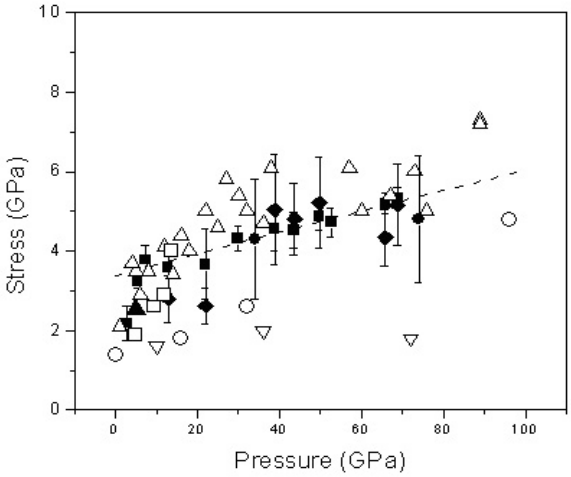


Figure 16. *Yield strength of tungsten from radial x-ray diffraction compared with values from shock compression (downward triangle[241], open circles[242, 243]) and quasi isentropic loading (upward triangles[241].*

Non-Hydrostatic Stress on Crystals and Polycrystals – The core of the contribution of **Rudy Wenk's** group at **Berkeley** is to study the influence of non-hydrostatic stress on crystals and polycrystals, particularly at high and ultrahigh pressure and investigate the effects on anisotropic physical properties. The ansisotropy in polycrystals is largely determined by preferred orientation (texture) and texture evolves during deformation and is modified during recrystallization and phase transformations. In phase transformations an enigmatic "texture memory" has been observed in many systems which is one aspect this group is trying to understand. Towards these goals, they are using synchrotron diffraction, particularly DACs in radial geometry and recently also multianvil systems, and time-of-flight neutron diffraction. The experimental data are in the form of 2D diffraction images and 1D diffraction spectra and new methods, based on the Rietveld procedure, have been developed to extract quantitative information about texture and stress.

In addition to the work at HPCAT (16-ID-B) experiments were performed at APS (GSECARS 13-BM-D, 13-ID, and BESSRC 11-ID-C), ALS, HASY, ESRF (ID-13 and ID-15B); LANSCE (HIPPO

and SMARTS), ILL (D19), ISIS (ENGIN-X). Some of the research was more methodological, improving experimental techniques (*e.g.* DAC gasket technology, neutron furnaces) and data processing. **Wenk's** group also was able to document strain distribution in the DAC, using copper as an example. 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.

Among materials $MgSiO_3$ perovskite turned out to be extremely interesting, displaying different texture types depending on conditions and starting material. So far **Wenk's** group could 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 changes during heating (recrystallization). A systematic investigation is the subject of CDAC supported graduate student **Lowell Miyagi**'s PhD thesis. In a recent collaborative study at HPCAT, the **Berkeley** and **Princeton** groups demonstrated that strong textures can be produced in the post-perovskite phase in germanates. The 110 texture is compatible with [001] pencil glide which makes sense since [001] is the direction of the octahedral chains in the structure.

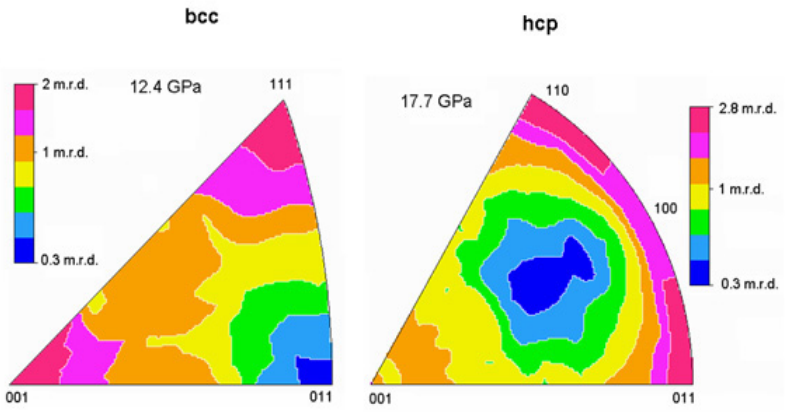


Figure 17. *Orientation relationships during the bcc-hcp Fe transformations measured with a radial DAC*[116].

Texture changes during phase transformations further confirmed a strong variant selection in many systems (Fe, Zr, Ti, and quartz; Fig. 17). **Wenk's** group attributes it 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. Textures that develop during deformation have profound implications for seismic anisotropy in the earth. They have used 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 core mantle boundary.

Crystal Grain Growth – CDAC graduate student **Nicholas Cunningham** (**University of Alabama-Birmingham**) has shown that Pr metal at high pressure undergoes dramatic grain growth as the metal passes through the fcc to α-U structural phase transition[31]. At 16.0 GPa smooth diffraction rings indicate a highly crystalline material with small particle sizes for the hR24 (fcc) phase of Pr (Fig. 18). The metal transforms to the fcc phase from the ambient pressure dhcp phase at 4 GPa. Diffraction data were obtained at HPCAT Sector 16-ID-B. At 18.9 GPa, the diffraction pattern shows significant grain growth as the fcc-to-alpha uranium phase transition is completed, as evidenced by large and distinct spots in the diffraction rings. The volume collapse across the transition is 9.1%. There is, however, no evidence of any particular orientation in the grain growth, as might be expected with standard texturing effects. Within about a 4 GPa increase in pressure, the grain growth begins to be suppressed, and at 28.5 GPa, the randomized, homogeneous and polycrystalline metal is clearly restored. The grain growth appears to be a general characteristic of the formation of the α-U phase in different materials as opposed to an effect associated with the large volume collapse.[31]

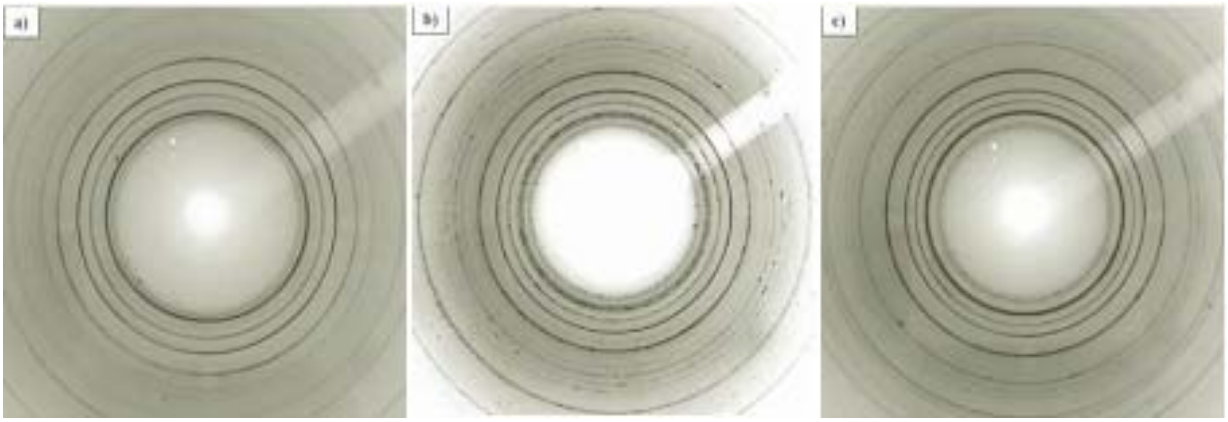


Figure 18. *Evolution of x-ray diffraction of Pr across its volume collapse. (a) Smooth diffraction rings for the hR24 phase at 16.0 GPa, slightly below the transition to the* α *-U structure. (b) Dramatic grain growth at 18.9 GPa showing spotty pattern. Close examination reveals that the affected rings all belong to the emergent* α*-U phase. (c) A return to continuous diffraction rings showing near random distribution of grains at 28.5 GPa*[31].

A collaboration between students **Jim Devine** and **Wendy Mao** at the **University of Chicago** and **Jenny Pehl** at **Berkeley** provided the first texture data for silicate perovskite at 43 GPa, from which deformation mechanisms could be deduced by comparing experimental patterns with simulations[115] Similar experiments on Fe revealed the of anisotropy changes during phase transformations and deformation of iron with pressure including the conclusion that basal slip is a significant slip system in ε-Fe at high pressure[116]. As mentioned above, **Tom Duffy**'s group measured the shear strength of cubic silicon nitride, which is 12 GPa at 67 GPa. Boron suboxide is also a promising new superhard solid; a shear strength of 14 GPa at 65 GPa was obtained[77].

Synergy Between Static and Dynamic Compression and Theory – Characterization by combined shock and dynamic experiments on fundamental materials provides the opportunity for major advances in the understanding of 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[117, 118]. The high-pressure optical properties to the far-IR range were characterized[39]. There is now interest in extending these measurements to dynamic compression. More important, the fabrication of large single crystal CVD diamond at **Carnegie** provides the potential for new studies of the elastic-plastic response of diamond on dynamic compression. The **Carnegie** and **SNL** groups are now collaborating on feasibility studies in this area. Related studies of interfaces and cracks under pressure will be investigated in Year Three with the picosecond vibrational SFG technique in **Dana Dlott**'s lab at **Illinois** together with new DACs developed at **Carnegie**.

The developments described above have provided an important opportunity within CDAC to develop a synergy between experiment (both static and dynamic compression) and first-principles theory for advancing the understanding of elastic-plastic behavior. **Ronald Cohen's** group has developed a non-collinear tight-binding model for iron, which gives very good results compared with first-principles calculations and experiment, along with Monte Carlo simulations developed by **Burkhard Militzer. Cohen's** group is collaborating closely with **Michael Oritz's** group at **Caltech** to perform lamination and finite-element modeling of strain driven phase transitions in iron. This work is being carried out in collaboration with the ASC group at **Caltech** and the Center for Simulation of Dynamic Response of Materials. **Cohen** is performing large scale linear response calculations on the ALC supercluster at **LLNL**. He and **Carnegie** postdoc **Xianwei Sha** are using these results to obtain elastic properties of iron as functions of pressure and temperature. This group is already providing information that can test predictions the thermoelastic properties of Fe, both with regards to elastic constants at room temperature as well as texture effects important for

understanding dynamic compression. In the next year, this group will explore the elastic constants at high temperatures in iron and important components needed for the ASC work. At the present time, there are no high-temperature shear data for hcp-Fe, except for the theoretical studies.

2.5 Electronic and Magnetic Structure and Dynamics

Hydrogen at High P-T Conditions – Studies of the behavior of hydrogen over a broad range of conditions continues within CDAC. Direct measurements of electrical conductivity (up to 210 GPa) and optical measurements (to ~300 GPa)[119, 120] also confirm that low-temperature solid hydrogen is non-conducting (at and below 300 K)[121] though it exhibits metallic-like conductivity in the high-temperature fluid at 140 GPa[122]. Due to the absorption threshold of diamond near 5 eV, the hydrogen band gap could only be implied indirectly through measurements of refractive indices. Recent breakthroughs in high-pressure x-ray Raman spectroscopy at HPCAT have enabled researchers to access the rich electronic information above 5 eV[21]. The pressure dependencies of electronic spectra (*e.g.*, band gap and excitons), above the diamond absorption threshold are being directly measured using IXS at HPCAT. These studies will be essential for helping to understand the static and dynamic compression results[119, 120].

In Year 3, CDAC will focus efforts on extending the maximum pressure on hydrogen and related systems. This effort will complement continuing activities at the Z facility (**SNL**) and eventually at NIF (**LLNL**) in producing and characterizing the dense plasma by laser shocks. CDAC hopes to extend x-ray diffraction and measurements of orientational information on the ordered crystal structure of hydrogen II and III, complementing recent neutron studies[123]. High-pressure x-ray Raman spectroscopy will probe the pressure dependence of the low energy excitons, which is important for possible condensation into the ground state (*e.g.*, to form an excitonic insulator).

Bonding and Electronic Structure of Low-Z Materials – Spectroscopic features near core electron absorption edges measured by x-ray absorption (XANES) or electron scattering (EELS) reveal rich information about bonding character. Such measurements of low-*Z* elements, however, have never been accessible for high-pressure studies, as the pressure vessels completely block the soft x-ray (<4 keV) or electron beams. These techniques were first applied to graphite in a CDAC collaboration between **Carnegie** and **Chicago**[124] and then to h-BN[22]. Most recently, the technique was applied to molecular oxygen[125], CO_2 [126, 127], and nitrogen[128]. High-pressure near *K*-edge spectroscopy of the entire second row of elements and near *L*-edge spectroscopy from Na to transition elements is now possible. A variety of novel pressure-induced phenomena in low-*Z* systems include the possible pairing in dense Li described above, the departure from simple metallic behavior in dense Na, metallization and breakdown of B icosahedra, the bonding changes in graphite to a diamond-like form[129, 130], magnetism and metallization of O_2, hydrogen-bond symmetrized ice, and transformations in LiH, BeH_2, $B_{10}H_{14}$ and BeO. These projects will be pursued in Year 3.

The high-pressure behavior of the plasmon of elemental Na was examined to 20 GPa, and the increase of the Na plasmon energy with decreasing r_s was observed. The measured dispersion values agree well with the RPA calculation. Valence band emission studies of Ge indicate strong correlation effects within the valence band in the semiconducting phase below 10 GPa[131]. The group has also conducted high *P-T* studies of the band gap and dielectric response function of H_2O (liquid and various forms of ice) in collaboration with **Chang-sheng Zha** at **Cornell**[132].

Magnetic Transitions – Magnetism in *d*- and *f*-electron metals plays a major role in controlling the physical and chemical properties of these materials as well as high *P-T* phase stability. Combining x-ray spectroscopy with megabar pressure provides a unique opportunity to systematically these phenomena in combination with theory, and to study the origin of the large number of phase transitions and the associated changes in their electronic structures. Resonant inelastic x-ray scattering (RIXS) can be used to probe specific elementary excitations, for example in *d* and *f* electron metals. The **Carnegie** group has pursued these studies with **Choong-Shik Yoo** at **LLNL** and **Chi-chang Kao** at **NSLS**.

The **Carnegie** group has measured NRIXS spectra of Fe over a broad range of conditions. Measurements to 50 GPa in He media[133] supplement previous nonhydrostatic experiments in $Fe_{0.93}Ni_{0.07}$ (110 GPa) and pure Fe (153 GPa), and allow them to derive the phonon density of states (DOS) and put constraints on elastic constants and thermodynamic parameters of hcp Fe. In collaboration with **Alexander Goncharov** (then at **LLNL**), the **Carnegie** team performed Raman measurements on Co metal that show evidence of coupling between the optical E_{2g} phonon and 2-magnon excitations.

The **Fultz** group at **Caltech** received two beam time allocations by CDAC to investigate hyperfine magnetic fields (HMFs) in hcp Fe alloys under pressure. These nuclear forward scattering experiments were performed to test a novel explanation why zero HMF is observed in hcp Fe, whereas *ab-initio* calculations show that hcp Fe should be antiferromagnetic (Fig. 19). The proposed cancellation of core electron polarization and conduction electron polarization is a delicate balance that can be upset by impurities such as Ni in the local neighborhood of Fe atoms. Values of ~30 KG were calculated for HMFs by Wien2K in the same way as the zero HMF was calculated for pure hcp Fe. Measurements on hcp Fe-Ni at 77 K and at 11 K showed zero HMF, however. Small HMFs would produce an oscillating spectrum analogous to the spectrum at the top of Fig. 19. **Ronald Cohen** at **Carnegie** is investigating the possible role of quantum fluctuations in producing this result.

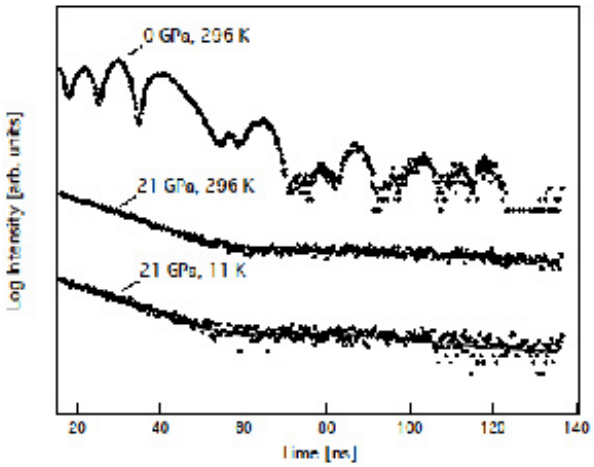


Figure 19. *Synchrotron Mössbauer spectra of Fe-8% Ni. At 21 GPa the sample is hpc, at ambient pressure it is bcc*[244].

Neutron experiments carried out by the **Carnegie** team and CDAC collaborators at the Intense Pulse Neutron Source (IPNS, **ANL**) and LANSCE (**LANL**), reveal surprising new findings in $Fe_{1-x}O$ (Fig. 20). Variable *P-T* neutron diffraction techniques were applied to investigate the magnetism of the rhombohedral phase of $Fe_{1-x}O$ (wüstite) above 15.0 GPa, a long standing controversy and fundamental problem for this material. Magnetic peaks similar to those at 180 K at ambient pressure were expected to be observed in the high-pressure rhombohedral phase; however, they are not evident in the high-pressure diffraction patterns (to 20.3 GPa at 300 K). The lack of magnetic peaks indicates the absence of long-range magnetic order in $Fe_{1-x}O$ under these conditions (perhaps above T_N). This result indicates the need to reconsider the interpretation of high-pressure Mössbauer studies and the mechanism of the high-pressure phase transitions in $Fe_{1-x}O$[41]. Moreover, the team's recent zone-axis synchrotron x-ray diffraction experiments on single crystals reveal that $Fe_{1-x}O$ has a long-range defect-cluster order-disorder transition around 14.0 GPa, and existence of pressure-induced multiple phase transformations occurs above 35.0 GPa[134, 135]. These results indicate that $Fe_{1-x}O$ has very complex behaviors under compression, requiring a combination of many techniques to investigate the interactions of charge, spin, lattice, orbital moment, and defects in this system. This research was also conducted in partnership with the **University of Arizona**.

As described in the highlights listed above, a team at **LLNL** and HPCAT led by **Choong-shik Yoo** found evidence for an isostructural, first-order Mott transition in MnO at 105±5 GPa, based on high-resolution x-ray emission spectroscopy and angle-resolved x-ray diffraction data. The

pressure-induced structural and spectral changes provide a coherent picture of MnO phase transitions from paramagnetic *B*1 to antiferromagnetic distorted *B*1 at 30 GPa, to paramagnetic *B*8 at 90 GPa, and to diamagnetic *B*8 at 105 GPa. The last was interpreted as a Mott transition, accompanied by a significant loss of magnetic moment, a ~6.6% volume collapse and the insulator-metal transition as demonstrated by recent resistance measurements[8].

Electronic Transitions in Simple Oxides – A **Carnegie** team that included **Jung-Fu Lin**, **Viktor Struzhkin**, and **Steve Jacobsen** together with colleagues from HPCAT recently reported new insights into the behavior of iron at high *P-T* conditions. Under the extreme pressure and temperature conditions of the lower mantle (400–1,800 miles below the surface), iron undergoes an unusual electronic transition wherein the outermost valence electron, rather than remain unpaired in its own separate orbital, pairs-up with another electron of opposite spin in the same orbital forming a so-called low-spin state. The team monitored the spin-state of iron in the most abundant non-silicate oxide material of the lower mantle, magnesiowüstite–(Mg,Fe)O, to over 100 GPa (one megabar), and discovered that the spin-state transition is associated with a rather drastic change in the material's elastic properties. While monitoring the spin-state of iron, the mineral's rate-of-change in volume upon compression was also measured using x-ray diffraction, which allowed them to estimate the density and bulk-sound velocity contrast across the electronic transition. The phenomenon should be observable seismically in Earth's lower mantle[9].

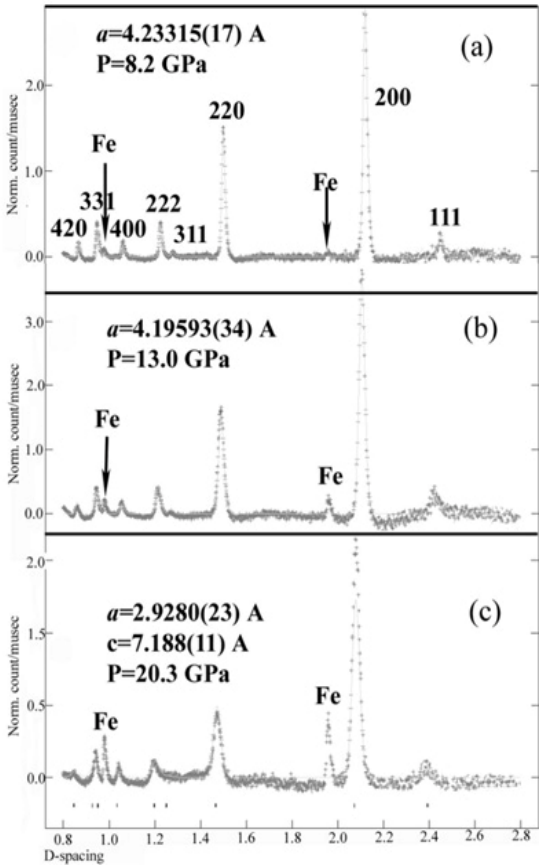


Figure 20*. Neutron diffraction of FeO at 8.2 GPa, 13.0 GPa, and 20.3 GPa[41].*

Nuclear forward scattering (NFS) studies in FeO from 150 K to 600 K up to 20 GPa at HPCAT carried out by a group from **Carnegie** provided determination of phase transition from nonmagnetic B1 structure to magnetic rhombohedral structure of FeO. The resistivity has been measured in compressed wüstite ($Fe_{0.94}O$) in experiments to 180 GPa between 4 and 300 K give unambiguous evidence for a transformation from semiconducting to metallic behavior at high pressure. Room temperature x-ray emission studies in FeO show disappearance of the satellite feature in the stability region of the metallic phase. Thus, direct magnetic measurements are required to establish the nature of magnetism in the high-pressure phase. The group collected extensive set of synchrotron Mössbauer data at high pressures and high temperatures (laser heating and external heating), which allowed determination of the magnetic phase diagram of FeO over an extended pressure range. The results indicate a magnetic phase in FeO is stable up to 200 GPa at room temperature. They were also able to detect magnetic signatures at 90 GPa and almost 2000 K, which leads to the conclusion that NiAs-type phase of FeO may be magnetic[136], as predicted by **Ronald Cohen's** group[137].

XES clearly indicates that CoO transforms to the low-spin state. Raman measurements to 70 GPa have been performed at 20 K. Magnetic excitations have been followed up to the highest pressure, and unambiguously indicate that the transition at 40-60 GPa occurs between magnetic

phases. These IR and x-ray emission measurements in oxides will continue in Year Three.[136] This system is also being studied theoretically by **Ronald Cohen's** group at **Carnegie.**

High-Pressure Superconductivity - A variety of studies of high-pressure superconductivity are being addressed in high-pressure experiments at CDAC using resistivity[138] and magnetic susceptibility techniques[139] in the multimegabar range. These approaches have provided detailed and accurate investigations of novel superconductors, including new metals formed from insulating molecular and elemental substances at very high pressure [140-146]. Pressure effects on superconductivity in copper-oxide superconductors continue to be the subject of intensive research. The pressure dependence of the superconducting transition temperature T_c in $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystals ranging from the highly underdoped through the nearly optimally doped to the highly overdoped level have been investigated using magnetic susceptibility at **Carnegie**[147]. The **Carnegie** group also carried out $T_c(P)$ measurements in He pressure media on Hg-1201 with different oxygen doping. The single crystal samples this group has received from **J. Karpinski** show an unusual magnetic background in the second harmonic. Both magnetic susceptibility and resistivity studies are in the planning stages; it is crucial for understanding pressure effects in transition metals and high-T_c cuprate superconductors.

High-pressure investigations of the high-temperature superconductor MgB_2 by Raman scattering were combined with measurements of T_c and lattice parameters up to 57 GPa. An anomalously broadened Raman band at 620 cm^{-1} was observed and assigned to the in-plane boron stretching E_{2g} mode. The pressure dependencies of the E_{2g} mode and T_c reveal anomalies at 15-22 GPa. The anharmonic character of the E_{2g} phonon mode, together with its anomalous pressure dependence and that for T_c, are interpreted to be the result of a phonon-assisted Lifshitz electronic-topological transition (ETT)[148]. The newly-developed inelastic x-ray scattering in a DAC provides a novel possibility to investigate the single crystal properties of MgB_2 under high pressure. The studies of the Γ-M dispersion branch under compression may provide valuable information on the possible pressure-induced electronic topological transition in the material (or alternatively, the pressure-tuned Kohn anomaly). The **Carnegie** group has investigated the phonons in MgB_2 using DAC techniques. The diamond anvils and MgB_2 single crystal samples were oriented with the help of x-ray single-crystal diffraction. The meaningful measurement to make is along Γ-M direction. Regarding the diamond background, this group tried to avoid the low energy part of the acoustic phonon branches trying to work near the diamond zone boundary. Measured relative pressure-induced energy changes are more prominent close to Γ point and are much less away from the Γ point. This group also tried to measure E_{2g} phonon dispersion. However, the broad and weak E_{2g} band is very close to the strong optical phonon from diamond anvils and consequently is much harder to extract from available experimental data. They were able to observe also several acoustic phonons in MgB_2. Further analysis of experimental data is underway.

Transition metal nitrides are intriguing compounds due to their high melting points and hardness, and some have relatively high superconductivity temperatures at ambient conditions. Last year the **Carnegie** team performed high-pressure measurements on single crystals of HfN, ZrN, and NbN[149]. For NbN, T_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 under high-pressure 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.

2.6 High *P-T* Chemistry

Understanding the chemistry of materials in the stockpile includes problems that range from the high *P-T* chemistry of explosives, metals in contact with reactive low-*Z* materials such as H_2 and H_2O, and complex composites (*i.e.*, interfaces), all of which may change appreciably as materials age. Specifically, the chemistry of hydrogen is important for stockpile aging as well as development of containment strategies in static experiments at high *P-T* conditions. New hydrogen containing

compounds have also been discovered[150], including recently found hydrogen-rich ices important for understanding the uptake of hydrogen in high-density phases.

New Reactions and Compounds at High Density – Prompted by the seminal theoretical work at **LANL** and **LLNL**[151, 152] and subsequent experimental studies[153], great progress was made by the **Carnegie** group during the past year with the synthesis of polymeric nitrogen above 150 GPa and its low-temperature recovery at ambient *P*[154, 155]. Work on new nitrogen phases and structural/EOS parameters to megabar pressures[156] is ongoing. The structure of the polymeric form was determined in jointly at HPCAT and the ESRF[53, 157]. Last year, the **Carnegie** group also examined a related transformation in NaN_3 to 160 GPa at 120-3300 K[157]. The results may be compared with the new high-pressure phases observed in other nitrogen-rich molecular materials[158-161]. Studies of metal hydrides continued[162].

Investigations of the kinetics of chemical reactions at high *P-T* conditions (*e.g.,* >50 GPa and >1000 K) are crucial for furthering the understanding of detonation and associated processes. Information on the EOS of reactants and products is an essential starting point, but this needs to be extended to probe the energetics of transition states and reactive intermediates, particularly in dense fluids. High-pressure FTIR spectroscopy with conventional sources has been extremely useful (*e.g*., at **LLNL**), and the high-pressure synchrotron IR technique developed by **Carnegie** at its dedicated beamline at the NSLS provides an enormous advantage over conventional FTIR spectroscopy, as demonstrated by numerous studies[146]. The method is now fully developed for high *P-T* studies and ready to apply to a broad range of problems in stewardship science.

Polymerization of Formic Acid – Raman, infrared, and x-ray diffraction measurements, with *ab initio* calculations on formic acid reveal that formic acid polymerized under pressure (Fig. 21). A team from **LLNL** working at HPCAT, led by **Alexander Goncharov** found an infinite chain $Pna2_1$ structure to be a high-pressure phase at room temperature. The data suggest that the symmetrization and a partially covalent character of the intrachain hydrogen bonds above approximately 20 GPa. Raman spectra and XRD patterns indicate a loss of long-range order at pressures above 40 GPa, with a large hysteresis upon decompression. The results are consistent with three-dimensional polymerization of formic acid[15]. This study won a Chemistry and Materials Science Associate Directors Award from **LLNL**.

The behavior of hydrogen bonds under strong compression has been studied in formic acid[15]. The x-ray diffraction measurements have been combined with Raman and IR spectroscopy and also *ab initio* and classical calculations. This group finds that at about 20 GPa the hydrogen bonds linking formic acid molecules into chains become symmetric. The hydrogen atoms sit midway between two oxygen atoms on neighboring molecules forming partially covalent bonds to both of them. These conclusions are substantially based on the results of measurements of the lattice constants under pressure performed at the IDB station of HPCAT.

Further compression results in a loss of translational order and true polymerization of formic acid which is evident from total disappearance of Bragg reflections and narrow vibrational excitations. This result is confirmed by this team's MD simulations of the amorphous phase that show the formation of interchain C-O-C ether bonds between polymeric fragments. Since the covalent ether bonds are stronger than hydrogen bonds, this explains the substantial hysteresis found in samples compressed above 40 GPa.

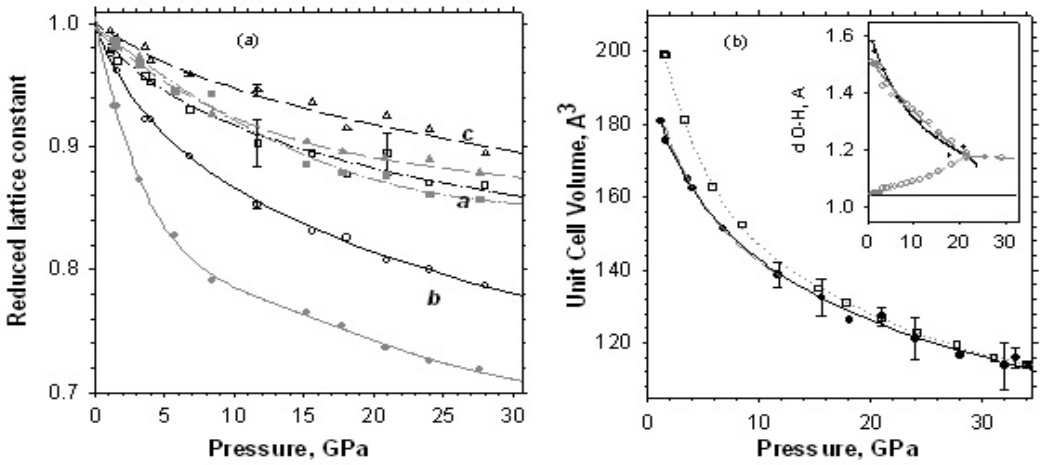


Figure. 21 . *(a) Reduced lattice constants of formic acid as a function of pressure. Gray lines and symbols- theory, black lines and symbols- experiment; (b) Unit cell volume as a function of pressure. Inset to (b): pressure dependence of O-H bond distances. Filled symbols and solid lines- experiment. Open symbols and gray lines- theory*[15]*.*

The above static high-pressure chemical studies provide an important benchmark for the interpretation of shock data, as demonstrated for the high *P-T* breakdown of CO_2[163, 164] and CH_4[165-167]. Close interactions with **Giulia Galli**'s group at **LLNL**[168] have also been established for these studies.

New dense high-nitrogen materials framework structures have been discovered. There has been considerable interest in the creation of new nitrides, motivated by the search for new superhard compounds, electronic materials (such as superconductors), and optoelectronic materials. In collaboration with a French team, the **Carnegie** group synthesized the first nitride of a noble metal[169]. The material has intriguing physical properties, including very high incompressibility, and it can be recovered at ambient conditions. CDAC college intern **Andrea Young** has discovered other new nitrides[170] and is spending the summer of 2005 at the ICTP in Trieste doing theoretical calculations with **Sandro Scandolo** and will be entering graduate school in condensed matter physics.

Novel Hydrogen Storage Materials – Another type of novel high-pressure chemistry was discovered in clathrate hydrates. Last year, a detailed neutron diffraction study has performed at LANSCE in collaboration between scientists at **LANL**, **Carnegie**, and **Rutgers** (including several students). Above 130-160 K the guest D_2 molecules were found in the delocalized state, rotating around the centers of the cages. Decreasing temperature results in the rotation freezing followed by a complete localization below 50 K. This work also complements an LDRD project on clathrates at **LANL**, which involves the **Carnegie** group. New studies include inelastic neutron scattering carried out by **Carnegie**[171]. At high pressure, hydrogen also forms a series of crystalline molecular compounds with methane. $(H_2)_4CH_4$ contains the largest amount of hydrogen of any known compound. The **University of Chicago** and **Carnegie** team demonstrated that this solid could be brought to near ambient pressure at low temperatures[172].

A theoretical description based on sophisticated state-of-the-art *quantum Monte Carlo* (QMC) methods is required to understand the stability of these materials. Ongoing work at **Carnegie**, led by **Burkhard Militzer** using QMC[173]as well as auxiliary fields QMC[174] to describe the energy landscape that the different storage materials provide for the hydrogen molecules, path integral MC[175] as well classical molecular dynamics to study absorption and desorption dynamics of the H storage process using the derived EL, and theoretical studies of how the stability of the

different clathrate cage structures can be enhanced in order to stabilize storage materials at high temperature and lower pressure. Much of this work benefits from active collaboration with theorists at **LLNL**. Supported by a modest grant from DOE, this work benefits significantly from the infrastructure established and maintained by CDAC.

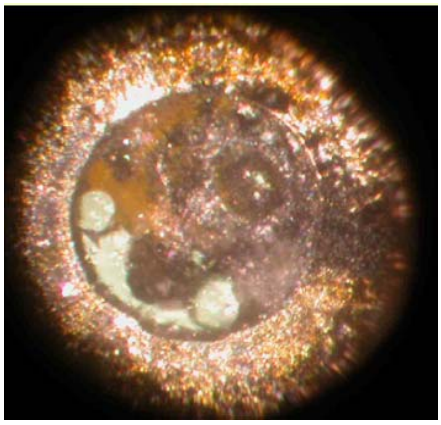


Figure 22. *Methane gas synthesized from wüstite, calcite and water at high temperatures and pressures in the diamond anvil cell. Bubbles formed in the mixture (bottom, left and near the center in the photomicrograph above) upon decompression to 0.5 GPa after laser heating at 5.7 GPa give a Raman spectrum consistent with the formation of methane[4].*

Hydrocarbon Formation and Stability at High P-T Condition – Last year, our *in situ* observations of hydrocarbon formation were carried out via carbonate reduction at upper mantle pressures and temperatures[176]. Methane was formed from FeO, $CaCO_3$-calcite and water at pressures between 5 and 11 GPa and temperatures ranging from 500 to 1500°C (Fig. 22). The results are shown to be consistent with thermodynamic calculations of the relevant chemical reactions based on thermochemical models and *ab initio* theory. The study demonstrates the existence of abiogenic pathways for the formation of hydrocarbons in the Earth's interior and suggests that the hydrocarbon budget of the bulk Earth may be larger than conventionally assumed. The study was carried out as a collaboration between **Indiana University-South Bend**, **Harvard, Carnegie**, and **LLNL**, including **Larry Fried**, **Michael Howard**, and **Sorin Bastea**. The study represented a novel application of the CHEETAH code, which was developed to predict detonation processes and properties of energetic materials. The work received a great amount of attention in the popular press and world wide[176].

Interface Dynamics Under Pressure – **Dana Dlott's** group at **Illinois** is using an ultrafast nonlinear vibrational spectroscopy technique termed broadband multiplex vibrational sum-frequency generation spectroscopy (SFG) to understand the dynamics of interfaces subjected to high dynamic and static pressures. The dynamic high pressure experiments involve watching a laser-generated shock front pass over molecules at an impedance-matched interface, providing picosecond temporal and angstrom spatial resolution. The static experiments involve developing the instrumentation needed for SFG studies in diamond anvils in order to look at aging effects at interfaces found in high-pressureerformance plastic-bonded explosives of special importance to the NNSA mission, such as PBX-9501.

James E. Patterson originated an experiment to study shock compression with femtosecond time resolution and angstrom spatial resolution. The crucial element of this experiment is the use of SFG spectroscopy which sees a layer of atomic groups only 1.5 Å thick. Through a combination of experiments and simulations, **Patterson** showed that chains with even and odd numbers of carbon atoms respond quite differently to fast compression by a 1.5 GPa shock. He defended his dissertation at the end of 2004 and has taken a postdoctoral position in **Yogendra Gupta's** laboratory at **Washington State University**. This work has been continued by postdoctoral student **Wentao Huang**, who has developed a laser pulse-shaping apparatus that gives better control over the shock generation process. He has used this apparatus to measure the mechanical strength of an alkane monolayer with fast dynamic loading.

Hackjin Kim, a visiting professor from **Chungnam University**, began work on energetic materials interfaces in 2004. Much of the interesting phenomena involved impact initiation of plastic-bonded explosives at interfaces between crystals or between crystals and binders. However a detailed understanding of the structures of these interfaces is lacking. Working with materials provided by **Randall Simpson** at **LLNL** and **Dan Hooks** at **LANL**, **Kim** has obtained the first surface vibrational spectra of energetic materials. Specifically he has looked at the main ingredients of PBX-9501, namely HMX crystals and estane binder (Fig. 23). **Kim** has measured the spectra of both the CH_2 and NO_2 groups on the crystal surface. They have characteristically different frequency shifts and linewidths from the same groups in the bulk crystal. In addition **Kim** has measured the spectra of the estane surface. Estane is a block copolymer with soft segments and hard urethane segments. His measurements showed that the surface has more of the hard urethane segments than the polymer bulk. Finally, he has obtained spectra of the HMX-estane interface. The HMX vibrational transitions at this interface are frequency shifted by their proximity to the estane. This project has been taken over by **Eric Surber**, a recent Ph.D. from **Arizona State University**.

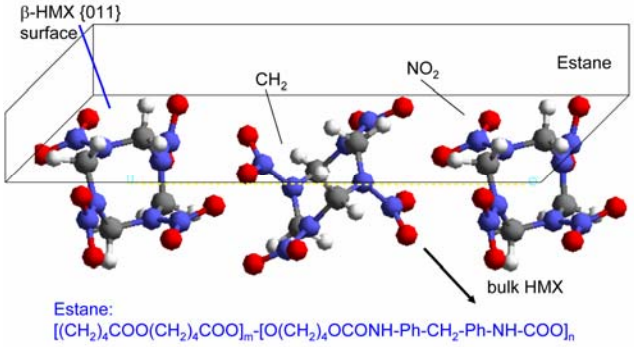


Figure 23. *Schematic of the interface between the {011} face of an HMX crystal and estane binder. SFG spectra see only the one-half of the HMX molecule at the crystal surface plus the molecular groups at the estane surface.*

The interface shock compression experiments demonstrate that **Dlott's group** has developed a new technology platform for dynamic shock compression measurements with time and space resolution needed for detailed comparison with shock simulations (Fig. 24). Future work will be focused on two areas: (1) better control of the shock compression process by computer-controlled laser pulse shaping; and (2) development of new molecular systems. At present this group is working on two new systems. The CO molecule bonded to a Pd surface is a model system that they expect to have an extremely fast and sensitive response to shock compression. A thin layer of interfacial water on the surface of a self-assembled monolayer will let this group study the effects of shock compression on water, which is expected to lead to interesting hydrogen-bonding dynamics resulting from the disruption of the water structure.

The high-explosive interface work has just reached the stage where many interesting materials can be studied. This group is working on studying different orientations of HMX and RDX crystals and their interactions with estane with and without nitroplasticizers, as well as other binders. Aging of energetic materials will be studied by looking at these interfaces while raising the temperature and the pressure. The group is running feasibility studies to determine geometries that are most likely to work in a DAC. The problem is propagating the extremely intense femtosecond pulses needed for SFG through the diamond anvil at a high angle of incidence with the sample, without severe distortion.

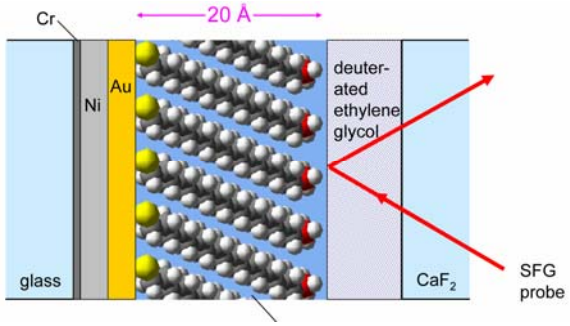


Figure 24. *Schematic of shock compression experiment to study the large-amplitude motions of molecules with angstrom spatial resolution. Vibrational sum-frequency generation selectively probes motions of the terminal CH_3 groups of a self-assembled monolayer of long hydrocarbon chains with 1 ps time resolution as they are driven into the contact liquid by a femtosecond laser-driven shock moving from left to right.*

Nanophase and Superhard Materials – Important progress has been made in CDAC in

the quest for new superhard materials with different mechanical and chemical properties optimized for cutting and shaping a great variety of hard metals, ceramics and rocks, has continued. Bonding changes related to mechanical properties have been monitored by high-pressure IXS[22, 124] in graphite and BN, as discussed above. Efforts continue to explore theoretically predicted superhard materials such as carbon nitride[177, 178]. As described above, shear strength can be estimated from information on sample thickness and pressure gradient measured by x-ray imaging and XRD[179, 180], or determined directly through high-pressure radial XRD[181, 182]. Properties of high-pressure synthetic diamonds can be characterized in-depth by using synchrotron radiation[183], and the use of various superhard materials, *e.g.*, cubic zirconia[184], moissanite[117, 185], and CVD diamond[186] as high *P-T* anvils have been tested in synchrotron radiation experiments. Diamond is a good example of a high-pressure material that can be synthesized through a low-*P* metastable process (CVD)[187, 188]. The work on CVD diamond will be discussed below.

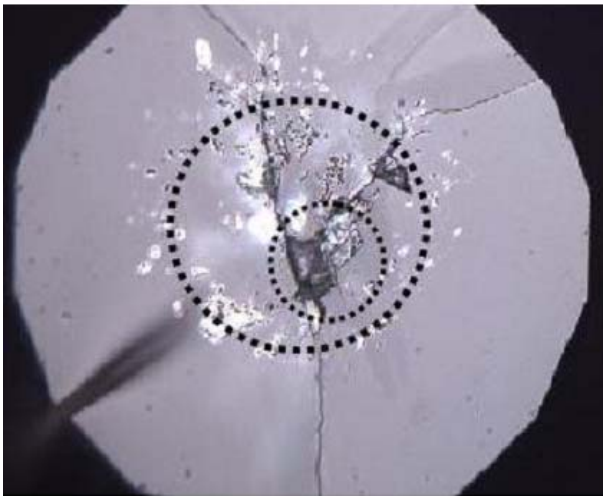


Figure 25. *Photomicrograph showing indentation (crack in center and related radial crack lines) of the diamond anvil by the high-pressure hexagonal polymorph of cold-compressed carbon nanotubes. The large circle represents the gasket hole; the small circle highlights the indentation mark with the depth of 3 μm(e.g., estimated from microscopy) at the center of the DAC[189].*

Cold compression of carbon nanotubes at 75 GPa results in the formation of a superhard hexagonal carbon polymorph that has a different structure than hexagonal diamond (Fig. 25)[189]. This new phase is quenchable to ambient pressure and has an experimentally determined bulk modulus of 447 GPa, slightly higher than that of cubic diamond (442 GPa). Formation of the superhard material cracks the diamond anvils used in the synthesis, and leaves a 3 μm indentation in the surface of the anvil. The larger circle shows the position of the stainless steel gasket used to contain the sample during compression. Comparison of the Raman spectra of various carbon materials shows conclusively that the phase is unique and not cubic or hexagonal diamond. This was a collaboration between **LANL**, **Cornell**, and **Carnegie**[189].

There is growing interest in the behavior of nanostructured composite materials under pressure. A group at **UNLV** working in collaboration with scientists at CDAC and HPCAT investigated nanostructured composites at high pressure to study the pressure-induced phase transitions expected to occur in the nanocrystalline phase of the composite. This group's primary interest was to identify any new phase and investigate its stability. *In situ* synchrotron radiation x-ray diffraction studies were performed on a nanocrystalline composite on compression up to 45 GPa and on successive decompression. The optically transparent material contained nanometer-sized single crystalline phase homogeneously dispersed within an isotropic host matrix. The pressure-evolution of x-ray diffraction patterns was consistent with a low-to-high density phase transition in the nanocrystalline phase of the composite. The results reveal the first reported pressure-induced phase transition arising in the nanocrystalline phase of a glass-ceramic composite that involves transition form a thermodynamically stable to an unstable phase, maintained after pressure release, by the densified host glass matrix.[190]

A renewed interest in β-Ga_2O_3 has arisen since it has potential applications in optoelectronic devices. β-Ga_2O_3 belongs to the group of transparent oxides with the widest band gap and it exhibits both conduction and luminescence properties. The amount of oxygen vacancies induced in this material depends mainly on the growth atmosphere, and determines the electrical character of the compound, which can vary from insulating to conductive. Furthermore, the magnetism of the conduction electron spins in this material exhibits an original memory effect within a wide range of temperatures from 4 K to at least room temperature. *In situ* x-ray diffraction studies were performed on β-Ga_2O_3 up to 70 GPa and on successive decompression. Pressure-induced structural transformations and the effect of hydrostatic and non-hydrostatic conditions on the pressure evolution of β-Ga_2O_3 were examined.[191]

High-Pressure X-Ray Diffraction of Fluoropolymers – EOS information for polymeric materials is important for several reasons including scarcity of experimental data at high pressure and temperature, a pervasiveness of these materials in the modern technologies, and large number of applications in which these materials are exposed to high pressure and/or high temperature, environments. Studying polymer microstructure and properties under conditions is largely under-explored, but is essential for understanding their uses, failure mechanisms, and predicting replacement materials. There are several on-going programs at **LANL**, and in collaboration with DOD labs, working to develop accurate EOS for polymeric materials. An important aspect of achieving accurate EOS is a thorough understanding of polymer crystalline structure and associated phase transformations within pressure/temperature regimes of interest. Several of the semi-crystalline polymers of interest are fluoropolymers, including poly(tetrafluoroethylene) (PTFE), poly(chloro-trifluoroethylene) (Kel-F81), poly(chloro-trifluoroethylene-*co*-vinylidene fluoride) (Kel-F800) and poly(vinylidene fluoride) (PVDF). Some of these materials are used as binders in energetic materials (explosives).

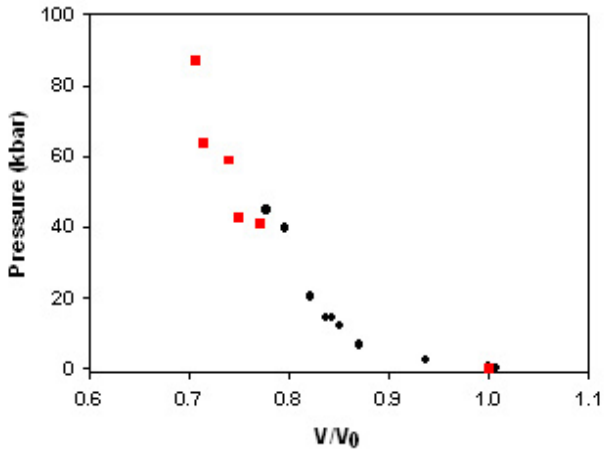


Figure 26. *EOS of PTFE: isothermal static compression data (black circles) compared to shock Hugoniot loci (red squares)[30].*

Dana Dattlebaum (**LANL**) has examined PTFE at HPCAT. The material this group is investigating is approximately 40% crystalline, and the brightness of the source at APS, as well as the high-pressure-specific equipment and tools at the HPCAT beamline have been essential to successfully interrogating the phase behavior of this material at high pressure. By coupling high-pressure Raman spectroscopy with physical analysis to acquire thermodynamic properties, and x-ray diffraction experiments at HPCAT, this group is successfully developing a thermodynamically consistent EOS for PTFE. PTFE is a semi-crystalline polymer with a complicated low-*P* phase diagram. At room temperature, its crystalline regimes exist in a helical form with 15 atoms per 180° twist, phase IV. At < 19°C, the helix is tighter with 13 atoms per 180° twist, phase II. At "high pressure," > 0.6 GPa, the helix is flattened into a planar zig-zag crystal III. In recent months, this group has indexed the phases and extracted cell volume as a function of pressure (manuscript in preparation). Both low-*P* crystalline phases (II and IV) were best fit to triclinic space groups. The "high-pressure" phase III (> 0.65 GPa) was adequately fit to several equivalent monoclinic space

groups. Preliminary analysis suggests that the new phase that they have discovered at even higher pressures may be orthorhombic. A pressure-volume curve for PTFE derived from this analysis compared to dynamic (shock) data is shown in Fig. 26. The relation between the static isothermal and shock data is reasonable, particularly when invoking viscoelasticity to describe the behavior of amorphous domains under high strain-rate conditions such as shock loading.

Very recent work at HPCAT has started to interrogate the phase behavior of the high explosive binder, Kel-F 800. Kel-F 800 is a copolymer of (chlorotrifluoroethylene) (PCTFE) and (vinylidene fluoride) (PVDF). The copolymer contains significantly more amorphous fraction than bulk polymers of either monomer. So far, this group sees no evidence of crystalline phase transitions in Kel-F 800 to 6 GPa. Finally, new and developing work will focus on an investigation of the high-pressure phase behavior of a class of fluorinated terpolymers named "THV" (Dyneon). These are similar in nature to Kel-F 800 and PTFE, and they anticipate similar successes with this class of materials.

Semiconductor Quantum Dots at High Pressure – In separate measurements of the near infrared absorption and fluorescence of lead selenide quantum dots **David Sander** and his group at **LANL** have found that there is a large shift of the fluorescence wavelength and the absorption to lower energies as the pressure is increased. A similar effect, but with the opposite direction of the wavelength shift has also been seen in cadmium selenide quantum dots. There are several possible explanations, one being a phase transition in the crystal structure of the quantum dots at high pressure. There is evidence that phase transitions in quantum dots may not occur at the same conditions as the bulk materials. A second possible explanation is that the electronic band structure shifts with pressure lead to a decreased separation between the conduction and the valence band. This could be something like a Mott-Hubbard transition. In their first run at the advanced photon source, they used a DAC with the same hydrostatic medium as this group has used for the infrared absorption measurements, chloroform. They found that the chloroform crystallized, and the resulting diffraction peaks obscured the lead selenide peaks. The group plans to return and use 1) an alternate solvent, methyl cyclohexane as a suspension medium for the quantum dots, 2) a more concentrated suspension of quantum dots in the chloroform, 3) a modified holder to heat the cell sufficiently to melt the chloroform.

3. EDUCATION, TRAINING AND OUTREACH

3.1 CDAC Graduate Students and Post-doctoral Associates

The education, training and outreach mission of CDAC is crucial not only for the future health and vitality of the National Labs but for national security in general, and a sizable portion of CDAC funding goes toward graduate student support. Students and post-doctoral fellows within CDAC are conducting cutting-edge research in world-renowned academic institutions and are utilizing state-of-the-art facilities to complete their thesis work. CDAC graduate students will therefore be well-prepared for future challenges and job opportunities within the NNSA/DP Lab complex. In Year Two, the following graduate students were supported by CDAC:

Princeton:	**Claire Runge**
	Zhu Mao
Caltech:	**Alex Papandrew**
	Matt Lucas
Chicago:	**James Devine**
	Wendy Mao
	Chris Seagle
Berkeley:	**Jenny Pehl**
	Lowell Miyagi
	Sergio Speziale (Postdoctoral)
	Sebastien Merkel (Post Doctoral)

Alabama: **Nick Cunningham**
Wei Qiu
Joel D. Griffith
Carnegie: **Brad Chen**
Marcus Origlieri

The CDAC student support goal of Year 2 was met, as fourteen students were supported in the Center, including two students at **Carnegie**. In addition, two graduate students, **Kimberly Tait** from the University of Arizona, and **Amy Lazicki** from the **University of California, Davis** are supported by **LANL and LLNL,** respectively, and are working directly with the high-pressure groups. **James Patterson** has taken a post-doctoral position at the **Institute for Shock Physics**, **Washington State University**, and is continuing his work in the area of stewardship science.

The Berkeley group has been supported by visiting students from **Università di Trento** (**Ivan Lonardelli** and **Gloria Ischia**) and from Dresden (**Ingwar Huensche**). **Ivan** is returning to Berkeley as a postdoctoral scholar. Two postdoctoral Miller fellows, **Sergio Speziale** (PhD Princeton) and **Sebastien Merkel** (PhD Lyon) are actively involved in working on CDAC-related aspects of the research program. The group is also reaching out beyond **Berkeley**, introducing graduate students **Jim Devine** and **Wendy Mao**, from **University Chicago**, to texture analysis from synchrotron images. Close collaboration with the Geophysical Lab continues; new collaborations have been started with **Tom Duffy** and **Atsushi Kubo** (Princeton; post-perovskite), **Martin Kunz** (ALS; perovskite deformation), **Yanbin Wang** and **Norimasa Nishiyama** (APS; D-DIA experiments) and **T. Barton** (**LBNL**; phase transformation theory).

During Year 2, visiting investigator **Hackjin Kim** continued work in the **Illinois** group, supported in part by CDAC. Also, CDAC post-doctoral associate **Duanwei He** remains in the high pressure group at Los Alamos, and **Wyoming** postdoctoral associate **Kristina Lipinska-Kalita** has continued her work in the high-pressure program of the High Pressure Science and Engineering Center at the **University of Nevada-Las Vegas**, after working at HPCAT and **Carnegie**, both post-doctoral associates remaining involved in stewardship science projects.

CDAC graduate students work on a wide variety of problems in materials science, physics, chemistry and high-pressure mineral physics and geophysics, all of which provide backgrounds ideal for tackling important problems in stewardship science. 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.[192-194]).

Publications and presentations involving CDAC-supported students and post-doctoral associates in Year 2 are listed below.

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Chen, X. J., High-pressure superconductivity and mechanical properties of nitrides, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).
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Yan, C. S., Y. C. Chen, S. S. Ho, H. K. Mao and R. J. Hemley, Large single crystal CVD diamonds at rapid growth rates, *The 10th International Conference on New Diamond Science and Technology* (AIST, Tsukuba, Japan, May 11-14, 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
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
S. Demouchy
L. S. Dubrovinsky
D. J. Frost
Anastasia P. Kantor
I. Y. Kantor
Catherine A. McCammon

BIOCARS-Advanced Photon Source
K. Brister
Brookhaven National Laboratory
G. L. Carr
C. C. Kao
Lisa Miller
Bulgarian Academy of Sciences
I. K. Bonev
I. Mitov
Daniela Paneva
Rossitsa D. Vassileva
California Institute of Technology
S. Kung
H. Su
California State University at Channel Islands

Tabitha Swan-Wood
Case Western Reserve University
J. Van Orman
Chinese University of Hong Kong
H. Q. Lin
CLCR Rutherford Appleton University
W. G. Marshall
Cleveland State University
J. Vitali

Colby College
Elizabeth Littlefield
Colorado College
P. Cervantes
Kristin M. Chynoweth
T. D. Atkinson
Columbia University
D. Walker
E. Cottrell
Cornell University
W. Bassett
C. S. Zha
Drexel University
M. W. Barsoum
European Synchrotron Radiation Facility, France
F. Berberich
T. Le Bihan
M. Mezouar
F.E.E. Gmbh, Germany
D. Rytz
Friedrich-Schiller-University, Germany
F. Langenhorst
Geoforshungzentrum, Potsdam
Monika Koch-Müller
H. J. Reichmann
George Washington University
Lauren Borkowski
C. Cahill
M. Frisch
Georgia Institute of Technology
X. Wang
Z. L. Wang
GSECARS, Advanced Photon Source
P. J. Eng
M. Newville
V. B. Prakapenka
M. Rivers
S. Sutton
Ecole Normale Superieure, Lyon
P. Gillet
EPFL, Switzerland
H. Berger
L. Forro
G. Margaritondo
Florida A&M University
R. Little
Florida International University
S. K. Saxena
H. P. Liermann
H. Yang
Harvard University
D. R. Herschbach
S. Rekhi
Sarah T. Stewart-Mukhopadhyay
Indiana University – South Bend
H. P. Scott

Institute for Earth Sciences, Acad. Sinica, Taiwan
E. Huang
Institute of Geochemistry, Chinese Academy of Sciences
M. Chen
X. Xie
Institute for High Pressure Physics, Troitsk
V. Denisov
A. G. Gavriliuk
M. Yu. Popov
I. A. Trojan
Institute for Problems of Chemical Physics, Chernogolovka Russia
E. B. Gordon
Institute for Solid State Physics, Chernogolovka
Valentina F. Degtyareva
N. I. Novokhatskaya
M. K. Sakharov
Institute für Mineralogie and Petrolographie, Switzerland
W. van Westrenen
Institutio di Gioscienze e Georisorse, Italy
L. Ottolini
Instituto Potosino de Investigación Cientifífica y Tecnológica, Mexico
T. Terrience
James Franck Institute, University of Chicago
Y. Feng
E. D. Isaacs
R. Jaramillo
T. N. Rosenbaum
Japanese Synchrotron Radiation Research Institute
K. Funakoshi
Japan Marine Science Center
S. Nagayoshi
N. Sata
Japan National Defense Academy, Tokyo
Y. Yoshimura
Jilin University, Changchun
G. Zou
Johns Hopkins University
Y. Ding
D. R. Veblen
Karl-Franzens-Universität Graz, Austria
J. K. Dewhurst
S. Sharma

Kent State University
C. C. Almasan
Laboratoire Leon Brillouin, France
I. N. Goncharenko
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
K. Syassen
H. Zhang
Moscow State University
B. N. Feygelson
Nagoya University
T. Okuchi
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
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
Heather Watson
Rutgers University
Martha Greenblatt
M. V. Lobanov
Royal Institution, London
P. McMillan
E. Soignard
St. John Fisher College
Kristina M. Lantzky
Scripps Oceanographic Institute
I. Gan
I. Gertsman
J. E. Johnson
T. Lin
Soliel, France
R. Fourme
Steacie Institute for Molecular Science, Canada
S. Patchkovskii
Stanford University
Tanja Cuk
SUNY-Stony Brook
J. Chen
Jennifer King
B. Li
L. Li
J. B. Parise
L. Wang
D. J. Weidner
Technological Institute for Superhard and Novel Carbon Materials, Russia
N. R. Serebryanaya
Texas Christian University
R. Senter
Texas Tech University
Y. Ma
V. Levitas
E. Selvi
A. White
J. Sandhu
Tokyo Institute of Technology, Japan
K. Hirose
T. Kombayashi
Universidad Complutense de Madrid
J. Santamaria
M. Varela
Università di Roma Tre, Italy
G. Della Ventura

Università di Trento, Italy
L. Lutterotti
G. Mariotto
Università G. D'Annunzio, Italy
Gianluca Iezzi
Universität Bonn, Germany
Winfried Kockelmann
N. Zotov

Universitat de Valenci, Italy
D. Errandonea
Universitat Politècnica de València, Spain
F. J. Manjòn
Université Catholique de Louvain, Belgium
X. Gonze
University College London, UK
D. Dobson
University of Alaska
T. Trainor
University of Arizona
R. T. Downs
D. Krishnamoorthy
A. Krishnamurthy
M. Origlieri
C. Prewitt
Kimberly Tait
University of Arkansas
A. Khanna
University of Bristol, UK
H. Darwish
A. E. Mora
J. W. Steeds
University of California, Berkeley
G. Ischina
R. Jeanloz
S. Merkel
W. B. Montgomery
Sergio Speziale
University of California, Davis
D. M. Krol
Brian Maddox
W. E. Pickett
R. T. Scalettar
University of California, Los Angeles
Abby Kavner
Anat Shahar
Sarah Tolbert
Michelle Weinberger
University of California, Riverside
H. Green
Larissa Dobrzhinetskaya
University of Chicago
W. Schildkamp
University of Colorado
C. M. Holl
J. R. Smyth
H. Spetzler
University of Connecticut
P. D. Mannheim

University of Edinburgh
J. Loveday
R. J. Nelmes
University Firenze, Italy
R. Bini
M. Ceppatelli
D. Chelazzi
M. Santoro
V. Schettino
University of Hawaii
G. M. Amulele
M. H. Manghnani
L. Ming
S. Sharma
S. Tkachev
University of Illinois
J. D. Bass
H. Hellwig
W. Huang
A. S. Lagutchev
Jie Li
Jennifer M. Jackson
University of Louisville
G. A. Lager
University of Manitoba, Canada
F. Hawthorne
University of Maryland
A. J. Campbell
University of Michigan
Wendy Panero
L. Stixrude
University of Missouri, Kansas City
B. Chen
E. P. Gogol
M. B. Kruger
J. Murowchick
University of Nevada-Las Vegas
A. L. Cornelius
M. Daniel
C. L. Gobin
E. Kim
R. S. Kumar
Kristina Lipinska-Kalita
Patricia E. Kalita
J. McClure
M. Nicol
T. Pang
Y. Shen
W. Stanberry
I. Tran
O. Tschauner
University of Nevada-Reno
D. Chandra
S. Chandra
R. Chellapa
University of New Mexico
C. Agee
University of Northern Florida
L. V. Gasparov

D. Arenas
University of Paris VI
J. Badro
G. Fiquet
Chrystele Sanloup
University of Tennessee
M. Anand
L. A. Taylor

University of Texas, Arlington
S. Sharma
University of Tokyo
S. Merkel
University of Toronto
M. Fujihsaki
University of Tsukuba
K. Matsuishi
University of Warsaw, Poland
W. Grochala
University of Warwick, UK
D. L. Carroll
M. L. Newton
University of Western Ontario, Canada
S. R. Shieh
University of Wyoming
S. Sampath

Verkin Institute, Kharkov
Y. A. Freiman
M. A. Strzhemechny
S. M. Tret'yak
Vernadsky Institute, Moscow
M. A. Nazarov
Virginia Polytechnic Institute
R. J. Angel
B. E. Hanson
Carla Slebodnick
Nancy L. Ross
J. Zhao
Waseda University, Tokyo
Y. Ohki
Washington State University
J. E. Patterson
Woods Hole Oceanographic Institution
N. Shimizu

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 **Steve 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 2004-2005, the following students participated in this program (Fig. 27).

2004:

Lora Armstrong, University of Michigan
Phase Relations in Pyrolite at Mantle Conditions
Mike Krawczynski, Brown University
Hydrous Synthesis of Aluminum-Bearing Silicate Perovskite
Rebekah Graham, University of California–Santa Barbara
Path Integral Monte Carlo Simulations of Hydrogen Melting at High Densities
Maureen Moses, San Diego State University
Fractionation of Platinum Group Elements into Molten Iron

2005:

Edward Banigan, Georgetown University
Equations of State of $MgAl_2O_4$ Spinel
Elizabeth Littlefield, Colby College
Effects of Water on the Behavior of $MgSiO_3$ Clinoenstatite 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 H_2-He Mixtures
Catherine Tarabrella, West Virginia University
Crystal Structures of CsI and CsCl at High Pressures

Figure 27. *Summer interns working on CDAC projects as part of the Carnegie Summer Intern Program. Top Left: Edward Banigan (Georgetown University). Top Right: Elizabeth Littlefield (Colby College). Bottom Left: Lesandra Rosario (Universidad Metropolitana, Puerto Rico). Bottom Right: Catherine Tarabrella (West Virginia University).*

In 2004, CDAC supported **Andrea Young** from Columbia University for work on the noble metal nitride project[170].

In Year 2, **Tom Duffy**'s group at Princeton supported **John Vermylen**, an undergraduate student. **Vermylen**, who graduated in the spring of 2005, was awarded an NSF fellowship for graduate study in geophysics at Stanford beginning in the fall of 2005.

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 2004, **Carnegie** scientists had the opportunity to work with two talented students from Maryland on projects related to the electronic structures of solids at high pressure. In 2005, two students from Washington, DC and one student from New York worked on various projects with **Carnegie** scientists (Fig. 28). **Jacob Cohen** and staff scientist **Viktor Struzhkin** looked for superconductivity in compressed sodium. He also worked with **Ronald Cohen** on visualizing different exchange correlation functionals in $PbTiO_3$. **Cheng Chin** worked with **Chih-Shiue Yan** on the CVD diamond project. **Daniel Cohen** worked with **Ronald Cohen** on studying the quantum effects on a phase transition. Although during the school year such students may not be paid for their participation, summer stipends for such talented students are provided by individual research sponsors from other grants or by the **Carnegie Institution**:

2004:

Kevin Gan, Wootten High School (now at Harvard University)
Superconductivity in Dense Lithium
Simon Kung, Winston Churchill High School (now at California Institute of Technology)
High-pressure Properties of Boron Nitride

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
Quantum Effects on a Phase Transition

Jacob Cohen, Yeshiva of Greater Washington
Superconductivity in Compressed Sodium; Exchange Correlation Functionals for $PbTiO_3$

Figure 28. *2005 high school summer interns at Carnegie. Left: Jacob Cohen (Yeshiva of Greater Washington). Center: Cheng Chin (Forest Hill High School, New York). Right: Daniel Cohen (Yeshiva of Greater Washington).*

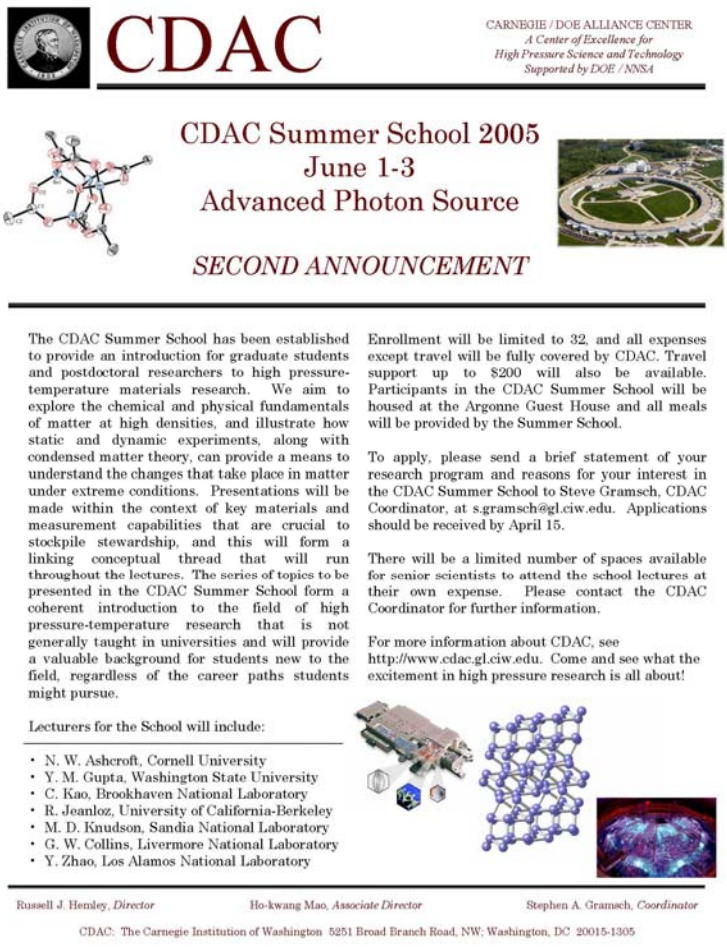
In addition, CDAC Coordinator **Steve Gramsch** teaches an Advanced Placement Chemistry class at the César Chávez Public Charter High school in the District of Columbia, a rigorous college preparatory school in the heart of the nation's capital. Four students from this class in their junior year formed a small group under **Steve Gramsch**'s direction to do independent study in the area of crystallography. These students are **Yamel Alcantara**, **Veronica Cisneros**, **Evert Orinion**, and **Chenty Reyes**. These students have now graduated, and two of them have gone on to undergraduate study in the sciences. A new group of students working on crystallograpy will be forming at the Chávez School in September 2005.

3.5 CDAC Summer School

The first CDAC Summer School, held June 1-3, 2005 at the APS, was a great success. 33 young scientists from around the country attended and were taught by leading scientists from academia and the National Labs about the fundamental science and current problems in high-pressure materials science (Fig. 29).

The aims of the School were to provide an introduction for graduate students and postdoctoral researchers to high *P-T* materials research, including fundamentals not typically taught in university courses, while at the same time introducing them to the techniques, problems, and materials important in the field.

Lectures given by top scientists from academic institutions around the country and five National Labs explored the chemical and physical fundamentals of matter at high densities, and


CDAC

CARNEGIE / DOE ALLIANCE CENTER
A Center of Excellence for High Pressure Science and Technology
Supported by DOE / NNSA

CDAC Summer School 2005
June 1-3
Advanced Photon Source

SECOND ANNOUNCEMENT

The CDAC Summer School has been established to provide an introduction for graduate students and postdoctoral researchers to high pressure-temperature materials research. We aim to explore the chemical and physical fundamentals of matter at high densities, and illustrate how static and dynamic experiments, along with condensed matter theory, can provide a means to understand the changes that take place in matter under extreme conditions. Presentations will be made within the context of key materials and measurement capabilities that are crucial to stockpile stewardship, and this will form a linking conceptual thread that will run throughout the lectures. The series of topics to be presented in the CDAC Summer School form a coherent introduction to the field of high pressure-temperature research that is not generally taught in universities and will provide a valuable background for students new to the field, regardless of the career paths students might pursue.

Lecturers for the School will include:

- N. W. Ashcroft, Cornell University
- Y. M. Gupta, Washington State University
- C. Kao, Brookhaven National Laboratory
- R. Jeanloz, University of California-Berkeley
- M. D. Knudson, Sandia National Laboratory
- G. W. Collins, Livermore National Laboratory
- Y. Zhao, Los Alamos National Laboratory

Enrollment will be limited to 32, and all expenses except travel will be fully covered by CDAC. Travel support up to $200 will also be available. Participants in the CDAC Summer School will be housed at the Argonne Guest House and all meals will be provided by the Summer School.

To apply, please send a brief statement of your research program and reasons for your interest in the CDAC Summer School to Steve Gramsch, CDAC Coordinator, at s.gramsch@gl.ciw.edu. Applications should be received by April 15.

There will be a limited number of spaces available for senior scientists to attend the school lectures at their own expense. Please contact the CDAC Coordinator for further information.

For more information about CDAC, see http://www.cdac.gl.ciw.edu. Come and see what the excitement in high pressure research is all about!

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

CDAC: The Carnegie Institution of Washington 5251 Broad Branch Road, NW; Washington, DC 20015-1305

Figure 29. *Announcement for the 2005 CDAC Summer School*

demonstrated how static and dynamic experiments, along with condensed-matter theory, can provide a means to understand the behavior of matter under extreme conditions.

Presentations were made within the context of key materials and measurement capabilities that are crucial to stockpile stewardship and the missions of the NNSA Labs, forming a linking conceptual thread that ran throughout the lectures, beginning with introductory lectures on the first day and moving to the more specialized techniques and problems. All in all, it provided an important and coherent introduction to the field and provided a valuable background for students new to the field. The students were highly engaged, with considerable discussion throughout the lectures.

Students – CDAC Summer School students came from universities throughout the United States. Of the 33 students, 11 were female and 16 were U.S. citizens. A detailed list of students and their home institutions is given below:

Alice Acatrini, New Mexico State University/LANL (Postdoctoral Student)
Muhetaer Aihaiti, Carnegie Institution of Washington (Postdoctoral Student)
Resul Aksoy, Texas Tech University (Graduate Student)
Can Aydiner, Iowa State University/LANL (Postdoctoral Student)
Cindy Bolme, Massachusetts Institute of Technology/LANL (Graduate Student)
Lauren Borkowski, George Washington University (Graduate Student)
Jon Brenizer, University of Illinois (Graduate Student)
Raja Chellappa, University of Nevada-Reno (Graduate Student)
Bin Chen, University of Illinois (Postdoctoral Student)
Jinarong Chen, University of Louisville (Graduate Student)
Alfredo Correa, University of California-Berkeley/LLNL (Graduate Student)
Tanja Cuk, Stanford University (Graduate Student)
Nicholas Cunningham, University of Alabama-Birmingham **(CDAC Graduate Student)**
Erik Emmons, University of Nevada-Reno (Graduate Student)
Lili Gao, University of Illinois (Graduate Student)
Rafael Jaramillo, University of Chicago (Graduate Student)
Zsolt Jenei, University of Stockholm/LLNL (Graduate Student)
Matt Lucas, California Institute of Technology **(CDAC Graduate Student)**
Wendy Mao, University of Chicago **(CDAC Graduate Student)**
Zhu Mao, Princeton University **(CDAC Graduate Student)**
C. David Martin, SUNY-Stony Brook (Graduate Student)
Lowell Miyagi, University of California-Berkeley **(CDAC Graduate Student)**
Jiang Qian, Los Alamos National Laboratory **(CDAC Graduate Student)**
Wei Qiu, University of Alabama-Birmingham **(CDAC Graduate Student)**
Claire Runge, Princeton University **(CDAC Graduate Student)**
Tarik Saleh, University of Tennessee (LANL)
Chris Seagle, University of Chicago **(CDAC Graduate Student)**
Emre Selvi, Texas Tech University
Kimberly Tiat, University of Arizona/LANL (Graduate Student)
Nenad Velisavljevic, University of Alabama-Birmingham (Graduate Student)
Yuejian Wang, Texas Christian University (Graduate Student)
Michelle Weinberger, University of California-Los Angeles (Graduate Student)
Rui Zou, Rensselaer Polytechnic Institute (Graduate Student)

Many students were from CDAC Partner Universities, but an impressive number came from outside of CDAC (called CDAC Collaborating Universities; Fig. 30). Thus the School served a very important role of outreach and enhancing the alliance between DOE/NNSA and academia. A number of students are also already doing research at the National Labs. Travel, accommodations, and registration costs for all students were provided by the core CDAC budget.

Figure 30. *Students, lecturers, and observers of the 2005 CDAC Summer School at the Argonne National Laboratory*

Lecturers – Lectures in the CDAC Summer School were given by thirteen different scientists during the three days of the school, with three of these lecturers giving two lectures each. The following list gives the lecturers, their institution, and the titles of the lectures they presented.

Lecturer	Institution	Lecture Title
Neil Ashcroft	Cornell University	1. Fundamentals of Matter at High Densities 2. Mainly Dense Hydrogen
Kimberly Budil	Department of Energy/NNSA	Stewardship Science
Paul Chow	HPCAT/Advanced Photon Source	Inelastic X-ray Scattering: Framework for Understanding Electronic Excitations
G. W. Collins	Livermore National Laboratory	Using Lasers to Study Extreme States of Matter
Dana Dlott	University of Illinois	Laser-Driven Shock Waves and Molecular Spectroscopy
Larry Fried	Livermore National Laboratory	Modeling Chemical Transformations Under Extreme Conditions
David Funk	Los Alamos National Laboratory	Ultrafast Studies of Shock-Induced Chemical and Physical Transformations
Yogendra Gupta	Institute for Shock Physics, Washington State University	1. Introduction to Shock Compression 2. *In-Situ* Measurements with Shock Compression Techniques
Michael Hu	HPCAT/Advanced Photon Source	Applications of X-ray Spectroscopy: Nuclear Resonant Scattering with Synchrotron Radiation
Raymond Jeanloz	University of California-Berkeley	Static and Dynamic Compression/Overview of Key Materials
Chi-Chang Kao	National Synchrotron Light Source, Brookhaven National Laboratory	1. Synchrotron Radiation and Beyond 2. Fundamentals of X-Ray Spectroscopy

Marcus Knudson	Sandia National Laboratories	Shock Compression and Pulsed Power Methods
Ho-kwang Mao	Carnegie Institution of Washington	Static High Pressure Techniques: Diffraction Methods
Burkhard Militzer	Carnegie Institution of Washington	First Principles Simulations
Adam Schwartz	Livermore National Laboratory	Physics, Materials Science, and Chemistry of Actinides
Yusheng Zhao	Los Alamos National Laboratory	High Pressure Neutron Diffraction

Each lecture was 50 minutes in length, with 20 minutes in between lectures for discussion and a break. Discussions following the lectures were lively and focused on student questions and comments. Copies of all presentations have been compiled and are being distributed to all participants (and other interested parties).

Observers – The School also served as a unique introduction to high-pressure materials science for more advanced researchers (including many of the lecturers!). Though the focus of the School was on the students, other scientists attended the lectures (as observers) to further their knowledge of the field. These scientists included:

Arunkumar Bommannavar, HPCAT/Advanced Photon Source
Yang Ding, HPCAT/Advanced Photon Source
Dhanesh Chandra, University of Nevada-Reno
Michael Lerche, XOR/Advanced Photon Source
Hans-Peter Lierman, HPCAT/Advanced Photon Source
Jung-Fu Lin, Carnegie Institution of Washington
Reginald Little, Florida A&M University
Haozhe Liu, HPCAT/Advanced Photon Source
Yue Meng, HPCAT/Advanced Photon Source
Agnes Mao, Carnegie Institution of Washington
Vitaly Prakapenka, University of Chicago/GSECARS
Guoyin Shen, University of Chicago/GSECARS
Maddury Somayazulu, HPCAT/Advanced Photon Source

Response and Outlook – The student reception to the program of lectures was overwhelmingly positive, with many compliments on the outstanding quality of the lectures and discussions, the favorable location at the Argonne Guest House, and the opportunity for extended discussions both between lectures and at mealtimes. The demand for another such opportunity appears to be high, as many students inquired whether there will be another school next year. Fitting the same number of lectures into a longer time period with time for some hands-on experience in x-ray diffraction and spectroscopy at HPCAT may be considered for future schools. It was also suggested that CDAC should consider publishing a book or series of volumes in this area.

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.

Visitors	Affiliation	Project	Date
Lauren Borkowski M. Frisch	George Washington University	X-ray diffraction	July, 2003-present (ongoing)
Michelle Weinberger	University of California – Los Angeles	Brillouin of nanoparticles	October 18-27, 2003
Y. Feng	University of Chicago	Sample loading, Raman	November 4-6, 2003
N. Cunningham	University of Alabama – Birmingham	Diffraction training, HPCAT	January 8-15, 2004

Kristina Lipinska-Kalita	University of Wyoming	Sample loading, Raman	February-April, 2004
Jenny Pehl	University of California – Berkeley	Gas loading basics	March 6-8, 2004
Jennifer Jackson	University of Illinois	Gas loading for APS experiments	March 19-24, 2004
D. Dolan	Sandia National Laboratory	Diamond work	April 21-22, 2004
J. Lie	University of Illinois	Gas loading basics	May 19-21, 2004
D. Chandra	University of Nevada – Reno	Diamond cell sample preparation	June 14-21, 2004
L. Zhang	Institute of Physics, Southwest Jiatong University, China	Diffraction	July 4, 2004-June 20, 2005
Becky Streetman	Los Alamos National Laboratory	Sample Loading, U2A prep	July 18-30, 2004
Y. Freiman	Verkin Insitute, Ukraine	Quantum transitions in hydrogen	July-August, 2004
M. Manghnani G. Amulele	University of Hawaii	Gas loading	August 19-20, 2004
S. Sheih	National SK University, South Korea	Ammonia at high pressure	September 12-15, 2004
A. Goncharov	Lawrence Livermore National Laboratory	Water/Raman	September 14-22, 2004
E. Schwegler	Lawrence Livermore National Laboratory	First principles simulations of water under pressure	September 21-22, 2004
G. Zou	Jilin University	Superhard Materials	October 8-22, 2004
Valentina Degteyareva	Institute for Solid State Physics, Chernogolovka	High pressure crystallography	October-December, 2004
D. Chandra R. Chellappa	University of Nevada – Reno	Polyalcohols/thermal storage materials	October-November, 2004
Jennifer Jackson	University of Illinois	Gas Loading	November 1-6, 2004
A. Goncharov	Lawrence Livermore National Laboratory	Raman studies of water	January 24-30, 2005
Tanja Cuk	Stanford University	Hi T_c Superconductors under pressure (transport properties)	January-May, 2005
W. Grochala	University of Warsaw, Poland	Novel Ag-F compounds metal-insulator, magnetism, superconductivity	January-February, 2005
W. D. Kraeft	Greifswald University, Germany	Seminar on the EOS of dense plasmas	January 7-8, 2005
E. B. Gordon	Institute for Problems of Chemical Physics RAS, Chernogolovka, Russia	Excess electrons in nonpolar dielectrics	February 4-7, 2005
C. Tulk	Oak Ridge National Laboratory	Preparation of neutron diffraction experiments	February 27 2005
J. Crowhurst	Lawrence Livermore National Laboratory	Gas loading of ammonia	March 10-14, 2005
M. Wanic K. Van Coille D. Verschueren	Bettonville	Bettonville Combi Laser system	March 15-18, 2005 March 7-15, 2005 March 14-18, 2005
Y. Huang	Army Research Laboratory	Brillouin spectroscopy	April 22, 2005

A. Gavriliuk	Institute for High Pressure Physics, Russian Academy of Sciences	Fe-containing garnets and borates	April-June, 2005
R. Chellappa	University of Nevada – Reno	$LiAlH_4$ at high pressure	May 2-12, 2005
H. Swarovski D. Fritz M. Snyder	Swarovski Crystal	Diamond analysis	July 8, 2005
Igor Lyubutin	Institute of Crystallography, Russian Academy of Sciences	Magnetic collapse in transition metal oxides at high pressures	July 22-August 4, 2005
Jennifer Ciezak	NIST; Aberdeen Army Laboratory	Raman laboratory	July 27, 2005 August 17-18, 2005 September 8, 2005-ongoing
J. Post M. D. Fuller Davia Kramer	Smithsonian Institution Fuller & Associates Jewelry Appraisal Laboratories	Diamond analysis	August 19, 2005
Don Clas Richard Clark	Morgan Crucible	Diamond analysis	August 31, 2001

3.7 High Pressure Seminar Series

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

Speaker	Affiliation	Topic	Date
S. Prosandeev	NIST	First order Raman spectra of double perovskites	June 9, 2004
T. Jenkins	Syracuse University (now Carnegie)	Short, strong hydrogen bonds examined by vibrational inelastic neutron scattering and computational methods	June 22, 2004
W. Grochala	University of Warsaw	Hydrogen storage for transportation. Challenges and tasks of chemistry	July 7, 2004
J. E. Patterson	University of Illinois	Spectroscopic study of shock-induced molecular dynamics at a metal-liquid interface	July 16, 2004
K. Hayashi	Kobe Steel, Japan	Developments in homoepitaxial CVD diamond films	July 19, , 2004
Y. Freiman	Verkin Institute, Ukraine	Entropy-driven reentrant phase transitions in solid hydrogens	August 10, 2004
G. Zou	Jilin University	Pure phases of C_3N_4 synthesized under high pressure and high temperature	October 22, 2004

T. Okuchi	Carnegie	Hydrogen bonding and molecular dynamics of compressed liquid methanol by DAC NMR	November 23, 2004
Wendy Mao	University of Chicago	Mineral physics at the core-mantle boundary	December 2, 2004
R. Cohen	Carnegie	High-pressureerformance computing requirements for the computational solid earth sciences	December 21, 2004
A. Zaitsev	City University of New York	New developments and applications of diamond	January 28, 2005
W. Grochala	University of Warsaw	From two-electron electromerism towards a novel, mnemonic device	February 4, 2005
E. B. Gordon	Institute for Problems of Chemical Physics, Russia	Excess electrons in nonpolar dielectrics	February 14, 2005
Tanja Cuk	Stanford University	Angle-resolved photo emission as a probe of electron-phonon coupling in high Tc superconductors	February 25, 2005
M. Wanic K. Van Coille D. Verschueren	Bettonville	Shaping and cutting diamond with the Bettonville Combi Laser	March 14, 2005
Z. Wu	Carnegie	Pressure-induced anomalous phase transitions and colossal enhancement of piezoelectricity in $PbTiO_3$	April 1, 2005
R. Caracas	Carnegie	First-principles calculations of major minerals present in the Earth's lower mantle: perovskite and post-perovskite	April 8, 2005
B. Militzer	Carnegie	Simulations of dense helium fluid at shock conditions	June 9, 2005
X. J. Chen	Carnegie	Superconductors under pressure: Why do we care?	June 24, 2005
I. Tamblyn	Dalhousie University, Canada	Simulation of hydrogen-helium mixtures in planets	July 21, 2005
I. Lyubutin	Institute of Crystallography, Russian Academy of Sciences	Magnetic collapse in transition metal oxides at high pressures	August 4, 2005
J. Post	Smithsonian Institution	Smithsonian Diamonds	August 19, 2005
T. Jenkins	Carnegie	Recent advances in High Pressure Neutron Spectroscopy and use in Hydrogen Storage Research	September 9, 2005

3.8 SSAAP Symposium

On August 23-24 2005, the Second Annual SSAAP Symposium was held in Las Vegas on the **UNLV** campus. This symposium was an opportunity for CDAC faculty, students, and post-doctoral associates as well as several university collaborators to be brought together. It was also an opportunity for all personnel involved with CDAC to interact with scientists and students from other groups supported by SSAAP and to learn about other research supported by the program. In total, there were 26 posters presented by CDAC-affiliated people at the meeting, mostly at the student poster section:

Aihaiti, M., Brillouin scattering studies of hydrides and ferroelectrics, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Chellappa, R., High pressure Raman spectroscopy studies on pentaerythritol, neopentylglycol, and $LiAlH_4$, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Chen, X. J., Neutron diffraction studies of FeO up to 25 GPa, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Chen, X. J., High-pressure superconductivity and mechanical properties of nitrides, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Chen, X. J., Superconductivity of NbN under pressure, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Chen, X. J., Irreversible phase transition to black silane, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Emmons, E., Dynamic studies of phase transitions in f-electron materials using photoluminescence spectroscopy, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Gramsch, S. A., Overview of CDAC, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Hemley, R. J., New developments at CDAC - The Carnegie/DOE Alliance Center: A center of excellence in high pressure science and technology (invited), *Stewardship Science Academic Alliances Program Symposium* (Las Vegas, NV, August 23-24, 2005).

Kalita, P. E., C. L. Gobin, R. J. Hemley and K. Lipinska-Kalita, High pressure-induced phase transition in b-Ga_2O_3: in situ synchrotron x-ray diffraction studies up to 70 GPa, *Stewardship Science Academic Alliances Program Symposium* (Las Vegas, NV, August 23-24, 2005).

Lazicki, A., A new high-pressure phase of Li_3N: Stability of the N_3 Ion to 200 GPa, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Liermann, H. P., Current and future experimental techniques at beamline 16 BM, High Pressure Collaboration Access Team: Simultaneous high-pressure, -temperature powder and single crystal x-ray diffraction, combined with in situ fluorescence and Raman spectroscopy, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Liermann, H. P., White beam Laue studies at beamline 16 BM-B, High Pressure Collaboration Access Team, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Lipinska-Kalita, K. E., P. E. Kalita and R. J. Hemley, High pressure-induced phase transition in a nanostructured composite: In situ synchrotron x-ray diffraction investigations, *Stewardship Science Academic Alliances Program Symposium* (Las Vegas, NV, August 23-24, 2005).

Lipinska-Kalita, K. E., High pressure-induced phase transition in a nanostructured composite: In situ synchrotron x-ray diffraction investigations, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Lipinska-Kalita, K. E., High pressure-induced phase transition b-GA_2O_3: In situ synchrotron x-ray diffraction studies up to 70 GPa, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Liu, Z., A high-pressure microspectroscopy beamline at the NSLS, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Meng, Y., HPCAT ID beamline overview, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Meng, Y., The power of an integrated approach in high-pressure research, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Meng, Y., Advances in high-pressure x-ray spectroscopy, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

Miyagi, L., Berkeley CDAC collaborations in texture analysis of Earth materials at high pressures, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 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).

Song, Y., Pressure-induced transitions in silane, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 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).

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).

Zhao, Y., High preessure neutron diffraction at LANSCE, *Second Annual SSAAP Symposium* (Las Vegas, NV, August 23-24, 2005).

4. TECHNOLOGY DEVELOPMENT

4.1 High *P-T* Experimental Techniques

CDAC is dedicated to advancing 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[195, 196], gas-guns[197], and magnetic compression methods[198] and continued refinements of DAC techniques at the NNSA/DP Labs form a natural complement to activities within CDAC[121, 199]. Advances made in high-temperature methods at ultrahigh pressure are providing new links to dynamic compression experiments. The Nd-YLF double-sided laser method[200, 201] has been extended to include CO_2 laser heating as well as simultaneous Raman spectroscopy[16, 46]. The technique developed in CDAC has been adapted and is now in place in the labs of **Choong-shik Yoo** and **Joe Zaug/Jonathan Crowhurst** at **LLNL**. Resistively-heated DACs, which provide a temperature accuracy of ±5 K, have been extended to >1000 K at megabar *P*, even for hydrogen[202]. New composite gasketing techniques, developed in collaboration with **LANL**, have substantially increased the available sample volumes[203, 204].

Nuclear resonant inelastic x-ray scattering (NRIXS) spectroscopy of iron at high temperature and pressure has been used to provide independent confirmation that the Planck radiation function is a reliable indicator of the temperature in the laser heated DAC. Using the principle of detailed balance and the peak intensities from the NRIXS data, the absolute temperature of the iron-57 sample at 58 GPa and elevated temperatures was determined. The data show that the Planck function and the temperature as measured by NRIXS are good agreement up to at least 1700 K[205].

Non-linear optical methods adapted for high- *P* multiphoton spectroscopy, photoionization, and CARS spectroscopy in DACs at **Carnegie** and **LLNL**[206] are complemented by a wide array of non-linear optical methods developed at **Illinois** that are being applied to high-pressure problems. This includes the recent breakthrough at **Illinois** in the use of vibrational sum-frequency generation (SFG) to probe molecules at interfaces as described above; the system can now be applied to investigate the structure, chemistry and aging properties of molecules at interfaces and crack propagation relevant to stockpile stewardship. As described above, **James Patterson**, the student who worked on this at **Illinois** joined **Yogesh Gupta**'s DOE-supported shock physics center at **Washington State**. The work sets the stage for future high-pressure developments, including the use of free-electron lasers and combined static/laser shock methods.

New Cell Designs – With accuracy of other properties needed for stockpile stewardship. changing support leveraged by CDAC, **Carnegie** has dedicated a significant effort toward the development of new classes of devices for high *P-T* materials science[185]. The **Carnegie** group continued to perfect processes to fabricate single crystal diamonds by microwave plasma CVD by epitaxial growth on diamond substrates at very high growth rates. During the past year, crystals up to 12 mm in thickness have been fabricated. Significant progress in CVD single crystal diamond was made possible by close collaboration with LANL[18]. As grown, the material has high fracture toughness and on annealing its hardness can increase dramatically, reaching values some 50% higher than conventional diamond[18]. As may be expected, the new diamond can be used to generate multimegabar pressures. This was demonstrated in Year One by CDAC graduate student **Wendy Mao** in a **Chicago**-**Carnegie** collaboration[186]. Additional studies of the strength and annealing effects were also carried out this year. Annealing samples were also studied in detail by a variety of spectroscopic methods[207]. Most recently, a 10-carat, half-inch thick single-crystal diamonds have been produced (Fig. 31). The team has also made colorless single-crystal diamonds, transparent from the ultraviolet to infrared wavelengths with their CVD process[208, 209].

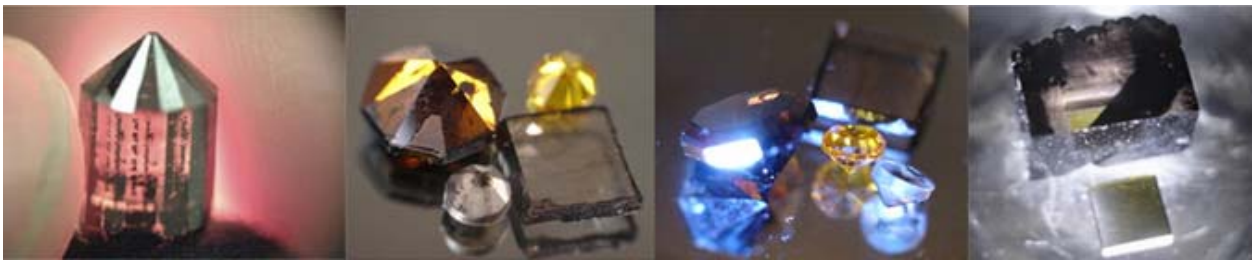


Figure 31. *CVD Diamonds created at* ***Carnegie****. Far left: 5-carat CVD diamond laser-cut from a 10-carat single crystal. Center: a variety of different single crystal CVD diamonds that have been produced by the team. Far right: 4 x 4 x 1.5 mm³ single-crystal diamond block formed by deposition on 6 {100} faces of a substrate.*

Yogesh Vohra's group at **Alabama-Birmingham** continues to develop complementary designer anvil technology as part of CDAC. An isotopically enriched ^{13}C homoepitaxial diamond layer of 6±1 μm thickness was grown on top of a brilliant cut diamond anvil by CVD deposition process for application as a pressure sensor. This isotopically enriched diamond tip was then used in conjunction with a natural isotopic abundance diamond anvil to generate high pressure on the sample. **Vohra's** group provides a calibration for the ^{13}C Raman mode of this extremely thin epitaxial layer to 156 GPa using ruby fluorescence and the EOS of Cu as secondary pressure standards. The nonlinear calibration of the ^{13}C Raman mode pressure sensor is compared with similar calibrations of ^{12}C Raman mode 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 also allow calibration to even higher pressures.[210]

As discussed above, the recently developed moissanite (single-crystal SiC) anvil cell (MAC) has become a useful device for achieving both high pressure and large sample volume in an anvil cell[185]. In a collaboration between **UC Santa Cruz**, **Indiana University–South Bend**, and **Carnegie**, tests were carried out to 53 GPa using moissanite anvil cells (MAC) combined with synchrotron radiation. No significant change of the transmission spectra through the moissanite anvils was observed over the pressure range studied[39]. As a further test, the infrared spectrum of $Ru_3(CO)_{12}$ was measured up to 27 GPa with a MAC; the pressure dependences of the infrared-active C-O stretching modes normally obscured by diamond anvils are readily observed[211]. These developments continue to strengthen the world-leading high-pressure synchrotron IR program this group maintains at the NSLS[212-214]. CDAC has supported several important upgrades of the facility. A growing number of NNSA Lab scientists and students are using this facility.

<u>High-Pressure Magnetic Methods</u> – Further optimization of magnetic techniques were made at **Carnegie** during the past year. Data on the pressure limit of superconducting T_c measurements along with the pressure limit in experimental attempts to achieve metallization in H_2 were explored. With continuing concentrated efforts they expect to be able routinely perform experiments in the 300 GPa range, and hopefully measure the predicted superconducting signals from metallic hydrogen within five years. Nuclear magnetic resonance (NMR) is a well-developed spectroscopic method at megahertz radio frequencies (rf). There have been few applications to high pressure in DACs because of the intrinsic low sensitivity. However, NMR provides unique information about local environments surrounding nuclear spins that complement other spectroscopic methods. Major developments in high-pressure NMR were made at **Carnegie**[215-217]. They constructed a new type of probe for nuclear magnetic resonance spectroscopy in the DAC[215, 216] consisting of a high-inductance solenoid coil and tuning capacitors. The solenoid rf probe was quantitatively evaluated for its radio frequency field homogeneity and its sensitivity. This group found that it gives a practically uniform rf field and better sensitivity than the previous most sensitive probe, making NMR at higher pressure more practical.

High-pressure Kβ x-ray fluorescence[218] and high-pressure Mössbauer spectroscopy[219,220] are complementary to magnetic susceptibility measurements. Measurements of Kβ x-ray fluorescence in Fe_3O_4 (magnetite) to 80 GPa, show clear evidence of spin collapse at 60 GPa, compatible with available Mössbauer data[221]. Further improvements in nuclear inelastic resonant x-ray scattering [which has been used to study Fe[145,222] and FeO[223]] 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.

4.2 Facilities at Brookhaven, LANSCE, and Carnegie

New generations of x-ray sources providing orders of magnitude higher brilliance have led to the major leaps that have fundamentally improved the temporal, spatial, and energy resolution of existing measurements and enabled new studies previously considered inaccessible. 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. This makes possible new classes of experiments on small samples to megabar pressures[146]. High-pressure IR measurements are being performed at the U2A beamline at NSLS, which is also managed and operated by this group. This facility was upgraded from the previous U2A facility with higher IR flux and the addition of new instrumentation. The beamline has a Bruker IFS 66v spectrometer, Bruker II IR microscope, 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 beamlines at X17C and the newly created X17B3 for high *P-T* diffraction, which are currently managed by **Carnegie** under the NSF COMPRES consortium. Both monochromatic and polychromatic diffraction can be performed with equipment that includes single-crystal and powder diffractometers, energy dispersive detectors, microbeam primary and secondary collimators, K-B focusing optics, micropositioners, optical alignment system, and ruby fluorescence systems. 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.

High P-T Neutron Scattering – Neutron probes have several unique advantages for the study of materials and phenomena of great importance at high pressure for stockpile stewardship, and are complementary to synchrotron x-ray and laser optical probes. (1) In all static high-pressure experiments, the diagnosis probe must be able to penetrate through the strong pressure vessel to reach the samples and the sample signal must be allowed to exit the vessel to reach the detector. In general, optical probes can be used only with colorless, gem-quality diamonds or hard gemstones, and x-ray probes can only pass through low-Z materials such as the diamond and the Be gaskets, thus severely restricting the high-pressure vessel design. Neutron radiation is far more penetrating to most materials. (2) It can detect and distinguish between hydrogen and its isotopes, important to stewardship science as pure elements and in compounds. (3) Neutrons can easily probe thick layers of heavy elements and radioactive materials that pose problems for x-ray methods. (4) Neutrons are an ideal probe for phonon dynamics: at low energies, they provide high resolution (±0.1 meV) ten times better than x-rays, and approaching some optical spectroscopy methods, but their high momentum can also probe the dispersion across the entire Brillouin zone while the low momentum optical probes are essentially limited to zone-center phonons. (5) Neutrons can probe magnetic moments that are crucial for *d*- and *f*-metals. (6) Neutrons probe a very large Q (in $Å^{-1}$) range and reveal in-depth crystallographic information. The most severe technical problem is the lack of neutron intensity to probe these minute samples under pressure, which has limited the application of neutron methods to 25 GPa with Paris-Edinburgh (P-E) cells and 43 GPa with DACs. The equally important infrastructure problem is the lack of a focused high-pressure program and research community.

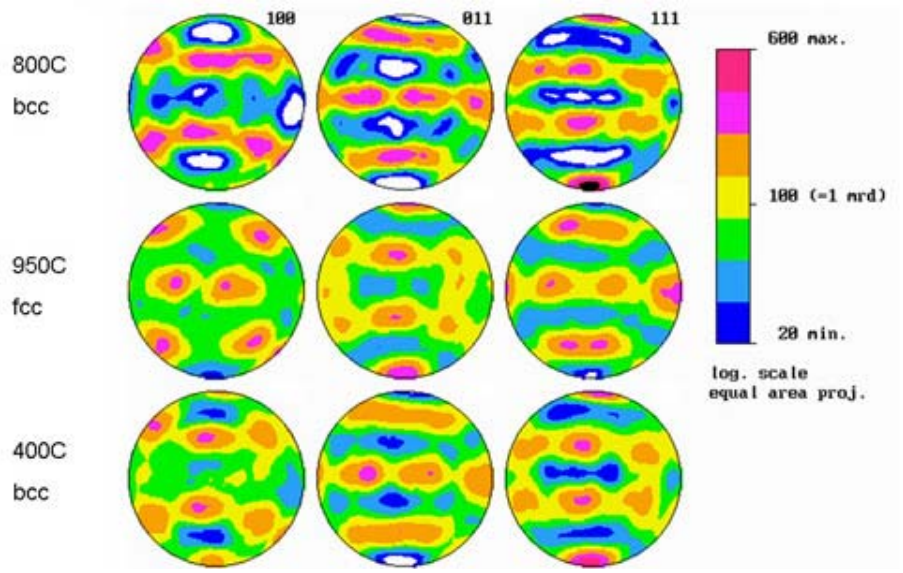


Figure 32. *Orientation relationships during phase transformations: bcc-fcc Fe transformation measured in situ with neutron diffraction (HIPPO diffractometer at LANSCE)*

CDAC is helping to spearhead the development of high-pressure neutron scattering at LANSCE. In Year One, processing procedures for TOF neutron diffraction data for textures, both with the Rietveld method and an automatic peak extraction method were streamlined[42, 43]. **Rudy Wenk's** group at **Berkeley** developed similar standard procedures for direct image analysis of synchrotron diffraction data with the Rietveld method[224-226]. At **LANL**, the group investigated with HIPPO and vacuum furnace anisotropy changes during heating, particularly texture changes during phase transformations of hexagonal metals (*e.g.,* Fig. 32)[34-36]. With the **Carnegie** and **LANL** teams, methods for radial high-pressure experiments with HIPPO were developed to investigate textures with CDAC graduate student **Jenny Pehl** spending an extended period at **LANL** to work with instrument scientists **Sven Vogel** and **Darrick Williams**, advancing the methods of quantitative data analysis[43]. Research with HIPPO and SMARTS is being continued with new student **Lowell Miyagi** addressing phase transformations under applied as well as residual stress, using the α–β quartz transformation as a model system but also applying it to metals such as iron[33]. This research will continue in Year Three. Both the *in situ* texture measurements with neutrons and synchrotron x-ray figure prominently in recent reviews[227-229].

As described last year, a collaboration between **Carnegie**, **Chicago**, **Rutgers**, and **LANL**, the D_2 clathrate hydrate crystal structure was determined as a function of temperature and pressure by neutron diffraction at LANSCE[10]. Other experiments concerned the structure of wüstite-$Fe_{0.93}O$ at high pressure mentioned above. Powder neutron diffraction measurements were performed to 12 GPa using large gem-moissanite (SiC) anvil cells, also at LANSCE[230]. The required sample volume for high-pressure neutron diffraction is dramatically reduced to several cubic millimeters. Other studies examined the unusual high-pressure behavior of glasses. For example, a **Carnegie**, **Wyoming**, **ANL**, and **ORNL** team carried out the combined *in situ* x-ray and neutron-diffraction study of GeO_2 glass, described earlier[6].

Finally, the **Carnegie** group and scientists at **Stony Brook** (led by **John Parise**) and **ORNL** (led by **Christopher Tulk**), are constructing the dedicated high-pressure instrument (SNAP) at the country's Spallation Neutron Source (SNS), which will be the world's most powerful neutron source when the facility is completed at **ORNL** in 2007. The project will 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 Two of its five-year plan. The first meeting of the SNAP instrument development team took place at LANSCE in April, 2003. The meeting was hosted by **Yusheng Zhao** (**LANL**) and involved a number of CDAC members, including **Brent Fultz and Neil Ashcroft** (CDAC Advisory Committee Member). The second annual SNAP meeting was held at the new SNS facility in July 2005 and was attended by many CDAC Academic and National Lab Partners.

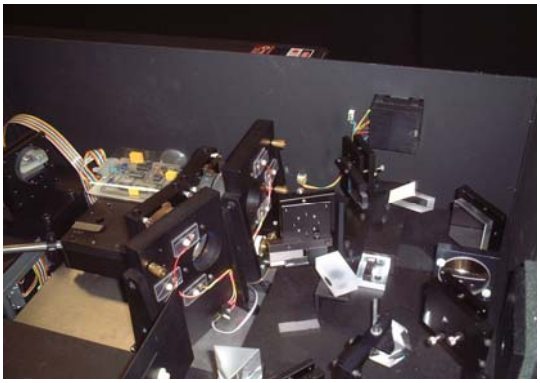


Figure 33. *Sandercock type Tandem Fabry-Perot interferometer at* ***Carnegie****.*

The **Carnegie** labs continue to be an important resource for the high-pressure community. In addition to the technical progress made at the HPCAT facility, important upgrades have been initiated and completed at many facilities used by CDAC. Upgrades and new facilities include those in general high *P-T* technology, for example new DAC designs (cryogenic to high temperatures); spectroscopy for new high *P-T* laser heating /Raman/ IR/Brillouin (Fig. 33); and elasticity with an improved high pressure GHz ultrasonics system (Fig. 34). These facilities and instrumentation upgrades made possible by the CDAC grant. Additional developments were made in the **Carnegie** CVD anvil facility (5 kW CVD system for large anvil fabrication and the addition of a 6 kW CVD system and a second 5 kW system), the dedicated high-pressure NMR laboratory (200 MHz widebore), and at the NSLS Facilities (upgraded high-pressure IR U2A beamline). These improvements were supported by other grants and by **Carnegie** funds.

4.3 Construction and Commissioning at HPCAT

HPCAT was launched in 1999 to reclaim the United States' lead in high-pressure synchrotron science. The construction and commissioning phase of HPCAT development is nearing completion. The multiple synchrotron x-ray and allied techniques have been developed and integrated with DACs, focusing on a unified scientific goal – exploring the rich behavior of materials under extreme pressures and temperatures. The current technology of high-pressure x-ray diffraction has been drastically improved; intriguing high-pressure structures can now be studied with an accuracy and sophistication that rival ambient structural determinations. A plethora of novel synchrotron x-ray spectroscopic techniques has been introduced and applied, many of them for the first time, for high-pressure

Figure 34. *Gigahertz ultrasonic interferometer for high-pressure studies of single-crystal elasticity DAC at* ***Carnegie****.*

applications. Direct probing of the fundamental electronic structure and phonon dynamics that were inaccessible for high-pressure research in the past has now been enabled. The facility is unleashing the full power of high-pressure study in numerous scientific disciplines, allowing CDAC researchers to tackle a range of grand challenges in various directions, including stockpile stewardship. Reviews of the use of synchrotron facilities to study materials under extreme conditions, including planetary interiors, were written[214, 231].

Figure 35. *Clockwise from top left: The construction of a diffractometer in 16BM-D; the x-ray diffraction station at 16ID-B of HPCAT provides state of the art techniques, including micro-focused beam, area CCD and image plate detectors, and in-situ double-side laser heating, for high-pressure and high-temperature x-ray diffraction studies; the setup in 16Id-D. The NFS, XRS, RXRS, and XES have been successfully commissioned in ID-D, and will become operational in 2006; the setup in 16ID-D. The NFS, XRS, RXRS, and XES have been successfully commissioned in ID-D, and will become operational in 2006; the BDCM monochromator installed in 16ID-A, allowing single undulator beam to be split into two branches: one for spectroscopy experiments at 16ID-D station, and the other for micro-diffraction experiments at 16ID-B. The BDCM is a horizontally deflecting monochromator delivering beam to the ID-B station. Si<220> crystals are mounted in the monochromator and the energy range is 24 keV to 35 keV. The crystals are water cooled. The horizontal offset from the main beam is 1 meter outboard. Bimorph mirrors focus the beam to 15 μm X 10 μm in the ID-B station.*

There have been many technical developments at HPCAT during the past year (Fig 35). At the ID-D experimental station dedicated to inelastic x-ray scattering at high pressure has made a number of technical advances. There is now a dedicated emission spectrometer that will be fully commissioned in the near future. In addition, the high resolution capability continues to improve with work being done to achieve 1 meV energy resolution for nuclear forward scattering measurements. In the past year, **Paul Chow** and colleagues at HPCAT did their first low-

temperature NFS measurement with the sample at high pressure and low temperature (10K). In August of 2005, this group made their first test of compound focusing of the beam, achieving a beam size of 10 μm (vertically) x 25 μm (horizontally) using a second set of K-B mirrors. In the last part of 2005, they will continue to upgrade their capabilities.

The bending magnet beamline BM-B completed a full years' operation during which a number of pilot experiments were conducted to crystallize plans for the completion of BM-C and BM-D. The station was then shut down for allowing the beam pipe carrying the inboard part of the fan to be set up. This was subsequently radiation tested and verified by the APS thus allowing BM-C to become operational. During the coming month, the end station BM-D will be verified and the last station in HPCAT will become operational. The group at HPCAT intends to start this BM-D as a white beam station but add monochromaters operating in large energy ranges. BM-B will continue to be the workhorse for doing routine Energy Dispersive X-ray Diffraction measurements that have not only benefited users at HPCAT but also users from other sectors now conducting high-pressure research. Based on the experimental studies on powder and single crystals using white beam Laue techniques, it has been decided that studies will continue with the same 3 circle geometry (twotheta-omega-chi) in BM-D with the option of adding an additional circle for the area detector. The 1-meter long K-B mirror will be set up shortly and this will allow focus of the full vertical beam. They intend to keep their options open in doing double focusing in this direction and also focus in the horizontal direction using a 200 mm long mirror. Their studies at BM-D showed that it is possible to achieve a 5 um focal spot quite easily. This group plans to carry out a number of studies at low temperatures (using a flow type liquid He cryostat) and at high temperatures (using a resistively heated diamond cell) and correspondingly, the BM-D station will have an on-line Raman system capable of measuring ruby fluorescence, 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.

During Year Two the sample preparation lab at HPCAT was significantly rearranged and upgraded to make it more user-friendly and efficient. Microscope upgrades include on axis illumination for efficient sample loading, analog camera view for teaching purposes, and large working distance microscopes to accommodate different DAC. The setup of the Be-drilling facility that is heavily used be all beam lines at HPCAT as well as other sectors around APS has also been upgraded. HPCAT is able to provide all common internal standards used for pressure measurements (*i.e.* Au, Ag, Pt, ruby) and pressure media (methanol/ethanol, NaCl, CsCl, silicon oil, Al). This is particularly important for training of new users that are often unfamiliar with the different choice of pressure standards and media.

The team at HPCAT has also worked on providing support for a wide range of resistive heating techniques. For that purpose, different power supplies are offered and thermocouple measurement and recoding equipment that can be easily integrated with the Beamline operations have been set up. Also provided is a facility to rebuild and reassemble different resistive heaters as well as thermocouple assemblies. This also includes a furnace to fire ceramics insulations. In addition, HPCAT has developed a state of the art Ruby/Raman facility that provides pressure measurements up to 250 GPa. However, the system also provides interchangeable Raman at 514 nm and 488 nm that has recently been used to measure high quality Raman spectra to verify the formation of super hard nitrides synthesized at high-pressure and temperature. A similar system will also be available at the end of 2005 for online measurements.

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 academic groups, including the synchrotron beamlines and the CDAC high-pressure labs. CDAC members meet at the monthly HPCAT meetings at APS. There are also frequent visits to at 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. In particular, the CDAC Summer School discussed in Section 3.5 and SSAAP Meetings outlined in Section 3.8 were very successful in providing a forum where a number of possible research collaborations between graduate students from academic groups and NNSA Lab personnel were discussed.

- ***Experiments performed at HPCAT.*** The integrated HPCAT facility, including the ID and BM hutches, as well as the off-line high-pressure lab and infrastructure at APS has turned out to be an excellent a forum for interactions. 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.*** Likewise, the technique development program at **Carnegie** provides an additional meeting ground for interactions. This has been enhanced by the additional office and lab space provided by the Institution. More than 20 visitors came this year, including one day to several week stays (for training, sample loading, or specific measurements).

Figure 36. *Screen shot of the CDAC website, http://cdac.gl.ciw.edu*

- ***Visits to other facilities.*** The unique facilities at the NSLS (*e.g.*, the **Carnegie** synchrotron IR beamline U2A) provided a useful platform for interactions. There were 51 different users this year. The first SNAP workshop took place at **LANL** in April 2004. The second was held at the Spallation Neutron Source (SNS) in June 2005; many CDAC personnel attended.

- ***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 students, post-doctoral fellows, and staff were able to interact together. Moreover, they have provided the CDAC also facilitated workshops and activities throughout the high-pressure materials science community (*e.g.* SNAP COMPRES laser heating workshop, and CDAC Summer School).

- ***Jointly supported students and post-doctoral fellows.*** Center students and post-doctoral scientists are actively involved in all aspects of these interactions, and will be well prepared for careers in research related to stewardship science, including positions at NNSA/DP Labs. Though no formal studentships and post-doctoral positions jointly supported by CDAC and the Labs were created, CDAC facilitated research for Lab students and post-doctoral fellows (*e.g.* travel support). Further, a number of postdoctoral fellows at the various CDAC nodes have been working on CDAC-related projects.

- ***Sabbatical leaves for NNSA/DP scientists at CDAC.*** Opportunities have been created for NNSA/DP scientists to take sabbatical leaves at CDAC nodes. With its location in Washington, **Carnegie** provides a multi-disciplinary research environment close to DOE headquarters and other government agencies. Again, this program will be promoted further in the coming year; several potential possibilities have been discussed at the various CDAC meetings.

- ***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. This is bringing closer interaction between CDAC and SNL. 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.

The CDAC website, located at *http://www.cdac.gl.ciw.edu*, serves as a primary source of information to the CDAC community and the public (Fig. 36). 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 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 produced by CDAC.

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, CDAC now is a 20% 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 60% (LLNL H-Division, 20%, CDAC, 20%, UNLV, 20%), thereby significantly increasing its ability to steer future developments at the facility.

CDAC beam time is allocated based on the membership shares of each of the contributing members. At this point, ID-B and ID-D are 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** (35% of remaining time), CDAC (20%), **LLNL** H-Division (20%), **University of Nevada-Las Vegas** (20%), and **University of Hawaii** (5%). At this point, that means approximately 20 shifts per beamline in a typical run period (about 200 shifts). During Year 2, 20 proposals were submitted for beam time through CDAC (14 from National Lab scientists and 6 from Academic Partners). Each of these proposals was granted beam time from the CDAC allotment. A detail of those who obtained beam time at HPCAT and the experiments they performed is given in Appendix II.

To obtain beam time through CDAC, a General User Proposal is first submitted to the APS online system. These proposals are evaluated by an APS committee for scientific merit, and the APS makes recommendations about which proposals should be offered time under the GUP program. These recommendations are passed along to the appropriate beamline personnel who evaluate the proposals for technical feasibility at the specific beamline. After the GUP time is awarded, remaining proposals from CDAC partners and collaborators are gathered by the CDAC staff and every effort is made to offer time to each of these proposals. Despite the fact that there were more proposals allocated beam time by CDAC in Year Two than in Year One, it was just possible to accommodate all CDAC requests for beam time. 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 beam time.

With APS delivering beam ~200 days annually, the four beamlines of HPCAT will have a total of 800 days of beam time among which 100 days will be open to general users of the entire high-pressure research community, and 100 days will be for HPCAT maintenance and internal development, leaving 600 days distributed according to members' shares, represented by all interested groups of NNSA/DP Labs, Divisions, and Universities, to allocate the 120 days (30 days each from 16ID-B, 16ID-D, 16BM-B, and 16BM-D) of CDAC beam time among individuals of these groups. The goal has been to ensure that all reasonable proposals among the CDAC participants are awarded appropriate beam time. In fact, each of the NNSA Lab scientists who requested it received beam time during the past year.

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**, **Neil C. Holmes**, **Andy K. McMahan**, **John A. Moriarty**, **Choong-Shik Yoo**, and **David A. Young**. UC-Davis graduate student **Amy Lazicki** has 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**, **Jon Eggert**, **William Evans**, **Sam Weir**, and **Joe Zaug**. **Dan Farber and Reed Patterson** have both been particularly active at HPCAT during the past year, with two visits each, to work on projects closely tied to **LLNL** Stewardship Science programmatic goals. The following people have been working on collaborations within CDAC or have interacted closely with CDAC scientists: **Bruce Baer**, **Sorin Bastea**, **Jim Belak**, **Jen Blank**, **Larry Boercker**, **Stanimir Bonev**, **Brian Bonner**, **Ricky Chau**, **Jonathan Crowhurst**, **Hynchae Cynn**, **Larry Fried**, **Alexander Goncharov** (now at **Carnegie**), **Michael Howard**, **Valentin Iota-Herbei**, **Bernie Kozioziemski**, **Magnus Lipp**, **Riad Manaa**, **Andy McMahan**, **Jeff Nguyen, Florent Occelli**, **Tadashi Ogitsu**, **Jae-Hyun Park**, **Robert Rudd**, **Eric Schwegler**, **and Randy Simpson**. Under CDAC there have been exciting new collaborations with these other groups, divisions, and directorates at **LLNL**[176].

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, **Alan Hurd**, and scientists **Robert McQueeney**, **Robert von Dreele**, and **Yusheng Zhao** are interacting with CDAC. In addition to neutron scattering, **Yusheng Zhao**'s group has been instrumental in characterizing the new CVD diamond material developed at **Carnegie**. Other **LANL** collaborators and contacts include **William Anderson**, **Robert Heffner**, **Robert Hixson**, **Rachel Hixon, David Moore**, **David Schiferl**, **J. Smith**, and **Carlos Tomé**. **Brent Fultz** has collaborated for several years with scientists at the Lujan Center and MST, and **Dana Dlott** interacts regularly with **David Moore**'s spectroscopy group. Other **LANL** scientists involved in ongoing collaborations with CDAC include **Bob Sander**, **Becky Streetman**, **Dana Dattlebaum,** former CDAC postdoctoral associate **Duanwei He**, **Gary N. Chesnut**, **Aaron Koskelo**, **A. C. Lawson**, **Luc Daeman**, **Konstantin Lokshin**, **Christian Pantea**, **Jiang Qian**, **and Kimberly Tait**. New collaborations begun in Year 2 include those with **Zhongwu Wang, Didier Saumon**,

and **David Funk**. In addition, in Year 2 **Joanna Casson** and **Lilliana Sanchez** have joined other **LANL** high pressure personnel for diffraction experiments at HPCAT.

SNL – There have been new initiatives proposed between the **Carnegie** group and **George Samara**'s group on piezoelectrics. 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. Others investigating collaborative projects with CDAC personnel include **Lalit Chabildas, Mike Furnish, and Tracy Vogler**.

Other Labs – There are also collaborators at other facilities: *e.g.*, groups directed by **J. Robertson** (ORNL), **Christopher Tulk** (ONRL), **Gene Ice** (ORNL), **Ercan Alp** (APS), **Chi-chang Kao** (BNL), and **G. Larry Carr** (BNL). 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. **William B. Daniels** (formerly of Delaware) is a Visiting Investigator at **Carnegie**. **Sebastien Merkel** joined the Berkeley group as a Miller Fellow. **Luca Lutterotti** (Trento, Italy) and **Siegfried Matthies** (Dresden) are planning extended visits to Berkeley to further develop the Rietveld texture code for quantitative analysis and particularly refining it to study the elastic behavior of textured materials[224, 232, 233].

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 two years, the following former post-doctoral fellows have set up teaching programs as new assistant professors (or the equivalent):

Mark Frank (Northern Illinois University; from Carnegie)
Eugene Gregoryanz (University of Edinburgh; from Carnegie)
Boris Kieffer (New Mexico State; from Princeton)
Jie Li (University of Illinois; from Carnegie)
Yanzhang Ma (Texas Tech; from Carnegie)
Henry Scott (Indiana University South Bend; from Carnegie)
Anurag Sharma (Renssalear Polytechnic Institute; from Carnegie)
Sean Shieh (University of Western Ontario; from Princeton)
Yang Song (University of Western Ontario; from Carnegie)
Sarah Stewart-Mukhopadhyay (Harvard; from Carnegie)

Each of these young scientists is an active collaborator and is training new students. Their students are already active in CDAC, using CDAC facilities and contributing to meetings.

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. 37. CDAC directly supports the HPCAT facility and graduate students with 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.

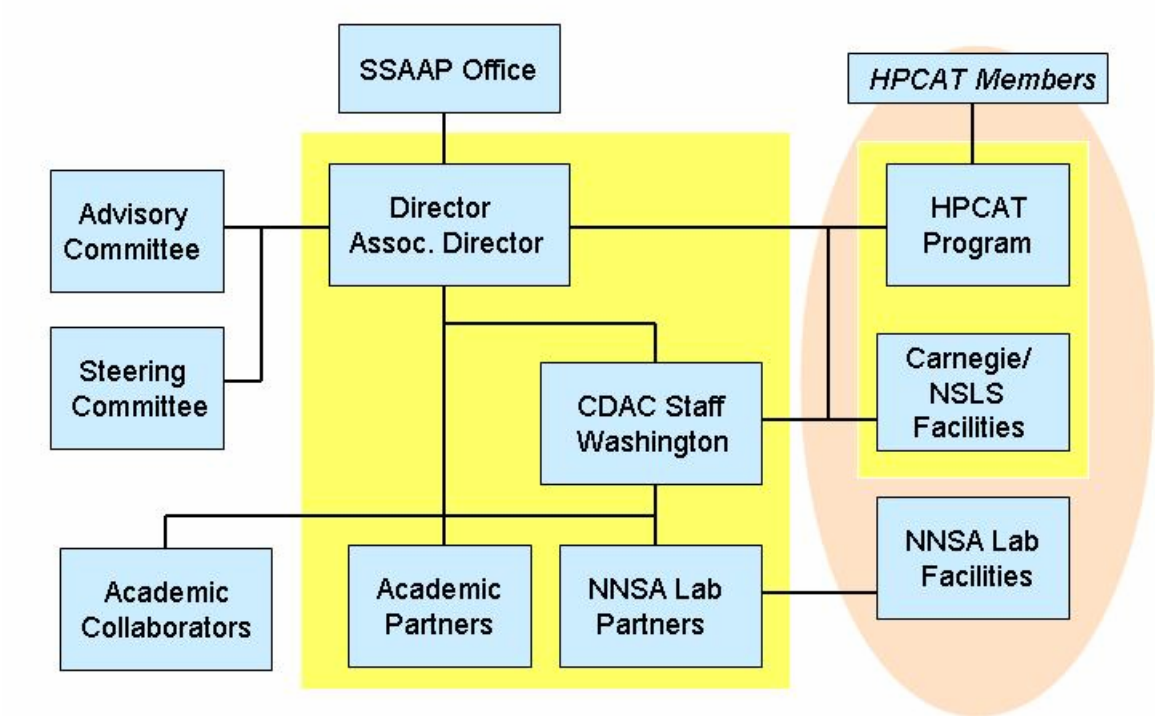


Figure 37. *CDAC organizational chart. The yellow area designates the principal components of CDAC. The oval area encompasses the three different groups of experimental facilities associated with CDAC.*

At **Carnegie** the CDAC staff 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
- **William Daniels** Senior Visiting Fellow
- **Premyslaw Dera** Crystallography
- **Yingwei Fei** Geochemistry and Petrology
- **Alexander Goncharov** Optical Spectroscopy
- **Dudley Herschbach** Senior Green Fellow
- **Burkhard Militzer** Computational Theory
- **Viktor Struzhkin** Electronic and Magnetic Properties

Alexander Goncharov led many CDAC projects as as staff member at **LLNL** and joined **Carnegie** in July 2005. He will continue the strong collaborations begun between CDAC and the CMS directorate in his new position at CDAC.

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
- **Stephen Gramsch** CDAC Coordinator/Research Scientist
- **Eugene Gregoryanz** Research Scientist
- **Jung-Fu Lin** Lab Manager/Research Scientist

- **Morgan Phillips** Administrative Assistant
- **Maddury Somayazulu** Research Scientist

As mentioned earlier, **Jung-Fu Lin** joined **LLNL** as a Lawrence Fellow in July 2005. Also, **Eugene Gregoryanz** took a position at the **Centre for Science at Extreme Conditions** at the **University of Edinburgh, Scottland** in September of 2005. **Olga Degtyareva** and **Maddury Somayazulu** joined CDAC as Research Scientists at **Carnegie** during the summer of 2005 and are responsible for serving CDAC visitors and training them 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 postdoctoral associates at **Carnegie** supported by the Institution, other grants, or outside fellowships worked on CDAC tasks during Year 2. Their contributions also include training CDAC students and visitors in high-pressure experimental techniques:

- **Muhetaer Aihaiti (Ahart)**
- **Jinyang Chen**
- **Olga Degtyareva**
- **Yang Ding**
- **Lars Ehm**
- **Michael Furlanetto**
- **Steve Jacobsen**
- **Tim Jenkins**
- **Yang Song**
- **Mario Santoro**

Notably**, Michael Furlanetto** joined the LANSCE division at **LANL** as a post-doctoral fellow in October 2004.

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. Eggert** (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 committee are invited to attend the monthly CDAC/HPCAT meeting and many interact frequently with the Director and Associate Director.

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 **Gouyin Shen** from **University of Chicago/GSECARS**. 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.

6.3 First Year Review

On May 7, 2004, the Year One 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 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)
- **Daniel Häusermann** (HPCAT Technical Overview)
- **Stephen Gramsch** (Education, Training and Outreach)
- **Choong-shik Yoo** (LLNL)
- **Yusheng Zhao** (LANL)
- **Marcus Knudson** (SNL)
- **Brent Fultz** (Caltech)
- **Dana Dlott** (Illinois)
- **Tom Duffy** (Princeton)
- **Dion Heinz** (Chicago)
- **Yogesh Vohra** (Alabama-Birmingham)
- **Hans-Rudolf Wenk** (UC-Berkeley)

Review Panel:

- **Kimberly Budil** (DOE/NNSA)
- **G. W. (Rip) Collins** (LLNL)

- **Alan Hurd** (LANL)
- **Chi-chang Kao** (BNL)
- **Marcus Knudson** (SNL)
- **Christian Mailhiot** (LLNL)

7. PLANS FOR YEAR THREE AND BEYOND

7.1 Year Three Work Statement

Technique Development – 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. Electron and phonon band structures and transport measurements will be developed at simultaneous high *P-T*. Pulsed laser heating experiments and time resolved measurements of IR reflectivity and electrical conductivity, as well as x-ray diffraction, will also be explored. 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. Developments launched in Year 2 will be completed including the new opportunities in combined static and dynamic compression.

Scientific Program – CDAC 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. 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. 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. 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. Real time SFG measurements will be obtained to reveal the chemistry of polymer binder energetic material interfaces. 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. 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. Expansion of full investigations to other key materials will be integrated with dynamic compression studies and theoretical models (*e.g.*, ASC).

Education and Training – Support for education and training of the proposed 14 graduate students will continue, and CDAC will provide either full or partial support for postdoctoral fellows working on CDAC-related projects. The summer school/workshop program will be continued. A workshop or retreat to plan for the educational program for CDAC beyond year three will be held, following reviews by the Advisory Committee.

7.2 CDAC Phase II

As discussed above, the Center can boast accomplishments that include personnel training and scientific advances, as well as construction, maintenance, and operation of user facilities for NNSA Lab scientists. Nevertheless, already in Year Three we see the need to enhance aspects of the program, many of which exceeded our expectations. These issues were discussed and endorsed by the CDAC Advisory Committee at its meeting on May 31, 2005. We need to take advantage of rare opportunities with an expanded program that includes an increase in the number of formal partners in the Center. The proposed enlargement of CDAC in Phase II will allow the Center to serve a unique role in providing support to university groups where high *P-T* materials science student training critical to the NNSA Lab missions is taking place.

Complementing the CDAC-Academic and CDAC-Lab groups, the CDAC-Collaborators group consists of a large number of institutions who do not receive formal student funding from CDAC but benefit mainly from the network of CDAC facilities through award of beam time, have received training within CDAC, and/or have taken part in CDAC events (*e.g.*, the Annual meeting). In some cases, travel funds for students have been made available to these groups. Examples include groups at the following universities: **University of Wyoming**, **Texas Tech University**, **University of Nevada-Reno**, **University of Hawai'i**, **Rennsalear Polytechnic Institute**, **University of California-Los Angeles**, **Indiana University-South Bend**, **Harvard University**, **New Mexico State University**, and **George Washington University**. As mentioned above, over 120 institutions throughout the world can be counted as CDAC-Collaborators. Many are led by excellent young faculty who are training very good students but have limited resources and need the benefit of joining CDAC as formal partners.

Current Needs – Despite these advances and accomplishments, we believe this is only the beginning: we can and will do much more. Before we can take CDAC to the next level, we need to address the following issues:

- **Support for the larger U.S. community that we have nurtured** – The CDAC-Academic group has had remarkable impact on the nation's high-pressure community. For example, in just the last 3 years, 14 students or post-doctoral fellows trained at **Carnegie** alone have become Assistant Professors and established thriving high-pressure research programs where they are training students. Many of them could benefit greatly from more formal participation in CDAC and in using CDAC/HPCAT facilities.
- **More beam time for CDAC at HPCAT** – Demand for beam time at HPCAT is ever increasing as this community has grown and the unique advantage of the facility to NNSA science becomes fully appreciated. The success is putting great pressure on the availability of beam time for NNSA/Lab scientists. We need to continue supporting our partners (both Academic and Lab), while at the same time conducting outreach to new users (*e.g.*, establishing new CDAC collaborators).
- **Improved support for users at HPCAT/CDAC** – Together with the growth of the users at HPCAT, there is a need to increase user support. However, there is a shortage of personnel. One beamline scientist needs to be on call for each experimental hutch (*i.e.*, one for each of the four), 24 hours a day to support users. These beamline scientists will be required to train new users. These needs extend to **Carnegie** as well: we have found it is often important to have a dedicated scientists train students, post-docs, and visitors who have little experience with particular techniques first at **Carnegie** and then move to HPCAT (or **NSLS**) for experiments.
- **Continued high *P-T* technique development** – The technology in the field is undergoing major advancement, with emerging high *P-T* static methods, confluence of static and dynamic techniques, the application of new laser methods, the development of new devices (*e.g.*, based on CVD diamond), and plans for time-resolved synchrotron/laser experiments. On

the other hand, CDAC does not have the required funds to even to start these projects; instead the Center's current budget is focused on direct student support and training.

- **Enhanced communication** – As we have developed over the last three years, we have found it necessary to improve our infrastructure to enhance communication. This includes enhancing training and advisor/student interactions at the beamlines, where it is now possible with modern instrumentation to interact in 'real time' during experiments. Such real time interactions are now done at European facilities very effectively, allowing multiple interested parties to help with experiments from their home institutions. Another important example is to improve communication across the many nodes of the Center, including interactions between facilities as well as between all of the Labs, partners, and collaborators. We also seek greater input on the regular basis from the Standing and Advisory Committees, but currently these groups cannot take part because of limited band pass of current connections. (Alternatively, we sometime borrow a system at **Carnegie** owned by NASA, but this is often not available and it serves only **Carnegie**). All of this improved communication is becoming more and more important with increases in travel costs.

The following would greatly extend the capabilities of CDAC as it moves from a three-year to a five year program:

- **Extension to a Five Year Cycle** – Our annual reviews by NNSA, as well as feedback from the general community, have strongly endorsed our program. Our Advisory Committee has enthusiastically recommended continuation of the program beyond the three year time frame originally envisaged. Both future planning within the Center and nurturing career considerations for CDAC-supported personnel require a long-term perspective within the program.
- **Increase in the number of partners** – One of the most striking consequences of CDAC was the creation of a large network of the CDAC collaborators – that is, beyond the six academic groups identified as the original partners. We now have over 120 collaborating institutions. With limited resources, we have successfully leveraged and drawn together a highly motivated community which has very successful student training programs in high *P-T* materials science and which would be of great benefit to the DOE/NNSA Labs. We have supported training and research in these groups by giving them access to the CDAC-managed beamlines, the **Carnegie** managed facilities, and attendance at CDAC/SSAAP activities. Establishing this broader infrastructure requires the funds and flexibility to select top groups which have expressed strong interest in formally joining CDAC in order to provide continuing student support. Due to the differences in costs of students at these universities (tuition, stipends, cost of living), this growth in the number of CDAC students would be accomplished with variable size contracts.
- **Enlarge the CDAC share at** HPCAT – Beam time at HPCAT is becoming extremely competitive with the growth in the field. With the increase in the number of partner would be accompanied by an enlargement of the CDAC share at HPCAT. The current program CDAC is a 20% member of HPCAT (10% from CDAC-Academic, 10% from National Labs). With an increase in CDAC partners by 50%, the CDAC membership in HPCAT would go to 30%. We would divide this equally between the National Lab and CDAC Academic groups; that is, 10% of additional beam time would be guaranteed to general CDAC and would be competed for by both groups. This could give CDAC NNSA/Lab scientists up to 50% more beam time. The 10% share would come from **Carnegie's** share, which would formally drop from 45% to 35% (the total beam time will increase significantly over the next two years, as we move from one fully commissioned hutch to four simultaneously operating hutches).
- **Additional CDAC support scientists** – The success of pioneering studies and student trainings at state-of-the-art facilities strongly depends upon on-site expert help and support. We will create a beamline scientist position at HPCAT for an expert in high-pressure x-ray

science and technology. This beamline scientist will be dedicated to CDAC research and will support both CDAC-Lab and CDAC-Academic groups on all beamlines, including training of new groups as well as supporting more experienced groups with particularly challenging experiments. The beamline scientist will also serve as a liaison to the NNSA Lab scientists and help them prepare for each HPCAT visit. To help with the training of new partners and growing number of collaborators, **Carnegie** will hire a second CDAC research scientist, who is an expert in overall high-pressure science and technology. In addition to help CDAC students, post-docs, and visitors at the **Carnegie** facility, this person will also travel to HPCAT, **NSLS**, and **LANSCE** as needed to help CDAC collaborators at these facilities.

- **Instrumentation development** – We have demonstrated that we can work quickly to bring new experimental techniques on line to be used at the Labs and at our facilities, but we do not the funds to carry this out. For example, despite the importance of the CVD diamond project to the shock-wave community, we were unable to grow crystals for tests in dynamic compression experiments during the past year because funds were not available (funding to get this started is pending through a separate SSAAP grant). We will establish a discretionary fund to seed new projects as they develop. Examples where this could be used are in doing feasibility studies table top laser shock experiments at **Carnegie**, time resolved and shock compression tests at HPCAT or NSLS, and testing new high *P-T* cells at LANSCE. These funds could be used for developing prototype equipment or supporting personnel short-term (*e.g.*, in NNSA Labs) for developing instrumentation and new experiments.
- **Infrastructure at Carnegie facilities** – With so many parts to CDAC, a fast broadband video conference is simply essential within the Center. We will increase communication with the acquisition of state-of-the art video networking capabilities (*e.g.*, the Argonne-based Access Grid). The facility will be used to enhance student training at facilities (*e.g.*, the facility can be configured to allow remote access to experiments, so advisors can help students at those facilities from their home institutions). This facility will be used for all monthly CDAC/HPCAT meetings, allowing Partners, Steering and Advisory Committee Members, and other interested parties (including NNSA people) to take part in meetings without the inconvenience and expense of travel. The facility can also be used by the administrators at the various institutions to improve the efficiency (*e.g.*, with subcontracts, payments, and invoices). Finally, there is increased use of the **Carnegie**-managed synchrotron infrared beamline U2A at the NSLS, a facility that complements HPCAT and the other beamlines at the APS (which has no infrared spectroscopy). Modest funds are required to fully support U2A, which is principally funded by the NSF.

APPENDIX I: CDAC Publications and Presentations for Year Two *

A. CDAC Publications

Ahart, M., A. Asthagiri, R. E. Cohen, J. L. Yarger, H. K. Mao and R. J. Hemley, Brillouin spectroscopy of relaxor ferroelectrics and metal hydrides, *J. Mat. Sci. and Engineering A*, submitted.

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

A. HPCAT (APS)

A large part of the first year budget was dedicated to the completion of construction and commissioning of the HPCAT facility. In addition to the 20% membership obtained by CDAC in HPCAT, the support generated by SSAAP funding made possible significant scientific productivity of this state-of-the-art high-pressure facility. Asterisks denote work done with beam time available through CDAC.

User Name	Affiliations	Project	Dates
B. Grocholski V. Lee R. Yu R. Williams	UC Berkeley	Partitioning of radioactive elements into planetary cores	August 4-6, 2004
H.K. Mao Wendy Mao D. Heinz	Carnegie Chicago	Olivine and perovskite-laser heating at high pressures	August 6-7, 2004
Olga Degtyareva M. Sakharov	Carnegie	High-pressure study of the Cu_5Zn_8 structure	August 8-10, 2004
P. Dera	Carnegie	Single crystal microdiffraction on BM-B	August 8-11, 2004
R. Wenk G. Shen	UC Berkeley GSECARS, APS	Laser heating and radial diffraction, ** commissioning	August 11-13, 2004
Y. Song	Carnegie	High-pressure diffraction study of sodium azide	August 14-16, 2004
N. Velisavljevic G. Amulele J. Zhu M. Maghnani	Alabama Birmingham Hawaii	High-pressure diffraction study of ceramics (WC, B4C, SiC)	August 16-19, 2004
J. Lin A. Young	Carnegie	High-pressure diffraction study w/LH of silicate perosvkite	August 19-20, 2004
XRN School 10 Students	Various Schools	High-pressure powder diffraction study of gold powder	August 20-21, 2004
L. Ehm P. Dera	Carnegie	High-pressure diffraction study of Nepheline and Pseudobrookite	August 21-23, 2004
R. Patterson	LLNL	High-pressure diffraction study of heavy metals	August 23-24, 2004
Y. Fei A. Corgne L. Zhang M. Frank K. Wheeler	Carnegie NIU Columbia	Ht/High-pressure diffraction study of magnesiowüstite	August 24-26, 2004
Yue Meng	Carnegie	Instrumentation development/HP/LH	October 8-December 20, 2004
Y. Ding H. Liu	Carnegie	Zone-axis high-pressure diffraction study of graphite	October 10-12, 2004
B. Maddox V. Iota	LLNL	High-pressure XES study of gadolinium	October 13-16, 2004
H. K. Mao Wendy Mao G. Zou	Carnegie Chicago Jilin U.	Ht/high-pressure diffraction study of olivine	October 16-23, 2004
Y. Feng	Chicago	EDXD of crystalline Cr	October 16-23, 2004

E. Gregoryanz	Carnegie	High-pressure diffraction of nitrides	October 20-22, 2004
M. Pravica C. Parado E. Romano Z. Quine Kristina Lipinska-Kalita	UNLV	High-pressure diffraction of erbium	October 22-25, 2004
R. Kumar A. Cornelius H. Giefers	UNLV	High-pressure diffraction study of Yb, titanate & niobate	October 22-25, 2004
P. Dera	Carnegie	SXD of muscovite	October 22-25, 2004
P. Dera B. Downs	Carnegie Arizona	Single crystal XRD	October 23-25, 2004
J. Lin S. Jacobsen	Carnegie	High-pressure diffraction spectroscopy study of magnesiowüsite and silicate perovskite	October 23-29, 2004
O. Tschauner	UNLV	High-pressure diffraction study of silicate & oxides	October 24-25, 2004
V. Struzkin	Carnegie	XES of perovskite	October 28-November 1, 2004
R. Patterson C. Aracne	LLNL	Ht/High-pressure diffraction study of heavy metals Th, U, Pr, Nd and/or Tm	October 27-29, 2004
N. Cunningham K. Hope	U.Alabama, Birmingham	Ht/High-pressure diffraction study of praseodymium and Gadolinium	October 29-30, 2004
H. K. Mao Wendy Mao	Carnegie Chicago	Ht/High-pressure diffraction study of orthpyoxers	October 30-31, 2004
E. Gregoryanz Olga Degtyareva	Carnegie	Ht/High-pressure diffraction study of NA	October 30-31, 2004
P. Dera	Carnegie	SXD White Beam	October 30-31, 2004
L. Ming J. Balogh	Hawaii	High-pressure diffraction study of BC & BC3	November 3-6, 2004
R. Kumar	UNLV	RIXS studies on Yb compounds	November 4, 2004
H. K. Mao Wendy Mao	Carnegie Chicago	Ht/High-pressure diffraction study of olivine	November 6-8, 2004
L. Ehm S. Speziele	Carnegie UC Berkeley	XRD commissioning at BM	November 8-11, 2004
Amy Lazicki	LLNL	RIXS study of gadolinium	November 9-15, 2004
R. Wenk Jenny Pehl	UC Berkeley	High-pressure diffraction study	November 8-12, 2004
B. Maddox	LLNL	RIXS commissioning study on ID-D	November 9-15, 2004
D. Farber Chantel Aracne	LLNL	High-pressure diffraction study of Pu	November 12-13, 2004
Dana Dattelbaum Kimberly Tait D. Williams	LANL	High-pressure diffraction study of perovskite	November 13-16, 2004
Kimberly Tait	LANL	High-pressure diffraction study of perovskite/clathrate	November 13-16, 2004
Y. Feng	Chicago	EDXD atudy of Cr on BM-B (Commissiong)	November 17-22, 2004
B. Manoun N. Phatak	Florida International	High-pressure diffraction study of carbide and nitride	November 17-21, 2004

M. Pravica H. Giefers	UNLV	XRS commissioning study of PETN on ID-D	November 21-25, 2004
H. K. Mao Wendy Mao	Carnegie Chicago	Ht/High-pressure diffraction study of orthpyoxeres	November 21-22,2004
W. Pravica	Wright College	XRS commisoning study of N containing Cpds	November 22, 2004
E. Gregoryanz	Carnegie	XRS commissioning study of N_2	November 26-29, 2004
S. Merkel	UC Berkeley	High-pressure diffraction study of iron powder	November 27-29, 2004
H. Cynn B. Baer W. Evans C. Yoo M. Lipp	LLNL	Ht/High-pressure diffraction study of Pu239	November 27-30, 2004
H. K. Mao Wendy Mao	Carnegie Chicago	Ht/High-pressure diffraction study of orthpyoxeres	December 3-5, 2004
E. Gregoryanz Olga Degtyareva	Carnegie	Ht/High-pressure diffraction study of Na	December 3-5, 2004
M. Manghnani S. Mariappan X. Honej G. Amulele	Hawaii	Ht/High-pressure diffraction study of B4C, Wc SiC	December 5-16, 2004
E. Rapacki	US Army	DOD-TARDEC-UH ID-D commissioning	December 7-8, 2004
E. Gregoryanz Olga Degtyareva	Carnegie	High-pressure diffraction study of binary alloys fromCu-Zn, In-Bi, Pb-Bi	December 10-11, 2004
A. Goncharov	LLNL	Ht/High-pressure diffraction study of water	December 14-16, 2004
R. Kumar H. Giefers	UNLV	High-pressure diffraction study of titanate and heavy fermion compounds	December 18-21, 2004
M. Somayazulu D. Hausermann	Carnegie	XRD and commissioning	January 31,2005
H.K. Mao Yue Meng J. Liu Y. Li W. Mao G. Shen	Carnegie University of Chicago	Laser heating XRD study of (Fe-Mg)SiO_3 and (Fe, Mg)O	February 3-8,2005
O.Tschauner	UNLV	Powder diffraction study of silica, copper and fullerene C_60	February 4-5,2005
Y. Ding P. Chow	Carnegie	Al plasmon under pressure	February 4-10, 2005
Olga Degtyareva R. Caracas E. Gregoryanz	Carnegie	HP/ HP diffraction studies on sodium crystal structures	February 10-12, 2005
M. Pravica W. Pravica	UNLV Wilbur Wright College	X-ray Raman spectroscopy of RDX and HMX	February 11-13, 2005
H.K. Mao Y. Ding	Carnegie	HP O_2 K-edge spectroscopy by inelastic XR scattering	February 16-18, 2005
Y. Song	Carnegie	HP/XRD measurement of silane and germane	February 17-18,2005
M. Pravica W. Pravica Kristina Lipinska-Kalita H. Giefers	UNLV	X-ray powder diffraction study of PETN, elemental Erbium, GaO, FeSnx alloys, $AgAbTe_2$, $LaSrFeO_3$ And PrN.	February 18-21,2005

A. Lazicki B. Maddox	LLNL	X-ray Raman scattering on N-edge of Li_3N	February 20-24, 2005
H.K. Mao W. Mao	Carnegie University of Chicago	XRD study of Fe-Mg partitioning between silicates and oxides at lower mantle *P-T* conditions	February 22-25,2005
E. Gregoryanz	Carnegie	HP/ Inelastic x-ray scattering in Nitrogen	February 24-27, 2005
B. Baer M. Lipp H. Cynn W. Evans	LLNL	XRD/scattering techniques at high *P-T* of Be, and O_2	February 25-28,2005
Olga Degtyareva R. Caracas E. Gregoryanz	Carnegie	HP/ HP diffraction studies on sodium crystal structures	March 3-4, 2005
Y. Fei A. Corgne L. Zhang	Carnegie	*P-V-T* EOS of magnesiowüsite up to core-mantle boundry pressure	March 5-6,2005
J.F. Lin M. Somayazulu	Carnegie	X-ray diffraction of H_2O in an externally heated cell	March 4-8, 2005
M. Pravica M. Nicol H. Giefers W. Pravica O. Tschauner Kristina Lipinska-Kalita	UNLV	X-ray powder diffraction studies of PETN, elemental erbium, GaO and FeSnx alloys	March 9-13, 2005
Wendy Mao	University of Chicago	High-pressure/temperature studies of (Fe, Mg)SiO3 during nuclear resonant inelastic ex-ray scattering	March 10-14, 2005
A. Cornelius R. Kumar M. Jacobson	UNLV	High-pressure studies of UCu2Si2 and CeCu2Si2 and Manganites	March 11-13, 2005
Olga Degtyareva R. Caracas E. Gregoryanz	Carnegie	High-pressure/temperature diffraction studies on crystal structure and melting behavior of sodium using the ruby system.	March 17-18, 2005
J.F. Lin V. Struzhkin	Carnegie	High-pressure x-ray diffraction on H_20	March 22-24, 2005
Tanja Cuk H. K. Mao M. Somayazulu X. Chen V. Struzhkin	Stanford Carnegie	Powder x-ray diffraction on Bi_2Sr_2Ca	March 22-25, 2005
A. Gavriliuk V. Struzhkin	Russian Acad. Of Science Carnegie	In-situ x-ray diffraction study of $Y_3Fe_5O_{12}$, $FeBO_3$ and $GdFe_3(BO_3)_4$ at high and low pressure	March 22-24, 2005
G. Chesnut Dana Dattelbaum	LANL	High-pressure x-ray diffraction of metals and polymers	March 24-26, 2005
A. Papandrew A. Yue I. Halevy	California Institute of Technology	High pressure and low temperature study of nuclear Forward scatteringon Fe-Ni alloys	March 25-29, 2005
A. Goncharov	LLNL	*In-situ* x-ray diffraction of water at elevated pressures and temperatures	March 26-28,2005
O. Tschauner	UNLV	Nuclear resonant foraward scattering on 57Fe containing silicate	March 29, 2005

R. Kumar A. Cornelius C. Gobin	UNLV	High pressure NRIXS studies on La_1, $3Sr_2$, $3FeO_3$	March 29-30, 2005
Olga Degtyareva	Carnegie	High-pressure/*T* diffraction studies on sodium crystal structures	March 29-April 1, 2005
L.C. Ming P. Zinin X. Liu M. Manghnani	University of Hawaii	High-pressure/temperature and XRD study of BC and BC_3	April 6-9, 2005
J.F. Lin V. Struzhkin	Carnegie	X-ray emission spectroscopy of magnesiowüstite at high pressure	April 6-8, 2005
V. Struzhkin A. Gavriliuk	Carnegie Russian Academy of Science	XES of $BiFeO_3$ and $GdFe_3(BO_3)_4$ under pressure	April 8-10, 2005
M. Manghnani X. Hong G. Amulele L.C. Ming	University of Hawaii	EOS by XRS of *in-situ* laser heating and stoichiometry in B_4C	April 9-11, 2005
Wendy Mao	University of Chicago	XES of (Fe, Mg) SiO_3 at high pressure	April 10-15, 2005
E. Goncharov	Carnegie	High-pressure/temperature diffraction studies on sodium crystal structures	April 12-13, 2005
L. Ehm	Carnegie	High-pressure/temperature investigations on dolomite, calcite and aragonite	April 13-14, 2005
H. Cynn	LLNL	High-pressure/temperature study of f-metal behavior in He-gas controlled membrane DAC	April 15-20, 2005
V. Iota-Herbei B. Maddox	LLNL	XES study of gadolinium foil, europium foil and europium nitride	April 16-20, 2005
M. Hu	Carnegie	XES commisioning	June 1, 2005
H.K. Mao G. Shen J. Shu	Carnegie	Fe-Mg portioning between silicates and oxides at lower mantle *P*/*T* conditions	June 7, 2005
O. Tschauner J. McClure C.S. Zha	UNLV Carnegie	Determination of *PVT*-EOS using an internal resistive heating technique	June 7-9, 2005
C.S. Zha	Carnegie	*PVT*, EOS of MgO, Au, Pt, NaCl	June 8-9, 2005
V. Iota-Herbei	LLNL	XES OF neodymium and praseodymium under high pressure	June 9-10, 2005
M. Pravica A. Kinsey Kristina Lipinska-Kalita Z. Quine E.D. Romano H. Giefers J. McClure E. Sokol C. Gobin	UNLV	X-ray powder diffraction study of Sn/Fe alloys, elemental erbium, GaO, and metal hydrides	June 9-13, 2005
T. Tyson	New Jersey Institute of Technology	Exploration of a pressure induced high spin to low spin transition in manganites	June 14-15, 2005
R. Kumar A. Cornelius M. Jacobson	UNLV	XES experiments on $YbAl_3$ and Yb organic complexes at high pressure	June 17-19, 2005

B. Edwards P. Martin K. Brister	Wayne State University University of Chicago	Protein structures under elevated pressures	June 18-20, 2005
G. Chesnut K. Zhuravlev R. Schaller R. Sander J. Pietryga	LANL	High pressure x-ray diffraction of tetrafluoroethylene, cerium, copper, tungsten, titanium and zirconium.	June 23-25, 2005
Wendy Mao	University of Chicago	XES of (Fe, Mg) SiO_3 at high pressure	June 26-28, 2005
H. Sheng W. Luo H. Liu	John Hopkins University Carnegie	Study of the atomic size effect on metallic glass formation using high pressure	June 29-July 2, 2005
C. Runge A. Kubo	Princeton	XRD of Cr_2O_3 at high pressure and high temperature	July 7-9, 2005
W. Evans V. Iota-Herbei J.F. Lin A. Lazicki M. Hu P. Chow	LLNL	High-pressure x-ray Raman spectroscopy of H_20, CO_2 and LI_2O	July 7-11, 2005
V. Struzkin	Carnegie	Nuclear inelastic scattering in pure iron, iron alloys and oxides	July 13-16, 2005
R. Kumar A. Cornelius	UNLV	Nuclear forward scattering experiments on FeSi and $FeSi_2$ at high pressure	July 16-17, 2005
Olga Degtyareva Cathy Tarabella	Carnegie	Melting curve and crystal structures of sodium	July 15-18, 2005
C.S. Yoo H. Cynn M. Lipp W. Evans B. Baer	LLNL	F-metal behavior at high pressure and high temperature using He-gas controlled membrane DAC	July 20-25, 2005
X. Chen Olga Degtyareva V. Struzkin H.K. Mao	Carnegie	High pressure structural study of Silane and Germane	July 25-28, 2005

B. U2A Infrared Beamline (NSLS)

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

User Name	**Affiliations**	**Project**	**Dates**
H. Liu	HPCAT	Study of stability of hydrous minerals and perovskites under high pressure by infrared and Raman spectroscopy (Proposal #: 5011)	August 3-7, 2004
C. Yan	Carnegie	Mid- and far-infrared studies of CVD diamonds (Proposal #: U9158)	August 11-14, 2004 August 26-28, 2004

D. Klug J. Tse	National Research Council of Canada	Far- and mid-infrared studies of symmetric hydrogen bond formation in clathrate hydrates (Proposal #: 5284)	August 16-18, 2004
J. Zhang	University of California – Riverside	IR spectroscopy of faulted eclogite samples	August 19-20, 2004
P. Cervantes	Colorado College	High-pressure infrared absorption of natural and synthetic FeS_2 powder (Proposal #: 5281)	Sepember 1-5, 2004 October 6-9, 2004
Gianluca Iezzi* G. D. Ventura*	Dip. Scienze della Terra, Univ. CHIETI, Italy Dip. Scienze Geologiche, Univ. ROMA, Italy	Towards a model for high-pressure phase transition from $P2_1/m$ to C2/m synthetic amphiboles by IR spectroscopy (Proposal #: 5386)	Sepember 9-11, 2004
W. Liu	SUNY	Elasticity and EoS of hydrous $(MgFe)_2SiO_4$ at the mantle conditions	Sepember 20, 2004
H. Long	SUNY	Investigation on cell assemblies for mantle rheology (Proposal #: 1132)	Sepember 23, 2004
K. Syassen	Max-Planck-Institute, Stuttgart, Germany	Infrared reflectivity/transmission spectroscopy of SnO under high pressure	Sepember 24-2, 2004
Z. Liu H. K. Mao	Carnegie	FTIR studies of post perovskite	Sepember 28-October 3, 2004
Y. Wang	Guangzhou Institute of Geochemistry, Chinese Academy of Sciences	Micro-scaled compositional changes of marine shale, carbonate and coal during the hydrolysis process	October 12-18, 2004
Y. Song	Carnegie	High-pressure FTIR measurements of solid hydrogen (Proposal #: 3616)	October 21-22, 2004
T. Tyson	New Jersey Institute of Technology	High-pressure Raman scattering measurements on manganites	October 25-31, 2004
Z. Liu	Carnegie	Far-IR FTIR studies of H_2O up to 80 GPa	November 3-24, 2004
Y. Lee T. Vogt	Brookhaven	High-pressure IR/Raman experiment on gas-sorption in zeolites (Proposal #: 1132)	January 10, 2005 February 10-17, 2005
S. Jacobsen S. Demouchy	Geophysical Lab University of Minnesota	A synchrotron-IR study of OH in silicate perovskite (Proposal #: 3853)	January 12-15, 2005
S. Shieh H. W. Huang T. Y. Kuo	Princeton University National Cheng Kung University, China	The spectroscopic study of hydrous phases at high pressure	January 18-22, 2005
Y. Song	Carnegie	High-pressure FTIR measurements of solid hydrogen (Proposal #: 3616)	January 27-31, 2005 May 2-7, 2005 June 11-12, 2005

Gianluca Iezzi	Dip. Scienze della Terra, Univ. CHIETI, Italy	Synchrotron FTIR spectroscopy of synthetic amphiboles at high pressure	February 1-5, 2005 February 9, 2005
Z. Liu	Carnegie	Far-IR spectroscopy of ice at high pressure	February 25-28, 2005
G. Lager J. Chen	University of Louisville	High-pressure infrared studies of hydrogarnet and OH-topaz	February 29-March 6, 2005
B. Chen	University of California – Berkeley	High-pressure XRD and IR study of polytypically disordered nano-ZnS	March 9-12, 2005 July 29-August 4, 2005
Z. Liu	Carnegie	High-pressure far-IR spectroscopy of D_2O	March 14-21, 2005
Z. Liu	Carnegie	Synchrotron far-IR spectroscopy of KBr and CsI up to 70 GPa	March 24-30, 2005
N. Hyatt J. Hriljac M. Colligan	University of Sheffield, UK University of Birmingham, UK	High-pressure Raman and infrared studies of layered perovkites	March 31-April 9, 2005
T. Zhou	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	April 18-20, 2005
S. Jacobsen	Carnegie	A synchrotron-IR study of OH in silicate perovskite (Proposal #: 3853)	April 21-23, 2005
J. Chen	University of Louisville	High-pressure infrared studies of hydrogarnet and OH-topaz	April 25-28, 2005
T. Tyson P. Gao	New Jersey Institute of Technology	High-pressure Raman scattering measurements on manganites	June 2-3, 2005
A. Khanna	University of Arkansas	High-T/P investigations in lead and bismuth borate glasses by infrared spectroscopic techniques (Proposal #: 4333)	June 6-10, 2005
Z. Liu	Carnegie	Test new HDAC	June 13-15, 2005
S. Jacobsen Elizabeth Littlefield	Carnegie Colby College	A synchrotron-IR study of OH in silicate perovskite and wadselyite (Proposal #: 3853)	June 20-22, 2005
H. Scott A. Ratkiewicz	Indiana University – South Bend	Hydrocarbon production by the reduction of calcite at high P/T (Proposal #: 1725)	July 10-15, 2005
L. Wang T. Kennell	SUNY	Water in nominally anhydrous mantle minerals (Proposal #: 1912)	July 18, 2005
G. Lager	University of Louisville	High-pressure infrared studies of hydrogarnet and OH-topaz	July 19-20, 2005 August 10-13, 2005
M. Vaughan L. Wang	SUNY	IR studies of MgO	July 21, 2005
Z. Liu	Carnegie	Assembly the custom IR/Raman microscope	July 22-25, 2005
P. Allen M. Kwang L. Wang T. Sun	SUNY	FTIR studies of MgFeO	July 28, 2005
J. Bass J. Wang	University of Illinois – Urbana-Champion	Quantitative analysis of hydrogen content of high-pressure phases and its effect on elastic properties	August 15-22, 2005

		(Proposal # 4230)	
T. Zhou	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	August 25-27, 2005

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).

User Name	Affiliations	Project	Dates
J.Hu	Brookhaven	Set up Laue experiment for single crystal study	August 4-9, 2004
H. Liu	HPCAT	Ag_2O_2, As_2O_5 at high-pressure	August 5-8, 2004
J.Hu	Brookhaven	Test with quartz crystal	August 12-16, 2004
J. Shu	Carnegie	Chromite in He	August 16-22, 2004 August 25-29, 2004
J.Hu	Brookhaven	Re-set up microscope for Laue experiment	August 29-September 5, 2004
S. Sheih	Princeton	NaCl, MgO, Au	September 12-16, 2004
P. Dera	Carnegie	Test SCD program	September 21-23, 2004 September 29-October 1, 2004
J. Shu	Carnegie	Chromite phase transition	September 23-27, 2004
J.Hu	Brookhaven	Test SCD program	October 1-4, 2004
D. Shim S. Rekhi J. Santihan S. Luadra	Massachusetts Institute of Technology	Crystal structure and crystal chemistry of perovskite-structured materials at high pressure	October 7-11, 2004
I. Halevy	Nuclear Res. Center Negev(Israel)	Hf-Ir compressibility	October 12-17, 2004
J. Hu	Brookhaven	Align mirrors	October 16-17, 2004

N. Velisavljevic W. Qiu P. Baker N. Cunningham	University Alabama – Birmingham	Structural and magnetic studies on rare earth metals at megabar pressures using designer DACs	October 19-23, 2004
Y. Ma E. Selvi	Texas Tech University	High-pressure study of tetragonal boron B-192	October 27-November 1, 2004
Tatinan Prozorov	University of South Carolina	Catalyzed alanates at high-pressure	October 29-31, 2004
H. Rong	Chinese Academy of Geological Sciences	Study of microinclusions in diamond from chromite of peridotite, Tibet, China	November 4-12, 2004
J. Xu	Carnegie	Structure of single-crystal wüstite (FeO) under high-pressure & low-temperature	November 12-22, 2004
S. Shieh	Princeton University	Strength and elasticity of hydrous phases at high pressures	January 17-21, 2005
J. Xu Y. Li X. Liu J. Hu	Carnegie Brookhaven	Megabar Nb and Pd	January 25-31, 2005
F. Jiang Zhu Mao Claire Runge A. Kubo T. Duffy	Princeton University	New application of radial x-ray diffraction technique at high-pressure	February 2-7, 2005
J. Provis	The University of Melbourne	Reaction kinetics of geopolymerisation	February 7-11, 2005
J. Hu	Brookhaven	Alignment	February 11-14, 2005
Q. Guo	Beamline	alignment of x-ray system	2/23-2/24/2005
J. Hu	Brookhaven	Alignment	February 23-24, 2005
W. Qiu P. Baker N. Velisavljevic	University Alabama – Birmingham	Structural and magnetic studies on rare earth metals at megabar pressures using designer diamond anvils	February 25-28, 2005
C. Martin	SUNY – Stony Brook	Phase transition of $NaMgF_3$	February 25-28, 2005
J. Chen G. Lager	University of Louisville	Affect of X- and Z-site substitutions on the high-pressure behavior of hydrogarnet	March 2-5, 2005
Q. Guo	Brookhaven	4-laue mono system alignment	March 5-7, 2005
J. Hu	Brookhaven	align mono-beam to 23keV	March 10-15, 2005
Y. Ma R. Lu R. Aksoy E. Selvi	Texas Tech University	High-pressure Study of tetragonal Boron B-192	March 15-20, 2005

J. Patterson C. Aracne J. Akella H. Cynn	LLNL	Phase diagrams, thermal EOS and structural changes of f-electron metals with designer diamond anvils and double sided laser heating	March 22-25, 2005
J. Hu	Carnegie	Nano $BaTiO_3$	March 30-April 4, 2005
Z. Liu	Carnegie	KBr	April 3-4, 2005
D. Shim J. Santillan S. Lundin S. Rekhi	Massachusetts Institute of Technology	Crystal structure and crystal chemistry of perovskite-structured materials at high pressures	April 7-11, 2005
F. Li J. Hu	Institute of Physics, Chinese Academy of Sciences	Nano-material	April 11-17, 2005
Z. Liu	Carnegie	H_2O+CH_4	April 19-20, 2005
J. Hu	Brookhaven	Align to EDXD	April 20-22, 2005
J. Shu	Carnegie	Single crystal chromite	April 22-25, 2005
J. F. Lin J. Shu	Carnegie	Elasticity and texture of magnesiowüstite in the Earth's lower mantle	April 27-May 2, 2005
C. Martin	SUNY – Stony Brook	Phase transition of $NaMgF_3$	April 29 – May 1, 2005
Q. Guo	Brookhaven	4-Laue monochromater setup	May 1-7, 2005
J. Xu, J. Hu	Carnegie	Single crystal structural determination at high pressure using synchrotron white x-ray beam	May 3-7, 2005
Q. Guo	Brookhaven	Single crystal Si wafer	June 12-13, 2004
J. Shu	Carnegie	Single crystal CH_4-III	June 15-18, 2005
N. Velisavljevic N. Cunningham W. Qui	University Alabama – Birmingham	Crystal structure and compressibility of transition metal nanoparticles under high pressures and high temperatures	June 21-26, 2005
Q. Guo	Brookhaven	Single crystal Si wafer	July 19-22, 2005
F. Chen Zhu Mao A. Kubo	Princeton University	New application of radial x-ray diffraction technique at high pressure	July 19-24, 2005
T. Tiberiv B. Chen F. El-Ghussein	University of Missouri UC – Berkeley	High pressure properties of nano TiO_2	July 26-29, 2005
J. Hu	Brookhaven	Align mono-beam 30.49 keV	August 3-8, 2005
B. Li W. Liu	SUNY – Stony Brook	Mantle silicates at high-pressure/temperature	August 6-10, 2005
Y. Ma R. Aksoy E. Selvi	Texas Tech University	Diamond powder, MoS, WS	August 11-21, 2005
D. Shim J. Santillan S. Lundin S. Rekhi	Massachusetts Institute of Technology	Crystal structure and crystal chemistry of perovskite-structured materials at high-pressure	August 25-29, 2005

References

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