

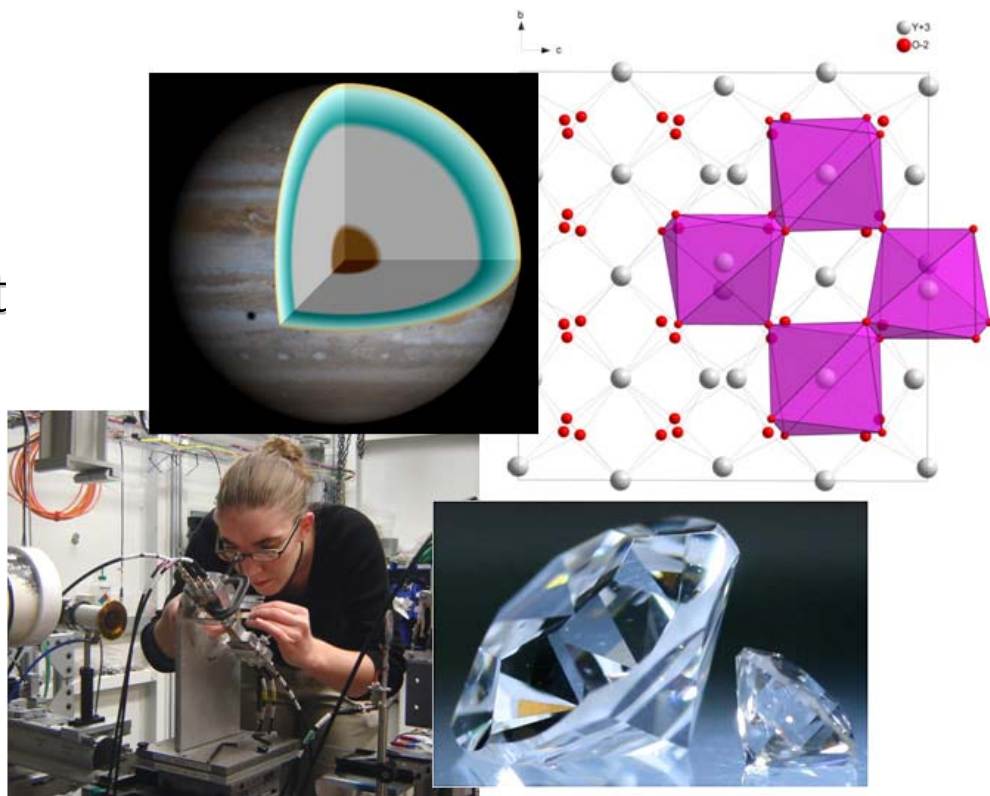


CDAC

CARNEGIE/DOE ALLIANCE CENTER

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

**Annual Report
2009-2010**



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

2009-2010 ANNUAL REPORT

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On the Cover

Clockwise from top left: 1) Investigations into the deep interiors of the gas giant planets such as Jupiter will be possible with dynamic compression experiments on methane, hydrogen and deuterium to be carried out at the National Ignition Facility. The experiments, which are now in the planning stages, will also be important in the coordination of dynamic and static compression measurements, a key CDAC goal. 2) The familiar bixbyite structure of Y_2O_3 undergoes varying compression behavior depending on the particle size. Nanoscale diffraction experiments at the Advanced Photon Source were made possible by technical advances at the HPCAT sector. 3) Improvements in diamond growth by chemical vapor deposition (CVD) are opening up new experimental capabilities in both static and dynamic compression. CVD diamond grown at Carnegie is both stronger and tougher than natural diamond. 4) Graduate student education is a central feature of the CDAC program, and support is provided for students such as Lisa Mauger, from the group of Academic Partner Brent Fultz at Caltech, to carry out forefront research at the APS and other state-of-the-art national user facilities toward their dissertation research. Lisa is studying the anharmonic behavior of phonons in bcc iron at high temperature.

1. OVERVIEW

The last two decades have been witness to a remarkable success in maintaining a safe, secure, and reliable nuclear deterrent based on scientific understanding rather than explosive nuclear testing. Central to this program of stockpile stewardship is the continued need to advance fundamental knowledge of the behavior of materials in a broad range of environments. The study of materials under extreme conditions of pressure and temperature is a key component of that enterprise. Indeed, research on materials in extreme environments driven by national security needs is leading to new discoveries that are opening up altogether new vistas on fundamental physics, chemistry, and materials science.

Throughout its history, the Carnegie Institution has promoted and supported fundamental science important for both the “betterment of mankind”¹ and for the security of our nation.²⁻³ The Carnegie-DOE Alliance Center (CDAC) was founded in 2003 as part of that tradition under the Stewardship Science Academic Alliances (SSAA) program of DOE/NNSA to bring together academic and National Laboratory groups to meet the need for an increased understanding of materials under extreme conditions, and to train the next generation of scientists in this area of research. Through a coordinated program of high *P-T* materials science research, education and training, and technique development (Fig 1.), CDAC supports critical underpinnings of stockpile stewardship. In our seventh year, we continued to make important advances in each of these areas of our program even as we

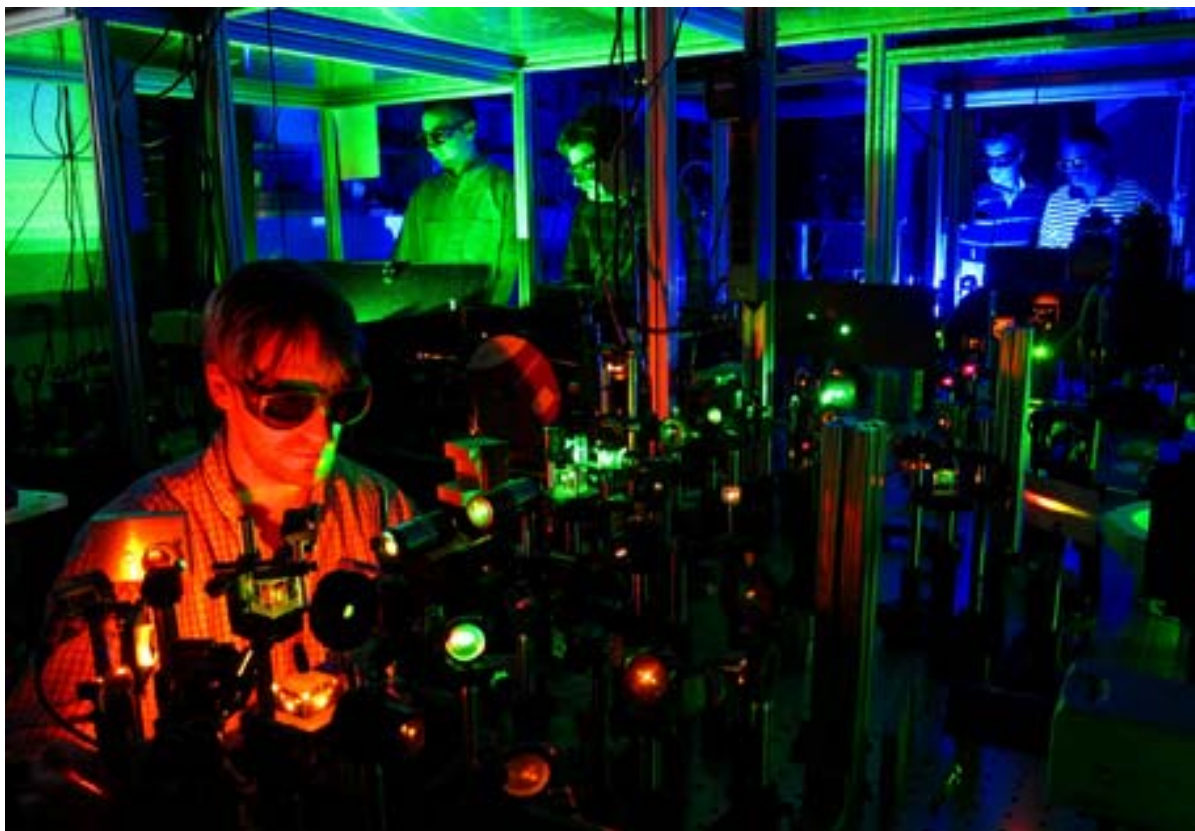


Figure 1. Exploring new applications of table-top laser systems is an important goal of CDAC. **Carnegie** research scientist **Timothy Strobel** (foreground) uses a pulsed laser system in one of the spectroscopy facilities supported by CDAC at the Geophysical Laboratory. Three pulsed laser sources are on the table before him: a pulsed green laser for Raman spectroscopy, a pulsed infrared (invisible) laser for rapid laser heating, and a pulsed supercontinuum broadband source for optical absorption studies. In the background, postdoctoral associate **Allen Dalton** and staff scientist **Alexander Goncharov** work on an ultrafast laser system for thermal conductivity measurements (left), and visiting investigator **Stewart McWilliams** and research scientist **Maddury Somayazulu** collect Raman scattering data using a continuous blue laser (right).

sought to broaden our scientific scope. This report covers the activities of the Center during the second year of our second five-year phase of funding as part of the SSAA program.

1.1 Extending the Scope of Extreme Conditions Science

One of the outstanding strengths of the CDAC program is the diversity of scientific interests in high P - T materials science pursued by CDAC personnel. This broadly-based effort has paid important dividends in all three areas of our Center's activities. CDAC research groups are investigating high pressure and pressure-induced structural optical, electronic and magnetic phenomena in a wide range of materials including metals, alloys, dense oxides, molecular systems and polymers, and composites and explosives; in bulk, on surfaces and at interfaces. Accordingly, the range of high pressure experimental techniques employed within CDAC is also very broad. In addition to measurements unique and specific to each laboratory, CDAC personnel take advantage of the capabilities – and support for NNSA science – available at DOE Office of Science (SC) user facilities at the Advanced Photon Source (APS), Argonne National Laboratory (ANL, Fig. 2), the National Synchrotron Light Source (NSLS), Brookhaven National Laboratory (BNL) and the Lujan Neutron Scattering Center at LANSCE (an NNSA facility) at Los Alamos National Laboratory (LANL). CDAC involvement in these SC national user facilities underscores one of the most important goals of the Center, which is to realize and promote partnerships between DOE/SC and DOE/NNSA programs.

Research groups within CDAC carry out a wide variety of investigations concerned with the effects of high pressures and high temperatures on material properties. From the beginning, a staple of our Center's activities has been investigations into the structures, equations of state, and magnetic and electronic properties of materials at high P and T under static compression, which

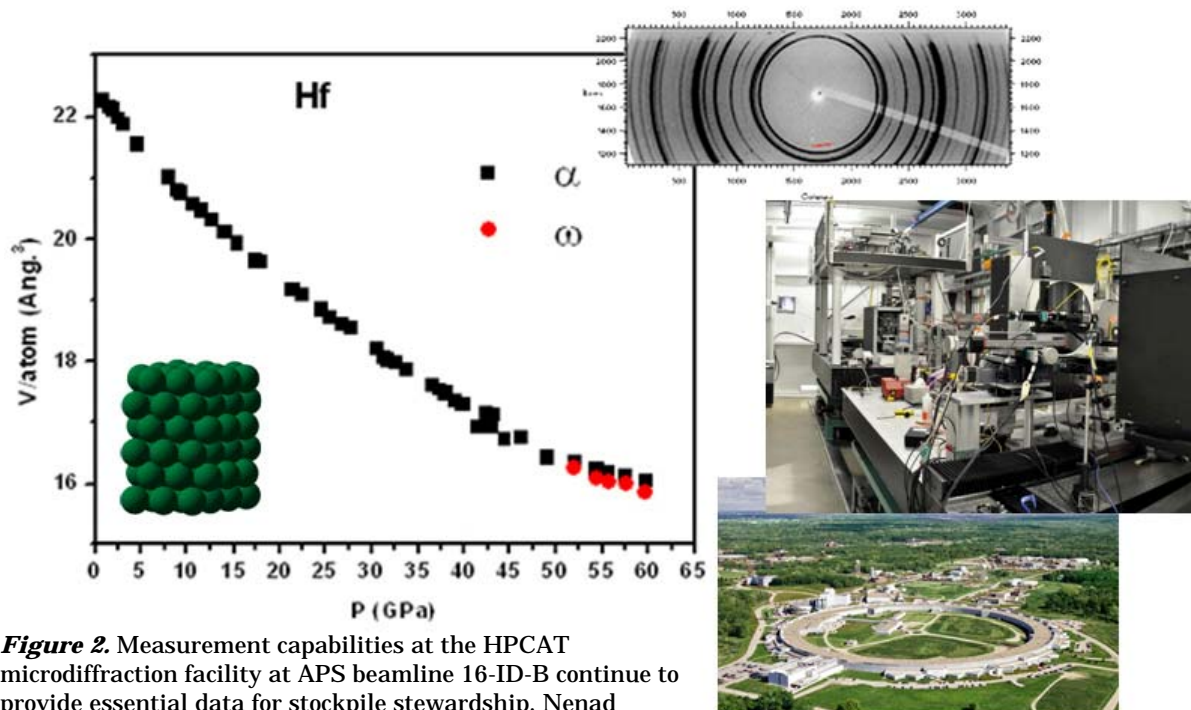


Figure 2. Measurement capabilities at the HPCAT microdiffraction facility at APS beamline 16-ID-B continue to provide essential data for stockpile stewardship. Nenad Velisavljevic (LANL) recently investigated the α - β transition in Hf metal and carried out diffraction measurements up to 60 GPa. The sensitivity and resolution available for these experiments allowed the phase transition to be observed at 40 GPa, much lower than in previous investigations. Left: P - V data for Hf metal (thermally annealed). Top right: Raw diffraction data showing splitting of peaks (in red) at the onset of the α - β transition. Middle right: Interior of the 16-ID-B hutch at HPCAT, which houses two separate tables for different types of microdiffraction experiments, including a third table holding the laser heating optics (upper background). Bottom right: Aerial view of the Advanced Photon Source.

provide critical data for code validation and tests of fundamental theory. CDAC scientists maintain active research programs investigating these aspects of metals, alloys, oxides, and hydrides even as research groups tackle new superconductors, metallic glasses, superhard materials, and transducers (Fig. 3) with special properties. Specialized techniques such as time-domain thermoreflectance and gigahertz interferometry, designed specifically for static compression measurements in diamond anvil cells (DACs) have been developed within CDAC. Added to such long-standing tools as x-ray and neutron diffraction and x-ray spectroscopy, these new techniques are leading to more complete structure-property information relevant to extreme conditions than has been previously available, while at the same time our traditional experimental methods become ever more optimized for measurements at extreme conditions. In addition, new chemistry that challenges our established understanding of chemical combination continues to appear at high P and T , not only in the bulk, but at interfaces and surfaces as well. Such studies are leading to new materials with unexpected compositions, and are stimulating new work aimed at exploring the Periodic Table in unprecedented depth and detail.

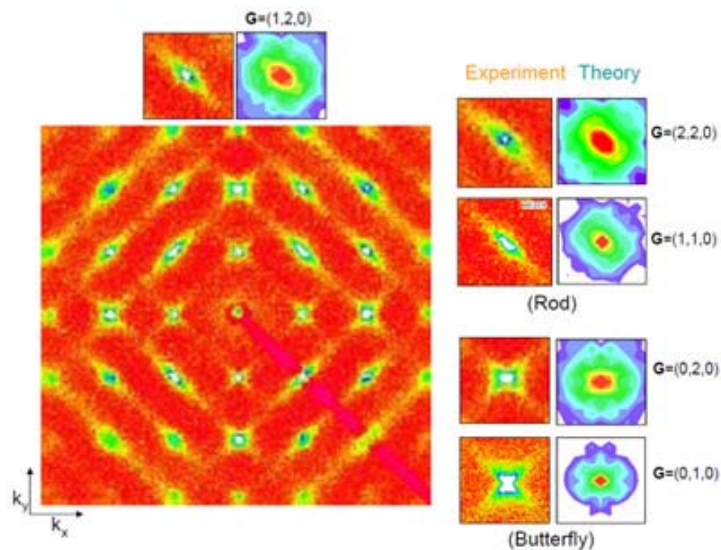


Figure 3. Diffuse x-ray scattering in the relaxor phase of $Pb(SC_{0.4}Nb_{0.6})O_3$, a potential new ferroelectric material.¹⁰

During 2009-2010, CDAC counted among its Academic Partner group 19 faculty from leading high pressure research groups throughout the country (see Box 1). The Center is managed at

- David Cahill (University of Illinois)
- Dana Clott (University of Illinois)
- Robert Downs (University of Arizona)
- Thomas Duffy (Princeton University)
- Rod Ewing (University of Michigan)
- Brent Fultz (California Institute of Technology)
- Steven Jacobsen (Northwestern University)
- Raymond Jeanloz (University of California – Berkeley)
- Abby Kavner (University of California – Los Angeles)
- Kanani Lee (Yale University)
- Jie Li (University of Michigan)
- Jung-Fu Lin (University of Texas) *new partner in Year 7
- Wendy Mao (Stanford University)
- Wendy Panero (Ohio State University)
- Surendra Saxena (Florida International University)
- James Schilling (Washington University in St. Louis)
- Yogesh Vohra (University of Alabama – Birmingham)
- Hans-Rudolf Wenk (University of California – Berkeley)
- Jeffrey Yarger (Arizona State University)

Box 1. CDAC Academic Partners for Year 7.

Carnegie by **Russell Hemley** (Director), **Ho-kwang Mao** (Associate Director), **Stephen Gramsch** (Coordinator) and **Morgan Phillips** (Administrative Assistant).

CDAC Academic Partners are joined by a group of Laboratory Partners, which represent the high pressure research groups at the three DOE/NNSA Laboratories. Laboratory Partners benefit from beam time for both programmatic work and individual research projects at CDAC facilities and serve as valuable points of contact in the National Laboratories for Academic Partners and their students. In addition, Laboratory Partners participate on the CDAC Steering Committee, which is charged with ensuring that the set of Academic Partner programs currently supported by the Center are aligned with DOE/NNSA

scientific objectives as well as the needs for the education and training of scientists in experimental methods that are relevant to the National Laboratories' mission. Through our many education and outreach activities (Fig. 4), Laboratory Partners are able to accurately convey to CDAC graduate students the many facets of work in the National Laboratories. This exposure is invaluable to students who contemplate a career at the DOE/NNSA Laboratories upon graduation or at some point in the future (Fig. 7).



Figure 4. Scenes from the 2010 Short Course on High-Pressure Synchrotron Techniques, co-hosted by CDAC and HPCAT. Clockwise from top left: CDAC graduate student **Madison Barkley (Arizona)** discusses her poster with **Carnegie** postdoctoral associate **Dan Hummer**; CDAC graduate students **Sally Tracy** and **Lisa Mauger (Caltech)** listen to a lecture presented by their advisor **Brent Fultz**; **Reinhard Boehler (Carnegie)** shares some insights on his years in the high pressure field at a cocktail hour before dinner; short course attendee **Brendt Hyde (Royal Ontario Museum)** and CDAC graduate student **Jeffrey Piggot (Ohio State)** attend a lecture presented by **Paul Chow (HPCAT)**; CDAC graduate students **Yun-Yuan Chang (left, Northwestern)** and **Jue Wang (Princeton)** discuss his poster during the Friday evening poster session; CDAC partner **James Schilling (Washington University)** presents his lecture on electronic and magnetic properties of materials.

An essential part of the scientific progress that CDAC has made since 2003 has been the array of experimental facilities that we support. Each of our facilities has made impressive advances over time in the challenge to push forward the technical frontier of high P - T research, which has paid dividends in terms of scientific progress, outreach and education, and technique development. Specialized facilities at **Carnegie** have been created and improved over the last seven years for sample preparation and high P - T spectroscopic, diffraction, and transport measurements at high P and T , and these facilities are available to the CDAC community. These are combined with the continued advances in diamond growth by chemical vapor deposition (CVD) and new device developments including novel anvil designs.^{4,5}

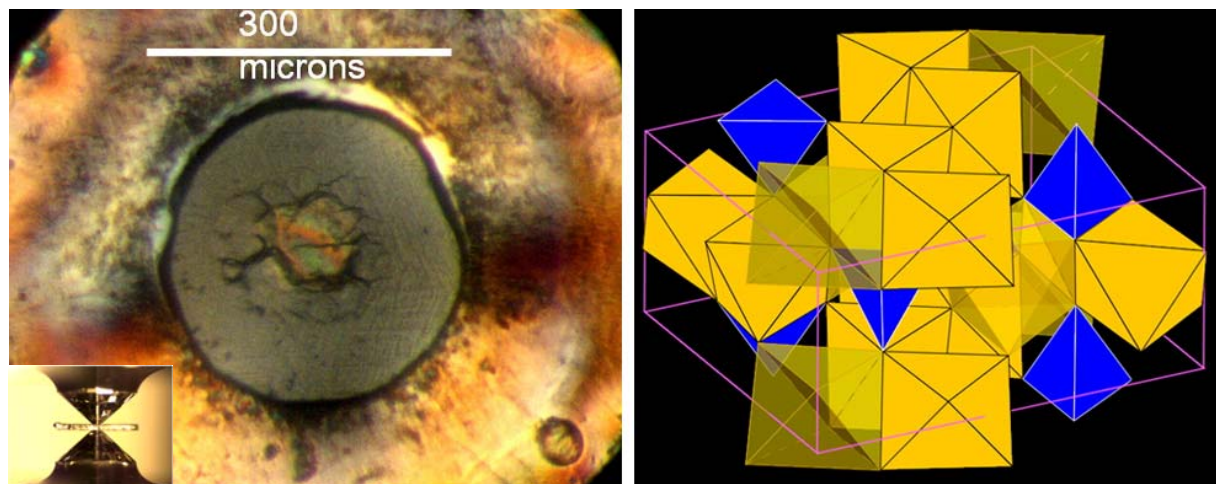


Figure 5. Top left: Emerging techniques at HPCAT such as high-pressure single crystal diffraction using the white-beam Laue method allow rapid collection of crystal structure data with beam sizes down to $5 \times 5 \mu\text{m}^2$. Norbergite crystal in a diamond anvil cell (DAC) at 2.5 GPa in a 4:1 methanol-ethanol pressure medium. Top left inset: One of the many types of diamond anvil cells in use at CDAC. Top right: Norbergite $\text{Mg}_2\text{SiO}_4 \cdot \text{Mg}(\text{OH},\text{F})_2$ Orthorhombic $Pnma$ $a = 4.71 \text{ \AA}$ $b = 10.27 \text{ \AA}$ $c = 8.74 \text{ \AA}$. Bottom right: Carnegie Summer Scholar **Amanda Lindoo** (**Augustana College**) at the 2010 Fall AGU Meeting.



The push toward accurate measurements of material properties at ever higher pressures and temperatures relies critically on the availability of state-of-the-art synchrotron sources. Larger facilities specifically designed for high pressure research, managed by Carnegie and supported by CDAC, **HPCAT** (APS) and **U2A** (NSLS) are world-leading experimental stations with the technical capabilities and personnel expertise necessary to continue advancing the frontier of extreme conditions science. Under the leadership of recently promoted program director **Guoyin Shen**, the High Pressure Collaborative Access Team (HPCAT) is dedicated to the development of spectroscopic and diffraction techniques critical to the advancement of the high P - T research frontier. The facility has reached the mature stage, with the original goal of four simultaneously operating beamlines having been realized, and with recent technical advancements allowing each of the four beamlines to operate independently of each other. While new techniques are continuously under development at HPCAT (Fig. 5) and existing techniques are perfected, the facility now accepts General User Proposals (GUPs) for all four beamlines. At this point, more than 619 different users have carried out experiments at HPCAT since its initial commissioning activities.

Through its mission of promoting high pressure research at additional beamlines at the APS, the High Pressure Synergetic Center (HPSynC) initiative has after two years become an important resource for building the high pressure research community through its dual program of technique development and scientific outreach. The outstanding success of the high pressure work carried out

thus far at HPCAT has provided the need for additional measurement and imaging techniques that can best be developed in collaboration with other beamlines. Taking advantage of the special technical capabilities of selected sectors at the APS has extended the high pressure research capabilities of several of these beamlines and in the process increased awareness of the scientific importance of extreme conditions research at the APS. HPSynC has to date yielded a number of collaborations and important new experimental methods that will be significant in addressing problems of relevance to the NNSA mission.



Figure 6. Carnegie Institution of Washington President **Richard Meserve** speaking at the 2010 SSAA Program Symposium held at Carnegie headquarters (pictured at bottom).

Complementing the diffraction and spectroscopic tools available at HPCAT, the infrared beam line U2A at the NSLS has become a key facility in the CDAC program. Managed by Carnegie research scientist **Zhenxian Liu**, U2A provides for the complete optical characterization of diamond cell samples from the vacuum UV to the far IR. Through its recent upgrades, the U2A station is now used as a critically important probe of local structure and dynamics for a number of CDAC groups.

Since the start of CDAC in 2003, one of the key goals of the Center has been to integrate static and dynamic studies of materials. To this end, CDAC has made synchrotron beam time and facility space available at NSLS and APS for the first synchrotron radiation measurements of dynamic compression. Now, CDAC personnel are actively involved in the development of experiments to be carried out at Z (**Sandia National Laboratories**) and NIF (**Lawrence Livermore National Laboratory**) and in the planning for the MaRIE facility at **Los Alamos National Laboratory**. At the smaller scale, laser-driven shock compression studies are also underway or are in the planning stages in several CDAC laboratories. This multi-scale effort at merging static and dynamic compression methods promises to provide a wealth of important information on materials behavior at extreme conditions, including accessing conditions and states of matter not previously available with static or dynamic compression alone.

This report details the activities of the Carnegie-DOE Alliance Center; its Academic Partners, Laboratory Partners and University Collaborators, during the period from July 2009 through December 2010. The research of Laboratory Partners done outside of CDAC-supported facilities is not included.

1.2 Highlights from Year 7

Outreach and Training

- In Year 7, CDAC supported fully or in part the PhD thesis research of 27 graduate students in 17 Academic Partner groups across the Center. Also in Year 7, five students received the PhD degree with CDAC support, bringing to 21 the number of PhD degrees awarded in the area of high P - T materials science with support from the Center.

- In September 2010, CDAC collaborated with **HPCAT** to present the “Short Course on High Pressure Synchrotron Techniques,” which was designed for graduate students and postdoctoral researchers new to the field of high pressure research or to synchrotron work. The three-day program, which included a student poster session, was attended by 40 graduate students and postdoctoral researchers, including two students from European countries and one from Canada (Fig. 4).

- Three undergraduates carried out experiments in the **Carnegie** high pressure laboratories supported by CDAC during the summer of 2010 for work on projects in of high P - T materials science. All three will be presenting their work in national meetings during the current academic year (Fig. 5).

- During Year 7, CDAC Laboratory Partners have carried out experiments at HPCAT during all three run periods. Approximately one-third of available discretionary CDAC beam over the course of the year time has been devoted to both programmatic and individual research programs of our Laboratory Partners.

- For the third straight year, the SSAA Program Symposium was hosted by **Carnegie** at its historic administration building in downtown Washington, DC from January 20-22, 2010 (Fig. 6). The meeting drew participants from around the country in all three areas of the SSAA program (High Energy Density Physics, Low Energy Nuclear Science and Materials Properties under Extreme Conditions). CDAC graduate students presented 27 posters at the meeting

- In cooperation with the physics department at **Howard University** in Washington, the high pressure group at **Carnegie** hosted two high school students during summer 2010 for an intensive introduction to the practice of scientific research. Two other high school students from the Washington, DC area also joined the group for the summer.

- Support from the core CDAC grant has contributed to operations and technical upgrades at the HPCAT sector. The number of unique users at HPCAT has now grown to 619, which includes many CDAC students and Laboratory Partners. Of the 21 students earning the PhD degree with CDAC support thus far, 18 have carried out some of their dissertation research at one or more of the HPCAT beamlines.

- The May/June, 2010 issue of *Synchrotron Radiation News* focused on high pressure research (Fig. 8). Both of the technical reports in this special issue showcased CDAC-supported work and were coauthored by HPCAT and U2A beamline personnel, including **Zhenxian Liu**, **Guoyin Shen**, **Yang Ding**, and **Wenge Yang**, as well as CDAC Academic Partner from **Tom Duffy (Princeton)**.

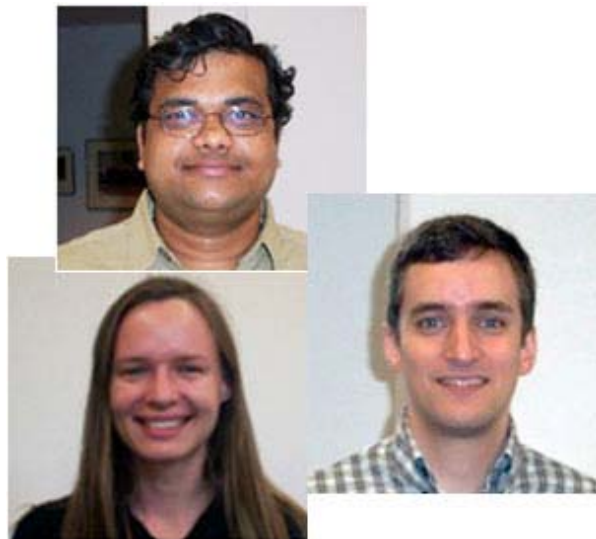


Figure 7. Three Carnegie/CDAC supported postdoctoral associates have accepted positions in the National Labs (pictured clockwise above). **Raja Chellappa** joined **LANL** in May. He is working with Dana Dattlebaum in the the Shock & Detonation Physics Group in the WX-9 division. He is studying structural phase transformations and decomposition behavior of energetic materials in a broad pressure-temperature regime. **Luke Shulenburg** joined the high energy density plasma theory group at **SNL** in July. His primary area of responsibility is the ab initio computation of materials properties under high pressure and temperature to be used in conjunction with the experimental work on the Z-machine. **Amy Lazicki** began work at **LLNL** in September. She joined the group of G. W. Collins to do laser shock compression studies of low-Z materials.

Scientific Breakthroughs

- CDAC graduate student **Michael Winterrose** from **Caltech** completed a comprehensive series of studies on the pressure-induced Invar behavior of Pd_3Fe , and showed that the Invar behavior in this material is due to a change in magnetism from a high-moment ferromagnetic state to a low-moment state with increasing pressure.⁷ Key nuclear resonant x-ray scattering measurements made in this work were carried out at **HPCAT**.

- Researchers from the group of CDAC Academic Partner **Rod Ewing** at **Michigan** have demonstrated a new method to detect and quantitatively measure pressure-induced atomic disordering in pyrochlore oxides. By careful analysis of diffraction peaks, it is possible to identify effects arising individually from defects on the cation and anion sites of a crystal structure. The work reveals a possible mechanism for photochemical reactions in these oxides.⁸

- Experiments carried out by CDAC graduate student **Walter Uhoya** from **Alabama-Birmingham** showed that the structure of the iron-based superconductor EuFe_2As_2 exhibits a negative compressibility (Fig. 9). Uhoya's experiments were carried out at **HPCAT** and employed designer diamond anvil technology for electrical resistance measurements under pressure, which showed a rapid increase in the superconducting transition temperature within the region of negative compressibility.⁹

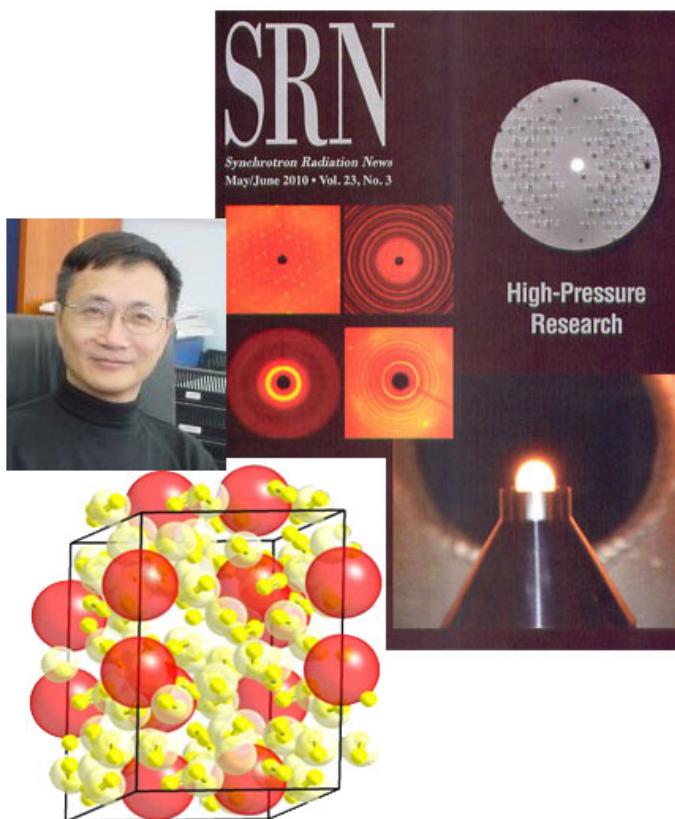


Figure 8. Clockwise from top: Cover of May/June 2010 edition of *Synchrotron Radiation News*; the crystal structure of $\text{Xe}(\text{H}_2)_7$; **HPCAT** Director **Guoyin Shen**.

- Using a combination of high pressure synchrotron x-ray diffraction and Raman and Brillouin scattering techniques, **Muhtar Ahart** at **Carnegie** and colleagues from **Sandia National Laboratories** reported on experiments revealing that the pressure-induced relaxor-to-ferroelectric crossover in disordered $\text{Pb}(\text{Sc}_{0.5}\text{Nb}_{0.5})\text{O}_3$ is a typical example of such phenomena in disordered perovskite systems. This behavior can be attributed to the relaxation of polar nanoregions in the bulk material. The work was begun in collaboration with the late **George Samara**, a member of the first CDAC Advisory Committee.¹⁰

- At **Carnegie**, **Xiao-Jia Chen** and co-workers carried out high pressure measurements of the superconducting transition temperature of $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10.8}$ and found that superconductivity can be induced in this material over two separate pressure ranges, indicating a pressure-driven competition between different states of electronic order.¹¹

- CDAC graduate student **Wenli Bi** from **Washington University in St. Louis** carried out x-ray magnetic circular dichroism experiments on Eu metal at Sector 4 of the APS and showed that the magnetism in the metal increases under pressure to 20 GPa, a result that confirms that Eu metal remains divalent in this pressure range.¹²

- In the **Wenk** group at **Berkeley**, CDAC graduate student **Jane Kanitpanyacharoen** has established the influence of temperature on the deformation mechanisms in the hexagonal metals Os, Hf, Zr, Sn and Cd. Using the D-DIA apparatus at HPCAT, she has shown that increasing temperature at high pressure reduces twinning activity.¹³

- Using two-photon inelastic x-ray scattering spectroscopy at HPCAT, CDAC Associate Director Ho-kwang Mao and co-workers carried out measurements on ⁴He that for the first time allowed a direct observation of the band gap.¹⁴

- Testing a theoretical prediction of superconductivity in compressed LiB, former **Carnegie** postdoctoral fellow and current LLNL postdoctoral fellow **Amy Lazicki** showed that the material exhibits structural changes at 5 GPa that appear to be related to the pressure-induced filling of Li-B antibonding states.¹⁵

- A combined team from **Berkeley** and **Carnegie** led by CDAC Academic Partner **Raymond Jeanloz** and CDAC Director **Russell Hemley**, and including **Paul Loubeyere** of the CEA, France and **G. W. (Rip) Collins** of LLNL, has been awarded time at the National Ignition Facility (NIF) for fundamental science experiments beginning in 2012. The Berkeley-Carnegie proposal, chosen from a group of 86 proposals initially under consideration, outlines work to be carried out on hydrogen and hydrogen-containing low-Z materials at the extreme conditions of pressure and temperature that can only be produced with NIF.

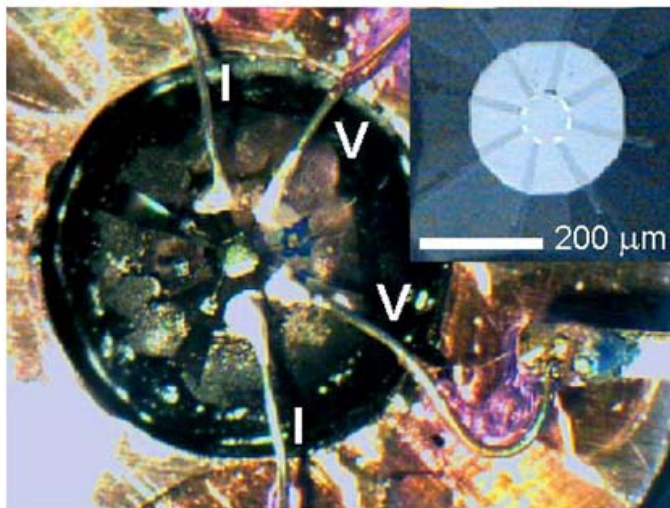


Figure 9. Designer diamond anvils for superconductivity measurements.⁹ Right: CDAC graduate student **Walter Uhoya (Alabama-Birmingham)**



Technique Development

- In the **Diott** group at **Illinois**, development is underway on a laser-launched flyer plate facility to study shock compression at much greater pressures and durations than are possible with femtosecond laser direct drive, and to investigate ignition processes in energetic materials. CDAC graduate student **Kathryn Brown** has led the effort to develop a novel method for generating a flat-top laser beam profile by spatial filtering with a commercially available mirror with a Gaussian reflectivity profile.¹⁶⁻¹⁷

- At HPCAT beamline 16-BM-B, beamline scientists **Dmitry Popov** and **Changyong Park** have recently commissioned a white beam Laue diffraction technique (Fig. 10). Feasibility studies carried out during the past year indicate that structure solution and refinement are possible with the technique on DAC samples. The white beam technique will help overcome limitations imposed on the diffraction experiment by the geometry of the pressure cell.

- Polishing techniques developed in the **Carnegie** CVD diamond group by CDAC Research Scientist **Chang-sheng Zha** have resulted in the capability to polish diamond surfaces to an RMS roughness of 0.48 nm, compared with a typical commercial RMS roughness of 8 nm.¹⁸

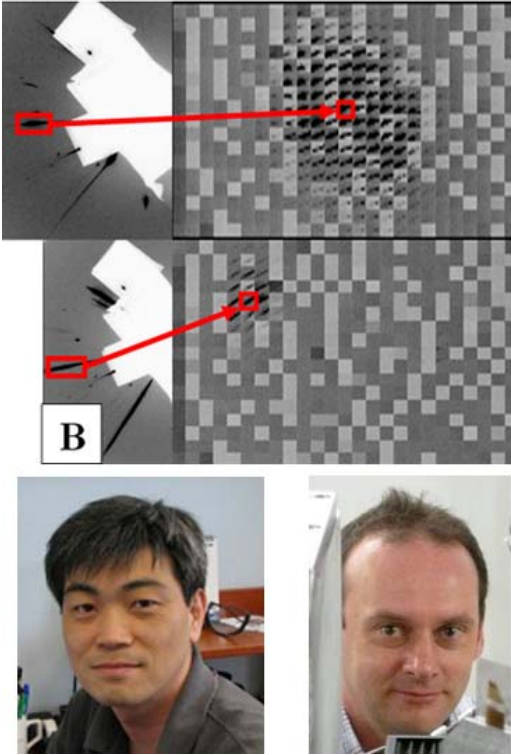


Figure 10. Top: Diffraction patterns taken of a single crystal in two different orientations with the white beam Laue microdiffraction apparatus at HPCAT beamline 16-BM-B. The white beam Laue technique allows for the collection of Bragg reflections produced by multiple x-ray energies in the same exposure and increases the amount of diffraction information available in a single experiment compared to monochromatic beam experiments. This is particularly important for DAC samples, in which the diffracted beam is limited by the pressure cell. Below: HPCAT beamline scientists **Changyong Park** (left) and **Dmitry Popov** (right).

- At **Carnegie**, a virtual control and data acquisition and analysis system to automate simultaneous Raman spectroscopy-laser heating experiments has been completed. The apparatus provides for a reduction of 90% in the time required to carry out these challenging experiments. The apparatus will now allow experiments on highly reactive or diffusive samples, which are impossible to perform in a manual operation mode.¹⁹

- **Lin Wang (HPSynC)** and co-workers from Carnegie and Stanford implemented the use of nanoscale diffraction capabilities at **HPCAT** and used the technique to show that the compression behavior of Y_2O_3 differs significantly depending on the size of the oxide particle.²⁰

- High-brilliance x-rays available at **HPCAT** were used by members of the **HPSynC** group to carry out the first time-resolved structural studies of nanoparticle growth. Nanoparticles of silver were grown at a GaAs substrate-AgNO₃ solution interface and diffraction measurements were taken with 30 ns resolution. This development opens up a new field of time-resolved measurements of nanoscale phenomena.²¹

- In academic partner **Steven Jacobsen's** lab at Northwestern University, CDAC graduate student **Yun-Yuan Chang** has used newly-developed GHz interferometry techniques to measure the shear moduli of diamond. Her ambient pressure measurements show a much narrower range of values in the measured the shear modulus of diamond as compared to other techniques, and provide lower uncertainties as well. The work establishes a benchmark for future high P - T work.

2. SCIENTIFIC PROGRESS

The CDAC research program is highly interdisciplinary, and as new research directions are pursued within the Center and existing ones are expanded, each of our six traditional focus areas have become ever more representative of the breadth of high P - T materials science. We retain this classification for the purposes of reporting, although most of the research results reported in this section may be classified under more than one focus area. This section describes scientific progress in the following general research areas.

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

2.1 High P - T Phase Relations and Structures

Information on the three-dimensional structure of materials provides the basic data necessary to understand the effect of extreme conditions on materials, and this area of research has always been a central feature of the CDAC research program. With state-of-the-art, high-resolution techniques for structural investigations available at academic partner nodes and at CDAC facilities, CDAC groups continue to make remarkable progress in carrying out challenging measurements at increasingly higher pressures and temperatures.

Static High-Pressure Behavior of $Gd_3Ga_5O_{12}$: Implications for Shock Compression –

One of the major themes of the CDAC research effort in the group of **Tom Duffy** at **Princeton** is to explore the connection between static and dynamic high-pressure phenomena. In general, static and dynamic experiments are highly complementary and static experiments can provide crucial information to allow a more complete and detailed interpretation of shock compression results. Recent shock compression experiments²² have reported that the dielectric oxide, gadolinium gallium garnet, $Gd_3Ga_5O_{12}$, (GGG) transforms to a virtually incompressible phase that is stiffer than shock-compressed sapphire or diamond above 170 GPa. This finding has potential practical relevance for shock reverberation and laser shock experiments.²²⁻²³ It also suggests that rare earth oxides could be new candidates for highly incompressible solids.

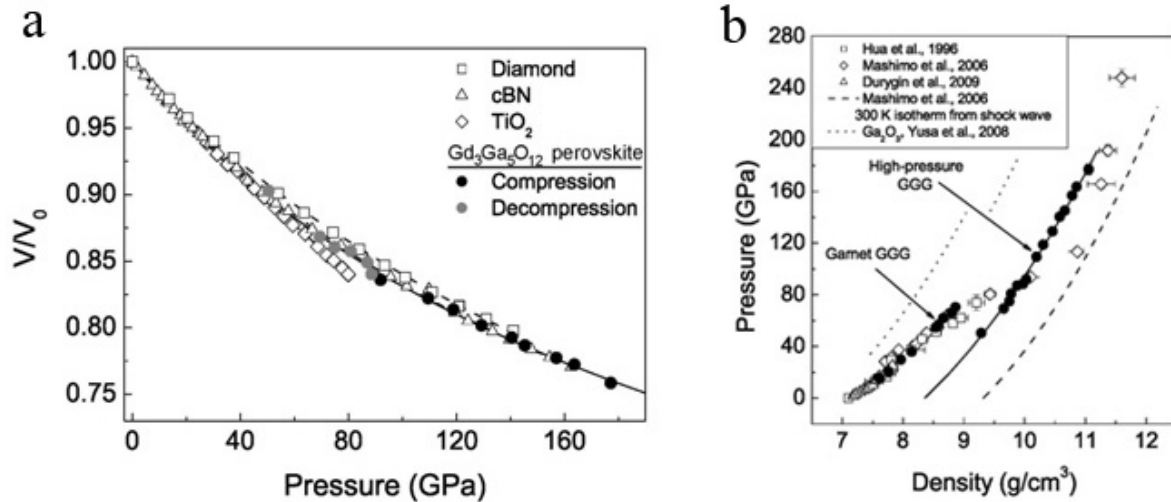


Figure 11. a) Equation of state of the cubic perovskite phase of gadolinium gallium oxide compared with those of other incompressible solids. b) Comparison of pressure-density relations for gadolinium gallium oxide from shock compression studies and the present work. Note that the Hugoniot curve and the static high pressure curve are nearly coincident, a result that has been observed for other incompressible solids such as Al_2O_3 .

CDAC graduate student **Zhu Mao** (now a postdoctoral fellow at UCLA) used the laser-heated DAC and synchrotron x-ray diffraction to investigate the phase stability and elastic properties of GGG to 180 GPa. Experimental results show that GGG is stable in the garnet phase from ambient pressure to 70 GPa at 300 K, and becomes amorphous at 86 GPa. A new high-pressure phase that can be indexed to a cubic unit cell was synthesized at 88 GPa after laser heating to 1500 K. This new phase matched the cubic perovskite structure with stoichiometry $(Gd_{0.75}Ga_{0.25})GaO_3$ and is stable up to 180 GPa. The bulk modulus, K_0 , and its pressure derivative, K_0' derived from fitting the measured P - V relations are 373 GPa and 4 (fixed), respectively. Compared with Hugoniot data for GGG, the results are consistent in that there is a structural transition to a phase with diamond-like compressibility above 90 GPa (Fig. 11a). However, the 300 K equation of state yields densities that are lower by 20% compared to the reduced shock isotherm (Fig. 11b). The density change observed is more consistent with typical values for garnet-perovskite transitions. Compared with the

P-V relations of other superhard materials, the high-pressure phase of $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ is slightly more compressible than diamond at low pressures, but its bulk modulus overlaps that of diamond within mutual uncertainties at 170 GPa (Fig. 11a). Overall, our results confirm the incompressible nature of the high-pressure phase of GGG and identify the high-pressure phase as an A-site ordered cubic perovskite structure.

Pressure-Induced Structural Transitions in Eu Metal to 92 GPa – CDAC graduate student **Wenli Bi** at **Washington University in St. Louis** has been collaborating with **Ravhi Kumar (University of Nevada, Las Vegas)** to fully analyze the results of the x-ray diffraction patterns on Eu metal obtained at HPCAT. The resultant analysis reveals that Eu undergoes four structural transitions: bcc \rightarrow hcp \rightarrow mixed phase \rightarrow orthorhombic (*Pnma*) under high

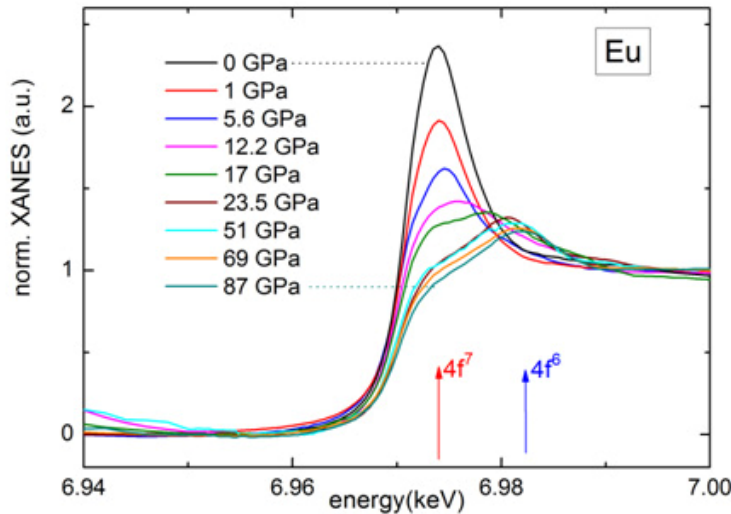
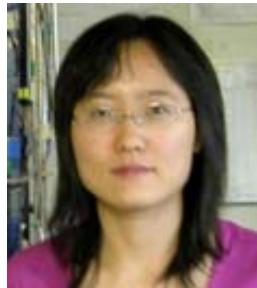


Figure 12. High pressure XANES spectra of the Eu L_3 edge to 87 GPa. Right: CDAC graduate student **Wenli Bi** (Washington University).



pressure to 92 GPa. The first two transitions from bcc to hcp at 12 GPa and from hcp to the Eu-III phase at 17 GPa agree well with the previous studies.^{12, 24} The new experimental data combined with density functional theory calculations by Richard Hennig (Cornell U.) and Yi Zhang (UNLV) show that above 18 GPa Eu gradually transforms into an orthorhombic phase (space group *Pnma*) through an intermittent monoclinic phase (*C2/c*). Above 66 GPa, the Eu structure is orthorhombic (*Pnma*). Above 66 GPa, the the structure of Eu is orthorhombic (*Pnma*) up to at least 92 GPa.

Previous L-III edge absorption and Mössbauer studies on Eu to 34 GPa indicate that Eu transforms into a mixed valent state in the bcc phase, the valence saturating at $\sim 2.64 \mu_B$ throughout the high-pressure Eu-III phase.²⁵⁻²⁷ To understand the valence state of Eu under extreme pressure, an

XANES experiment was carried out at the Eu L_3 edge up to 39 GPa at APS beamline 20-BM. However, no obvious transition from divalent to trivalent as claimed by J. Röhler²⁵ was observed. To confirm this result and investigate possible valence changes at higher pressures, **Wenli** carried out further experiments at APS beamline 4-ID-D up to 87 GPa with the help of **Daniel Haskell** and **Narcizo Souza-Neto**. In this experiment, one full anvil and one partially perforated anvil were used to reduce the absorption from the diamond in the transmission geometry. The experimental results (Fig. 12) show that the absorption peak intensity decreases under pressure in the bcc phase below 12 GPa. In the hcp phase above 12 GPa, the peak becomes broad and a double-peak feature begins to appear at higher pressures. No clear shift of the absorption edge was observed to 87 GPa (Fig. 12). The DFT-XANES simulations done by **Souza-Neto** to 18 GPa suggest that the changes in the spectral features under pressure are be structural in origin.

High Pressure Structural Studies on Tetravalent Metals – Continuing work on the Group IV transition metals, **Nenad Velisavljevic (LANL)** and **Neal Chesnut (Univ. of West Georgia)**, moved on to investigations on hafnium metal. Hafnium, like the other group IV metals Ti and Zr, undergoes a high pressure structural phase transition from a ductile α to a brittle ω phase.²⁸ Previous work has shown that the onset of the $\alpha \rightarrow \omega$ structural phase transition can be severely affected by such factors as experimental conditions (hydrostatic vs. non-hydrostatic) and both substitutional and interstitial impurity concentration.²⁹⁻³⁰ In addition, preferred crystal orientation, grain growth, transition kinetics, and other sample conditions at static high pressures can also limit the ability to detect the $\alpha \rightarrow \omega$ transition.³¹

Using the angle dispersive x-ray diffraction (ADX) technique at HPCAT, two Hf samples, one as received and the other temperature treated and annealed, were investigated. Integrated ADXD patterns, from collected image plate recordings taken during room temperature compression, show the $\alpha \rightarrow \omega$ structural phase transition in Hf, as expected. From the integrated patterns, the $\alpha \rightarrow \omega$ transition appears to start above 50 GPa. However, further investigation of the as-collected image plate pattern shows that the initial appearance of the ω phase could be occurring at pressures as low as 40 GPa. In many cases, detecting the onset of structural phase transitions from integrated patterns may be hindered by the ability to measure and resolve the diffracted beam intensity signal of the initially strong parent phase versus the weak daughter phase. However, it remains to be seen if the apparently sluggish evolution of the ω phase can be attributed to sample pressure gradients or intrinsic material properties.

In another set of experiments, simultaneous spectral reflectometry and x-ray diffraction measurements were performed on cerium metal. Cerium is known to undergo a number of structural phase transitions, and has a very rich phase diagram.³² Several of the observed transitions are driven by significant changes in electronic structure and in some instances are accompanied by a large volume collapse. In many cases, due to grain growth and other texture effects, high-pressure phases, especially at elevated temperature, are difficult to identify using x-ray diffraction alone. In collaboration with Jerry Stevens (NSTec), the LANL group collected multiple high pressure data sets at ambient and elevated temperatures. Initial spectral reflectivity data, collected at room

temperature, show substantial changes in reflectivity during pressure increase up to 25 GPa. Relative changes in reflectivity were correlated to structural changes in Ce, as determined by simultaneous x-ray diffraction measurements. By performing simultaneous spectral reflectometry and x-ray diffraction measurements it is possible to correlate data from two separate diagnostic tools in order to help identify structural phase transitions and possible

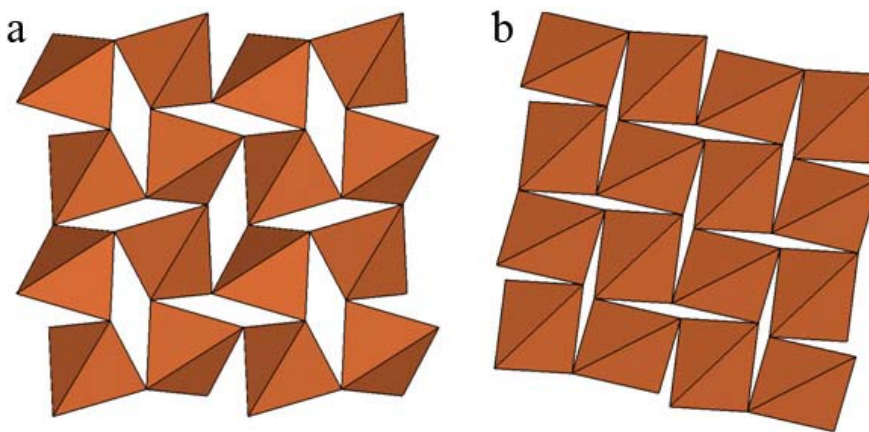


Figure 13. a) The structure of $\text{Be}(\text{OH})_2$ looking down $[001]$ and b) its high-pressure analogue (10.44 GPa) looking down $[00-1]$. At ambient conditions, behoite exhibits a unit cell of $a = 4.475 \text{ \AA}$, $b = 4.571 \text{ \AA}$, $c = 7.036 \text{ \AA}$ and space group $P2_12_12_1$. At 9.64 GPa, the high pressure polymorph has unit cell $a = 5.604(7) \text{ \AA}$, $b = 6.092(7) \text{ \AA}$, $c = 7.105(9) \text{ \AA}$, with space group $Fdd2$. Right: CDAC graduate student **Madison Barkley (Arizona)**.



new high P - T phases. The reflectivity data will also be used for comparison to similar measurements being performed in dynamic shock compression experiments.

The Crystal Structure of Binary FeAs under Pressure – Binary FeAs, in addition to being a common mineral, is a low-symmetry member of the recently discovered ferropnictide class of high-temperature superconductors. FeAs is magnetic at ambient pressure, with an ordering temperature near 70 K.³³⁻³⁴ High pressure transport measurements of FeAs carried out at LLNL by CDAC Laboratory Partner **Jason Jeffries** have revealed the magnetic transition to be robust and unchanging up to nearly 10 GPa, above which the features associated with the transition change, suggesting a loss of magnetism. Structural measurements of this orthorhombic system were carried out at HPCAT in an effort to determine if the apparent loss of magnetism is associated with a structural change. Angle-dispersive x-ray diffraction measurements of FeAs in Ne (pressure-transmitting medium) indicate that the ambient-pressure crystal structure persists to 25 GPa, well in excess of the pressure at which magnetism disappears. The bulk modulus was obtained by fitting the P - V data to a 3rd order Birch-Murnaghan equation of state. The experimental value of the bulk modulus can serve as a test for first-principles theoretical methods, which provide important insights into the structure-property relationships in this material and related compounds.

Structure of Be(OH)₂ at High Pressure – CDAC graduate student **Madison Barkley** at **Arizona** has carried out structural refinements on data obtained at APS Sector 13 (GSECARS) from a natural crystal of Be(OH)₂ (behoite) between 0.34 and 9.64 GPa. The data suggest an orthorhombic phase similar to that proposed by Miletich in an unpublished report. A structural model for the high pressure phase was obtained using a combination of simulated annealing and energy minimization methods. At 9.64 GPa, the high-pressure polymorph of Be(OH)₂ exhibits an orthorhombic unit cell $a = 5.604(7)$ Å, $b = 6.092(7)$ Å, $c = 7.105(9)$ Å, with space group $Fdd2$ (Fig. 13). Without heating, the high-pressure phase remains stable to 37.34 GPa, the highest pressure reached in the experiments.

Additional experiments carried out with cristoballite show that the well known reversible displacive phase transition to cristobalite-II, which occurs at approximately 1.8 GPa, can be suppressed by rapid pressure increase, leading to an overpressurized metastable state, persisting to pressures as high as 10 GPa. Single-crystal data have been used to refine the structure models of both cristobalite and the monoclinic high-pressure phase II over the range of pressure up to the threshold of formation of cristobalite XI (13 GPa), providing important constraints to assess the feasibility of two potential competing silica densification models, based on quantum mechanical calculations. Preliminary diffraction data obtained for cristobalite XI suggests that the currently assumed model is not correct.

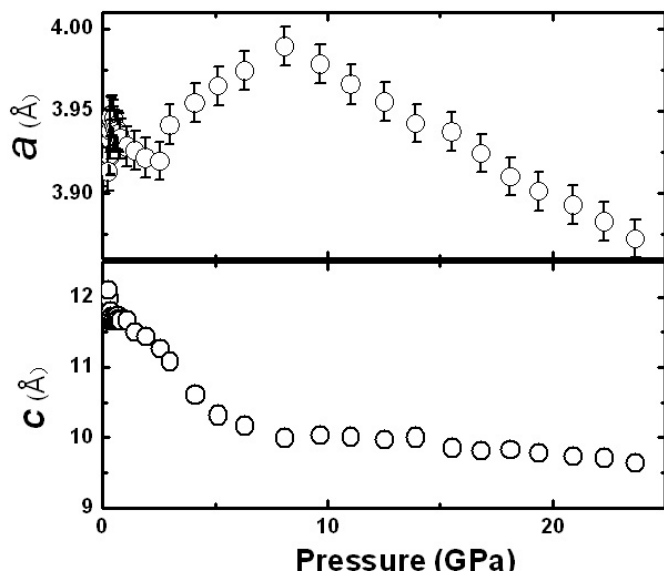


Figure 14. Measured lattice parameters for the tetragonal phase of EuFe_2As_2 as a function of pressure. A negative compressibility is observed for the a -axis and a maximum is observed at 8.5 GPa. The c -axis shows a rapid decrease with increasing pressure up to 8 GPa and a normal decrease with further increase in pressure. The error bars for the c -axis data series are smaller than the symbol size used in plotting.

The fact that the tetrahedrally coordinated Be(OH)₂ remains stable up to 40 GPa is remarkable, since in SiO₂ and most other chemical systems forming silica-like structures a transformation to an octahedrally coordinated phases occurs at pressures lower than 30 GPa. It appears that the

role of hydrogen is to act as an inhibitor in the phase change. This is possibly due to the strengthening of hydrogen bonds, an effect observed in other hydrous minerals including lawsonite $\text{CaAl}_2\text{Si}_2\text{O}_7(\text{OH})_2 \cdot \text{H}_2\text{O}$,³⁵ hibschite $\text{Ca}_3\text{Al}_2(\text{SiO}_4)_{1.5}(\text{OH})_{1.5}$,³⁶ chondrodite $2\text{Mg}_2\text{SiO}_4 \cdot \text{Mg}(\text{OH})_2$,³⁷ brucite $\text{Mg}(\text{OH})_2$ and portlandite $\text{Ca}(\text{OH})_2$.³⁸ Daniel *et al.*³⁵ suggest that the strengthening of hydrogen bonds is common in hydrous minerals and this causes decreased compressibility with increased pressure, and that the stability field of these minerals could be significantly enlarged toward higher pressures. If the hydrogen bonds are strengthened due to the packing of oxygen, then the O-H is weakened, and consequently the Be-O bond is strengthened. While behoite and cristobalite are isostructural at room conditions, they do not undergo the same sequence of high-pressure transformations.

Anomalous Compressibility Effects and Superconductivity in EuFe_2As_2 — The Vohra group at **Alabama-Birmingham** has been investigating the structural and magnetic phase transitions under high pressures in the iron/arsenic-based superconducting systems. As part of this research program, the crystal structure and electrical resistance of EuFe_2As_2 have been studied up to 70 GPa and down to 10 K using designer DAC methods.⁹ The room temperature compression of the tetragonal phase of EuFe_2As_2 ($I4/mmm$) results in an increase in the a -axis length and a rapid decrease in c -axis length with increasing pressure. This anomalous compression reaches a maximum at 8 GPa and the tetragonal lattice behaves normally above 10 GPa with a nearly constant c/a axial ratio. The rapid rise in superconducting transition temperature (T_c) to 41 K with increasing pressure is correlated to this anomalous compression, with a decrease in T_c observed above 10 GPa. Figure 14 shows the measured lattice parameters as a function of pressure, and illustrates these anomalous compression effects. The a lattice parameter shows an initial decrease with pressure to 2.6 GPa followed by an increase with increasing pressure with a maximum in the a -axis length at 8.5 GPa. A further increase in pressure beyond 8 GPa, results in a decrease in a and a normal compression behavior that continues to 70 GPa, the highest pressure reached in this experiment. This negative compressibility in the a -axis length is a very intriguing feature of the compression of EuFe_2As_2 , because the c -axis length shows a rapid decrease with increasing pressure up to 8 GPa and a normal decrease with further increase in pressure to 70 GPa. This project has been part of the Ph.D. thesis work of CDAC graduate student **Walter Uhoya**.

Collapsed Tetragonal Phase and Superconductivity in BaFe_2As_2 — High pressure x-ray diffraction and electrical resistance measurements have also been carried out on BaFe_2As_2 to 35 GPa and temperatures down to 10 K. At ambient temperature, a phase transition from the tetragonal phase to the collapsed tetragonal (CT) phase is observed at 17 GPa under non-hydrostatic conditions as compared to 22 GPa under hydrostatic conditions. The superconducting transition temperature increases rapidly with pressure up to 34 K at 1 GPa and decreases gradually with a further increase in pressure. The results suggest that T_c falls below 10 K in the pressure range of 16-30 GPa where the CT phase is expected to be stable under high pressure and low temperature conditions. Figure 15 shows the measured onset of T_c as a function of pressure up to 30 GPa and down to 10 K. T_c increases to a maximum temperature of 34 K

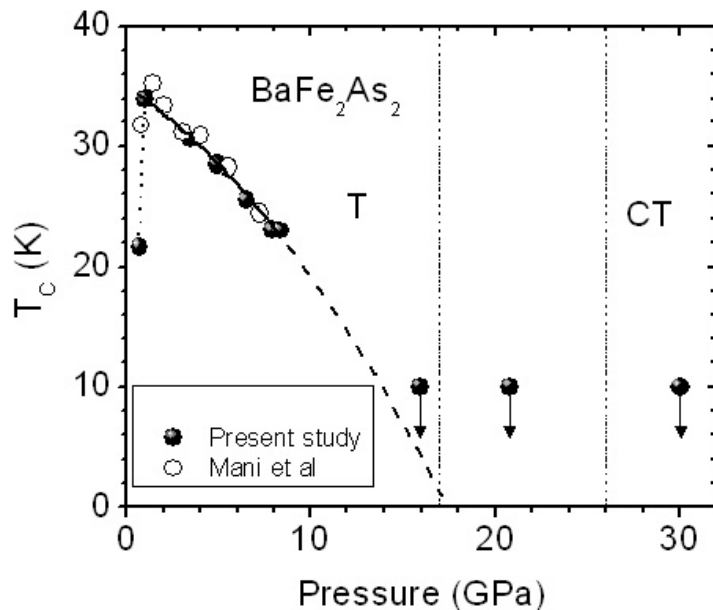


Figure 15. Measured superconducting transition temperature as a function of pressure for BaFe_2As_2 as obtained by electrical resistivity measurements.

at a pressure of 1.0 GPa and then decreases monotonically with increasing pressure from 1.0 GPa to 8.3 GPa. The pressure dependence of the superconducting transition temperature for single crystal BaFe_2As_2 under non-hydrostatic conditions is also compared to the earlier reported data³⁹ to a maximum pressure of 7 GPa in a solid pressure-transmitting medium and a good agreement is obtained. Figure 15 shows that the variation in T_c with pressure can be described by a second-order polynomial equation, which suggests that T_c decreases rapidly in the region where anomalous compressibility effects are observed in the a -axis. The extrapolation of the second order polynomial fit described above suggests that T_c approaches 0 K at 17 GPa and a non-superconducting state is achieved above this pressure, however, direct measurements below 10 K and in the pressure range of 15 to 30 GPa are needed to support this extrapolation.

Previous synchrotron diffraction data on a polycrystalline sample show that the T to CT transition occurs at 22 GPa at 300 K and 26 GPa at 33 K with a helium pressure medium. The phase transition therefore seems to be sensitive to the magnitude of uniaxial stresses, which may explain the scatter in transition pressure from 17 GPa to 22 GPa at ambient temperature. The region between vertical lines at 17 and 26 GPa, therefore, represents the pressure range over which this structural transition would seem likely to occur at low temperatures. Graphical points with down-pointing arrows in Fig. 15 indicate that the onset of T_c is suppressed to below the experimental temperature limit of 10 K in the pressure region where the T-CT phase transition occurs. Additional low-temperature experiments below 10 K are needed to precisely pinpoint the disappearance of superconductivity and correlate it to the stability of the CT-phase.

Formation of a Collapsed Tetragonal Phase in EuCo_2As_2 under High Pressure —

The structural properties of EuCo_2As_2 , an analogue of the Fe-As based superconductor EuFe_2As_2 , have been studied up to 35 GPa. At ambient conditions, EuCo_2As_2 ($I4/mmm$) has a tetragonal structure with a bulk modulus of 48 ± 4 GPa. With increasing pressure, the a -axis exhibits negative compressibility with a concurrent sharp decrease in c -axis length. The anomalous compressibility of the a -axis continues up to 4.7 GPa, at which point the structure undergoes a second-order phase transition to a collapsed tetragonal (CT) state with a bulk modulus of 111 ± 2 GPa. A strong correlation exists between the ambient pressure volume of the so-called "122" parent structures and

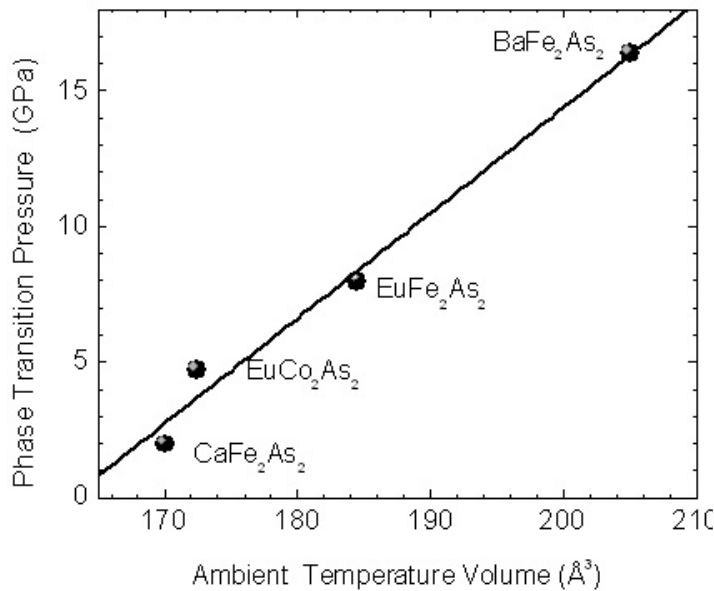


Figure 16. The correlation between ambient pressure volume for AT_2As_2 122 materials and their corresponding phase transition pressures from tetragonal (T) to collapsed tetragonal (CT) phases at 300 K.

the corresponding tetragonal to collapsed tetragonal phase transition pressures. Figure 16 shows the correlation between the observed zero pressure volume (V_0) for AT_2As_2 (122) materials ($A=\text{Ba, Eu, Ca}$ and $T=\text{Fe, Co}$) and their corresponding pressures for the phase transition from T to CT at 300 K. The variation shows a nearly linear increase in P_T with increasing V_0 .⁴⁰

Structural and Magnetic Phase Transitions in NdCoAsO —

As part of the program on iron/arsenic-based superconductors, the quaternary rare earth transition metal arsenide oxide NdCoAsO has also been studied.⁴¹ This compound is isostructural to the high temperature superconductor NdFeAsO . Four-probe electrical resistance measurements carried out in a designer DAC show that the ferromagnetic Curie

temperature and anti-ferromagnetic Néel temperature increase with increasing pressure, while x-ray diffraction studies done at HPCAT show a structural phase transition from the ambient tetragonal phase to a new phase at 23 GPa at 300 K. The NdCoAsO sample remained antiferromagnetic and non-superconducting down to 10 K and to the highest pressure achieved, 53 GPa. Figure 17 shows the measured four-probe electrical resistance of an NdCoAsO sample as a function of temperature between 10 K and 50 K and at various pressures from ambient to 53 GPa. All the measured resistance curves have been normalized to the resistance value at 50 K to compare the resistance minimum observed at low temperatures. The ordering of magnetic moments gives rise to additional scattering of electrons and an increase in the electrical resistance of the sample. The antiferromagnetic transition is marked by a minimum in electrical resistance at low temperature and is observed at 14 K at ambient pressure. The minimum in the resistivity is marked by arrows on Fig. 17 and is observed to shift to higher temperature with increasing pressure. The electrical resistance minimum also becomes less pronounced as the pressure is increased. The presence of the minimum at the highest pressure indicates that material remains anti-ferromagnetic to at least 63 GPa.

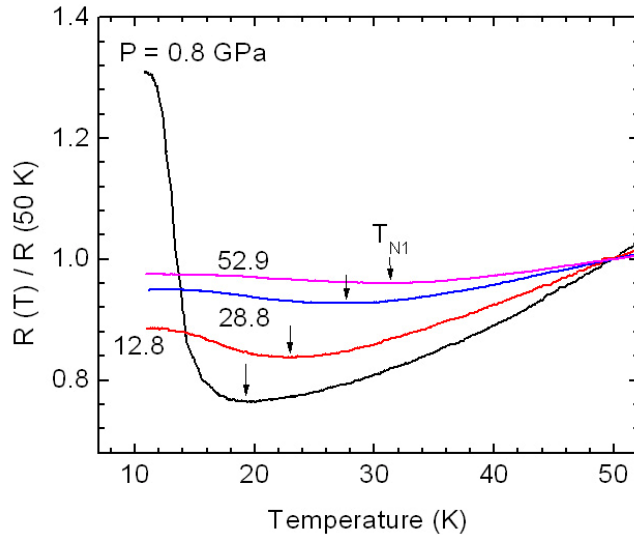


Figure 17. Temperature variation of the electrical resistance normalized to its value at 50 K for NdCoAsO at various pressures. The location of the Néel temperature is indicated by a minimum in the electrical resistance with respect to temperature (marked by arrows).

Pressure-Induced Magnetic Transitions in Cementite – During the past year, the group of CDAC partner **Jie Li** at the **University of Michigan** has investigated pressure-induced magnetic transitions in Fe_3C using neutron diffraction at the Los Alamos National Laboratory. The main goal of this work is to elucidate the nature of magnetic transitions in Fe_3C under high pressure, and to study the effect of temperature on such transitions.

Fe_3C has been a subject of intense study in the Earth sciences because it could be a significant component of the Earth's inner core, making it the largest reservoir of carbon in the planet. Testing the hypothesis of an Fe_3C -rich inner core requires knowledge on the phase stability, equation of state, and lattice dynamics of Fe_3C under high pressures and temperatures. Fe_3C has attracted widespread interest in materials science and condensed matter physics as well, because of its industrial application as a hardening agent in steel, and its Invar behavior similar to that of the classical Invar alloy $\text{Fe}_{0.65}\text{Ni}_{0.35}$.

A number of studies have shown that Fe_3C undergoes magnetic transitions upon compression, although the pressures of these transitions and their effects on the equation of state of Fe_3C remain controversial.⁴²⁻⁴⁶ In particular, recent synchrotron x-ray diffraction measurements on single crystals of Fe_3C in a neon pressure medium revealed two discontinuities in the compression curve between 1 bar and ~ 200 GPa (Fig. 18).⁴⁶ Mössbauer spectra indicate that the discontinuities are associated with loss of the magnetic moment. It is not clear, however, if the magnetic transitions are due to changes in spin state or long-range magnetic ordering of iron.

Neutron diffraction can, however, provide direct information on the periodicity of the nuclei and magnetic lattice, revealing long-range magnetic ordering in transition-metal alloys and compounds. Neutron diffraction is therefore complementary to Mössbauer spectroscopy, which probes the average local structure of Fe. Neutron diffraction, when coupled with high-pressure

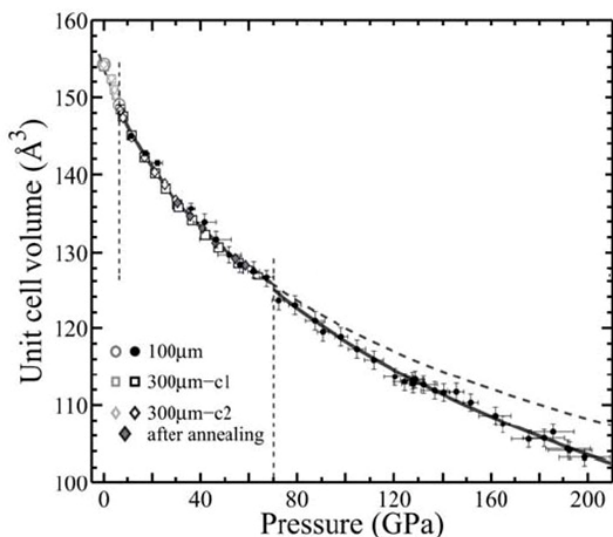


Figure 18. Unit cell volumes of Fe_3C as a function of pressure, revealing two pressure-induced magnetic transitions at ~ 6 GPa and ~ 70 GPa, respectively.

supply, and the temperature is monitored with dual thermocouples placed immediately next to the sample. Pressure is calibrated using the Decker equation of state of NaCl and/or graphite from the furnace. After reaching each desired pressure, the sample is heated at 450-600 K to ensure hydrostatic or semi-hydrostatic conditions in the cell. At each pressure, the data were collected for 3-6 h and the diffraction patterns were obtained by integrating the intensities from detectors mounted at diffraction angles of 90° .

Neutron diffraction patterns of Fe_3C were collected at pressures up to 7.5 GPa and temperatures up to 1073 K, in order to determine the magnetic structure and lattice constants of Fe_3C as a function of pressure and/or temperature. The data are currently under analysis, and the plan is to collect more data using the toroidal-type cell with pressures up to 10 GPa and temperatures up to 1500 K in a second experimental run in the near future. These experiments will take advantage of a gem-quality moissanite anvil cell that is currently under development at LANSCE and may achieve pressures over 20 GPa and temperatures down to 30 K. The experiments will allow an examination of the transition at ~ 6 GPa as well as a study of the structural variation in the Fe_3C phases as a function of pressure and temperature.

A parallel study was conducted to investigate the thermal equation of state, phonon density of states and Mössbauer characteristics of Fe_3C under high pressure.

techniques, is a powerful tool for studying pressure-induced magnetic transitions. In the current work, neutron diffraction data were collected using the High Pressure Preferred Orientation Diffractometer (HIPPO) at the Los Alamos Neutron Science Center (LANSCE), Los Alamos National Laboratory.

For neutron experiments at high pressure and high temperature, the toroidal anvil press (TAP-98) with a unique cell assembly developed at LANSCE (Fig. 19) was employed. In the cell assembly, a ceramic gasket is used for its high strength and thermal/electrical insulation, and the high temperature is achieved via internal resistance heating of a cylindrical graphite furnace, which ensures stability and homogeneity in the temperature distribution. Heating is controlled with a DC power

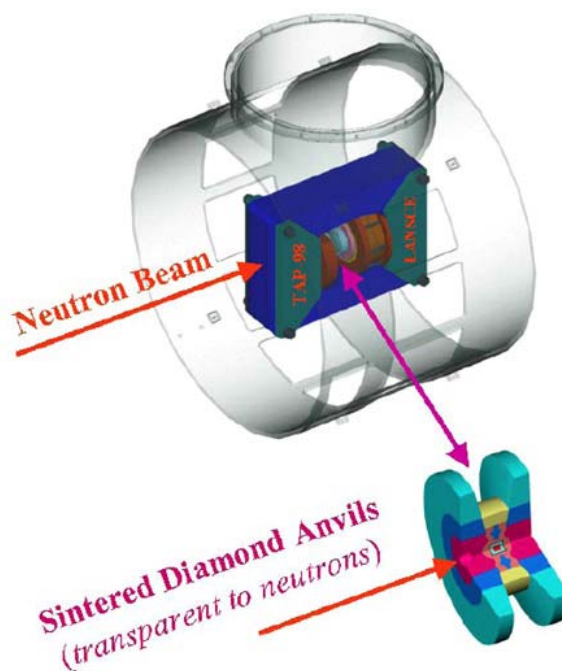


Figure 19. Schematic drawing of the TAP-98 press inside the HIPPO sample chamber. The composite curvature opening of the press frame and toroidal cell assembly design allow the maximum use of the $2\theta = 90^\circ$ diffraction windows available to HIPPO. Incident unpolarized thermal neutrons pass into the press and through one of the single-crystal moissanite anvils to the sample along the unique axis of the cell.

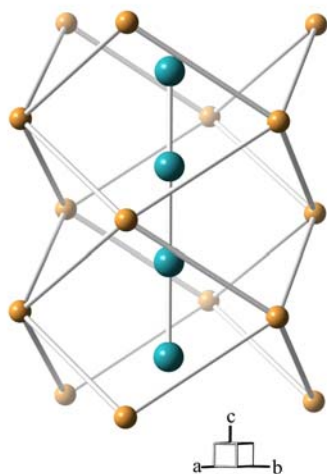


Figure 20. Sixfold column of Li atoms completely encasing one-dimensional, disordered and incommensurate chains of boron atoms.

The results from the neutron diffraction and synchrotron x-ray studies will be combined to elucidate the nature and consequences of pressure-induced magnetic transitions in Fe_3C and implications for the Earth's inner core.

Novel Properties of Compressed LiB – Interest in lightweight analogs of the novel superconductor magnesium diboride (MgB_2) has motivated a search for new high pressure phases in metal boride systems. In the case of lithium monoboride (LiB), a previously unknown series of high pressure structures, some of which are expected to exhibit superconductivity, has been predicted theoretically.⁴⁷ In an experimental effort begun at CDAC, **Amy Lazicki** led a search for structural changes in LiB related to the predicted novel behavior. The research involved CEA France, the Geophysical Laboratory, the University of California – Davis, and Washington State University. It was found that LiB becomes increasingly disordered, but maintains its ambient pressure structure (Fig. 20) up to at least 70 GPa.¹⁵ At 5 GPa, however, an abrupt change in the evolution of the c/a lattice parameter ratio was discovered, which is likely related to pressure-induced electronic filling of Li-B bonding states. Amy Lazicki is now a postdoctoral fellow at LLNL where she works on laser-driven dynamic compression experiments.

Pressure-Induced Disorder and Water Intercalation in Pyrochlore – Researchers from the group of CDAC Academic Partner **Rod Ewing** at **Michigan** and collaborators from the Geophysical Laboratory have demonstrated a new method to detect and quantitatively measure pressure-induced atomic disordering in pyrochlore oxides. This discovery provides new insight on the formation of defects at extreme conditions and reveals a possible mechanism for photochemical reactions in these oxides. Pressure-induced structural disordering, such as the substitution of elements or the formation of vacancies and other defects, is very common and is important to earth and material sciences. However, quantitative analysis of disordering at high pressure at the atomic scale is a very challenging problem from technical standpoint. In the particular case of pyrochlore oxides, cations and anions will form antisite defects and Frenkel pairs simultaneously at extreme conditions.

With x-ray diffraction data collected on the pyrochlore oxide $\text{La}_2\text{Zr}_2\text{O}_7$, at Beamline X17C at the NSLS, the group has shown that defects originating from the cation and anion sites in the pyrochlore

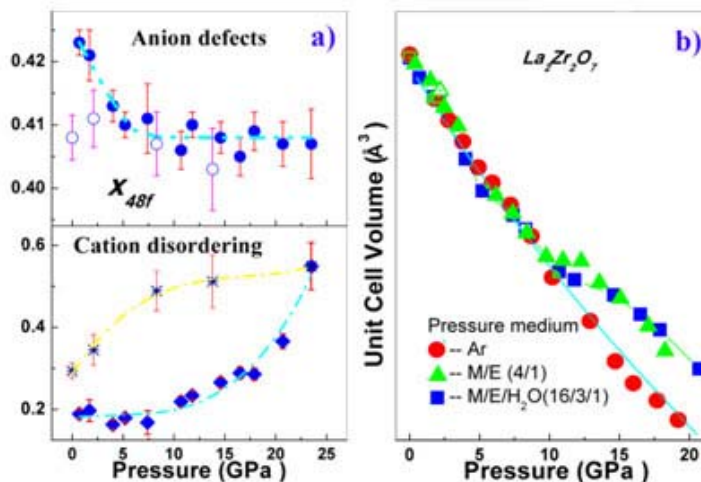


Figure 21. a) Pressure dependence of defects in $\text{La}_2\text{Zr}_2\text{O}_7$. Filled symbols, compression measurements; open symbols, decompression measurements. Top: variation of x ($48f$), the single free structural parameter in the pyrochlore structure, indicating increased disordering with pressure. Bottom, cation disordering between La^{3+} and Zr^{4+} with increasing pressure. b) Pressure-volume relationships for $\text{La}_2\text{Zr}_2\text{O}_7$ in various pressure-transmitting media. Water-containing media such as methanol-ethanol (green triangles) or methanol-ethanol-water (blue squares) result in anomalous expansion of the unit cell volume at high pressures.

structure have different influences on the individual diffraction peaks and their contribution can be quantitatively distinguished in the x-ray diffraction pattern (Fig. 21). Using the Rietveld refinement method, it was concluded that anion defects formed below 5 GPa and cation antisite defects dominated above 10 GPa. An anomalous lattice expansion was confirmed in the oxide at 10 GPa by x-ray diffraction, if a water-containing pressure medium is used. Water intercalation in pyrochlore oxides may be common during the process of either pressurization or ion irradiation, and it is mainly due to the formation of cationic defects. Some pyrochlore oxides such as $\text{La}_2\text{Zr}_2\text{O}_7$ have been used previously as catalysts for the photochemical splitting of water, a process that may be closely related to the formation of defects in the pyrochlore structure.⁸

A Pressure-Induced Phase Transition in FeGa Alloy – Giant magnetostriction in Fe – $x\%$ Ga alloys with $x = 15\text{-}27\%$ have attracted attention from both the scientific and industrial communities, and offers potential for future generations of sensors and actuators. A maximum in the magnetostrictive strain about 10 times greater than that of pure Fe is found at a Ga content of about 19%. The material also offers a unique combination of other properties including high mechanical strength, good ductility, and high imposed blocking stress, as well as exceptional weak field properties at moderate saturation fields. Accordingly, the alloy offers a large magnetoelastic energy density when used either in tension or compression. Both equilibrium and metastable phase diagrams for Fe– $x\%$ Ga have been reported. In the equilibrium diagram, a disordered body-centered-cubic bcc -Fe or A2 phase is in equilibrium with a face-centered-cubic fcc L12 ordered phase; whereas in the metastable diagram, the A2 phase is in a metastable equilibrium with a bcc DO3 ordered phase. However, there has been no work describing the effect of pressure on the properties of these materials. Figure 22 shows how the (110) Bragg peak evolves with pressure, with data obtained at HPCAT by **Carnegie's Muhetaer Ahart**, in collaboration with **C. DeVreugd** and **D. Viehland** from **Virginia Tech** and **P. Gehring** from **NIST**. The pressure dependence of the d-spacing shows that the crystal transforms from a cubic to a hexagonal structure, but at a pressure 10 GPa higher than in pure Fe. It appears from preliminary analysis that the transition is reversible.

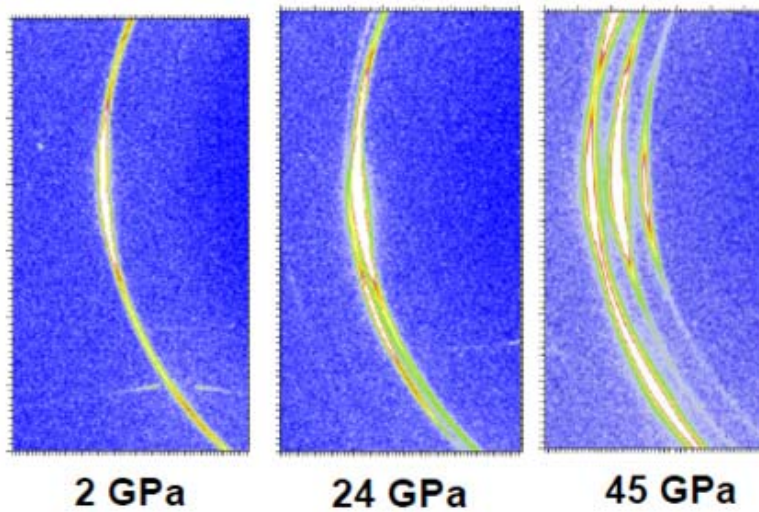


Figure 22. Splitting of the cubic (110) Bragg peak from an Fe-19% Ga sample with increasing pressure. Right: **Muhetaer Ahart** (Carnegie).



High-Pressure Phase Transition of Thauasite Containing Octahedral Si-OH – Formation of thauasite, $\text{Ca}_3\text{Si}(\text{OH})_6(\text{CO}_3)(\text{SO}_4)12\text{H}_2\text{O}$, is recognized as a precursor of sulfate attack in Portland cement, which weakens concrete in contact with sulfate-rich groundwater. In addition to having important implications for waste storage in concrete, the structure of thauasite is under investigation because it contains a highly unusual Si group in octahedral coordination with hydroxyl, OH. Undergraduate **Julia Swanson**, along with CDAC graduate student **Yun-yuan Chang** and faculty member **Steve Jacobsen** at **Northwestern** have identified a possible high-pressure phase transformation of thauasite using Raman spectroscopy. As shown in Fig. 23, upon compression

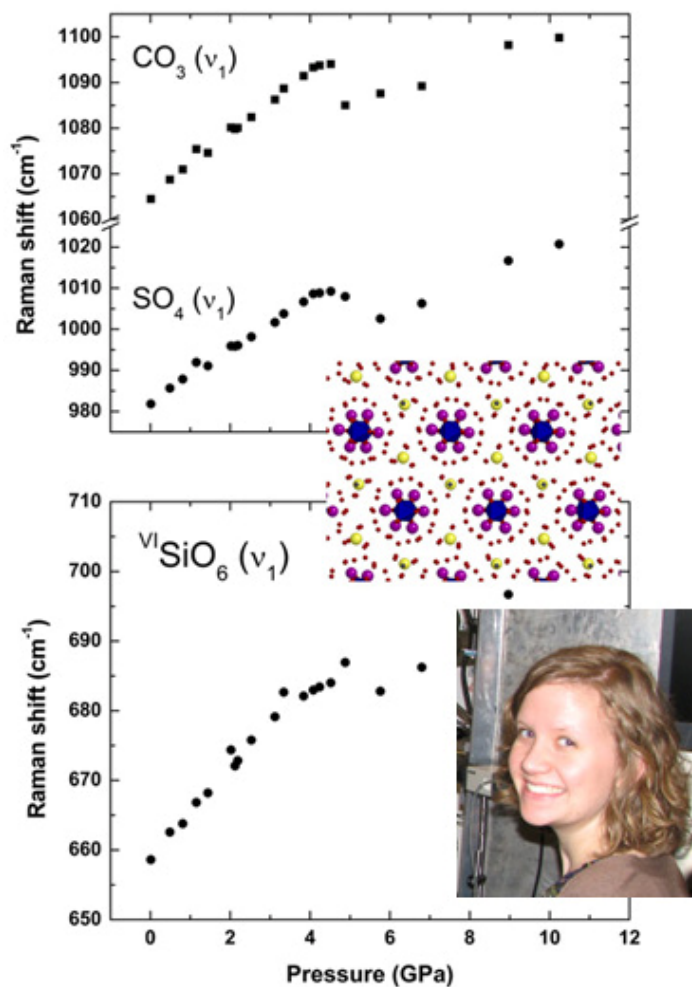


Figure 23. High pressure Raman spectroscopy of thaumasite. Inset: **Julia Swanson (Northwestern).**

Researchers **Timothy Strobel, Xiao-Jia Chen, Maddurry Somayazulu** and **Russell Hemley** have recently discovered a novel hydrogen rich compound, with approximate stoichiometry $\text{GeH}_4(\text{H}_2)_2$, that crystallizes from germane – hydrogen mixtures above 7.5 GPa.⁴⁸

Optical microscopy, spectroscopic and x-ray diffraction studies at high-pressure have been carried out in order to investigate the properties of the new compound under pressure. The measurements reveal multiple H_2 vibrons substantially softened from bulk solid hydrogen, and with increasing pressure, the frequencies of several Raman- and infrared-active H_2 vibrons decrease, indicating an anomalous attractive interaction for closed-shell, non-polar molecules. Synchrotron powder x-ray diffraction measurements show that the compound has a structure based on a face-centered cubic arrangement of GeH_4 molecules, with the H_2 molecules likely distributed between octahedral and tetrahedral interstitial sites. Above approximately 17 GPa, GeH_4 molecules in the compound become unstable with respect to decomposition products ($\text{Ge} + \text{H}_2$). The compound can be preserved metastably to ~27 GPa for several hours.

The new GeH_4+H_2 compound represents a class of hydrogen dominant materials, which like the $\text{SiH}_4\text{-H}_2$ phase discovered earlier,⁴⁹ are characterized by enhanced interactions between molecular components. The interaction between H_2 and GeH_4 suggests an unusual bonding mechanism which may be useful in the design of new hydrogen storage materials and novel high temperature

above 4 GPa, the symmetric stretching modes of the carbonate, sulfate, and Si-OH groups exhibit softening and subsequent recovery on further compression to 10 GPa. After the transition, the crystal remains optically intact with clean extinction, suggesting that a new pressure-induced crystalline phase has formed. In the coming year, students will repeat the experiment and conduct *in-situ* x-ray diffraction studies at HPCAT to determine the structure of the high-pressure phase, which may reveal a new dense structure containing significant amounts of carbon, sulfur, and hydrogen.

Compound Formation in Germane-Hydrogen under Pressure

Under pressure, simple molecular mixtures can crystallize as unique compounds characterized by a subtle interplay of intermolecular (*e.g.* van der Waals) interactions. Examples include hydrogen-rich molecular compounds which could be important in the development of new materials for energy storage and as possible high temperature superconductors, in understanding interstellar ices and to basic condensed matter physics. At **Carnegie**, a significant effort is underway to investigate the chemistry of these hydrogen-containing materials.

superconductors.⁵⁰ Compounds of this type provide examples of "chemical precompression" of molecular hydrogen,⁵⁰ and provide insight into the behavior of hydrogen at very high densities.

2.2 P-V-T EOS Measurements

Accurate modeling of materials at extreme conditions requires highly accurate P - V - T equation of state data. Diamond anvil cell methods for x-ray and neutron diffraction and sound velocity measurements are essential for stockpile stewardship applications in that they provide data that can be combined with that obtained in dynamic compression studies to more fully understand material properties at all relevant conditions. The full range of materials are explored in CDAC groups, from metals and crystalline solids to superhard materials and polymers, liquids and glasses.

Hardness of Zirconia and Hafnia – Zirconia (ZrO_2) and hafnia (HfO_2) are well-known components of modern ceramic materials, which lead to important industrial applications because of their interesting mechanical properties. Both oxides are also important as they follow similar structural behavior to TiO_2 , which has been studied recently in the group of CDAC Partner **Kanani Lee** at **Yale**. Previous experimental and theoretical studies predict different structural phase transition sequences under high pressure and/or temperature. The most recent first-principles computations predict that ZrO_2 and HfO_2 undergo the following sequence: baddeleyite \rightarrow OI \rightarrow OII (e.g., Ref.⁵¹) in good agreement with previous measurements.⁵² The OII phase of both oxides is dense with a high bulk modulus, approaching that of diamond. Previous work on ZrO_2 and HfO_2 shows several possibilities of the transition sequence as well as different phases in each sequence under high pressure and temperature, where tetragonal and cubic phases are also expected, as outlined in the work of CDAC graduate student **Yahya Al-Khatatbeh**.⁵²⁻⁵⁵ As with previous work on TiO_2 ,⁵⁶ a phase diagram of ZrO_2 ⁵⁷ and for HfO_2 (Fig. 24),⁵⁸ under high pressure and temperature have been constructed to help identify the possible phases and the transition sequence.

In general, it is expected that a material becomes harder with decreasing volume, either within a single phase, or across volume-reducing phase transitions. Thus, if high-pressure phases can be recovered at ambient conditions, this may provide a promising route for the synthesis of materials with

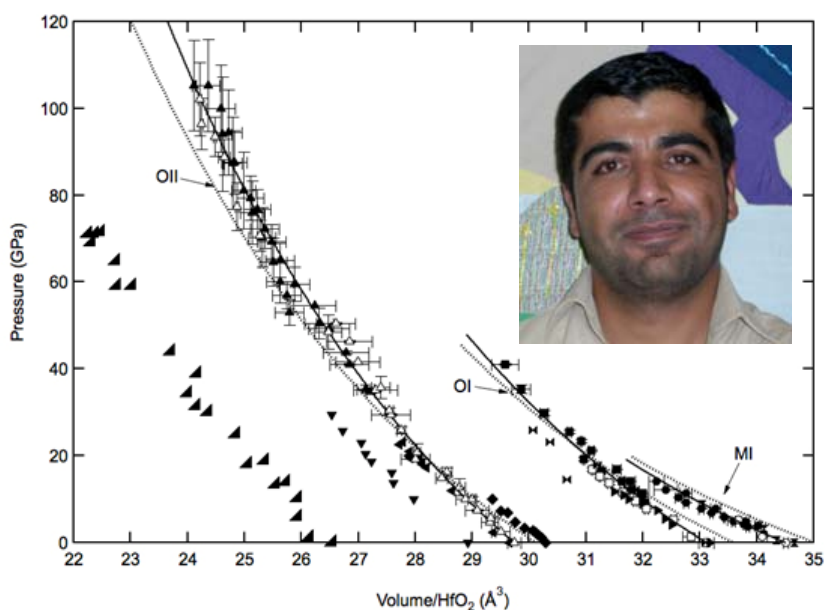


Figure 24. Pressure versus volume for one HfO_2 formula unit as determined by experiment. MI (circles), OI (squares), and OII (triangles). Volumes are shown under compression (solid symbols) and on decompression (open symbols). The solid curves show the experimental EOS, and the dotted curves show the predicted EOS from GGA calculations. MI: data are close to GGA calculations; for comparison, other experimental work is included (vertical bowties for Leger et al.,⁵⁴⁻⁵⁵ and diamonds for Desgreniers & Lagarec⁵²). OI: GGA calculations go through almost the data, especially at pressures > 10 GPa; for experimental work (horizontal bowties for Leger et al., 1993, right-handed triangles for Ohtaka et al., 2001 and inverted triangles for Desgreniers & Lagarec⁵²). OII: observed OII data up to ~ 105 GPa are in good agreement with GGA calculations especially at pressures < 50 GPa; for comparison, other experimental work is included (left-handed triangles for Ohtaka et al.,⁵⁹ and right-angled triangles for Desgreniers & Lagarec⁵²).

enhanced mechanical properties,⁶⁰⁻⁶¹ which would increase the pool of currently available superhard materials. On the one hand, if volumetric effects dominate hardness, then the bulk modulus is expected to be a suitable proxy for the mechanical strength of a material. On the other hand, if shear displacement is dominant, then the shear modulus should be a better proxy for the mechanical strength of a material.

The large volume decrease across the OI → OII phase transition as obtained from both experiments and calculations is ~10%. Present estimates, using scaling relations,⁶² indicate that both OII phases of ZrO₂ and HfO₂, while dense and quenchable, have a comparatively low mechanical hardness of ~10 GPa, which is comparable to MI and OI phases, and much lower than 40 GPa, a prerequisite for a material to qualify as superhard. The results also show that the shear modulus better correlates with hardness between phases than the bulk modulus.

Static Compression to Multimegabar Pressures Under Quasi-Hydrostatic

Conditions – The study of materials under static loading to pressures greater than 1 Mbar is hampered by the difficulty in achieving and characterizing a hydrostatic sample environment under such conditions. Use of helium or neon as a pressure transmitting medium is known to provide very good quasi-hydrostatic conditions to pressures up to at least 1 Mbar⁶³⁻⁶⁴ but its use at higher pressures has not been well explored. Accurate pressure calibration is a fundamental and critical

problem that limits the reliability of DAC experiments at ultrahigh pressures. Pressure errors are introduced by uncertainties in equations of state of pressure calibrants, discrepancies between pressure scales, and non-hydrostatic stress conditions in the DAC. The **Duffy** group at **Princeton** has carried out a series of experiments to pressures as high as 2.5 Mbar in order to (1) measure the equations of state of standard materials (Au, Pt, Ne, MgO, and NaCl) to provide accurate pressure calibration and cross-calibration of pressure scales to this pressure, and (2) characterize the differential stress when using neon, helium, or no pressure media up to these conditions.

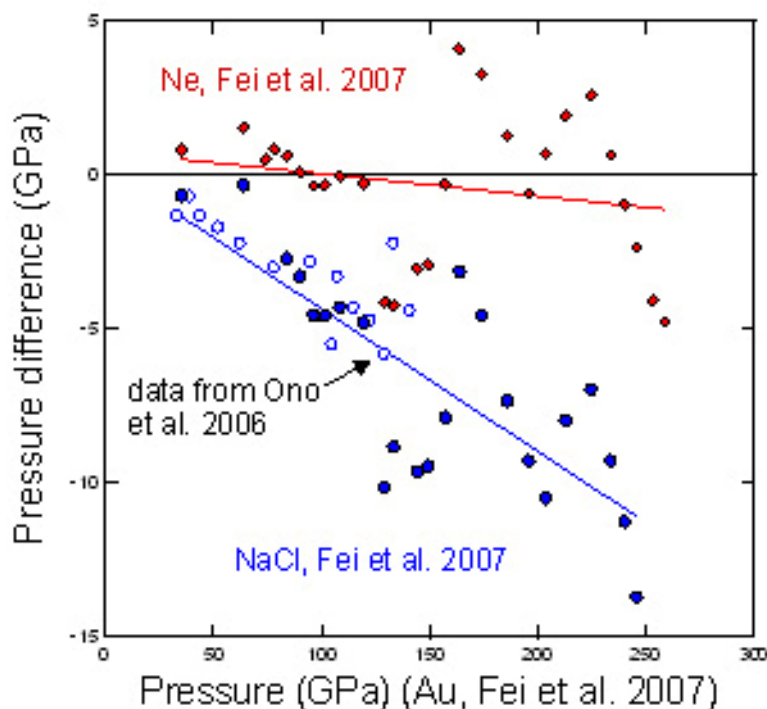


Figure 25. Comparison of pressure differences between gold, neon, and the sodium chloride B2 phase up to 259 GPa. In this work, the cross-calibration of these materials has been extended by a factor of 2 in pressure compared with earlier data. Neon and Au diffraction data yield consistent pressures to ultrahigh pressures, but NaCl B2 shows a systematically lower pressure. Right: CDAC graduate student **Susannah Dorfman** (Princeton).



In early experiments carried out by CDAC graduate student **Susannah Dorfman**, pressures indicated by MgO and Pt scales⁶⁵⁻⁶⁶ differed by as much as 10% above 200 GPa. Differential stress in the sample was estimated by applying lattice strain theory⁶⁷ to relative shifts in the positions of Pt diffraction peaks. Using the elastic anisotropy-pressure relationship

for Pt, values for differential stress in Pt range from 1-4 GPa, or a maximum of 2% of the peak pressure. Analysis of the diffraction peak widths confirmed that the increase in differential stress was small over the pressure range studied. A similar experiment on Pt and MgO in a neon medium to 175 GPa found the differential stress and peak widths do not differ significantly between the He and Ne media. By examining a Pt and NaCl mixture in helium to 188 GPa, the work was extended to cross-calibration of Pt, MgO and NaCl.

Subsequent x-ray diffraction experiments were carried out at HPCAT on mixtures of Au and NaCl in a neon pressure medium to 259 GPa (Fig. 25). Preliminary findings are that the Au and Ne pressure scales⁶⁸ remain consistent within 2% up to these pressures while the NaCl pressure scale diverges by more than 5%. It is now possible to cross-calibrate the Pt, MgO, Au, NaCl, and Ne pressure scales up to 2.5 Mbar. Quasi-hydrostatic conditions are maintained in the Ne medium above 2 Mbar, as evidenced by diffraction peak widths comparable to previous work in a He medium. Ne diffraction line shifts due to lattice strain indicate a yield strength for neon of ~6 GPa at 2 Mbar, in good agreement with previous work. However, the lattice strain results for other materials show complex behavior that prevents extraction of differential stress values. Further work will be directed towards better understanding the stress state under these extreme conditions.

Equation of State of Ammonium Nitrate – Ammonium nitrate (AN, NH_4NO_3) is perhaps the most widely used fertilizer and mining explosive in the world. In explosive applications, the ammonium nitrate prills are prepared so that they readily absorb ~6 wt% fuel oil forming an ammonium nitrate-fuel oil (ANFO) mixture. ANFO is known to be a non-ideal explosive with measured detonation velocities near 4 km/s.⁶⁹ While there have been numerous studies of the detonation properties of ANFO, there are limited reports of the EOS and initiation properties of pure AN.

AN is known to exist in at least 6 phases in addition to the melt as a function of temperature and pressure. Analysis of ADXD patterns at room temperature (298K) and elevated pressures reveal that the high pressure crystal structure(s) could be indexed as Phase IV, an orthorhombic phase ($Pm\bar{m}n$), with two molecules per unit cell, from ~0.4 GPa to 25 GPa, with an initial density of 1.726 g/cm³. While Sharma⁷⁰ and others⁷¹ have reported, and as has been observed in the group's own laboratory, changes in vibrational bands below 2 GPa that may be indicative of a phase transition, both the vibrational and x-ray structure analysis indicate any new phases must be closely related to the parent Phase IV. Comparison of the lattice parameters at 0.4 GPa with Hermann *et al.*,⁷² (ambient conditions, in parentheses): a (Å) = 5.748 (5.745), b (Å) = 5.428 (5.438), c (Å) = 4.937 (4.942), $V/\text{molecule}$ (Å³) = 77.02 (77.20) show good agreement. As the pressure was increased, the collapse of the b axis at pressures exceeding ~6 GPa, where the c/b ratio approached 1, consistent with Sandstrom, was observed.⁷³ The scatter in the determined lattice constants from separate experiments also increased in the pressure range of ~6-8 GPa, giving a

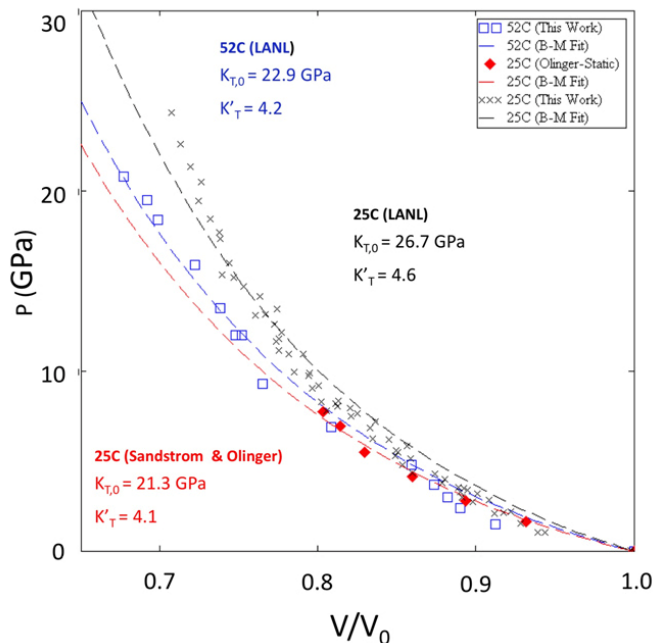


Figure 26. Normalized volume change of AN as a function of pressure at 25 °C and 52 °C. Hysteresis upon decompression is evident as the unit cell volume is not fully recovered. The fits of the isotherms to the Birch-Murnaghan semi-empirical fitting form are also shown, with the results of the fits given on the figure.

maximum estimate of the error (based on the scatter in the lattice constants propagated through to volume) of $\sim 7\%$. Further, as the temperature is increased, the collapse of the b axis is observed to occur at higher pressures. This may be indicative of a new tetragonal structure (and phase line) in the phase diagram.

Figure 26 shows the resulting isotherms for AN indexed to Phase IV at room temperature and 52°C . As expected, AN softens at warm temperature, and the bulk modulus drops by ~ 4 GPa between RT and 52°C . Also shown in the figure are B. Olinger and F. Sandstrom's data,⁷³ which within the pressure regime studied, are in good agreement with the LANL data. The isothermal bulk moduli and their pressure derivatives resulting from fits of the isotherms to Birch-Murnaghan EOS form are also shown on Figure 26. High pressure-high temperature Raman spectra were collected to support and lend insights to the x-ray diffraction results. At room temperature, the Raman spectra do not exhibit discontinuities or mode splittings suggestive of pressure-induced phase transitions, *e.g.* phase IV remains stable to very high pressures.

These new high pressure Raman and synchrotron XRD studies on AN have revealed a wealth of new information regarding the phase stabilities of various AN phases. A P - T diagram is being mapped based on the phase stabilities identified by these experiments; the phase boundaries exhibit steep slopes and the AN-IV phase is extraordinarily stable over a broad range of P - T conditions. Continuing work is devoted to exploring the extraordinarily steep melting line (at ambient pressure AN melts at 170°C while at 0.8 GPa it melts at $\sim 520^\circ\text{C}$) as well as the decomposition behavior as a function of pressure.

Pressure-Induced Changes in the Electronic Structure of PdN₂ – In a collaboration between **Carnegie** and **Livermore**, a combined theoretical and experimental study of the electronic structure and equation of state of crystalline PdN₂ has been carried out. PdN₂ forms above 58 GPa in the pyrite structure and is metastable down to 11 GPa. It has now been shown that the EOS cannot be accurately described within either the local density or generalized gradient approximations. The Heyd-Scuseria-Ernzerhof exchange-correlation functional (HSE06), however, provides very good agreement with experimental data (Fig. 27). The strong pressure dependence of the Raman intensities can be understood in terms of a similar dependence of the calculated band gap, which closes just below 11 GPa. At this pressure, the HSE06 functional predicts a first-order isostructural transition accompanied by a pronounced elastic instability of the longitudinal-acoustic branches that provides the mechanism for the experimentally observed decomposition. Based on an extensive Wannier function analysis, it is clear that the structural transformation is driven by a phase transition in the electronic structure, manifested by a discontinuous change in the hybridization between Pd d and N p electrons as well as a conversion from single to triple bonded nitrogen dimers. The results of this investigation suggest the existence of a critical point for the isostructural transition, at which massive fluctuations in both the electronic and structural degrees of freedom are expected.⁷⁴

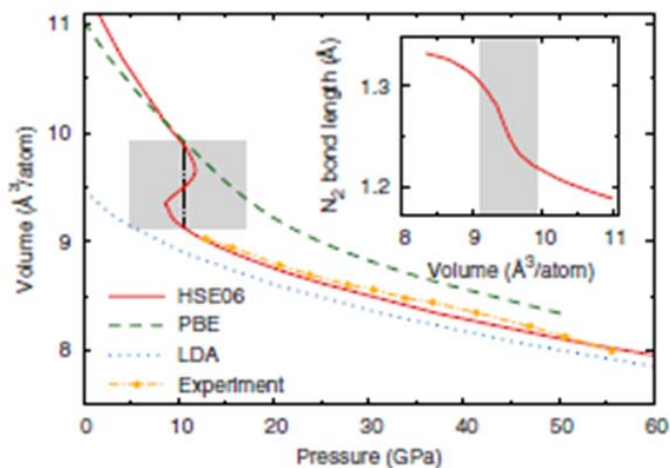


Figure 27. Equation of state for PdN₂ as obtained from theory (HSE06, red solid line, PBE, green dashed line, and LDA, blue dotted line) and experiment (yellow dash-dot line). Inset: nitrogen bond length as a function of atomic volume. Gray area indicates the two-phase region.

Equation of State Measurements on Glassy Materials – Magnesium orthosilicate (Mg_2SiO_4) is a major component of the Earth's upper mantle and plays an important role in models of the melt during the formation of the early planet. However, little is known about the melt structure and properties of Mg_2SiO_4 , primarily because of its high melting temperature of 2163K and the difficulty of performing high pressure x-ray experiments on these weakly scattering elements. In the **Yarger** group at **Arizona State**, some insight has been gained through the study of bulk Mg_2SiO_4 glass at high pressure, which can be synthesized from high temperatures using a containerless levitation technique (in collaboration with Chris Benmore and Richard Weber at ANL). The technique relies on capturing images of a polished flat glass in a DAC as a function of pressure. The glass is often coated with a thin layer of gold (10-100 nm thick) to improve the refractive index contrast and better define the edges of the sample. Care must be taken to insure a hydrostatic medium with no bridging of the polished sample between the two diamonds. The development of EOS measurements at high pressure is critical to understanding the thermodynamics of glasses and

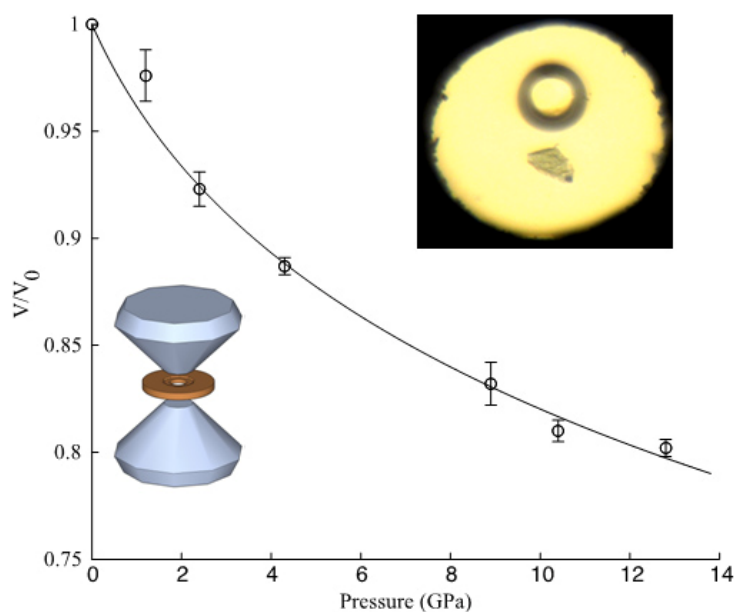


Figure 28. Top: Measured diamond anvil cell equation of state for gold-coated amorphous Mg_2SiO_4 in 14:3:1 methanol:ethanol: water at ambient temperature. Bottom: CDAC students from **Arizona State**, **Keri McKiernan** (left) and **Samrat Amin** (right).

liquids as well as being a requirement for proper scaling of x-ray and neutron diffraction data for pair distribution function (PDF) analysis.

In preliminary work, high-energy x-ray measurements on Mg_2SiO_4 glass up to pressures of 30 GPa were carried out using a perforated DAC, developed in part with technique development funding from CDAC. The average Mg-O coordination numbers were extracted from the experimental pair distribution functions assuming two cases (i) there is no change in Si-O coordination number with pressure and (ii) the average Si-O coordination number increases the same as for pure SiO_2 glass. Both analyses give similar results and show a gradual increase in the average Mg-O coordination number from 5 at ambient pressure to ~7 at 30 GPa. There is good qualitative agreement between the experimental structure and equation of state data (Fig. 28) for the glass compared to several recent molecular dynamics simulations carried out on liquid Mg_2SiO_4 . This work was performed by CDAC students **Samrat Amin** and **Keri McKiernan**.

A Primary Pressure Scale from First-Principles Theory – An accurate measurement of the pressure is a fundamental aspect of all high pressure experiments, and there is a need for continuous development of new and better pressure scales. Pressure calibration has generally relied on the experimentally-determined equations of state or spectroscopic properties of internal standards such gold or ruby. In recent work, a research team that includes the **Geophysical**

Laboratory's Ronald E. Cohen, along with colleagues from the **University of Illinois at Urbana-Champaign**, the **University of California – Berkeley**, and the **Cavendish Laboratory** has established a new pressure scale based on a high-accuracy solution to the underlying equations of quantum mechanics, which govern all material properties. In applying this first-principles approach, the group removed a key approximation employed in previous simulations, which has given their simulations an accuracy that rivals experiment.

The group developed an all-electron quantum Monte Carlo (QMC) method for solids that does not rely on pseudopotentials, and used it to construct a primary ultra-high-pressure calibration based on the equation of state of cubic boron nitride. The static contribution to the free energy was computed with the QMC method, and the phonon contribution was then obtained using density functional theory, which yields a high-accuracy calibration up to 900 GPa, and is directly applicable to experiments. The anharmonic Raman frequency shift was also computed with QMC simulations as a function of pressure and temperature, allowing optical pressure calibration. This all-electron method is applicable to first-row solids, providing a new reference for *ab initio* calculations of solids and benchmarks for pseudopotential accuracy.⁷⁵

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

For predicting the behavior of materials at extreme conditions, a knowledge of their vibrational properties is essential in that the thermodynamic information that may be extracted from such data provides another piece of the structure-property relationship. Synchrotron x-ray diffraction, x-ray spectroscopy and infrared spectroscopy are supplemented by laboratory Brillouin scattering techniques to investigate a wide variety of physical properties of alloys and semiconductors, crystalline solids, polymers and molecular materials.

Pressure-Induced Invar Behavior – At Caltech, CDAC graduate student **Mike Winterrose** completed studies of pressure-induced Invar behavior in Pd₃Fe. After the publication of the key initial observations,⁷⁶ the analysis of phonon modes in this material

under pressure were completed. The publication on phonons across the pressure-induced Invar transition in Pd₃Fe has been submitted to *Physical Review B*. In this work, the ⁵⁷Fe phonon partial density of states (PDOS) in L1₂-ordered Pd₃Fe was studied at high pressures by nuclear resonant inelastic x-ray scattering (NRIXS) measurements at HPCAT and density functional theory (DFT) calculations. As seen in Fig. 29, the NRIXS spectra showed that the stiffening of the ⁵⁷Fe PDOS with decreasing volume was slower from 12 to 24 GPa owing to the pressure-induced Invar transition in Pd₃Fe, with a change from a high-moment ferromagnetic (FM) state to a low-moment (LM) state observed by nuclear forward scattering. Force constants obtained from fitting to a Born-von Karman model showed a relative softening of the first-nearest-neighbor (1NN) Fe-Pd longitudinal force constants at the magnetic transition. For the FM low-pressure state, the DFT calculations gave a PDOS and 1NN longitudinal force constants in good agreement with experiment, but discrepancies for the high-pressure LM state suggest the presence of short-range magnetic order.

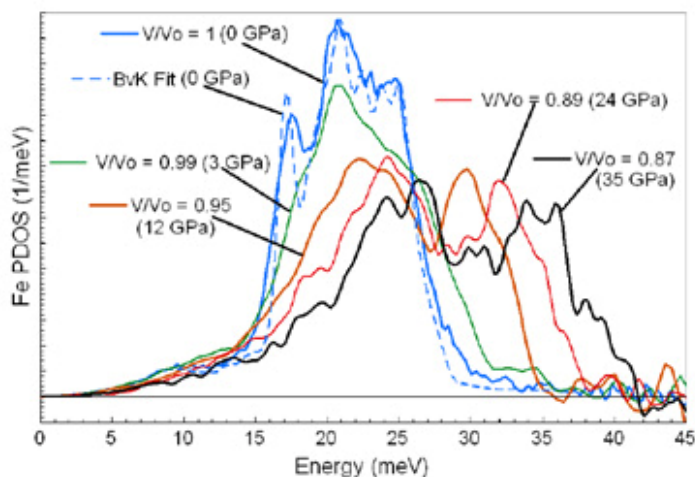


Figure 29. ⁵⁷Fe phonon PDOS from NRIXS measurements on L1₂-ordered Pd₃Fe. The Fe PDOS from a fit of the 0 GPa results to a Born-von Karman model is also shown (dashed line).

Anharmonic Behavior in bcc-Fe at High Temperatures – In the **Fultz** group at **Caltech**, nuclear resonant inelastic scattering experiments (NRIXS) have been performed on bcc ^{57}Fe at elevated temperatures, at both at HPCAT and XOR Sector 3 at the APS, by CDAC graduate student **Lisa Mauger**. The data were reduced to a phonon DOS using the PHOENIX software package. In the case of pure bcc-Fe, the partial phonon DOS is equal to the phonon DOS, and can be a direct measure of non-harmonic thermodynamic behavior.

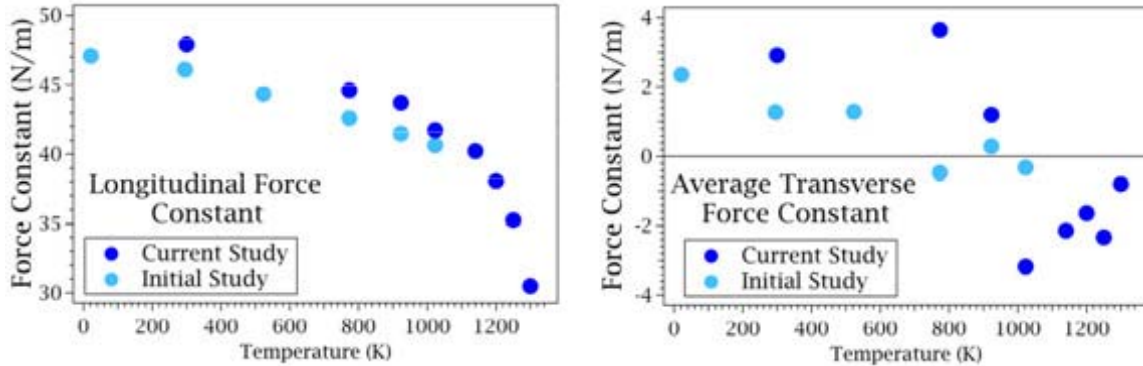


Figure 30. Optimized first-nearest neighbor Fe force constants are shown for a range of temperatures. The force constant tensors were projected onto the bonding axis for the longitudinal force constants. The transverse force constants are an average of the force constants perpendicular to the bonding axis. These force constants are compared with results from our earlier measurements on bcc Fe at lower temperatures.

A Born-von Karman model of lattice dynamics was used to interpret the thermal trends in terms of changes in interatomic force constants. The computational effort involved embedding the Born-von Karman model into a global optimization framework. Trial sets of force constants were generated randomly according to the differential evolution algorithm, and the resulting density of states (DOS) are compared with experimental data.⁷⁷ The process continued until the optimization converged to a single set of force constants – the “best fit” to the experimental NRIXS DOS. The optimization included atomic interactions up to fifth nearest neighbors. Each optimization used a 100 member populations and evolved for more than 100 generations, with the resulting sum of squared errors below 0.002 in all cases. These computations are still underway; current results for the trends for the first-nearest neighbor (1NN) force constants are shown in Fig. 30. (The second neighbor forces seem more constant with temperature, but show more scatter.) The data show an accelerating decline in the 1NN longitudinal force constant as the temperature increases beyond the Curie transition. Beyond 1000 K, the transverse 1NN force constant drops below zero, indicating the possibility of soft shear modes that may be related to the fcc-bcc martensitic phase transition.⁷⁸ These trends in the 1NN force constants are not consistent with a simple quasiharmonic interpretation of the phonon thermodynamics. The working hypothesis is that the anharmonicity at high temperatures is dominated by the change in the electronic DOS in Fe through the Curie temperature. When there are significant changes with temperature in the ability of conduction electrons to screen ion displacements in phonons, anharmonic behavior can result from electron-phonon interactions.

High Pressure Temperature Effects on Laves Phases – The cubic rare earth-iron Laves phases (C15 structure) have been studied extensively because of their interesting magnetic and magneto-mechanical properties, particularly giant magnetostriction. A famous example is the pseudo-binary compound $\text{Tb}_{0.3}\text{Dy}_{0.7}\text{Fe}_2$ (Terfenol-D), which shows giant magnetostriction with a high Curie temperature that saturates at moderate magnetic fields. When there is a strong coupling between shape and magnetism, magnetic effects on phonons are expected, but effects of magnetism on phonons are not well understood. The intricate interaction between the iron 3d electrons and the lanthanide 4f electrons should be affected significantly by pressure.

In the spring of 2010 CDAC graduate student **Jorge Muñoz (Caltech)** carried out NRIXS measurements at elevated temperatures (HPCAT) and pressure (APS/XOR Sector 3). The ^{57}Fe partial phonon DOS were measured for C15 RFe_2 ($\text{R} = \text{Tb, Dy, Er, Y}$) materials with different magnetostrictions, in a search for changes in phonons with pressure and temperature. The results are still being analyzed, but Fe phonon partial DOS curves at various pressures are presented in Fig. 31. Ancillary measurements of bulk modulus and thermal expansion at Caltech will give the parameters required to test for classical quasi-harmonic behavior, and any deviations will be interesting. The compounds TbFe_2 , ErFe_2 , and YFe_2 have similar Curie temperatures, (704, 578, 542 K, respectively⁷⁹), and all lose magnetism under pressures between 50 – 70 GPa at 300 K. The phonon DOS curves stiffen strongly with pressure, especially for TbFe_2 and YFe_2 .

The temperature dependence of the ^{57}Fe phonon partial DOS was measured on ErFe_2 , YFe_2 , and TbFe_2 from 300 K to 750 K. Over this range of temperatures, the softening of the phonon DOS is substantial. The Grüneisen parameters obtained from thermal expansion were large, approximately 4 for these compounds. Data from the literature,⁸⁰⁻⁸² also show that the Grüneisen parameter for some C15 compounds is around 4. It is tempting to attribute this behavior to magnetic and magnetoelastic properties, but other explanations are possible. ErFe_2 seems to show the same temperature dependence of the phonon DOS, and the same Grüneisen parameter, but does not stiffen so much under pressure as YFe_2 , and TbFe_2 .

Finally, diffraction data on ErFe_2 , YFe_2 , TbFe_2 and CeFe_2 under pressure show the C15 Laves phase to be stable over the pressure ranges of this work, and will be useful in determining a Grüneisen parameter from the pressure dependence of the phonon partial DOS. A major effort over the next year will be sorting out the systematic trends in these data, and relating the phonon thermodynamics to the magnetism and electronic structure.

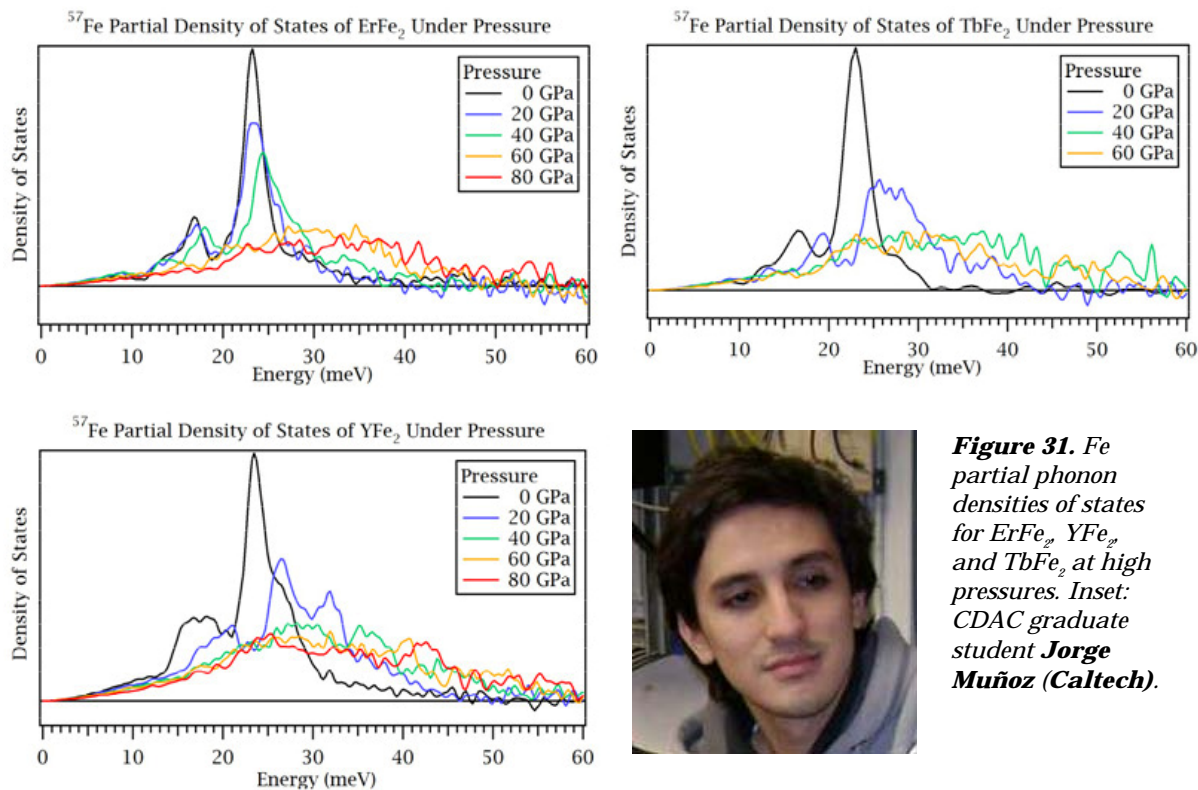


Figure 31. Fe partial phonon densities of states for ErFe_2 , YFe_2 , and TbFe_2 at high pressures. Inset: CDAC graduate student **Jorge Muñoz (Caltech)**.

Effects of Defects on Diamond Elasticity – Perfect crystals of any material are rare in nature or the lab, and this includes diamond. Point defects in crystals can modify material elastic properties at the atomic scale. Diamond is one of the most important materials in high-pressure

research and technology and knowledge of its elastic properties is critical to developing and modeling static and shock high-pressure experiments, as well as designing new materials with superhard properties. Having one of the highest shear moduli of any known material, diamond is also extremely challenging to measure accurately. CDAC graduate student **Yun-yuan Chang**, and partner **Steve Jacobsen** at **Northwestern University** are determining the elastic properties of a range of diamond materials using new GHz-ultrasonic methods along with a newly developed, hybrid optical micrometer for accurate length measurements. The results are providing improved values for diamond elastic constants (C_{ij}) and making it possible to scrutinize the variability in diamond C_{ij} reported in the literature, especially for CVD diamond.

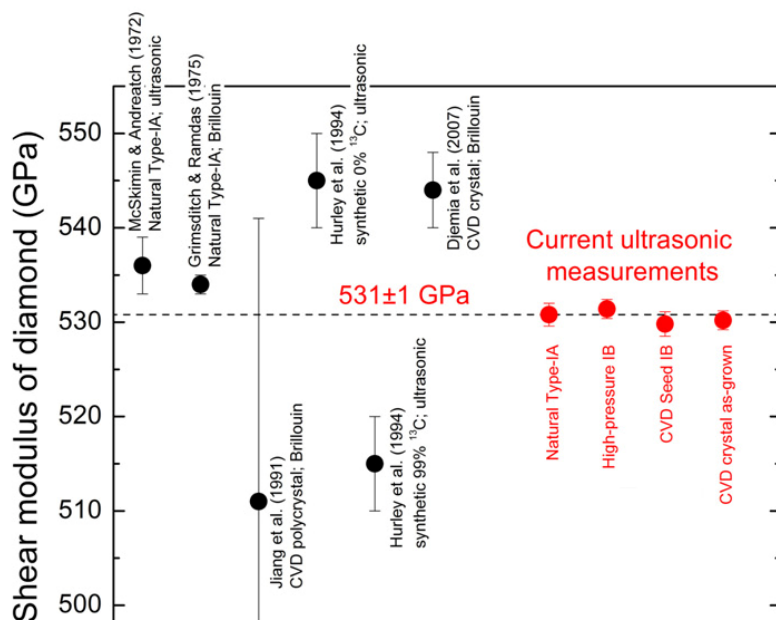


Figure 32. Reported shear moduli of diamond obtained with different methods. Right: CDAC graduate student **Yun-Yuan Chang** (Northwestern).



The optical micrometer, developed last year with CDAC support, uses sapphire lenses as both a double-contact point and optical port to view the contact area. One lens is tracked by a laser heterodyne interferometer. During Year 7, the new instrument has been tested using several grade00 gauge blocks. An example measurement of a 100 μm gauge block displays a value of $100.00 \pm 0.03 \mu\text{m}$, corrected for air temperature, pressure, and relative humidity.

Previous measurements of the shear modulus for various forms of diamond using different techniques give a range of values from about 510-545 GPa, with some examples shown in Fig. 32. Does the reported variability in shear modulus of diamond reflect differences in material properties, or measurement uncertainties? The current GHz-ultrasonic study suggests a much narrower range in diamond elastic properties between

various types of diamond, and provides lower uncertainty in STP-diamond elasticity measurements, a benchmark for future high P - T studies of diamond properties.

High P - T Thermoelastic Behavior of a Dual Oxide Composite Material: $\text{FeO} + \text{SiO}_2$ -

The Kavner group at UCLA is using some of the principles of composite properties to design and test materials for high pressure, high temperature equation of state measurements in the laser heated DAC in conjunction with x-ray diffraction. Since many high-pressure, high-temperature experiments rely on the presence of more than one material in the diamond cell sample chamber, by definition these experiments are actually composite experiments.

One approach is to leverage an Fe_2SiO_4 starting composition to synthesize *in situ* a well mixed FeO and SiO_2 assemblage and measure their relative equations of state directly at pressure and temperature conditions of the lower mantle. This approach seeks out a middle ground between measuring densities of single-phase materials, which is subject to large uncertainties in pressure

calibration, especially at high P and T , and measuring properties of complex multicomponent assemblages, which adds additional uncertainties due to variable chemistry and uncertain phase diagrams. This work forms part of the dissertation research of CDAC graduate student **Matt Armentrout**.

The results point to an inconsistency between previously determined high pressure, high temperature equations of state of SiO_2 ⁸³ and FeO ,⁸⁴⁻⁸⁵ as shown in Fig. 33. Therefore, at least one of these equations of state needs to be revised. Each choice has a very different outcome. If the existing SiO_2 equation of state is used as a pressure standard, the present wustite data and Seagle and Campbell's⁸⁶ wustite data cannot be reconciled with a single high pressure equation of state. However, if Seagle and Campbell's wustite equation of state is used as

the pressure standard; the current data combined with others' high P - T SiO_2 data yield a self-consistent equation of state for stishovite. Therefore, the preferred approach is to refine a high P - T equation of state for SiO_2 stishovite. The best fit to the Mie-Grüneisen-Debye equation of state of

stishovite yields $V_0 = 14.015 \text{ cm}^3/\text{mol}$, $K_0 = 299 \text{ GPa}$, $K' = 4$, $\theta_0 = 1160 \text{ K}$, $\gamma_0 = 1.28$ (3), and $q = 1.9$ (2).

Elasticity of Iron at Extreme

Conditions - Iron is the most abundant metal in the universe and in the planetary cores, and is an archetypal metal for understanding d - and f -band metals and compounds. Postdoctoral fellow **Zhu Mao** (Figure 34) and graduate student **James Liu** at **University of Texas - Austin** have conducted high-energy resolution inelastic x-ray scattering (HERIXS) and nuclear resonant inelastic x-ray scattering experiments (NRIXS) on hcp-Fe to measure its sound velocities and elastic anisotropies under high pressures and temperatures. The V_p - ρ (compressional

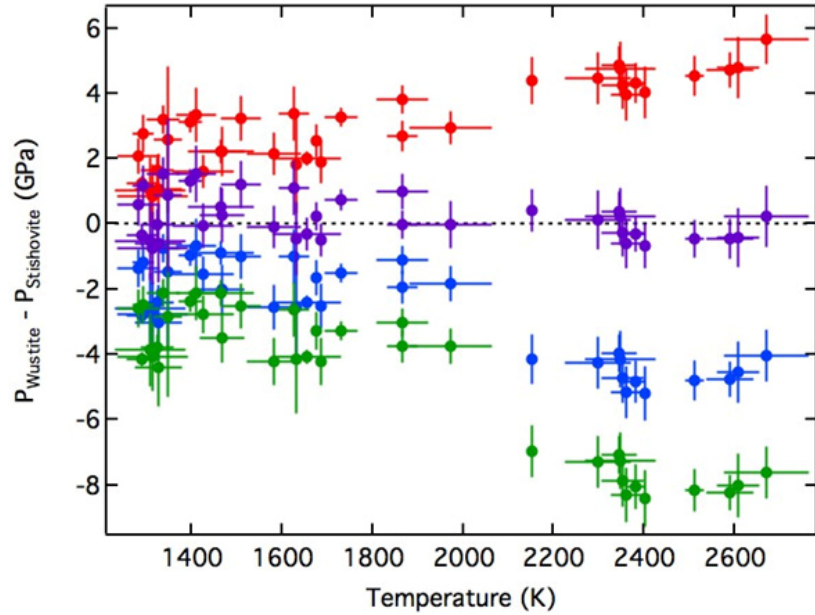


Figure 33. Pressure mismatch between stishovite and wustite as a function of temperature. Previously determined high pressure and temperature equations of state for stishovite and FeO were used to infer their pressures in our experiments. Three different high P - T equations of state for SiO_2 were used, corresponding to blue, green, and red data points. The results from a best fit equation of state are also shown (purple). Right: CDAC graduate student **Matt Armentrout (UCLA)**.

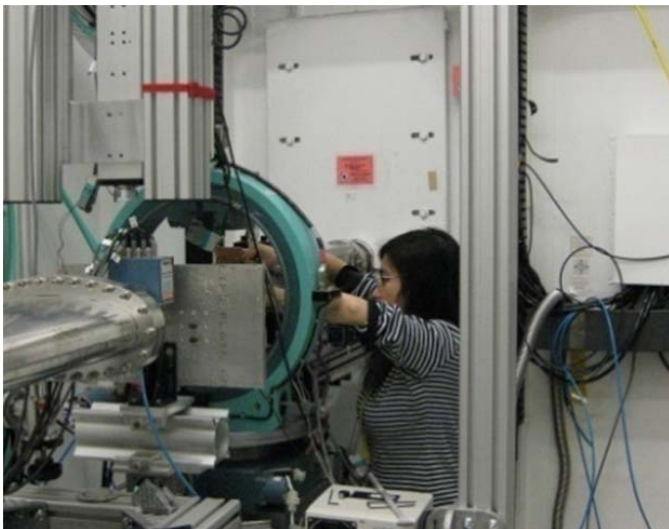


Figure 34. Postdoctoral **Zhu Mao (UT Austin)** working on the HERIXS experiments at the Advanced Photon Source.

wave velocity-density) data at a given temperature can be well described by an empirical power-law function with a concave behavior at higher densities, instead of the linear approximation.⁸⁷ Furthermore, high temperatures result in significant decreases in the V_p along the density profile of the Earth's core. This behavior significantly differs from that of Co and other transition metals, and thus calls for further theoretical understanding on the elasticity of *d*- and *f*-band metals and compounds under extreme environments.

2.4 Plasticity, Yield Strength, and Deformation

The field of extreme conditions research includes high strain rates as well as high pressures and temperatures, and material properties under high strain rates are of primary importance for stockpile stewardship applications. Strain-induced texture development in both metals and crystalline solids are studied by several CDAC groups, and these groups continue to pursue technical advancements in both data collection and analysis. Such investigations, carried out with both neutron and x-ray diffraction methods, provide insight into possible mechanisms for phase transformations in a wide variety of materials.

Combining Resistive and Laser Heating in DAC Deformation Experiments – Radial diffraction with the DAC has become an important technique for deforming materials at ultrahigh pressure. Deformation mechanisms are inferred from experimentally produced lattice strains and lattice preferred orientation observed *in-situ* at pressures relevant to the deep Earth. So far most of these experiments have been performed at ambient temperature. It is questionable whether room temperature studies are appropriate for extrapolation to behavior in planetary interiors where materials are deforming at both high pressure and temperature. In order to address this limitation the **Wenk** group at **Berkeley** has developed a laser heating system for radial DAC experiments and have applied the method to study *in-situ* phase transformation and deformation of bcc (•), fcc (•) and hcp (•) iron at a range of pressures and temperatures up to 30 GPa and 1900 K.⁸⁸



Figure 35. Left: Graphite heater within a DAC. Center: Resistive heating assembly with DAC cell set up inside and thermocouples attached. Right: Fe-Ni alloy sample at 2000 K inside a DAC.

Laser heating, while indispensable for many high temperature DAC experiments, has limitations. In particular, temperature gradients are severe and low temperatures cannot be applied. Thus, the group is also working on advancing resistive heating for the radial DAC geometry and has made significant progress at HPCAT⁸⁹ as well as at ALS 12.2.2. Figure 35 (left) displays a graphite heater assembled inside the DAC. A new resistive heating frame was developed to be light-weight, small and very flexible with membrane pressure control, large opening windows to allow radial diffraction geometry as well as laser heating pathway from the top (Fig. 35, center). A breakthrough was achieved in October 2009 in reaching 2000 K with Fe-Ni alloys (at 40 GPa with resistive heating, Fig. 35, right). In March 2010, the group was able to combine resistive and laser heating, and reach temperatures of 3000 K in ringwoodite. The new technique has been applied to investigate changes in deformation mechanisms in periclase, ringwoodite and Fe-Ni alloys as well as to study phase transformations in FeO (Fig. 36).

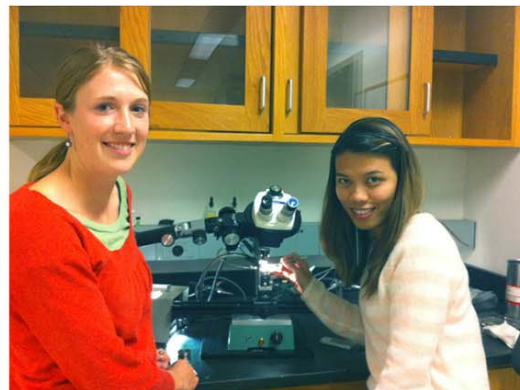
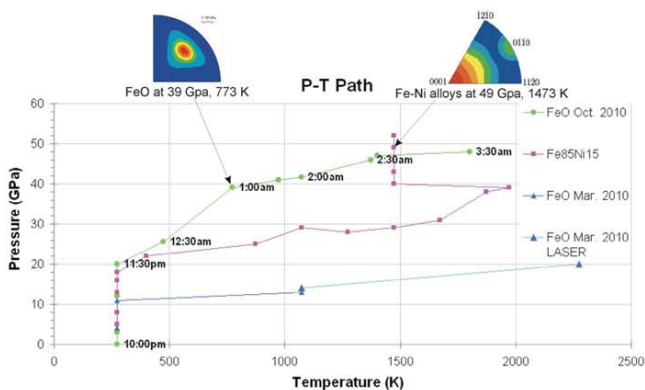


Figure 36. Left: P-T path of resistive heating experiment on FeO (green and blue) and Fe-Ni alloys (red). Increasing pressure to 20 GPa introduced the phase transformation from cubic to rhombohedral in FeO. Pressure and temperature were increased on the Fe-Ni alloys and resulted in a transformations from bcc (•), to fcc (•) and hcp (•) at a range of pressures and temperatures up to 52 GPa and 2000 K. Right: CDAC graduate students from **Wenk's** group at **Berkeley**, **Pamela Kaercher** (left) and **Jane Kanitpanyacharoen** (right).

The Role of Phase Transformations on Texture Changes in Uranium – The Wenk group continues to make use of the unique features of the HIPPO TOF neutron diffractometer at LANSCE to measure *in situ* texture changes during phase transformations. The research on zirconium⁹⁰ and titanium⁹¹ documented regular variant selection during the hcp-bcc-hcp transformation based on a Burgers relationship. Similarly, variant selection occurs in iron during the bcc-fcc transformation.⁹² Phase transformations occur in many low symmetry minerals as well and it is critical to understand the significance of applied stress during a phase transformation. For this reason the **Wenk** group has begun investigating a low-symmetry metal system. In *uranium* there are two phase transformations: orthorhombic (α) up to 660°C, tetragonal (β), from 668°C to 766°C and bcc (γ) above 766°C.⁹³ Does an orthorhombic crystal remember its orientation after transforming to a cubic structure?

In December 2009 the group performed experiments on U-0.7Ti with the D-DIA apparatus at the APS under varying temperature and pressure to induce phase transformations under stress. At high pressure this brittle material became ductile, and a very strong texture develops at 4 GPa and room temperature. In follow-up experiments with HIPPO, texture memory and variant selection without excessive grain growth was documented. Uranium is not only a fascinating system because of the low crystal symmetries but also because it has shape memory properties (U-Nb⁹⁴) and is relevant for NNSA science. This is a collaborative project between researchers at **LANL** (J. Bingert, D. Brown, S. Vogel), **APS** (Y. Wang) and **Berkeley**. New CDAC graduate student **Pamela Kaercher** is participating in this research.

Deformation Mechanisms in Hexagonal Metals – For some time the Wenk group has been interested in texture development in hexagonal metals, which have received a lot of attention in materials science due to important applications as light structural metals (Mg, Ti) and applications in the reactor industry (Zr, Hf). CDAC graduate student **Jane Kanitpanyacharoen** has extended these studies to osmium and zinc using radial DAC techniques. Contrary to Zn, where texture development is gradual and attributed to slip, a strong texture immediately develops in Os due to mechanical twinning. These observations were confirmed with D-DIA experiments on Hf, Zr, Zn and Cd. With D-DIA techniques, it has been shown convincingly that increasing temperature at high pressure reduces twinning activity (Fig. 37). These observations also apply to geophysics, because the inner core of the Earth is thought to be composed of hcp iron. At inner core conditions twinning is unlikely, but in high stress experiments it may dominate.¹³

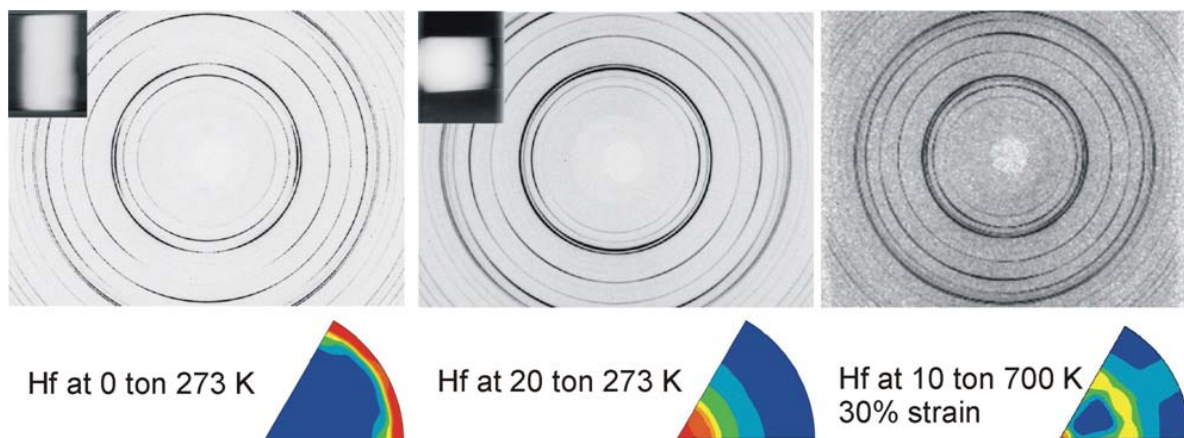


Figure 37. Deformation of hafnium as observed with a D-DIA apparatus.

Deformation Mechanisms in Postperovskite (pPv) and Anisotropy in the Lowermost

Mantle – MgSiO₃ pPv is thought to be a major phase in the Earth's lowermost mantle (D" region).

It is critically important to understand the plastic deformation properties of pPv in order to understand the rheology and seismic anisotropy of this region. Previous room temperature DAC deformation experiments to 150 GPa on MgGeO₃ pPv⁹⁵ and MgSiO₃ pPv⁹⁶ produced textures consistent with slip on (100) and/or {110} lattice planes. However, D-DIA experiments on the pPv analog CaIrO₃ identified (010)[100] slip.⁹⁷ To resolve this controversy it was necessary to perform new deformation experiments on MgSiO₃ pPv and MgGeO₃ pPv. It was observed that at large strains a texture evolves with a maximum at [001], which is consistent with (001) slip as confirmed with polycrystal plasticity simulations.⁹⁸ MgGeO₃ post-perovskite was synthesized and deformed in a DAC using both MgGeO₃ enstatite and MgGeO₃ perovskite as starting materials.⁹⁹ Different starting materials produce different transformation textures. Thus previous conclusions need to be revised. The new (001) slip system is compatible with observed seismic anisotropy in the D" zone, *i.e.* fast S-waves polarized parallel to the core-mantle boundary and an opposite anisotropy behavior for S-waves and P-waves.

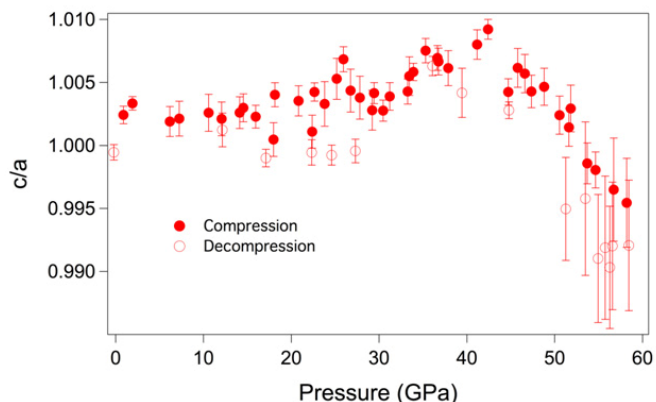


Figure 38. The *c/a* ratio (normalized to the room pressure *c/a* ratio) of WB₄ versus pressure showing collapse of the *c*-axis at about 42 GPa.

High Pressure Study of Ultra-Incompressible WB₄ – A high-pressure x-ray diffraction experiment on tungsten tetraboride, a new ultra-incompressible superhard material, was conducted by the **Kavner** group at **UCLA**. Angle-dispersive x-ray diffraction was carried out on Beamline 12.2.2 at the Advanced Light Source at Lawrence Berkeley National Laboratory. A third-order Birch-Murnaghan equation of state was used to fit the measured pressure-volume data. Using only the compression data, fitting the *P-V* relation yields $K_0 = 308(3)$ GPa with fixed $K_0' = 4.0$. Figure 38 shows that at ~ 40 GPa, the *c*-axis becomes more compressible, which suggests a reversible collapse of the *c* lattice parameter at this pressure. An additional set of high pressure experiments are planned to confirm this observation of structural changes in networked boron-based ultrahard materials.

2.5 Electronic and Magnetic Structure and Dynamics

Physical property measurements at extreme conditions are demanding from the technical standpoint, and improving the apparatus and methods for these types of experiments are ongoing in many CDAC groups. Both laboratory-based and synchrotron-based techniques for investigating electronic and magnetic properties are carried out in parallel with structural studies on key materials. The unprecedented accuracy and resolution of current measurement capabilities are now providing information on physical properties of materials at the level of electrons, and hold great promise for not only understanding existing materials, but also for the preparation of new materials as well.

High Pressure XMCD and Mössbauer Measurements on Eu Metal – Divalent Eu ($4f^7$) orders antiferromagnetically at ambient pressure with $T_N \approx 90$ K. Under pressure, if Eu transforms toward trivalent ($4f^6$), as reported in previous studies, the magnetism should be weakened. To help understand the pressure-induced valence change in Eu metal, **Wenli Bi** has studied the magnetism of Eu under pressure from XMCD experiments at APS beamline 4-ID-D with the help of **Daniel Haskell** and **Narcizo Souza-Neto**. The measurements were done at ~ 4.6 K in a continuous flow cryostat and under 4 T using a superconducting magnet. As shown in Fig. 39, the magnetism goes up drastically under pressure to 20 GPa and then decreases at higher pressures to 60 GPa. The increase

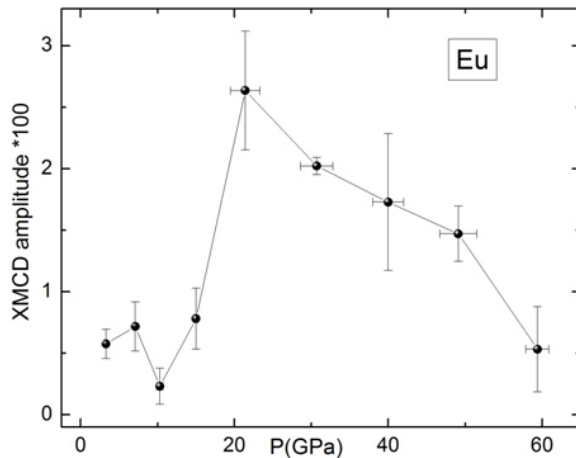


Figure 39. Amplitude of the XMCD signal to 60 GPa.

of magnetism to 20 GPa supports our conclusion from the above XANES experiments that Eu (see Section 2.1) remains divalent in this pressure range. To confirm previous results from the XANES and XMCD experiments, with the help of graduate student **Gilberto Fabbris**, along with **Erchan Alp** and **Jiyong Zhao** from sector APS Sector 3 (XOR), room temperature Mössbauer spectroscopy experiments were also carried out at beamline 3-ID, to 25 GPa. The isomer shift versus pressure agrees well with previous reports¹⁰⁰⁻¹⁰¹ where, however, there is concern that the data may have been interpreted incorrectly. Further room temperature and low temperature experiments to Mbar pressures are planned for the near future.

Magnetic Properties of Single Crystal EuO at High Pressure – At ambient pressure EuO orders ferromagnetically at 69 K. T_c goes up drastically under pressure with T_c higher than 200 K at 13 GPa.¹⁰² Above this pressure T_c decreases to ~ 140 K at 20 GPa. To study the ordering temperature under higher pressures and search for possible pressure-induced superconductivity, **Wenli Bi** measured the ac susceptibility under hydrostatic pressure to 46 GPa in a nonmagnetic DAC using He as pressure medium. The ferromagnetic transition was observed to 10 GPa. Above 10 GPa the ferromagnetic transition could not be resolved because the transition became broader, up to 46 GPa, the highest pressure reached in the experiment. No superconducting transition was observed between 4 K and 180 K up to 46 GPa.

High Pressure Magnetic Susceptibility Studies of Iron Pnictide Superconductors – EuFe_2As_2 exhibits interesting magnetic properties under pressure, ordering antiferromagnetically at ambient temperature with T_N near 19 K. A previous study to 12 GPa shows that EuFe_2As_2 first becomes superconducting in a very narrow pressure range (2.5 – 2.7 GPa) and then becomes ferromagnetic above 8 GPa.¹⁰³ To measure the Curie temperature at higher pressures and search for superconductivity, **Wenli Bi** and **Hunter Banks** at **Washington University in St. Louis** and visitor **Liling Sun** from the **Institute of Physics-Chinese Academy of Sciences**) carried out an

ac susceptibility experiment on a single crystalline sample provided by **K. Matsubayashi** in a nonmagnetic DAC (0.5 mm culet) under hydrostatic pressures to 48.5 GPa with He as pressure medium. Unfortunately, due to the small sample size (< 100 microns) necessary in the hydrostatic experiment, neither the antiferromagnetic nor the ferromagnetic transitions were observed. With a much bigger sample (~200 micron), the antiferromagnetic ordering could be clearly resolved. Over the measured pressure and temperature (4-70 K) range, no superconducting transition was observed.

Solid Solutions in the Iron-Pnictide Superconductor Systems – At ambient pressure EuFe_2As_2 orders antiferromagnetically while the solid solutions $\text{EuFe}_2\text{As}_{1.4}\text{P}_{0.6}$ and $\text{EuFe}_{1.715}\text{Co}_{0.285}\text{As}_2$ order ferromagnetically. The doped samples $\text{EuFe}_2\text{As}_{1.4}\text{P}_{0.6}$ and $\text{EuFe}_{1.78}\text{Co}_{0.22}\text{As}_2$ were previously reported to exhibit, in coexistence with the ferromagnetism, bulk superconductivity at ambient pressure. To study the magnetic properties and possible superconductivity in these samples under hydrostatic pressure, the temperature-dependent ac susceptibility of EuFe_2As_2 , $\text{EuFe}_2\text{As}_{1.4}\text{P}_{0.6}$, and $\text{EuFe}_{1.715}\text{Co}_{0.285}\text{As}_2$ were measured to hydrostatic pressures as high as 0.8 GPa. It was found that the magnetic ordering temperatures increase linearly with pressure at the rates +0.35(3), +2.4(1), and +2.0(1) K/GPa, respectively. In these measurements no evidence for superconductivity was found in any of the samples to 0.8 GPa in the temperature range 10-60 K.

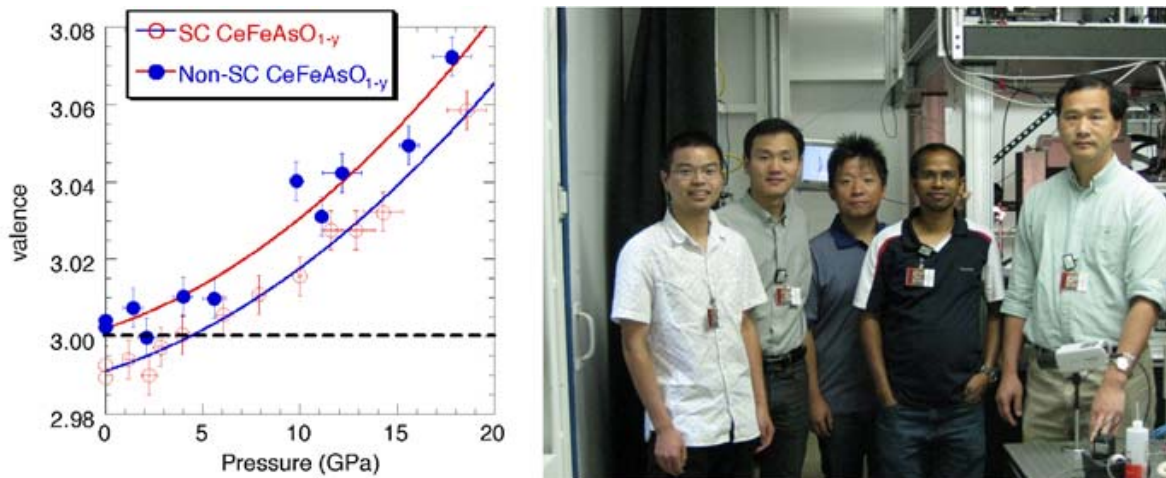


Figure 40. Left: Variation in the valence of Ce with pressure as determined with PFY-XAS spectra for superconducting CeFeAsO_{1-y} and non-superconducting CeFeAsO_{1-y} at 300 K. Solid lines are fits to the data assuming parabolic functions. The dashed line corresponds to a valence of 3.0. Right: **UT Austin** group at the APS.

Iron-Based Pnictide Superconductors at High Pressure and Low Temperature – Iron pnictide compounds—which are based on conducting layers of iron and arsenic—were discovered in 2008 to possess superconducting properties while under pressure and also upon doping. Tuning pressure provides a potent means to understand their properties. The iron arsenides such as AFe_2As_2 , where “A” denotes the alkaline-earth metals Ba, Ca, or Sr, displayed complicated structural, magnetic, and superconducting properties on and around the boundary between an antiferromagnetically ordered orthorhombic phase (AFM-O) and a superconducting phase (SC). The superconductivity is taking place at the iron layer where iron is in the Fe^{2+} state. The parent state of the ferropnictides forms a “spin density wave” type AFM strip phase. The **UT Austin** group of **Jung-Fu Lin** collaborates with Dr. H. Yamaoka and I. Jarrige of the Spring-8 and Dr. C. Jin and J. Wu of the Chinese Academy of Sciences to investigate the electronic structures of these superconductors under high pressures and low temperatures using resonant x-ray emission spectroscopy (RXES), x-ray absorption spectroscopy in the partial fluorescence mode (PFY-XAS), and synchrotron Mössbauer spectroscopy (SMS) at the Advanced Photon Source and the Spring-8 (Fig. 40). Results show that the valence of Ce in the related compound CeIrSi_3 rapidly increases at $P > 3$ GPa but is nearly constant until about 3 GPa, suggesting a possible scenario in which the hybridization destroys the superconductivity in CeIrSi_3 at high pressure.¹⁰⁴ The electronic and magnetic structures of the iron-

based arsenide superconductors (*e.g.*, BaFe₂As₂) have also been investigated using synchrotron Mössbauer and resonant x-ray emission spectroscopies at high pressures and low temperatures to understand the interplay between superconductivity and electronic/magnetic structures. Results show that pressure significantly decreases the Neel temperature of the “122” BaFe₂As₂ compound. These and related studies are underway using various synchrotron techniques available at the APS.

Bonding Changes in Hot Fluid Hydrogen at Megabar Pressures – Raman spectroscopy in the laser heated DAC has been employed to probe the bonding state and phase diagram of hot dense hydrogen up to 140 GPa and 1500 K. The **Carnegie** group, led by **Alexander Goncharov**, has discovered a pronounced discontinuous softening of the molecular vibron at elevated temperatures above 40 GPa along with a large broadening and decrease in intensity of the roton bands. These phenomena indicate the existence of a state of the fluid having significantly modified intramolecular bonding. Above 110 GPa it is found that that the change in this novel fluid becomes less pronounced. The results are consistent with the existence of a pressure-induced structural transformation in the fluid related to the presence of a temperature maximum in the melting line as a function of pressure. Fitted spectra at 1500 K and 1800 K (red lines in Fig. 41) were calculated with a model that explicitly accounts for thermal gradients in the sample region and discontinuities in vibron behavior; the dashed blue line shows the best fit of the data using a model without the vibron discontinuity. The red arrow points to the transition originating in the first excited vibrational state (1,2) in the 1500 K and 1800 K spectra.¹⁰⁵⁻¹⁰⁶

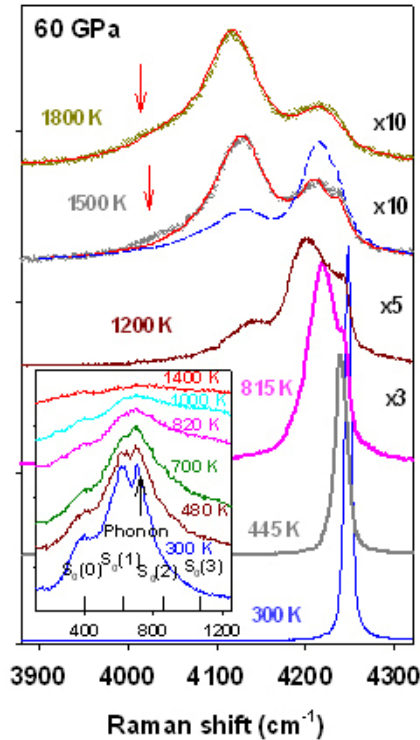


Figure 41. Spectra of hot dense molecular hydrogen at 60 GPa and 1500 and 1800 K. (See text). Inset: Vanishing of the E_{2g} phonon mode and broadening and diminishing of the $S_0(J)$ roton bands above 815 K. The vibron amplitude at 300 K is about five times larger than that of the strongest roton band.

Spin of Semiconductor Quantum Dots under Hydrostatic Pressure – Spin coherence dynamics of semiconductor CdSe quantum dots under hydrostatic pressure have been investigated by combining the ultrafast optical orientation method with the diamond-anvil cell technique. **Alex Goncharov** at **Carnegie** and co-workers from the **University of Maryland** have shown that the spin confined within quantum dots is observed to be robust up to several gigapascals, while electron and exciton Landé g factors show novel bistable characteristics prior to the first-order structural transition. This observation is attributed to the existence of a theoretically predicted metastable intermediate state at the nanoscale, for which there has been no previous experimental support. The results also reveal pressure enhanced fundamental exchange interactions for large-sized quantum dots with sizable anisotropy. These findings¹⁰⁷ provide insight into underlying mechanisms of long-debated nanoscale solid-state transformations in semiconductors and are also crucial for the development of future quantum information processing and manipulation based on spin qubits of quantum dots.

On the "Hidden Order" and Antiferromagnetic Ground State of URu₂Si₂ – Since its discovery over 25 years ago, the “hidden order” (HO) state of URu₂Si₂ has remained a perplexing mystery of condensed-matter physics.¹⁰⁸⁻¹¹⁰ Below $T_f=17.5$ K, the HO state is revealed in a variety of bulk measurements, but to date no satisfactory order parameter has been advanced to describe the nature of this ordered state. Under a modest pressure of 1.5 GPa,¹¹¹ the HO ground state yields to a

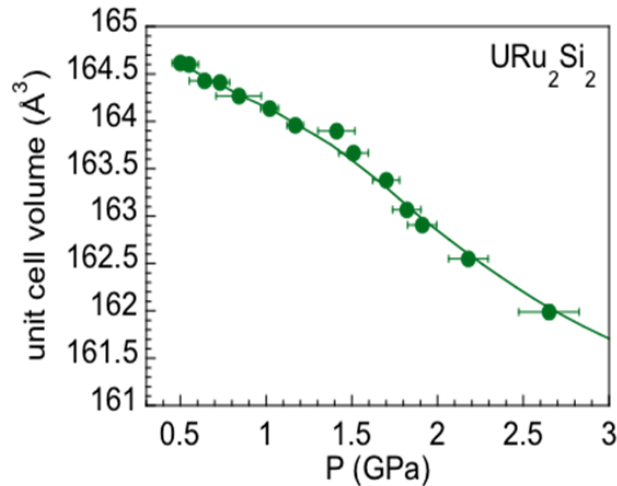


Figure 42. Pressure-volume relation for URu_2Si_2 illustrating a change in compression mechanism at approximately 1.5 GPa.

broken in proposed nematic ordering models of the HO state. A small kink in the compressibility of the sample appears near 1.5 GPa (Fig 42), the critical pressure where the paramagnetic, HO, and AFM states meet in the low-temperature region of the P - T phase diagram.

Pressure Reveals Hidden Insights in Ferroelectric Perovskites – Two new studies point to the important role that pressure plays in understanding and creating new ferroelectric materials. Lead-based relaxor ferroelectrics with complex perovskite structures exhibit a strong frequency-dispersive dielectric permittivity with a broad and smooth temperature dependence. Their high permittivity and high piezoelectric constants make them suitable for applications in devices for sonar or medical imaging. While extensive theoretical and experimental studies have advanced our understanding of relaxors, their properties are still poorly understood. These difficulties stem from the complexity of the materials, which have a high degree of compositional, structural, and polar disorder.

Using a combination of high pressure synchrotron x-ray diffraction, Raman and Brillouin scattering techniques, **Muhtar Ahart** and colleagues from **Carnegie** and **Sandia National Laboratories** report on experiments revealing that the pressure-induced relaxor-to-ferroelectric crossover in disordered $Pb(Sc_{0.5}Nb_{0.5})O_3$ is a typical example of such phenomena in disordered perovskite systems and that such behavior can be attributed to the relaxation of polar nanoregions in these materials. The pressure-dependent Raman bands are broad, which is a relaxor-specific spectral signature, and indicate a structural phase transition (Fig. 43). A significant softening in the longitudinal acoustic mode is also observed. The similarity in relaxation times found in the temperature and pressure dependencies show that the softening of the longitudinal acoustic mode may be attributed to electrostrictive coupling between polar nanoregions and acoustic modes. X-ray diffraction reveals that the material is characterized by two distinct pressure-volume compression curves below and above the phase transition pressure. This work is a tribute to co-author **George Samara** from **Sandia**. He was a leading figure in the field of ferroelectrics and was the first to demonstrate the importance of the pressure variable in understanding these important materials. He helped launch this CDAC collaboration but passed away in 2006.¹⁰

In a related study, **P. Ganesh** and collaborators from **Carnegie**, **NIST**, **Argonne**, and **Simon Fraser University** showed that correlations between chemically ordered regions, which act as polar nanoregions, are responsible for the relaxor behavior in complex relaxors and relaxor ferroelectrics such as $Pb(Mg_{1/3}Nb_{2/3})O_3$ and $Pb(Sc_{1/2}Nb_{1/2})O_3$, which are technologically important due to their colossal dielectric and/or piezoelectric response in the relaxor phase. The origin of the so-called relaxor phase in these materials, which show a frequency-dependent dielectric constant that deviates

long-range antiferromagnetic (AFM) ground state through a first-order transition.¹¹² Understanding the relationship between these two pressure-dependent ground states could provide clues to the nature of the ambient-pressure HO state. To this end, and combining temperature-dependent electron diffraction and x-ray diffraction in the DAC, **Jason Jeffries**, a CDAC laboratory partner from **LLNL**, has embarked on a series of experiments designed to probe the crystallography of URu_2Si_2 in the paramagnetic state, the HO ground state, and the pressure-induced AFM ground state.

Results show that the crystalline symmetry is conserved in all three electronic phases, and as well as a conservation of rotational symmetry, a symmetry that is

from the Curie-Weiss temperature behavior of normal ferroelectrics, has been a topic of debate for nearly half a century. A joint theoretical and experimental study was performed to explain the origin of the characteristic diffuse scattering observed in these materials in their ferroelectric, relaxor and paraelectric phases and investigate their temperature and pressure dependence. The findings suggest a possible route to engineer superior dielectric/piezoelectric materials by nano-engineering different types of chemically ordered regions that will enhance the correlations between the polar nanoregions.¹¹³

Direct Observations of the Band Gap of He under Pressure – Direct measurements of the band gap of solid helium (⁴He) at high pressure are beyond the capabilities of typical optical techniques. This is because the band gap and associated excitations are masked by absorption by the gasket and anvils of the pressure cell. Until now, there has not been an experimental technique with the energy range and resolution needed for these types of studies. As a result of new advances in two-photon inelastic x-ray scattering (IXS) spectroscopy, however, it is now possible to make these challenging measurements under pressure.

A group led by CDAC Associate Director **Ho-kwang Mao (Carnegie)** with scientists from **HPCAT, HPSynC, NIST, University of Chicago, Brookhaven, SLAC, and Stanford** has succeeded in probing the high-pressure electronic structure of helium at 300 K. Features of the electronic spectrum in the 20-40 eV range are accessible through measurements of the energy loss from high energy x-rays incident on a sample at high pressure. In addition, with IXS it is possible to measure the momentum transfer, which reveals the dispersion behavior of the excitations with pressure, giving rich information about the features the electronic structure of the solid.

Figure 44 shows the raw data from the IXS experiment at 13.4 GPa along with data from the Be gasket and the diamond anvils. Manipulation of the background spectra made it possible to extract the spectrum of He with greater clarity than has been possible before. In addition to the sharp exciton peak at 24.4 eV and a sharp absorption edge at 23.7 eV, additional features are now resolved at higher energy. Combined with data taken at a series of momentum transfers as well as theoretical calculations, the results show that the excitations in solid helium have a more complex

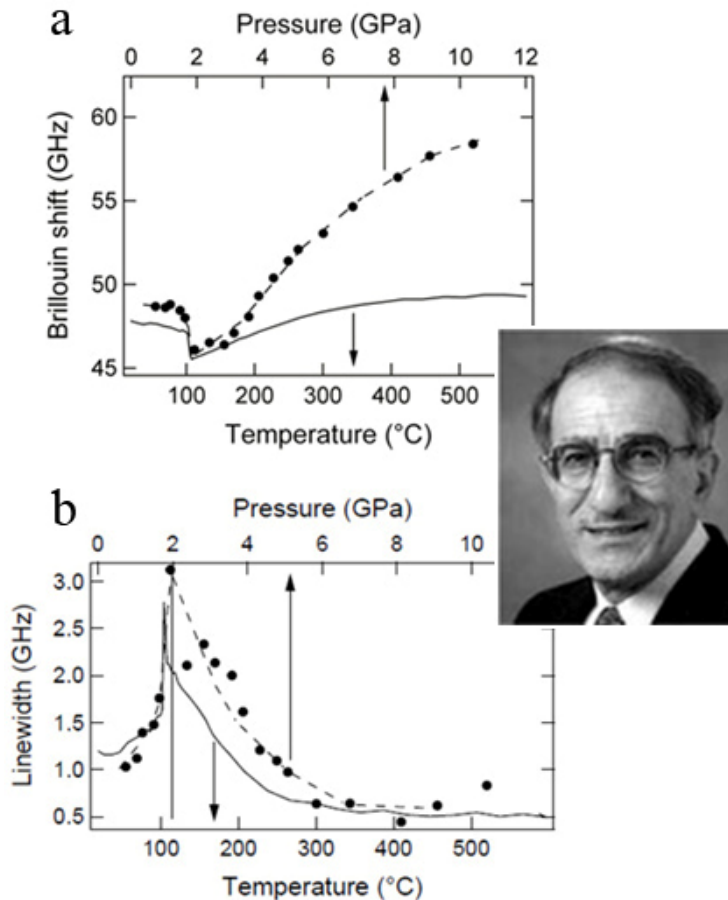


Figure 43. a) Pressure dependence of the longitudinal-acoustic-mode (circles). The symbols are data and the dashed curve is a guide to the eye. For comparison, the temperature dependence of the longitudinal-acoustic-mode is also plotted (solid curve). b) Pressure dependence of the linewidth of the longitudinal-acoustic-mode (solid circle). For comparison, the temperature dependence of the linewidth of the longitudinal-acoustic-mode is also plotted (solid curve). Inset: **George Samara (1936-2006)**.

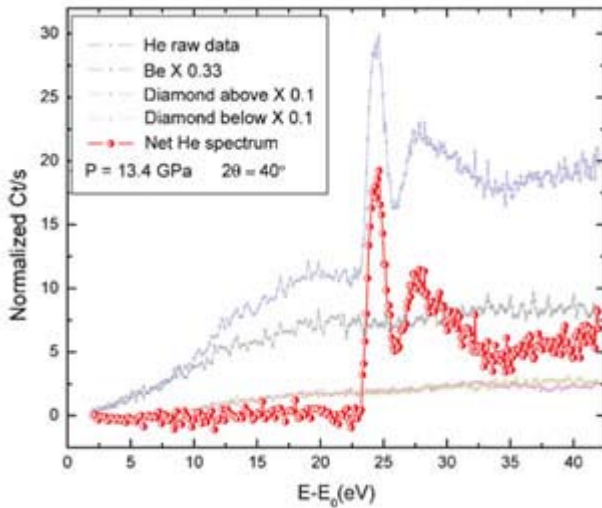


Figure 44. Raw data (top trace) and net data (red trace) from the IXS measurements on ^4He at 13.4 GPa. New features observed in this series of measurements include the excitations beyond 25 eV.

superconducting state can be induced under two different pressure regimes in a bismuth cuprate crystal of composition $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10.8}$, referred to as Bi2223. This material has a layered structure, with insulating bismuth-oxide layers sandwiching layers of strontium oxide, copper oxide, and calcium oxide. The outermost and inner copper oxide layers have different physical properties resulting in an imbalance of electric charge between the layers. It appears that this unusual two-step phenomenon comes from competition in electronic behavior between different kinds of copper-oxygen layers in the crystal.

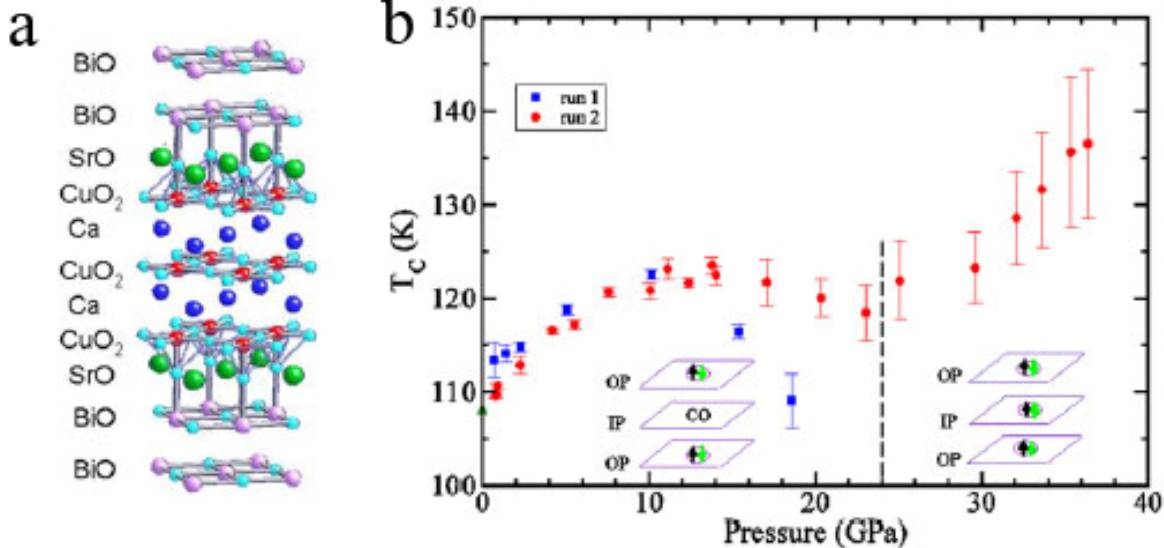


Figure 45. a) Structure of the Bi2223 cuprate conductor. Light blue spheres, copper atoms; red spheres, oxygen atoms. The two different types of copper-oxygen sheets in the structure lead to an imbalance of electronic charge. b) Variation of superconducting transition temperature with pressure. Different types of electronic order are shown schematically below the data. OP, outer planes; IP, inner plane. In the higher pressure range, condensed Cooper pairs exit in all three planes, while at lower pressure, competing order (CO) within the inner plane lessens the interaction between the two outer planes.

character than the Wannier or Frenkel types previously assigned on the basis of less highly resolved data.¹⁴

Superconducting Transition

Temperatures on the Rise – A superconductor exhibits no resistance to electrical current when cooled below the critical temperature T_c , and developing superconductors with the highest possible transition temperatures is currently one of the grand challenges in materials physics. Until now, the highest T_c values have been observed in copper oxide based materials known as cuprates. In fact, cuprates have provided the only examples of superconductors with transition temperatures above the boiling point of liquid nitrogen, 77 K. **Xiao-Jia Chen (Carnegie)**, along with researchers from **Carnegie, South China Institute of Technology**, and the **Max Planck Institute**, have unexpectedly found that the

One way of increasing the transition temperature of superconducting materials is to dope them by valence substitution into the parent material. Under normal pressure, the transition temperature of the optimally doped Bi2223 is 108 K. Chen and colleagues subjected doped crystals of the material to a range of pressures up to 36 GPa, the highest pressure yet for magnetic measurements in cuprate superconductors. The first increase in transition temperature was recorded at 10 GPa, with further increasing pressures resulting in lower transition temperatures. Then, surprisingly, at 24 GPa the superconducting state reappeared (Fig. 45). The transition temperature rose to 136 K at 36 GPa, which was the highest pressure attained in the experiment. Other research has shown that similar multilayered superconducting materials exhibit different electronic and vibrational behaviors in different layers, and suggests that 24 GPa represents a critical point at which applied pressure suppresses one type of electronic behavior and enhances another, in this case superconductivity.¹¹

3d Transition Metal Compounds at High Pressure – The group of CDAC partner **Wendy Mao** at **Stanford** is examining different aspects of transition metal oxides a high pressure using advanced x-ray scattering techniques. Several examples of this work are outlined in the following:

X-ray Absorption Spectroscopy of Fe₂O₃ at High Pressure – K-edge x-ray absorption spectroscopy in the partial fluorescence yield geometry has been used to look at the evolution of the pre-edge features of Fe₂O₃ at high pressure. This is a new technique that provides direct quantification of the change in crystal field energy as a function of pressure and during the electronic-magnetic transitions. With this technique, it was found that the crystal field energy of Fe₂O₃ increases monotonically with pressure from 1.4eV at ambient conditions to 1.85 eV at 48 GPa. Moreover, at pressures higher than the structural-electronic transition pressure (50 GPa), the pre-edge features significantly broaden, indicating a wider 3d band and a metallic state. Atomic multiplet, cluster diagonalization, and density-functional calculations were performed by **Tom Devereaux's** group at **SLAC National Accelerator Laboratory** and **Stanford University** to simulate the pre-edge absorption spectra, and showed good qualitative agreement with the measurements. The calculations showed that changes in the multiplet structure and hybridization are important for a quantitative estimate of the critical pressure. CDAC graduate student **Shibing Wang** has been the first author on a forthcoming publication on this topic.

High Pressure X-ray Emission Spectroscopy Study of Mn₂O₃ – Bixbyite (Mn₂O₃) is known to transform to the CaIrO₃ structure (space group *Cmcm*) at 30 GPa at ambient temperature. XES measurements indicate that the high spin to low spin transition is not completed up to 120 GPa, suggesting that some other mechanism is responsible for the phase transition.

LiMn₂O₄ at high pressure – LiMn₂O₄ with the spinel structure has attracted considerable attention as a cathode material due to its high power density, low cost, environmental friendliness, and facile synthesis. Since the electrochemical behavior of the material is strongly influenced by its structural/physical properties, studying the pressure-induced phase transitions in LiMn₂O₄ can serve as a diagnostic tool to provide a better understanding of the structure-property relationships and design improved lithium cathode materials. A recent study from the Mao group indicates that both bulk LiMn₂O₄ and well-characterized nanorods are extremely sensitive to deviatoric stress under nonhydrostatic conditions which result in a pressure-induced phase transition from a cubic phase to a distorted orthorhombic phase, driven by the Jahn-Teller effect. The manuscript (first author is graduate student **Yu Lin**) is in preparation to be submitted to *The Journal of Physical Chemistry C*.

Electronic Spin Transitions in Iron Oxides – Iron can exist in various valence states and form ferric and ferrous oxide compounds, which have been shown to undergo electronic spin transitions under pressure. The electronic spin transitions can in turn affect a wide range of physical and chemical properties of the iron oxide compounds under extreme conditions. Postdoctoral fellow **Zhu Mao** and undergraduate student **Caleb Jacobs** in the Lin group at **UT-Austin** are studying

the electronic spin and valence states of iron and their associated effects in (Mg,Fe)O, (Mg,Fe)SiO₃, and Fe₂O₃ under high pressures. In particular, the focus is on studying hematite (Fe₂O₃), an antiferromagnetic insulator under ambient conditions, as it is regarded as an archetypal Mott-insulator for the trivalent transition-metal oxides (TMOs), of which the majority crystallize in the corundum-type structure. The high-pressure phonon density of states of Fe₂O₃ across structural and electronic transitions has been investigated by nuclear resonant inelastic x-ray scattering spectroscopy and first-principles calculations. Drastic changes in elastic, thermodynamic, and vibrational properties in Fe₂O₃ occur across the Rh₂O₃(II)-type structural transition at 40-50 GPa, which are attributed to strong phonon-magnon coupling, leading to softening behavior in the THz acoustic phonons. The Mott insulator-metal transition occurring later in the Rh₂O₃(II)-type phase only causes nominal changes in the properties of the Fe₂O₃.

2.6 High *P-T* Chemistry

Investigations of chemical reactivity at extreme conditions are providing an increasingly important base of knowledge on the compositional aspect of materials behavior for stockpile stewardship applications. Reactivity patterns under both static and dynamic compression in a broad range of systems: small molecules, hydrogen-containing mixtures, organic molecules on surfaces, and complex systems of geochemical interest, including the diamond anvil cell itself, are the focus of vigorous investigations in many CDAC groups. The emergence of time-resolved measurement techniques for samples at extreme conditions holds great promise for revealing the kinetics of chemical reactions at high pressures.

Spectroscopy of Molecular Monolayers at Extreme Conditions – The **Dlott** group at **Illinois** aims to extend the study of molecular materials under extreme conditions of high temperature, static high pressure and dynamic high pressure to molecular monolayers.¹¹⁴⁻¹¹⁵ There are a number of reasons for doing this, among them that monolayers at high pressure provide new insights into the molecular dynamics of lubrication and adhesion, and monolayer spectroscopy of shock compression provides the ultimate in time and space resolution of the shock wave-molecule interaction. The concept of the shock monolayer technique is illustrated in Fig. 46. A shock is launched by a femtosecond laser pulse into an Au surface with a self-assembled monolayer (SAM). The shock propagates through the SAM and dissipates in an impedance-matched medium (typically ethylene glycol). The response of the shocked molecules is probed via nonlinear coherent vibrational sum-frequency-generation spectroscopy (SFG). The **Dlott** group has recently developed some energetic material simulants that mimic the functionalities of typical energetic materials in a SAM motif.¹¹⁶ As illustrated in Fig. 46, the method offers an unprecedented level of control over the shock-molecule interaction. These isomers of nitrobenzenethiol allow observation of how a shock, incident along different directions, excites nitro groups.

Recently, the group developed the "heat shock" technique, in which monolayers on a metal (typically Au) surface are flash-heated to a high temperature by femtosecond laser heating of the metal layer.¹¹⁷ The term "heat shock" is used to indicate that the heating process is not the ordinary diffusive heat conduction. Due to the short length scales, heat flows rapidly and ballistically

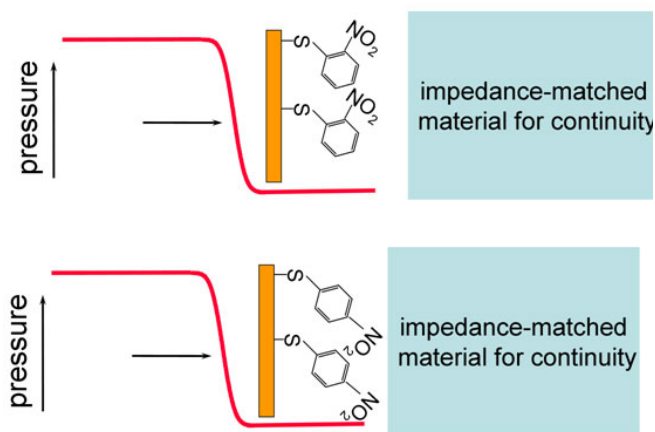


Figure 46. Schematic of a steep shock hitting a self-assembled monolayer of energetic material simulants that allow control of the shock-nitro orientation. Probing a monolayer with vibrational spectroscopy gives the high time and space resolution needed to understand shock initiation at a fundamental level.

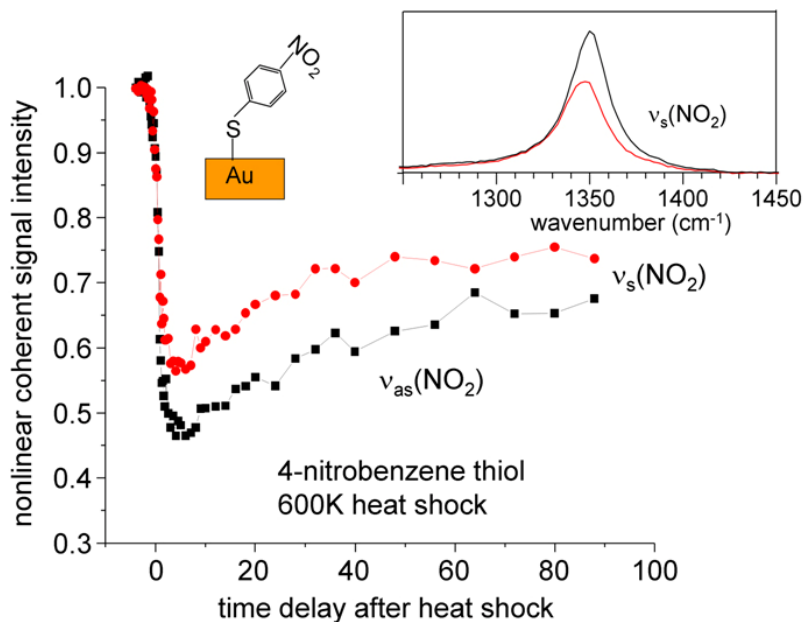


Figure 47. Response of nitro group of a SAM to a heat shock from 300 K to 600 K. Equilibrium is attained in 60 ps. The inset shows the nitro symmetric stretch lineshape. Right: CDAC graduate student **Kathryn Brown (Illinois)**.



along alkane chains.¹¹⁷ During the course of initial heat shock experiments, technical improvements have allowed implementation of a second generation of the shock monolayer concept, which will feature more powerful and spatially uniform shocks, better detection, and the possibility of preheating the shock molecules with a heat shock to enhance the chemical reactivity.¹¹⁸ The original spectra had a poor signal to noise ratio and also a large nonresonant background from the Au surface and from the windows and contact liquid. The heat shock has much better signals because there is no window. A newly-developed nonresonant suppression technique¹¹⁹ relies on temporal windowing of the unwanted nonresonant signal. Spectra with about 100x improved signal-to-noise ratios can be obtained from shocked molecules. Now CDAC graduate student **Chris Berg** is working on a laser upgrade to improve the shock drive pulse by

increasing its energy by ten, which requires a longer-duration drive pulse and an additional pulse picker to improve the contrast ratio. A second compressor is used to vary the drive pulse duration¹²⁰ up to 10 ps, and a microfabricated beam shaper is used to generate a flattop rather than Gaussian profile shock. In these second-generation experiments, the shocked monolayer vibrational spectra will be compared to static high temperature and high pressure monolayer measurements. After a period of many picoseconds, when the shock becomes hydrostatic and the molecular energy equilibrates, the molecules will have an actual temperature and pressure.¹²¹⁻¹²³ Prior to that time, shock dynamic effects will predominate. One cannot ordinarily heat a SAM above about 100°C due to decomposition, but with heat shock it is possible to create temperatures of hundreds of degrees for a few microseconds, which is faster than decomposition.¹²⁴ Figure 47 shows some heat shock data obtained by probing the nitro transitions which ultimately equilibrate at 600 K. The temperature is measured by detecting changes in reflectivity of the Au substrate. The lineshape in the inset for the symmetric nitro stretch shows a thermal redshift but little broadening. Also collaborating on this work were CDAC graduate student **Kathryn Brown** and summer undergraduate student **Elizabeth Friedman**.

Low-Temperature IR-Reflectivity of CH₄ – Light hydrocarbons such as methane (CH₄) are among the most important energy resources today. Knowledge of CH₄ properties and phase stability has applications ranging from stewardship science to identifying states of CH₄ on icy bodies of the outer solar system. At **Northwestern University**, CDAC graduate student **Kimberly Adams**, along with postdoctoral fellow **Sylvia-Monique Thomas** and CDAC Academic Partner **Steve**

Jacobsen are collaborating with **Carnegie's Maddury Somayazulu** and **Zhenxian Liu** to study the low-temperature IR-reflectivity of methane across phase changes in CH_4 . By examining broad-spectrum IR-reflectance, changes in CH_4 states are identified more readily than with typical IR-absorption spectroscopy.

In 2008, *Cassini* observations of Titan, Saturn's largest moon, revealed dark, lake-shaped patches through the 2 and 5 μm windows of Titan's atmosphere.¹²⁵ Interpreting these dark patches in terms of possible hydrocarbon lakes requires laboratory-based, IR-reflectivity of methane and ethane at relevant conditions. CH_4 was loaded into an optical cell with diamond windows for IR-reflectance measurements at 50-100 K on the U2A beamline at NSLS. At conditions below the critical pressure, co-existing states of vapor and liquid CH_4 was observed at temperatures down to 94 K, as shown in Fig. 48. Upon crystallization below 94 K, a dramatic increase in reflectance of CH_4 was observed at the diamond-sample interface (R_{sd}).

Whereas the position of characteristic absorption bands of CH_4 are insensitive to the phase state, darkening of liquid CH_4 in reflectance is consistent with Titan's observed dark surface features, which may represent large polar lakes forming seasonally through exchange with clouds and rain of methane where Titan's surface temperatures are within a few degrees of the triple point.

Spectroscopy of the Diamond-Water Interface – At **Illinois**, **Chris Berg** has also been working on methods for obtaining the spectrum of water at the water-diamond interface using sum-frequency generation. Early attempts were hampered by the use of polycrystalline CVD diamond, which has many interfaces that generate an optical background. In collaboration with **Carnegie**, a single-crystal diamond window has been obtained and polished. This work will continue on into Year 8.

Structural Evolution of Ammonia Borane (NH_3BH_3) at High Pressure – Ammonia borane (AB) has attracted considerable attention as a potential hydrogen storage material mainly due to its high gravimetric (19.6 wt %) and volumetric H_2 densities where H_2 can be released by three single steps. Over the past year, several groups have investigated its structural behavior and crystal chemistry at high pressure, combining a number of experimental techniques with theoretical calculations. These recent high pressure studies¹²⁶⁻¹²⁷ have produced somewhat contradictory results. Using Raman spectroscopy,¹²⁸ CDAC graduate student **Yu Lin** at **Stanford** performed a systematic investigation of the structural evolution of AB at high pressure in a DAC up to 15.0 GPa and room temperature by synchrotron x-ray diffraction. Two first-order phase transitions were identified. The **Mao** group is also collaborating with **Timo Thonhauser's** theory group at **Wake Forest University** on density functional theory calculations. At 1.6 GPa, the parent tetragonal structure

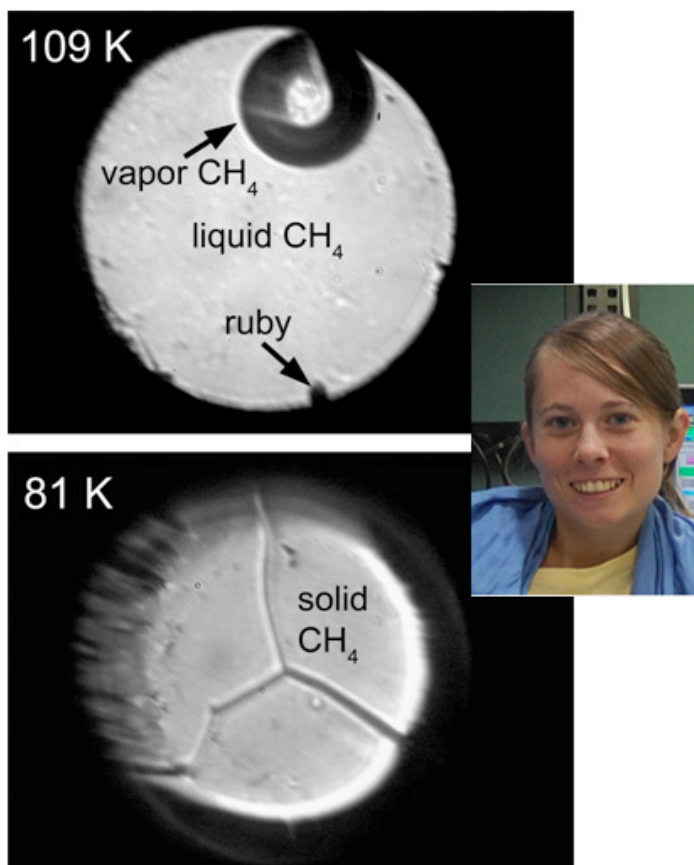


Figure 48. Sample of CH_4 passes through the triple point in an optical cell at NSLS-U2A. Inset: **Kimberly Adams** (Northwestern).

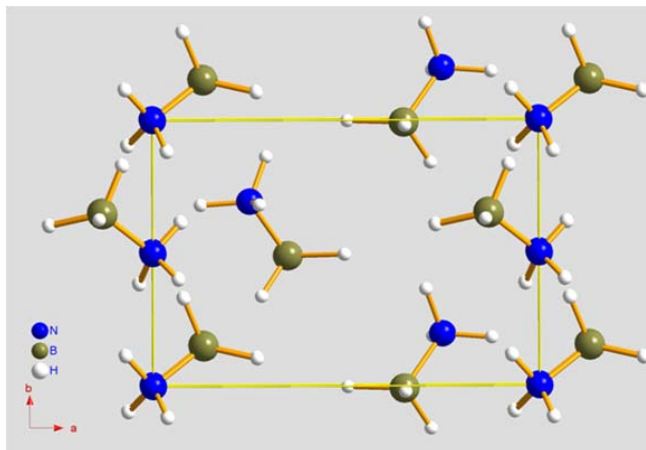


Figure 50. The crystal structure for the $P2_1$ phase of $\text{NH}_3\text{-BH}_3$. N, B and H atoms are denoted as blue, olive and white balls respectively.

nature of these glasses simply by applying pressure instead of by changing the composition. Structural transitions resulting from an increase in atomic coordination (Fig. 51) have been reported in a variety of amorphous materials, including amorphous ice and silica glass. This has been termed polyamorphism --- the transition from a low-density amorphous form to high-density amorphous form, much as crystals change structure, but here there is no ordered crystal structure.

Using a combination of high pressure synchrotron x-ray absorption spectroscopy and diffraction techniques, **Qiaoshi Zeng (Zhejiang University)** and colleagues from **Carnegie and Stanford University** report experiments that uncover the origin of the pressure-induced polyamorphism from a low-density amorphous state to high-density amorphous state in this class of materials. Studying $\text{Ce}_{75}\text{Al}_{25}$ metallic glass, the group observed the Ce 4f electrons transform from their ambient condition, localized state to an itinerant state at high pressure. There is an associated volume collapse of 8.6%, coinciding with the 4f delocalization. This new type of electronic polyamorphism in densely-packed metallic glass is dictated by the Ce constituent, and is distinct from the well-established structural polyamorphism in which densification is caused by coordination change and atomic rearrangement. These results have implications for understanding the behavior of other metallic glasses and is valuable for searching for polyamorphism associated with electronic transitions in other f-electron materials.¹²⁹

($I4mm$) undergoes a first-order phase transition to an orthorhombic phase $Cmc2_1$. As pressure is increased to 12.9 GPa, a new high pressure phase is observed and its space group determined as monoclinic $P2_1$ with powder diffraction data. Density functional theory is employed to complementarily optimize the positions of N and B atoms, as well as NH_3 and BH_3 groups. The crystal structure of the new $P2_1$ phase with four molecules per unit cell is shown in Fig. 50.

A New Class of Glass – Metallic glasses are attracting a great deal of attention at the cutting edge of current materials research. New experiments now show that one can drastically change the

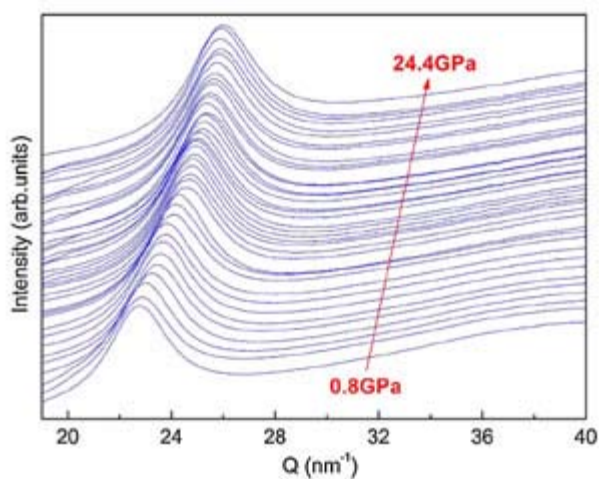


Figure 51. In situ high-pressure x-ray diffraction patterns of $\text{Ce}_{75}\text{Al}_{25}$ metallic glass from 0.8 to 24.4 GPa. The position of first sharp diffraction peak shifts to the higher Q values with increasing pressure as a result of densification.

3. EDUCATION, TRAINING, AND OUTREACH

CDAC places a heavy emphasis on education, training and outreach, in keeping with the goals of the SSAA program. In the following sections, we outline in detail the various components of this aspect of the Center.

3.1 CDAC Graduate Students and Post-doctoral Fellows

The main focus of the CDAC effort in its education, training and outreach mission is the support of graduate student preparation in the groups of the academic partners (Fig. 52). CDAC graduate students carry out their dissertation research on a wide variety of problems in high P - T research relevant to stockpile stewardship, through projects in the fields of materials science, physics and chemistry as well as high-pressure mineral physics and geophysics.

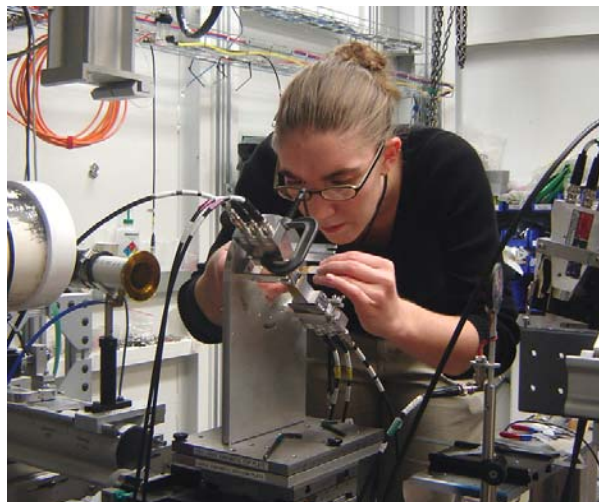


Figure 52. CDAC graduate student **Lisa Mauger** (Caltech).

The following graduate students in the research groups of CDAC Academic Partners received full or partial support of their graduate work through CDAC during 2009-2010.

Princeton (Duffy):

Susannah Dorfman
G. Jeffrey Finklestein

Caltech (Fultz):

Jue Wang
Lisa Mauger
Jorge Munoz
Michael Winterrose
Sally Tracy

Berkeley (Wenk):

Jane Kanitpanyacharoen
Pamela Kaercher

Alabama (Vohra):

Gopi Samudrala
Walter Uhoya

Illinois (Dlott):

Kathryn Brown
Chris Berg

Arizona State (Yarger):

Samrat Amin
Keri McKiernan (undergraduate)
Erin Oelker

New Mexico State/Yale (Lee):

Yahya Al-Khatatbeh (postdoctoral)
Joseph O'Rourke (undergraduate)

Florida International (Saxena):

Lyci George
Rostislav Hrubciak

UCLA (Kavner):

Matt Armentrout
Yun-yuan Chang

Northwestern (Jacobsen):

Kimberly Adams
Bin Chen

Illinois (Li/Michigan):

Berkeley (Jeanloz):

Arianna Gleason
Daniel Reaman

Ohio State (Panero):

Jeffrey Pigott

Arizona (Downs)

Madison Barkley

Washington Univ. (Schilling):
Stanford (Mao)

University of Texas (Lin)

Rod Ewing (Michigan)

David Cahill (Illinois)

Wenli Bi
Yu Lin
Shibing Wang
Jin Liu
Chang Lu
Caleb Jacobs (undergraduate)
Sandra Fernando
Scott Pray
Wen-Pin Hsieh

The full list of graduate students who have received the PhD degree with CDAC support since the beginning of the program in 2003 is as follows:

James Patterson (Illinois, 2004)
Raja Chellappa (Nevada-Reno, 2004)
Wendy Mao (Chicago, 2005)
Jenny Pehl (Berkeley, 2005)
Sergio Speziale (Princeton, 2005)
Tabitha Swan-Wood (Caltech, 2005)
Alexander Papandrew (Caltech, 2006)
Nenad Velisavjevic (Alabama, 2006)
Emre Selvi (Texas Tech, 2007)
Joanna Dodd (Caltech, 2007)
Matthew Lucas (Caltech, 2008)
Resul Aksoy (Texas Tech, 2008)
Lowell Miyagi (Berkeley, 2009)
Chris Seagle (Chicago, 2009)
Bin Chen (Illinois, 2009)
Zhu Mao (Princeton, 2009)
Lyci George (Florida International, 2010)
Michael Winterrose (Caltech, 2010)
Erin Oelker (Arizona State, 2010)
Arianna Gleason (Berkeley, 2010)
Yahya Al-Khatatbeh (New Mexico State, (2010)

Publications and presentations involving CDAC-supported students and postdoctoral fellows in Year 7 are listed below.

Student Publications

- Adams, K. A., S. D. Jacobsen, S. M. Thomas, Z. Liu, M. Somayazulu, and D. M. Jurdy, Visible and near-infrared reflectivity of solid and liquid methane: application to hydrocarbon lakes on Titan, *Planet. Space Sci.*, submitted.
- Al-Khatatbeh, Y., High-pressure behavior of transition-metal dioxides TiO_2 , ZrO_2 , and HfO_2 as determined by synchrotron x-ray diffraction and density functional theory, *Ph.D. Thesis, New Mexico State University, Physics*, (2010).
- Al-Khatatbeh, Y., K. K. M. Lee, and B. Kiefer, High-pressure behavior of TiO_2 as determined by experiment and theory, *Phys. Rev. B*, **79**, 134114 (2009).
- Al-Khatatbeh, Y., K. K. M. Lee, and B. Kiefer, Phase relations and hardness trends of ZrO_2 phases at high pressure, *Phys. Rev. B*, **81**, 214102 (2010).
- Al-Khatatbeh, Y., K. K. M. Lee, and B. Kiefer, Phase diagram up to 105 GPa and mechanical strength of HfO_2 , *Phys. Rev. B*, **82**, 144106 (2010).
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3.2 Undergraduate Student Summer Scholars

A number of university undergraduate students participating in the highly successful Carnegie Summer Scholars Program (Fig. 67) have worked in the high pressure group at Carnegie, and have carried out research with CDAC personnel. The Summer Scholars Program program, which is run by CDAC coordinator **Stephen Gramsch** and funded by the NSF, seeks to identify promising students who may not have had the opportunity to engage in research during the academic year. At **Carnegie**, such students experience a rigorous introduction to scientific research, and through the CDAC group meeting setting, are learning about the important problems in the field of high-pressure research. During the summers of 2009-2010, the following students worked with the Carnegie group.



Figure 53. 2010 Carnegie Summer Scholars.

2009:

Neil Foley, Carleton College

Fractionation of Sulfur Isotopes in the Formation of Mars

Zhili Liang, Lehigh University

Crystallization of Periodic Mesoporous Organosilicas

Alexander Savello, Emory University

Measurement of the Thermal Conductivity of (MgFe)SiO₃ Perovskite at High P and T

Angela Schad, University of Notre Dame

High Pressure Raman Studies of Ferroelectric Perovskites

2010:

Bethany Chidester, University of Toledo

A High Pressure Study of the NH₃-H₂ System to 13 GPa

Amanda Lindoo, Augustana College

High Pressure Crystal Chemistry of Norbergite

Michael Wong, University of California-Berkeley

Thermal Conductivity of Argon at High Pressure and Temperature

3.3 DC Area High School Outreach

Every year at **Carnegie**, several local high school students are hosted by CDAC and offered guidance in their science fair projects and in other areas of research. In 2009, **Emily Sandford** studied the Brillouin spectroscopy of polymers with **Muhetaer Ahart**, and **Claire Barkett** extended the work begun by **Jaqueline Rivera** in the previous year on Fe/Al solid solutions. In 2010, a partnership with **Howard University** in Washington, DC allowed the Carnegie group to host **Yasmine Kadry** and **Thomas Hittenger**; **Soren Scott** and **Winston Liu** also joined the Carnegie team in the summer of 2010. **Liu** was selected as a semi-finalist in the Siemens Science Talent Search, the fourth such student that Carnegie has hosted in recent years.

2009:

Claire Barkett, Good Counsel High School, Olney, MD
Low-Temperature Synthesis of Fe-Bearing Solid Solutions
(Now at High Point University, High Point, NC)

Emily Sandford, Glenelg Country School, Ellicott City, MD
High-Pressure Brillouin Spectroscopy of Polymers
(Now at Massachusetts Institute of Technology, Cambridge, MA)

2010:

Soren Scott, Bethesda-Chevy Chase High School, Bethesda, MD
Hydrogen Storage Materials at High Pressure

Yasmine Kadry, John F. Kennedy High School, Silver Spring, MD
Laser Heating of Materials at High Pressure
(Now at University of Maryland, College Park, MD)

Thomas Hittinger, Osbourn High School, Manassas, VA
High Pressure Raman Spectroscopy of Small Molecules

Winston Liu, Montgomery-Blair High School, Silver Spring, MD
Ethane-Hydrogen Mixtures at High Pressures

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

3.4 CDAC Collaborators

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 provided the leverage needed to work on a number of exciting new research directions. The CDAC collaborators to date include faculty and students from the following institutions:

Abdus Salam International Center for Theoretical Physics, Italy

M. S. Lee
S. Scandolo

Academia Sinica - Nanking, Taiwan

F. C. Hsu
L. Y. Huang
S. M. Rao
M. K. Wu
K. W. Yeh

Academy of Sciences of Moldova

E. V. Rusu
V. V. Ursaki

Albert-Ludwig University, Germany

J. Majzlan

Argonne National Laboratory

J. D. Almer
E. E. Alp
D. L. Brewster
Z. Cai
G. W. Crabtree
J. Gosztola

Argonne National Laboratory, cont'd.

D. R. Haefner

D. Haskel
E. Kaneshita
P. L. Lee
W. Liu
J. Mitchell
Y. Ren
S. D. Shastri
W. Sturhahn
Y. Sun
T. T. Truong
M. van Veenendaal
H. Yavas
J. Zhao

Arizona State University

C. J. Benmore
H. Bhat
E. Soignard
R. Sharma

Beijing University of Technology

X. D. Han

Bhabha Atomic Research Centre, India

S. N. Achary

A. K. Tyagi

Brookhaven National Laboratory

A. E. Bolotnikov
Y. Q. Cai
G. S. Camarda
V. Carcelen
Y. Cui
L. Ehm
S. Ghose
R. Gul
A. Hossain
R. B. James
K. Kim
G. Yang
Z. Zhong

California Institute of Technology

T. J. Ahrens
P. D. Asimov
W. A. Goddard, III
I. Halevy
J. M. Jackson
J. B. Keith
N. Kostandova
M. Kresch
C. W. Li
C. Ma
N. Markovsky
A. F. Yue

California State University – Northridge

R. Kundargi

Carnegie Mellon University

M. Widom

Case Western University

M. R. Chance
S. Rekhi

CEA Marcoule, France

C. Poinssot

Chinese Academy of Sciences

L. Bai
L. G. Bai
G. F. Chen
Z. Q. Chen
L. Chen
C. Dong
X. L. Dong
S. Jiang
C. Jin
C. Q. Jin
W. Li
X. D. Li
Y. Li
Z. Li
J. Liu
Q. Q. Liu
W. Lu
Y. X. Lv
L. L. Sun

Chinese Academy of Sciences, cont'd.

D. Tan
C. Y. Tu
N. L. Wang

X. C. Wang
W. Xiao
X. Xiong
L. Yang
Y. X. Yang
W. Yi
S. You
S. J. You
H. Yu
C. Zhang
D. Zhang
S. J. Zhang
Y. Zhang
Z. X. Zhao
Z. Zhu

Chinese University of Hong Kong

Y. L. Li
H. Q. Lin

City University of Hong Kong

C. Zhang
R. Q. Zhang

Columbia University

C. Y. Chin

**CNR-ISTM Istituto di Scienze e Technologie
Molecolari, Italy**

C. Gatti

Delaware State University

G. D. Gwanmesia

Duke University

P. M. Wu

East China Normal University

X. Ke

**Eindhoven University of Technology, The
Netherlands**

G. J. Kramer
R. A. van Santen

ETH Zurich, Switzerland

A. R. Oganov
C. W. Glass
Y. Ma

**European Synchrotron Radiation Facility,
France**

G. Aquilanti
G. E. Gonzalez
N. Guignot
M. Mezouar
S. Pascareli

Florida International University

J. Chen
V. Drozd
A. Durygin
R. S. Vennila
T. Yu

**Forschungszentrum Karlsruhe GmbH,
Germany**

E. G. Bardaji
M. Fichtner

Frank Laboratory of Neutron Physics, Russia

S. Matthies
GeoForschungsZentrum Potsdam, Germany

D. Rhede
S. Speziale
R. Wirth

George Mason University

H. W. Sheng

GSECARS

P. Dera
I. Kantor
B. Lavina
V. Prakapenka
M. L. Rivers
S. Sutton

Harbin Institute of Technology, China

J. G. Zhao

HASYLAB am DESY, Germany

C. Lathe

Hendricks High School, New Hyde Park, NJ

V. Jain

Indiana University – South Bend

H. P. Scott

**Indira Ghandi Centre for Atomic Research,
India**

T. R. Ravindran
N. Subramanian

Institute of Coal Chemistry, China

X. Y. Guo

Institute of High Pressure Physics, Russia

T. I. Dyuzheva

**Institute of Physical and Chemical Research,
Japan**

H. Yamaoka

**Japan Agency for Marine-Earth Science &
Technology**

K. Hirose
N. Sata

Japan Atomic Energy Agency

A. Ikeda-Ohno

I. Jarrige

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N. Hirao
Y. Ohishi
S. Tsutsui

Jilin University, China

G. Bao
Q. Cui
T. Cui
D. Duan
C. Gao
C. X. Gao
Y. Gao

Jilin University, China, cont'd.

J. Hao
W. W. Lei
D. Li
F. Li

J. Li

M. Li

Q. Li

S. Li

A. Lin

P. Lin

W. Lin

B. Liu

D. Liu

J. Liu

R. Liu

Z. Liu

L. Tang

H. Wang

H. Wang

K. Wang

L. Wang

P. Wang

R. Wang

T. Wang

G. Wen

Y. Xu

M. Yau

S. D. Yu

J. Yuan

R. Zheng

G. Zhou

Q. Zhou

P. Zhu

B. Zou

G. Zou

Y. Zou

Johns Hopkins University

Y. Q. Cheng

E. Ma

M. Xu

**Laboratoire de Planetologie de Grenoble,
France**

P. Beck

Lawrence Berkeley National Laboratory

K. Chen

T. Cuk

M. Kunz

N. Tamura

Lawrence Livermore National Laboratory

D. Aberg

N. Barton

J. C. Crowhurst

H. Cynn

P. Erhart

W. J. Evans

J. H. Klepeis

A. Lazicki

R. E. Rudd

Lawrence Livermore National Lab., cont'd.

F. J. Ryerson

B. Sadigh

S. T. Weir

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J. M. Zaug
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Technology, Russia**
A. I. Kolesnikov
A. G. Kutcherov
Los Alamos National Laboratory
R. Chellappa
L. L. Daemen
M. Hartl
D. He
K. A. Lokshin
Z. J. Lin
C. Pantea
J. Qian
C. Tome
S. Vogel
H. Xu
J. Zhang
Y. Zhao
Massachusetts Institute of Technology
K. Catalli
B. Grochalski
S. H. Shim
Max Planck Institut für Chemie, Germany
S. Japel
M. Ross
B. Schwager
**Max Planck Institute of Colloids and
Interfaces, Germany**
W. Lei
National Academy of Sciences of Ukraine
A. Grechnev
Y. A. Freiman
S. M. Tretyak
National Cheng Kung University, Taiwan
J. Kung
**National Institute for Materials Science,
Japan**
N. Tsujii
**National Institute of Advanced Industrial
Science and Technology, Japan**
H. Eisaki
A. Iyo
H. Kito
N. Takeshita

**National Institute of Standards and
Technology**
B. Burton
E. Cockayne
T. A. Jenkins
E. L. Shirley

**National Synchrotron Radiation Research
Center, Taiwan**
N. Hiraoka
H. Ishii
K. D. Tsuei
**National Technical University of Athens,
Greece**
C. Raptis
E. Stavrou
Naval Research Laboratory
J. L. Feldman
New Jersey Institute of Technology
H. Y. Chen
P. Gao
T. A. Tyson
New Mexico State University
B. Kiefer
Nihon University, Japan
H. Okada
H. Takahashi
Northern Illinois University
M. Frank
Northwestern University
Rebecca Fischer
Y. C. Tseng
Oak Ridge National Laboratory
D. L. Abernathy
J. M. Bai
M. V. Buchanan
L. A. Boatner
O. Delaire
E. Egami
C. L. Fu
P. Ganesh
D. Mandrus
M. A. McGuirre
J. J. Molaison
A. F. Moreira Dos Santos
B. C. Sales
A. S. Sefat
M. D. Stone
A. Subedi
C. A. Tulk
Ohio State University
D. M. Raeman
Okayama University, Japan
T. Okuchi
S. Yamashita

Osaka University
Y. Nakamoto
T. Okada
K. Shimizu
Pacific Northwest National Laboratory
T. Autrey

Pennsylvania State University

A. C. T. van Duin

Plainview Old-Bethpage John F. Kennedy High School

J. Yi

Polytechnic Institute of New York University

K. Levon

Princeton University

R. J. Cava

F. Jiang

A. Kubo

D. V. West

Rensselaer Polytechnic Institute

P. Keblinski

Royal Institute of Technology, Sweden

A. B. Belonoshko

Russian Academy of Sciences

V. F. Degtyareva

K. F. Frolov

A. Gavriiliuk

I. S. Lyubutin

S. G. Ovchinnikov

Y. S. Ponsov

S. V. Streltsov

I. A. Troyan

Rutgers University

S. W. Cheong

Y. J. Choi

Sandia National Laboratory

D. Dolan

M. Knudson

L. Shulenburg

Savannah River National Laboratory

D. Anton

P. Berseth

A. C. Stowe

R. Zidan

Sichuan University, China

H. Chen

D. He

Z. Li

F. Peng

J. Wang

J. Xu

Simon Fraser University, Canada

Y. Bing

Z. G. Ye

Sichuan University

H. Dong

D. He

Sincrotrone Trieste, Italy

M. Voltolini

South China University of Technology

Y. Pan

Southwest Jiaotong University, China

X. R. Liu

Stanford University

J. G. Analytis

M. Baldini

K. Bandyopadhyay

C. C. Chen

J. Chu

T. P. Devereaux

I. R. Fisher

C. C. Kao

B. Kalisky

J. R. Kirtley

K. A. Moler

Z. X. Shen

A. P. Sorini

A. Vailionis

T. Vanorino

Stony Brook University

Z. Chen

J. Hu

B. Li

S. Mueller

H. Nekvasil

A. R. Oganov

M. H. Rafailovich

B. Rigas

J. Sokolov

L. P. Wang

Y. Wang

D. J. Weidner

Z. Zhang

Texas Tech University

R. Aksoy

J. Chaudhuri

R. Knudson

R. G. Lee

D. Hou

Y. Ma

E. Selvi

H. Yang

Tohoku University, Japan

E. Ohtani

Tokyo Institute of Technology, Japan

M. Hirano

H. Hosono

Y. Kamihara

Y. Nakajima

Tsinghua University, China

X. Zhang

Umeå University, Sweden

B. Sundqvist

T. Wagberg

United States Army Edgewood Chemical Biological Center

E. D. Emmons

United States Army Research Laboratory

J. A. Ciezack

Universidad Complutense de Madrid, Spain

E. Buforn

M. Mattesini

Universidad Complutense de Madrid, cont'd.

M. Ramfrez
 D. Santamaria-Perez
 A. Udias
Universidad de Cantabria, Spain
 J. Gonzalez
 F. Rodriguez
Universidad de La Laguna, Spain
 J. P. Lopez-Solano
 A. Munoz
 P. Rodriguez-Hernandez
Università degli Studi di Trento, Italy
 L. Lutterotti
Università di Roma Tre, Italy
 G. Della Ventura
Università G. D'Annunzio, Italy
 G. Iezzi
Universität Bayreuth, Germany
 T. B. Ballaran
 L. S. Dubrovinsky
 D. J. Frost
Universität Duisburg-Essen, Germany
 W. Keune
Universitat de València, Spain
 D. Errandonea
 R. Lacomba-Perales
 J. Ruiz-Fuertes
 A. Segura
Universitat Jaume I, Spain
 A. Beltrán
 L. Gracia
Universitat Politècnica de València, Spain
 O. Gomis
 F. J. Manjon
 S. Ray
Université de Picardie, France
 P. Toledano
Université de Rennes I, France
 B. Bureau
Université des Sciences et Technologies de Lille, France
 S. Merkel
Université Paris Nord, France
 O. O. Kurakevych
 V. L. Solozhenko
Université Pierre et Marie Curie, France
 D. Antonageli
 J. Badro
 J. Siebert
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 Y. Gueguen
 C. S. Roiland
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 T. Rouxel
 J. C. Sangleboeuf
 J. Troles
 G. Yang
University of Alabama – Birmingham

G. Tsoi
University of Arizona
 O. Gulbitten
 E. A. King
 P. Lucas
University of Cambridge, UK
 M. A. Carpenter
University of California – Berkeley
 M. Bortolotti
 B. Buffett
 B/ K. Godwal
 B. Militzer
University of California – Davis
 N. Browning
 I. Arslan
 V. Ortalan
 W. E. Pickett
 S. Y. Savrasov
 G. Shen
University of California – Riverside
 L. F. Dobrzhinetskaya
 H. W. Green
University of California – San Diego
 M. B. Maple
 D. A. Zocco
University of Central Florida
 J. R. Croy
 R. B. Cuenya
 H. Heinrich
 A. Naitabdi
 L. K. Ono
University of Chicago
 P. Eng
 D. Heinz
 J. Hu
 I. Kantor
 N. Nishiyama
 Y. Wang
 W. Zhang
University of Colorado
 B. D. Haugen
 J. R. Smyth
University of Edinburgh
 O. Degtyareva
 E. Gregoryanz
University of Hawai'i
 R. Jia
 L. C. Ming
 P. V. Zinin
University of Illinois
 J. D. Bass
 J. A. Carter
University of Illinois, cont'd.
 B. Chen
 K. P. Esler
 Y. Fu
 H. Fujiwara
 L. Gao
 A. Lagutchev

Z. Wang
H. Yavas
University of Kiel, Germany
H. Katzke
University of Leeds, UK
G. E. Lloyd
University of Liege, Belgium
M. Ausloos
J. F. Fagnard
P. Vanderbemden
University of London, UK
F. M. Grosche
University of Maryland
M. Ouyang
Y. Tang
University of Michigan
U. Becker
M. Lang
V. Pointeau
L. C. Schuller
J. W. Wang
F. W. Zhang
J. M. Zhang
University of Missouri – Columbia
A. K. Speck
University of Montevallo
K. M. Hope
University of Nevada – Las Vegas
C. Chen
A. L. Cornelius
M. Galley
T. Hartman
P. E. Kalita
X. Ke
E. Kim
R. S. Kumar
S. Kumar
B. Lavina
K. Lipinska-Kalita
Z. Liu
J. McClure
M. Nicol
M. Pravica
S. N. Tkachev
O. Tschauner
P. F. Weck
B. Yulga
Y. Zhang
University of Nevada – Reno
D. Chandra
W. M. Chien
A. M. Covington
University of Nevada – Reno, cont'd.
J. C. Fallas
V. K. Kamisetty
E. F. Littlefield
University of Oxford, UK
A. T. Boothroyd
D. Prabhakaran

University of Pittsburg
J. K. Johnson
University of Saskatchewan, Canada
J. S. Tse
University of Sydney, Australia
S. P. Ringer
University of Texas – Austin
C. Jacobs
Z. Mao
University of Tokyo, Japan
T. Yagi
University of Toronto, Canada
N. Coombs
University of Trento, Italy
L. Lutterotti
University of Tsukuba, Japan
A. Hushur
S. Kojima
University of Warsaw, Poland
V. Drozd
M. Pekala
University of Western Georgia
M. Bishop
University of Western Ontario, Canada
Z. Dong
C. Murli
S. R. Shieh
Y. Song
K. Traikov
S. Xie
K. K. Zhuravlev
University of Wisconsin
A. Bengston
D. Morgan
Uppsala University
R. Ahuja
A. Blomqvist
P. Lazor
W. Luo
Washington State University
J. Y. Chen
M. Debessai
Y. M. Gupta
M. Kim
K. Perkins
K. M. Pitman
S. J. Turneure
C. S. Yoo
K. Zimmerman

Washington University, St. Louis
H. B. Banks
J. J. Hamlin
T. Matsuoka
Wayne State University
J. D. Cook
T. Stremmler

**Xian University of Architecture and
Technology, China**

K. Ding

Xiantian University, China

S. Xiao

Yale University

B. Kiefer

Yinnel Tech, Inc.

L. Li

Yonsei University, Korea

Y. Lee

D. Liu

Zhejiang University, China

Y. Z. Fang

J. Z. Jiang

H. B. Luo

X. D. Wang

F. M. Wu

Q. S. Zeng

3.5 Visitors to CDAC

Carnegie also receives many visiting scientists each year, who utilize 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. Such visitors often make informal presentations, which enrich the scientific work of the group as a whole.

Visitors	Affiliation	Project	Date
G. Shen	HPCAT	Seminar on "High pressure dimension in x-ray science"	September 10-11, 2009
Maria Baldini	Stanford University	Manganese oxide and LaMnO ₃ using Raman spectroscopy	September 11-18, 2009
G. Makhatadze	Rensselaer Polytechnic Institute	Seminar on "Specific volume changes of globular proteins upon unfolding. Implications for the <i>P-T</i> diagram of protein stability"	September 14, 2009
C. Cahill	George Washington University	Seminar on "Hybrid materials from the f elements: Synthesis, structure and spectroscopy"	September 21, 2009
C. DeVreugd	Virginia Tech	Visit to Raman and Brillouin laboratories with Muhetaer Ahart	September 22, 2009
S. Stishov	Russian Academy of Science	Seminar on "New studies of the magnetic phase transition in MnSi at ambient and high pressure"	September 28, 2009
G. Pradhan	IISc Bangalore	Talk on "Pressure induced phonon freezing in Zn _{1-x} Be _x Se ternary alloy"	September 28, 2009
E. Ohtani	Tohoku University	Visit with Yingwei Fei	September 28, 2009
M. Hudl Zuzana Konopkeva	Uppsala University	Superconductivity and thermal conductivity of Fe	September 28-October 30, 2009
Shibing Wang	Stanford University	Work with Xiao-Jia Chen	October 11-17, 2009
Q. Peng	California State University	Investigation of properties of pyroelectric material	November 2-30, 2009
Jie Li	University of Illinois	Work with Chang-sheng Zha	November 13, 2009
L. Bing	HPSynC	Superconductivity in YH ₃	November 16-20, 2009
A. Tsamaloukas	Rensselaer Polytechnic Institute	Work with Chang-sheng Zha	November 30-December 4, 2009
H. Yolin	Army Research Laboratory	Discussion with Muhetaer Ahart in regards to ARL	December 17, 2009

		supported projects	
Mengjing Xu	China University of Geosciences	Investigating the phase transformations of chromite at high pressure and temperature with Yingwei Fei	December 18, 2009- March 31, 2010
C. Park	HPCAT	Seminar on "Molecular processes at mineral-aqueous interfaces: New understanding with synchrotron x-ray probes"	January 11, 2010
W. Yang	HPSynC	Discussions with Reinhard Boehler and Ho-kwang Mao	January 17-22, 2009
J. Zhang	South China University of Technology	Diamond nanomaterials synthesis with Yingwei Fei and Russell Hemley	February 1, 2010- January 31, 2011
L. Bing	HPSynC	High-pressure superconductivity study of YH ₃	February 23-March 1, 2010
G. Zou B. Zou	Jilin Univesity	Research with Ho-kwang Mao	March 24-30, 2010
W. Wanene	University of Nevada – Reno	Research with Raja Chellappa	March 29-April 2, 2010
Lisa Mauger	Caltech	Sample loading	April 5-9, 2010
Surinder Sharma	Bhabha Atomic Research Center, India	Discussions with Maddury Somayazulu about high pressure carbon nanotube experiments	May 4-7, 2010
K. Lokshin	University of Tennessee	Work with Viktor Struzhkin	May 17-21, 2010
A. Gavriuliuk	Institute for High Pressure Physics, Russian Academy of Sciences	Work with Viktor Struzhkin	May 19-June 20, 2010
M. Weinberger	Lehigh University	High pressure/high temperature work with Yingwei Fei	June 1-15, 2010
Lisa Mauger	Caltech	Sample loading	June 9-10, 2010
R. Caracas	GSECARS	Visit with R. Hemley	June 10, 2010
Yuki Nakamoto	University of Osaka	Collaborative projects in high pressure research	June 15, 2010-June 15, 2011
R. Sussman	King's College – London/DeBeers Industrial Diamonds	Talk on "Growth and Applications of Diamond Grown By Chemical Vapor Deposition"	August 2, 2010
Tingting Qi	University of Pennsylvania	Talk on "DFT and MD modeling of ferroelectric perovskite materials for nonvolatile memory and high piezoelectricity applications"	August 3, 2010
M. Murakami	Tohoku University	Optical absorption of glass materials with A. Goncharov	August 4-18, 2010
R. Chellappa	LANL	Sample loading	August 5-10, 2010
M. Mahmood	Howard University	Collaborative projects with Alexander Goncharov	August 11, 2010- August 10, 2011
M. Weinberger	Lehigh University	Crystallizing monstructure composites with Yingwei Fei	August 16-September 4, 2010

W. Wannene	University of Nevada – Reno	UV-VIS absorption and Raman spectroscopy on BeReH ₉ , Li ₂ ReH ₉ , and NaReH ₉	August 23-September 3, 2010
S. Kamada	Tohoku University	Analysis of potassium partitioning between silicate and metals using FIB-SEM	September 9-23, 2010
P. Lazor	University of Uppsala	Gas loading and Raman experiments	September 20-October 1, 2010
S. Mikhail	University College – London	Raman spectroscopy studies	October 18-22, 2010
W. P. Hsieh	University of Illinois – Urbana Champaign	Thermoreflection system set-up with Alexander Goncharov	November 15-19, 2010
Q. Liu	Peking University	Partial melting of carbonated silicates with Yingwei Fei	November 15, 2010- January 31, 2011
C. Tulk B. Sips	Oak Ridge National Laboratory	Resistivity measurements of semi-conducting clathrates under pressure	November 22-26, 2010

3.6 Carnegie CDAC Group Meetings

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

Speaker	Affiliation	Topic	Date
O. V. Dolgov	Max-Planck-Institut für Festkörperforschung	Superconducting glue: Are there limits on T_c	September 17, 2009
Lucille Giannuzzi	FEI Company	DualBeam instrumentation and applications	October 20, 2009
S. McWilliams	Washington State University	Strength of diamond under shock compression from 0.1 to 1 TPa	October 30, 2009
T. Tani	Toyota Research Institute of North America	Microstructural design and fabrication of electronic ceramics	November 12, 2009
S. Jacobsen	Northwestern University	Earth's deep water cycle: From atomic to geophysical scales	January 12, 2010
Nita Sahai	University of Wisconsin – Madison	Organic acid adsorption and calcite growth/dissolution modification	January 26, 2010
N. Woodward	Department of Energy, BES	Overview of geosciences research in DOE Basic Energy Sciences	March 19, 2010
R. Potter	Pacific Northwest Laboratory	Thermodynamic analysis of process chemistry for regeneration of ammonia borane	April 1, 2010
Z. Lin	LANSCÉ – Lujan Center, LANL	Synthesis, characterization, and modeling of laminated ceramics and superhard materials	April 6, 2010

Y. Furukawa	Tohoku University	Variety of organic compounds synthesized by ocean impacts on the early earth	May 3, 2010
T. Mattsson	Sandia National Laboratory	Water from 10 Å to 10 Mm – understanding the structure of ice giants by first-principles simulations	May 6, 2010
J. Bass	University of Illinois – Urbana-Champaign	COMPRES: Consortium for materials properties research in earth sciences	June 10, 2010
Tingting Qi	University of Pennsylvania	DFT and MD modeling of ferroelectric perovskite materials for nonvolatile memory and high piezoelectricity applications	August 3, 2010
D. Phelan	NIST	Single crystal neutron scattering studies of lead zirconate titanate	October 8, 2010

3.7 2010 SSAA Symposium

For the third consecutive year, the SSAA Program Symposium was hosted by **Carnegie** at its historic administration building in downtown Washington, DC (Fig. 54). The meeting was held



Figure 54. Images from the 2010 SSAA Program Symposium.

from January 20-22 and drew participants from around the country. Individual grant recipients and center directors from the three divisions of the program (High Energy Density Physics, Low Energy Nuclear Science and Materials Properties under Extreme Conditions) gave updates on center or group activities and progress. CDAC Director **Russell Hemley** provided an overview of the CDAC program in his invited talk, and 12 CDAC graduate students presented posters at the meeting.

3.7 2010 Short Course on High-Pressure Synchrotron Techniques

Where does one go to learn the fundamental aspects of high pressure synchrotron work from experts in the field? To provide this opportunity, from September 15-18, 2010 CDAC and HPCAT co-hosted a short course entitled "High Pressure Synchrotron Techniques," designed for graduate students and postdoctoral fellows that may be new to synchrotron work. The goal of the Short Course program was to give an introduction to the fundamentals of high pressure science that are integral to the informed use of synchrotron facilities, but are not generally taught in university-level graduate programs.

Fifteen lectures were presented by CDAC partners and HPCAT and APS staff, with the morning lectures focusing on the fundamentals of high pressure science, synchrotron radiation, high pressure chemistry and physics, thermodynamics, and electronic and magnetic properties. Afternoon sessions were devoted to applied aspects of various types of high pressure synchrotron experiments, including diffraction, spectroscopy, laser heating, imaging, and time-resolved measurements (Fig. 55). Finally, the Saturday program included lectures on current topics: hydrogen storage, elasticity and rheology, and high-pressure mineralogy.

In all, 39 graduate students and postdoctoral fellows, both from within CDAC groups as well as other high pressure groups around the country, attended the lectures and participated in a poster session.



Figure 55. Short course attendees **Brendt Hyde** (*Royal Ontario Museum*) and CDAC graduate student **Jeffrey Piggot** (*Ohio State*) attend a lecture presented by **Paul Chow** (*HPCAT*).

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

Thursday, September 16th:

Ho-kwang Mao* (*Carnegie*), *Introduction to high-pressure research*
George Srajer (*Argonne*), *Synchrotron radiation and high pressure*
Choong-shik Yoo (*Washington State University*), *High-pressure chemistry*
Przemek Dera (*GSECARS*), *High-pressure diffraction*

Yue Meng* (HPCAT), *Laser heating at high pressure*
Stanislav Sinogeikin* (HPCAT), *Practical aspects of high-pressure experiments*
Reinhard Boehler (Carnegie), *High-pressure science: Future prospects (Keynote)*

Friday, September 17th:

Brent Fultz* (Caltech), *Thermodynamics*
James Schilling* (Washington University at St. Louis), *Transport properties*
Guoyin Shen* (HPCAT), *Science at HPCAT – Examples and opportunities*
Paul Chow* (HPCAT), *High-pressure spectroscopy*
Jin Wang (Advanced Photon Source), *Time resolved x-ray measurements*
Wenge Yang* (HPSynC), *High-pressure x-ray imaging techniques*

Saturday, September 18th:

Thomas Duffy* (Princeton University), *High-pressure mineralogy*
Maddury Somayazulu* (Carnegie), *Hydrogen storage*
Jihua Chen (Florida International University), *Elasticity, plasticity, and rheology*

Posters Presented at the 2010 Short Course on High-Pressure Synchrotron Techniques

- Armentrout, M. and A. Kavner, The equation of state of FeO + SiO₂ in the Earth's lower mantle, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Bi, W., G. Fabbri, J. S. Schilling, R. S. Kumar, A. L. Cornelius, Y. Zhang, C. Chen, R. Henning, N. M. Souza-Neto, D. Haskel, J. Zhao, E. E. Alp, A. Alsmadi, Y. Meng, and W. Yang, High-pressure studies of structure and valence in europium metal to 92 GPa, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Caron, L., B. Knors, M. Uitterhoeve, Z. Ou, N. T. Trung, J. C. V. Leitão, N. H. Dung, and E. Brück, Study of the nature of magnetoelastic phase transitions using hydrostatic pressure, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Chellappa, R. S., High P-T phase diagram of ammonium nitrate, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Dera, P. and J. Lazarz, Successive, pressure-induced development of bonding in NiAs compounds and polymorphism of NiP, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Dera, P., J. Lazarz, V. B. Prakapenka, M. Barkley, and R. T. Downs, New insights into the high-pressure polymorphism of SiO₂ cristobalite, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Dorfman, S. M., C. M. Holl, Y. Meng, and T. S. Duffy, Static compression to multimegabar pressure under quasi-hydrostatic conditions: Au and NaCl to 258 GPa in a Ne medium, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Fischer, R. A., A. J. Campbell, G. A. Shofner, O. Lord, V. B. Prakapenka, and P. Dera, Equation of state and B1/B8 phase transition in FeO, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Girard, J., J. Chen, P. Raterron, and C. Holyoke, Effect of water on the slip systems activity in the formation of olivine single crystals, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Konôpková, S. and P. Lazor, Characterization of P, T conditions and stress-strain state in the laser-heated diamond anvil cell, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Lin, Y., Compressional behavior of LiMn₂O₄ at high pressure, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Liu, J., B. Mysen, Y. Fei, H. Mao, R. J. Hemley, and J. Li, Temperature dependent mossbauer spectra of aluminous perovskite and implications for the Earth's lower mantle, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).
- Mauger, L., M. L. Winterrose, J. A. Munoz, P. Chow, and B. Fultz, Lattice dynamics across the pressure-induced invar transition in Pd₃Fe, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).

Pradhan, G. K., A. Kumar, U. V. Waghmare, C. Narayana, and S. K. Deb, Elastic and structural instability of cubic Sn_3N_4 and C_3N_4 under pressure, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).

Wang, J., R. F. Smith, J. H. Eggert, J. Montoya, G. Finkelstein, D. Braun, T. R. Boehly, G. W. Collins, and T. S. Duffy, Development of a platform for laser ramp compression of planetary materials, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).

Zhang, D., J. M. Jackson, W. Sturhahn, and Y. Xiao, Changes in the local environments of iron in orthoenstatite at high-pressures, *HPCAT/CDAC Short Course on High Pressure Synchrotron Techniques* (Argonne, IL, September 15-18, 2010).

3.8 Future of Dynamic Compression Science Workshop

At the "21st Century Needs and Challenges in Compression Science" Workshop held at the Bishop's Lodge Ranch in Santa Fe, NM September 23-25, 2010 CDAC Director **Russell Hemley** chaired the Static Compression Panel, which included CDAC Advisory and Steering Committee members, as well as several CDAC collaborators. The workshop was convened by LANL Staff Scientists **Dave Funk** and **Rusty Gray** to help chart the course of high-pressure science for the

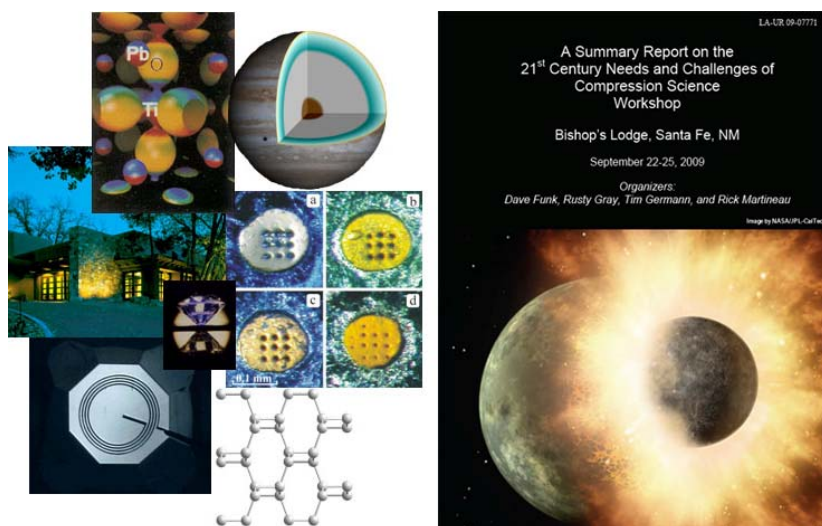


Figure 56. Right: collection of images representative of the topics discussed at the recent workshop on the future of dynamic compression science. Far left in the set of images: Bishop's Lodge Ranch in Santa Fe. Right: cover of the Summary Report from the Bishop's Lodge workshop.

coming decade, including opportunities at the proposed MaRIE facility at Los Alamos. The other participants on the Static Compression Panel were **Christian Mailhot** (LLNL, CDAC Advisory Committee), **Dana Dattlebaum** and **Yusheng Zhao** (LANL, CDAC Steering Committee), and CDAC collaborators **Reinhard Boehler** (Carnegie), **William Evans** (LLNL), **Malcolm McMahon** (University of Edinburgh), **Michael Pravica** (University of Nevada-Las Vegas) and **Adam Schwartz** (LLNL).

3.9 CDAC Research Presented at the APS March Meeting

The annual March meeting of the American Physical Society was held in Portland, Oregon from March 15-19, 2010 with CDAC researchers well represented among a number of sessions. Seven of the CDAC academic partner groups, along with **Carnegie** personnel, National Laboratory Partners and HPCAT/HPSynC staff presented 46 papers in 20 different sessions throughout the course of the meeting. Of particular interest was a series of four high pressure research focus sessions, in which the work of a wide cross-section of the CDAC community was included. Of the 45 presentations in these special focus sessions, 20 of these contained a CDAC component in the results. The scientific and technique development work of **Vohra's** group (Alabama) was featured twice in the focus sessions, and David **Cahill** (Illinois) also gave several presentations.

CDAC Scientists from **Carnegie** presented 9 talks. **Maddury Somayazulu** and **Tim Strobel** discussed their experimental work on the high-pressure behavior of the Xe-H_2 and $\text{SiH}_4\text{-H}_2$ systems, respectively. On the theoretical side, **J. G. O. Ojwang** and **Luke Shulenburger** presented new results on transition metal oxides and **P. Ganesh** gave a talk on first-principles studies on ferroelectric materials. Also representing **Carnegie** was **Angela Schad**, a 2009 Carnegie Summer

Scholar from the **University of Notre Dame**, who presented her theoretical work on Raman spectra of ferroelectric perovskites.

CDAC Laboratory Partners **Dana Dattlebaum (LANL)**, **Will Evans (LLNL)** and **Dan Dolan (Sandia)** also presented work from their respective high pressure groups. **Dattlebaum** spoke about the pressure-induced decomposition of hydrogen peroxide, while **Dolan** presented work on the P - T phase diagram of tin as determined from dynamic isentropic compression experiments. **Evans** was a co-author on four talks, and also chaired an important session that promoted new research and employment opportunities at the National Labs.

4. TECHNOLOGY DEVELOPMENT

Pushing the frontier of high P - T science requires a significant investment in technological development. At CDAC, each of the academic and laboratory partner groups pursue technology development to some degree. In the following sections, we present some highlights in this area that have been important to advancing the CDAC scientific program over the past year.

4.1 Technical Improvements at HPCAT

The HPCAT sector at the APS remains the centerpiece of the CDAC program. Not only does CDAC directly support the facility at the level of 30% of the operating costs on a yearly basis, many of the fundamental scientific advances made within CDAC have been a direct result of the cutting-edge capabilities available on the sector's four beamlines. Here we outline some of the recent developments made at HPCAT.

Dual Undulators in Canted Mode – The current undulator line at HPCAT contains two branches operating in two separate energy ranges. Because both branches use the same undulator source, the energies used by each branch of the beamline are coupled. To permit *independent*

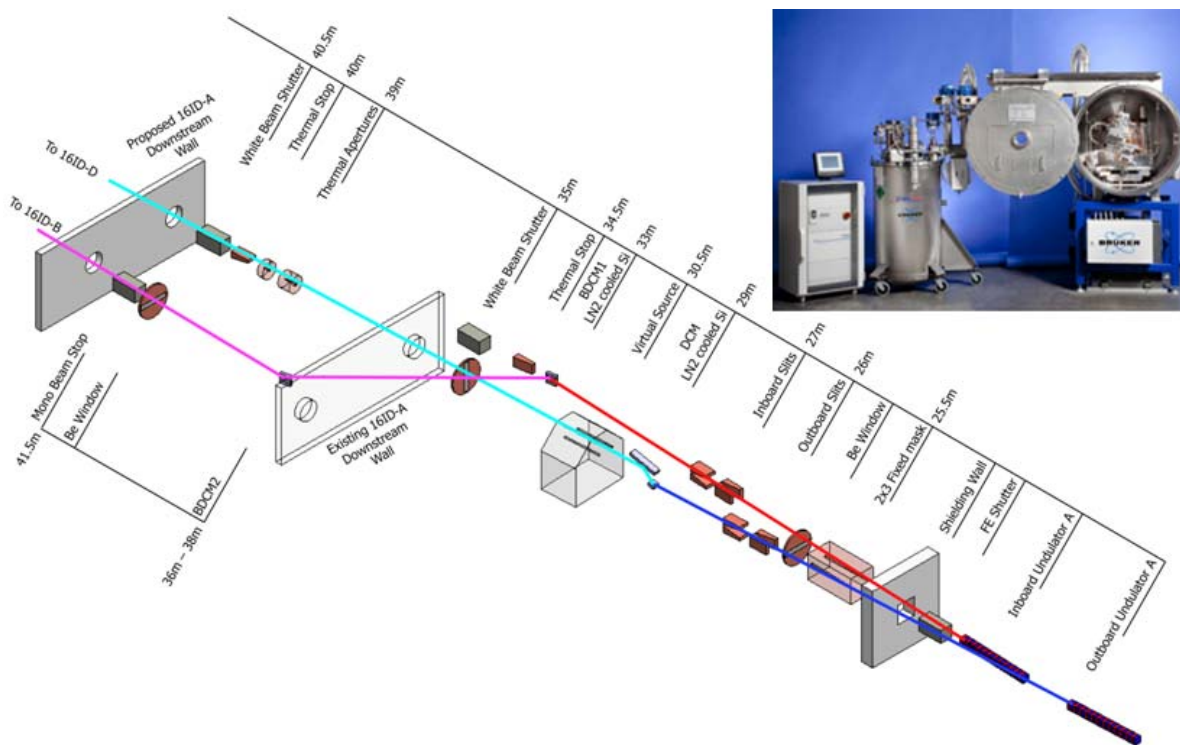


Figure 57. Layout of the optical components on 16-ID: Canted undulator sources with 1-mrad separation provide beams for two fully independent beamlines. The outboard branch will be used for high pressure spectroscopy and for enabling submicron probes; the inboard branch will be used for high pressure micro-diffraction studies.

operation, the 16-ID line is scheduled for canting the straight section in September 2011. This development was supported by the APS. The canted geometry (Fig. 57) will separate the beams by 1 mrad and allow independent undulator control, thereby providing optimal operation of both branches (16-ID-B and 16-ID-C,D,E) and increasing the usable ID beam time.

Two canted beams from the undulators will first go through the primary slits, and then will encounter the double crystal monochromator (DCM), the virtual source unit, the branching double crystal monochromator (BDCM), thermal apertures, and thermal beam stops, as shown in Fig. 57. Two new monochromators (*i.e.*, the DCM and BDCM) matching the canted geometry will be installed at 16-ID-A, the first optics enclosure, in 2011. The two monochromators will be from Bruker-Accel equipped with a liquid-nitrogen-cooled crystal assembly. The advantages of having new monochromators include high throughput (high flux), extended energy range, energy scanning capability, better beam focusing capability, more uniform beam profile for imaging, and significantly improved stability in both position and energy.

Beamline 16-ID-B: Laser Heating with a Fiber Laser Apparatus – Newly added fiber lasers at the beginning of 2010 have increased the total heating power up to 200 W, and offer a significantly improved heating stability (Fig 58). In addition, 16-ID-D now has laser profile shapers with the capability of modifying the output profile for different heating applications including a flat-top heating mode. The flat-top heating mode provides a spot size of 15 to 20 microns in diameter; together with the 5x5 x-ray beam size and 4x4 temperature sampling area, this setup further enhances the reliability of *in-situ* measurements. Other areas of improvement include centralized experiment control, automatic background subtraction in temperature measurement, and an automatic data logging system, all of which have contributed to operational efficiency and effectiveness.

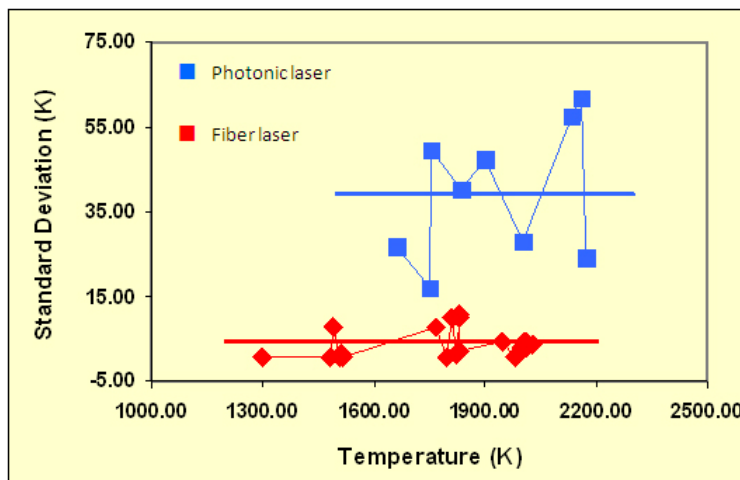


Figure 58. Stability of laser heating temperature with increasing temperature for a fiber laser compared with a standard laser apparatus.

New developments in pulsed laser heating with *in-situ* x-ray diffraction at HPCAT (in collaboration with **Reinhard Boehler** of **Carnegie**) have shown promise for studying melting related phenomena at high pressures. By synchronizing a laser heating pulse with the x-ray shutter, detector and temperature measurement, the effect of heating on crystal structure can be obtained from a single pulse heating or from the accumulation of a series of pulses.

Beamline 16-ID-D: Seven-Element Emission Spectrometer – Presently the x-ray emission spectrometer at 16-ID-D employs a single 100 mm diameter bent Si wafer as the analyzer at a 1m radius. Given the emission energy of interest, the (*hkl*) of the analyzer is selected to give the geometry closest to backscattering. The emission radiation is energy-analyzed at 90 degrees to the incident beam, and focused in to a point detector on a Rowland circle. In order to increase the efficiency of the spectrometer, the group is in the design stage of upgrading to multiple analyzers. The new design can house up to seven 100 mm diameter analyzers in the same Rowland circle geometry. With the proposed design, different modules of pre-aligned analyzers can simply be plugged in to measure the spectra of the element of interest and data collection efficiency will increase proportionally. This seven-element assembly matches the opening of most DACs.

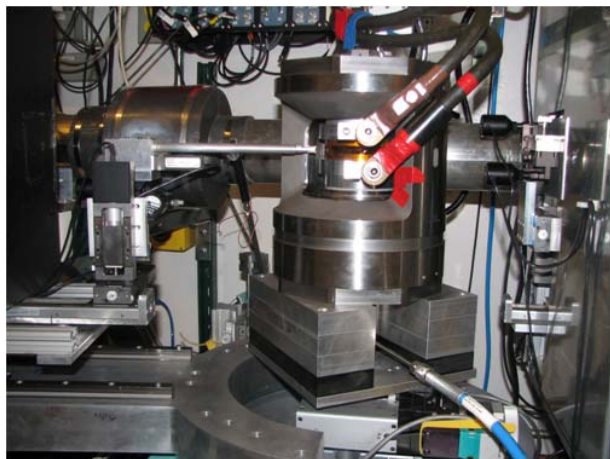


Figure 59. Paris-Edinburgh cell installed at beamline 16-BM-B for use in white beam mode.

DAC with reasonable collection times. In addition, for measurement of plasmons (collective excitations of the electron gas), where the momentum transfer needs to be well-defined, the 17-element analyzer allows for easy masking of the array. Sodium plasmons in a DAC have recently been measured in this way.

Beamline 16-BM-B: Paris-Edinburgh Cell – The Paris-Edinburgh cell (Fig. 59) provides a large sample size (1-2 mm) and high temperature conditions (up to 2700 K). The primary goal of this development program is to study liquid properties at high pressures. The feasibility for this type of measurement has been successfully demonstrated in the past year in collaboration with scientists from the **University of Chicago** and **Ehime University** in Japan. The maximum pressure and temperature ranges (with no gasket blow-out) are currently up to 7 GPa and 2500 K using WC-based anvils. Extending the pressure range remains one of the major goals for future development, which will be explored by using different types of anvils. With the current P - T coverage, many experiments have been performed for studying melt structures of albite, basalts, metal-borates, and germinates at high pressures. In the materials science area, metals and metal-alloy melting experiments combined with white beam radiography were tested. The new development of ultrasound velocity measurement in parallel with an improvement of the whitebeam radiography technique is currently planned for expanding the scientific application, for example, in determining equations of state for liquid phases. A table-top Si(111) channel-cut monochromator also has

Beamline 16-ID-D: 17-Element Backscattering Analyzer – The beamline staff at 16-ID-D has now completed the commissioning of the 17-element backscattering analyzer and has been routinely using it for x-ray Raman spectroscopy measurements. Measuring x-ray Raman signals from carbon in a DAC requires a small focused beam to prevent diamond scattering from contaminating the carbon sample signal. Using a 200 mm KB mirror to obtain a 10 micron vertical beam size reduces the incident flux on the sample, which makes it difficult to measure the weak signal from the carbon sample. The increased solid angle of the 17-element analyzer now allows measurement of carbon-based samples at high pressure in a

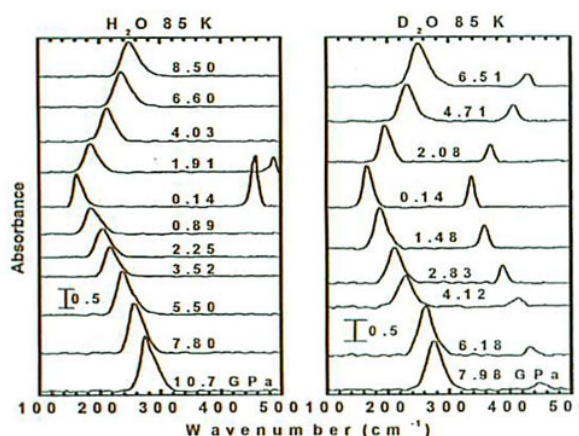
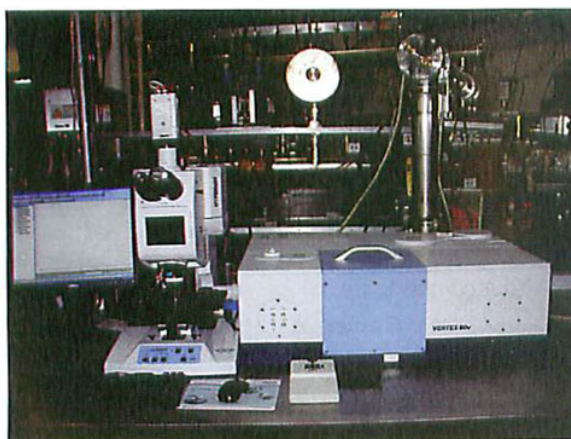


Figure 60. Top: Newly established U2A side station with Bruker Vertex 80v FTIR spectrometer and Hyperion 2000 IR microscope. Bottom: The plot indicates pressure dependence of far-infrared absorption spectra of H_2O and D_2O ice VIII obtained at 85 K.

been installed to enable switching between white beam and monochromatic beam experiments. The channel-cut monochromator system is dedicated to monochromatic transmission measurements for *in-situ* density determination and high-energy XANES. Methodology developments for this type of experiment are in progress.

CDAC Science in Synchrotron Radiation News – The May/June, 2010 issue of *Synchrotron Radiation News* focused on high pressure research. Both of the technical reports in the edition showcased CDAC supported work and were coauthored by CDAC supported beamline personnel, including **Zhenxian Liu, Guoyin Shen, Yang Ding, and Wenge Yang**, as well as CDAC Academic Partner **Tom Duffy (Princeton)**. The work of Brookhaven/NSLS and colleagues from Brookhaven, SUNY, Princeton, and Carnegie was featured in a report about high-pressure research at NSLS (Fig. 60). High-pressure research at the APS was the focus of a report by **Shen** and colleagues from HPCAT, the University of Chicago, APS, and HPSynC.¹³⁰⁻¹³¹

4.2 Infrastructure Development at Carnegie and Academic Nodes

Laser-Launched Flyer Plate Apparatus – The **Dlott** group at **Illinois** is developing a laser-launched flyer plate facility to study shock compression at much greater pressures and durations than possible with femtosecond laser direct drive, and to investigate ignition processes in energetic materials. With flyer plates, the shock duration will be in the 3-20 ns range and the impact velocities will be in the 0-9 km/s range, which in Al metal will generate a shock at ~700 GPa. Laser-launched flyer plates have found a variety of uses,¹³²⁻¹³⁵ but in this work, the focus will be on three applications for which these flyers are well suited: improved methods for measuring pressures and velocities, Hugoniot of thin film materials, and ultrafast spectroscopy of impact initiation of energetic materials.

The first year or two of this project will be devoted to technique development, which is being led by CDAC graduate student **Kathryn Brown**. The ability to launch a flyer is critically dependent on the ability to produce a very smooth flattop laser beam. In the initial phase of this work, the group developed a novel method to generate a flattop beam by spatial filtering with a

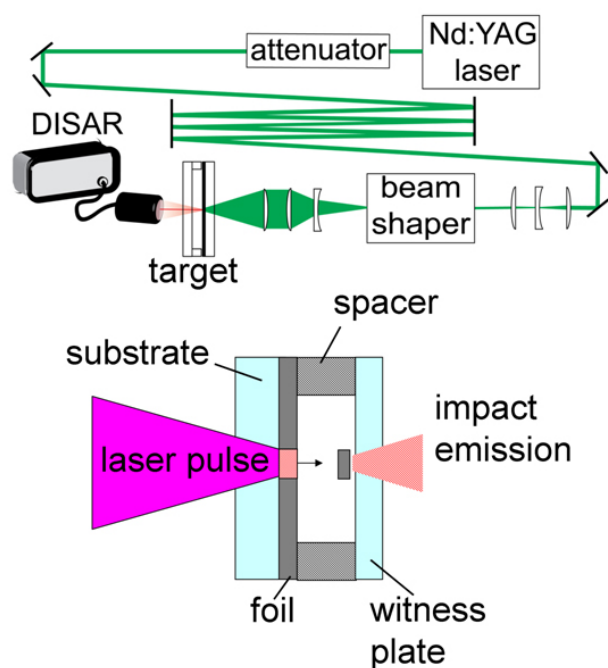


Figure 61. Optical layout for flyer launch and schematic of one element of the target assembly.

commercially available mirror with a Gaussian reflectivity profile.¹³⁶⁻¹³⁷ The beam was allowed to propagate 30 m, so diffraction smoothed out a lot of the spatial variation to produce an approximately Gaussian beam, and then the filter was applied. A Gaussian beam can be filtered with an aperture so only the uniform center is used, but the efficiency is low. The perfect variable reflectivity mirror is not available in a high power version, but that would generate a flattop beam having 67% of the input power. A Gaussian mirror can transmit a flattop beam with 30% of the input power and a super-Gaussian mirror with up to 45% of the input power.¹³⁷ The latter two are commercially available. After filtering there was 50 mJ available to launch. The concept of the launcher is depicted in Fig. 61. Flyers have been launched up to 4 km/s but now the typical flyer is 25 μm thick. The flight path is variable but typically 100 or 200 μm , the impact makes a consistent shock of 7 ns duration and the velocity ranges from 0-2 km/s.

The group has shown that impact emission results primarily from the gas that the piston-like flyer concentrates on its surface during flight and then impacts on the window. When Ar is used rather than air the emission is much more intense and when a vacuum is pumped the emission practically vanishes. A spectrogram of the Ar emission is shown in Fig. 62a, comprised of a continuum and line emission. This spectrum indicates there are two kinds of Ar emitting plasmas, a denser one that looks like a blackbody and a less dense one that looks like atomic emission. This is not what was predicted by Zel'dovich¹³⁸ but it is consistent with what Putterman¹³⁹ has seen in collapsing bubble emission. The 8 GHz DISAR does an excellent job of monitoring flyer plate launch, flight and impact, as illustrated in Fig. 62b. The flyer velocity is visible and also how it slows down upon impact.

Advancing Software for Analysis of Neutron Diffraction Data at LANSCE – The Rietveld analysis code “Materials Analysis

Using Diffraction” (MAUD), which Luca Lutterotti began developing during his post doctoral appointment at Berkeley,¹⁴⁰ has been greatly expanded. Among the new features are an improved approach for monoclinic crystal symmetry¹⁴¹ and a function that allows for turbostratic disorder.¹⁴² A webpage introduces new users to the complex procedures (<http://eps.berkeley.edu/~wenk/TexturePage/MAUD.htm>), and a recent publication describes, step by step, the analysis of TOF neutron diffraction spectra.¹⁴³

Virtual Experiment Control for High P-T Raman Spectroscopy – Double-sided laser heated DAC methods allow simultaneous *in situ* confocal Raman measurements of materials up to megabar pressures and high temperatures. At **Carnegie, Alexander Goncharov** and **Subramanian Natarajan** have developed a virtual control and data acquisition system to automate simultaneous Raman/ laser heating experiments. The system enables reduction of experiment time by 90% in comparison to manual operations, allowing measurements of high quality Raman spectra of even highly reactive or diffusive samples, such as hydrogen at extreme conditions, using continuous wave laser heating. These types of measurements are very difficult and often impossible to obtain in a manual operation mode. Complete data archiving and accurate control of various experimental parameters (e.g., on-the-fly temperature determination and self-adjusting data collection time to avoid signal saturation) can be done, and open up possibilities of other types of experiments involving extreme conditions. The apparatus is described in a recent publication.¹⁹

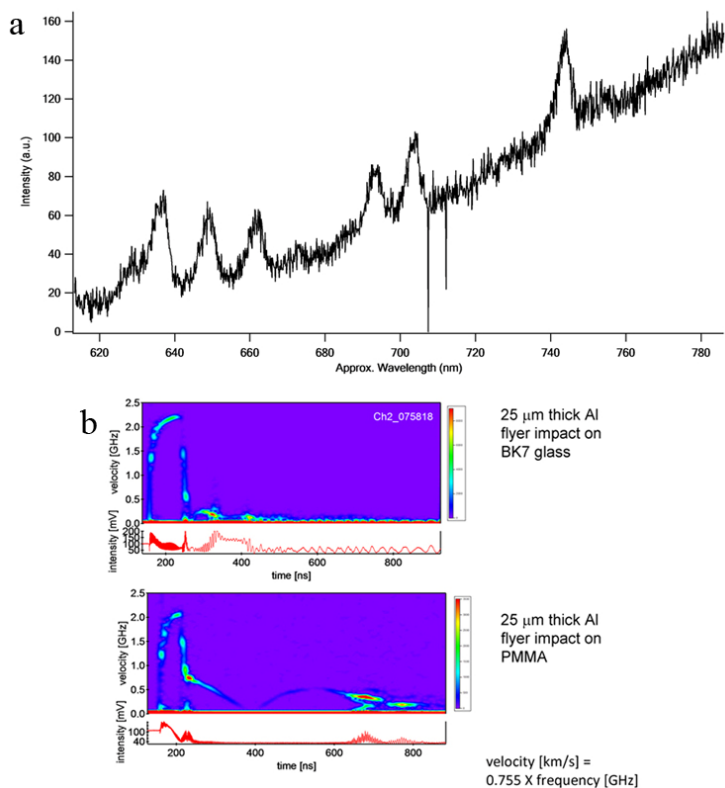


Figure 62. a), Emission spectrum (time-integrated) from flyer collision with the window, in an Ar atmosphere, showing discrete Ar transitions and a broad continuum. b) Interferograms and their Fourier transforms from flyer collision with glass and PMMA. After launch the speed runs up to about 1.5 km/s. After collision there is an ~25-35% drop in speed. This new speed is the velocity U_p of the shock drive. The shock lasts for ~7 ns. A viscoelastic unloading process is clearly seen in PMMA but not in glass.

Pulsed Laser Heating for Synchrotron X-ray Diffraction at High Pressures – The Carnegie group has also developed a method for *in situ* x-ray synchrotron diffraction measurements of samples heated by a pulsed laser in the DAC at pressure up to 60 GPa. Designed by **Alex Goncharov** in collaboration with the group at APS Sector 13 (GSECARS), the technique employs an

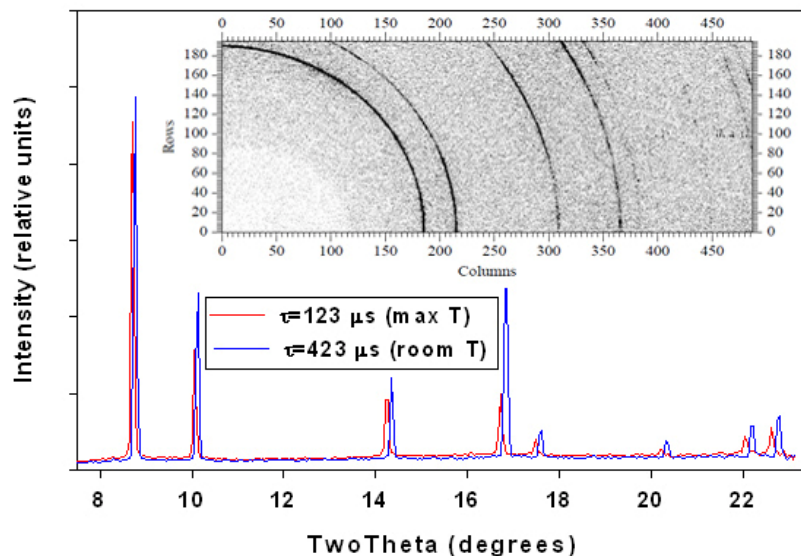


Figure 63. Time-domain laser heating x-ray diffraction experiments in platinum at 40 GPa (APS, GSECARS). Blue line – the pattern measured (with 1 ms time resolution) at the delay time well outside the laser pulse duration. Red solid line- the pattern collected at the delay time corresponding to the largest thermal expansion and hence the largest bulk sample temperature (3000 K). The inset shows the diffraction image corresponding to the pattern measured from the hot sample (red curve).

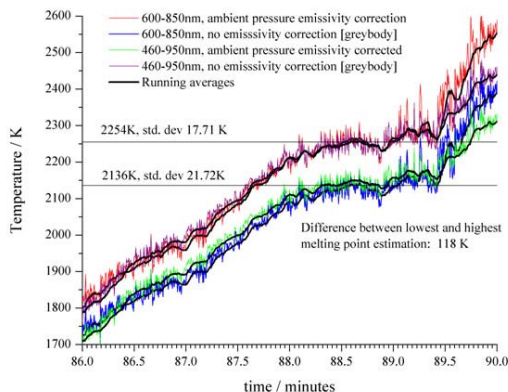
heating.¹⁴⁴ This novel technique offers a new and convenient way of fine tuning the maximum sample temperature by changing the pulse width of the laser (Fig. 63). This delicate control, which may also prevent chemical reactivity and diffusion, enables the accurate measurement of melting curves, phase changes, and thermal equations of state.

Laser Heated Diamond Anvil Cell Apparatus at FIU – The **Florida International** group, headed by CDAC Partner **Surendra Saxena**, has focused in the development and application of laser heating methods for DAC experiments. The temperature of a heated surface is normally measured using a non-contact spectroradiometric technique, in which the thermal radiation from the surface of the heated specimen is measured and fitted to the Plank equation. With the FIU apparatus, it is possible to measure a two-dimensional temperature distribution across a laser heated sample by scanning the image of the heated spot across the thin slit entrance of a spectrometer. The temperature measurement system is enabled using a software suite that integrates the control of individual laser heating system components and provides complete automation of the experiment in graphical user interface. Some of the key hardware components of the system controlled by the LH-DAC software suite are the half-wave plate for laser power control, laser power meter, an actuator for image scanning and a CCD camera for radiometric temperature measurement.

It is well known that there are many causes of error in this type of temperature measurement and therefore it is absolutely necessary to carefully calibrate the system using available standards. The intensity transfer function of the spectrometer is calibrated by measuring spectra of several metals at their known melting temperatures (*e.g.* platinum, and for higher temperatures, tungsten). Even with calibration, there are still often other sources of temperature

electronically modulated 2–10 kHz repetition rate, 1064–1075 nm fiber laser with 1–100 μ s pulse width synchronized with a gated x-ray detector (Pilatus) and time-resolved radiometric temperature measurements. This enables the time domain measurements as a function of temperature in a microsecond time scale averaged over many events, typically more than 10^3 . X-ray diffraction data, temperature measurements, and finite element calculations with realistic geometric and thermochemical parameters show that in the present experimental configuration, the temperature of a sample 4 μ m thick can be continuously monitored (up to 3000 K in the most recent set of experiments) with the same levels of axial and radial temperature uniformity as with continuous

Hotspot temperature history [increasing laser power]



Melting of Iron under high pressure

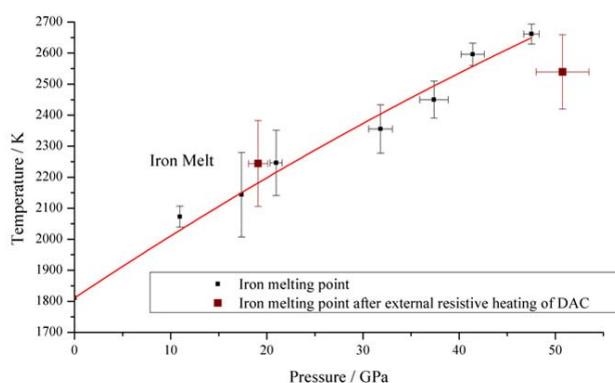


Figure 64. Left: Uncertainty in temperature for the LH-DAC system obtained by error analysis of the melting temperature. Right: Measurement of the melting curve of iron to 50 GPa, with data shown as black filled squares. Sample: $70 \mu\text{m}^2$ Fe foil, $20 \mu\text{m}$ thick; pressure medium: MgO dried at 1000°C ; pressure determination: ruby luminescence.

measurement errors, and an error analysis has been performed to determine the lower and upper bounds of various measurement errors. Temperature error can also be caused by an arbitrary choice of fitting parameters associated with the Plank equation. Often an unknown thermal emissivity creates a significant error in temperature measurement. By varying possible values of unknown fitting parameters (*e.g.* range of wavelengths to fit, sample emissivity function), the lower and upper bounds of the temperature measurement for a given sample and for a given temperature range are obtained (Fig. 64).

In the temperature calculation, the diamond cell and sample geometry are simulated in COMSOL, a MATLAB finite element analysis routine. Employing the approximate two-dimensional symmetry of the sample environment, the calculation speed can be increased by orders of magnitude. COMSOL obtains the temperature distribution by simultaneously solving the heat transfer partial differential equation at each of the nodes. The parameters that can be varied include laser power, laser beam width, thermo-physical properties of the sample, emissivity of the sample, sample thickness (and overall geometry), dimensions of the pressure chamber, thermo-physical properties of the pressure medium, gasket and diamonds, and surrounding temperature or boundary conditions.

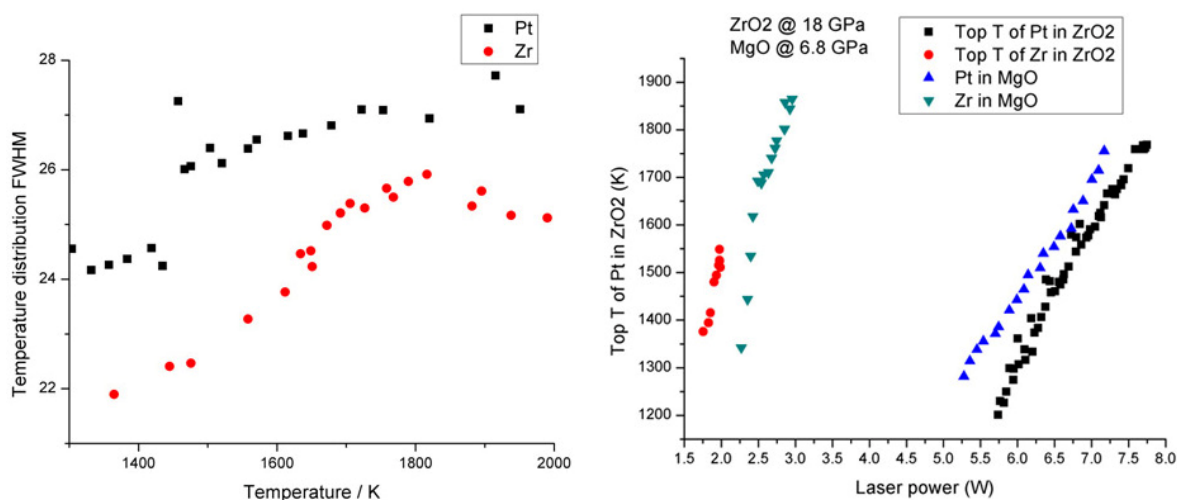


Figure 65. Left: FWHM of the hot spots at various temperatures, with Pt as compared to Zr. This initial result agrees qualitatively with theoretical calculations. Right: Variation of temperature with laser power for laser heating of Zr and Pt with different insulating media.

Thermal Conductivity of Materials in LH-DAC – A proof of concept experiment for measuring the thermal conductivity of materials in a DAC with CW laser heating has been undertaken. The first results show qualitatively that the experimental technique reproduces the theoretical prediction for thermal behavior of a material in a LH-DAC system. In this measurement, metal foils of Pt and Zr ($100 \times 100 \mu\text{m}^2$, $20 \mu\text{m}$ nominal thickness) were loaded into the DAC with MgO as the pressure medium.

During the actual laser heating, a succession of temperature distribution profiles is recorded at different times and at chosen laser power conditions. Temperature profiles were recorded in sequence at about 1-2 seconds apart. Each temperature profile is then fitted to a Gaussian function to approximate the FWHM of each temperature profile. This was done to qualitatively see how the hot spot spreads in each of the samples (Fig. 65).

Advances in CVD Diamond Growth and Characterization – Development work on the growth of single crystal diamond at **Carnegie** by the CVD process has advanced considerably during the past year. In particular, breakthroughs have been made in rapid growth (up to $200 \mu\text{m/hr}$) of high quality, large diamond single crystals, three-dimensional expansions of diamond single crystals, and diamond anvil restoration/enhancement for high pressure research.

The 2.3 carat colorless anvil shown in Fig. 66 was cut from a 13.5 carat diamond block grown at high growth rates (around $50 \mu\text{m/hr}$) in the absence of impurities other than hydrogen. UV-VIS absorption, Raman/photoluminescence spectroscopy and cathodoluminescence, birefringence topography are used to characterize the CVD diamond. The measurements show that the material has high optical quality and clarity, which makes it a promising material for high pressure windows, as shown in Fig. 67. Raman spectra show a large intensity ratio (above 5) of the second-order Raman peak to the background (Fig. 66). Luminescence measurements along the growth directions indicate that the color may be due to an unintentional leak of nitrogen.¹⁴⁵

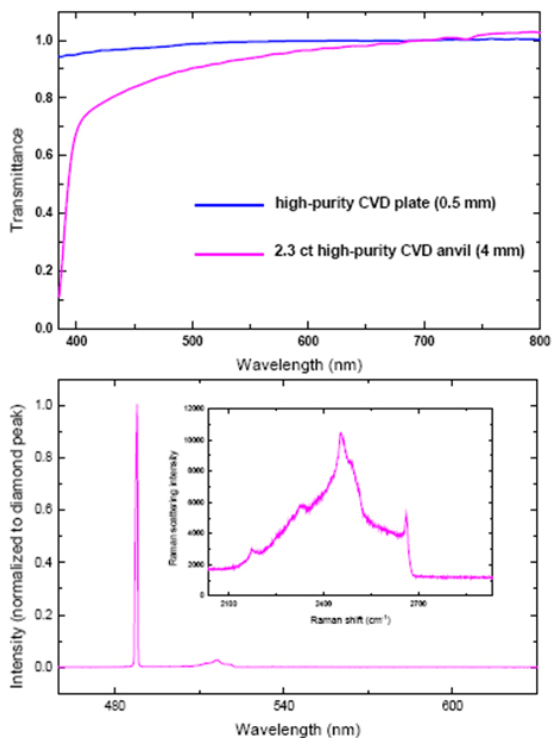


Figure 66. Left, 2.3 ct colorless single-crystal CVD diamond anvil beside a 0.25 ct anvil. Right, UV-visible transmittance and Raman spectra (excited by 457nm laser) of the 2.3 ct CVD diamond anvil. Inset: second-order Raman spectrum.

Because of the nature of homoepitaxial growth, the dimensions of grown CVD single crystal diamond are limited by the area of the single crystal diamond seeding substrates, which are normally synthesized by a high pressure-high temperature process. The typical area of these seeds is $\sim 8 \text{ mm} \times 8 \text{ mm}$.

The growth mechanism of diamond single crystals by the CVD process gives rise to new paths for making larger diamond. The addition of nitrogen to the reaction gas chemistry can significantly prompt the growth along the [100] crystallographic directions. The CVD group at Carnegie has been working on enlarging the dimensions of single crystal diamond by growing into the three orthogonal [100] type crystallographic directions. Starting from a 0.5 mm thick seeding substrate, after multiple growths in the [001] directions, a single crystal diamond ingot with dimensions of $13.8 \text{ mm} \times 13.4 \text{ mm} \times 15.7 \text{ mm}$ was synthesized. CVD seeding substrates with area up to $15 \text{ mm} \times 12 \text{ mm}$ were sliced out from this ingot along the [001] direction. The largest surface of these newly fabricated seeds are normal to the [100] crystallographic directions and can be used for the synthesis of a secondary diamond ingot, with expected dimensions of at least $15 \text{ mm} \times 15 \text{ mm} \times 15 \text{ mm}$, and consequently a $15 \text{ mm} \times 21 \text{ mm}$ seeding substrate: an increase in terms of usable area by a factor of five compared to the original seed.



Figure 67. Single crystal CVD diamond windows for small angle x-ray scattering studies at high pressure. Windows are 3.0 mm in diameter and 0.5 mm thick.

Diamond anvils, which are normally produced from natural diamonds, often break during high pressure experiments. Many times these breaks are small or localized only at the cutlet leaving the bulk of the diamond untouched. These cracks or defects compromise the diamond's overall strength because they can propagate under further stress. The CVD group at CIW has spearheaded a new way to restore damaged diamond anvils. The solution to salvaging the unscathed diamond is to remove the affected area and replace it with high quality CVD diamond. Laser sawing is then used to shape the raw product into anvil shapes, which are then polished. The CVD diamond layers produced by this process were studied by photoluminescence and UV-Vis absorption, which showed that the optical quality of these layers are comparable to (or even better) than type IIA diamond,

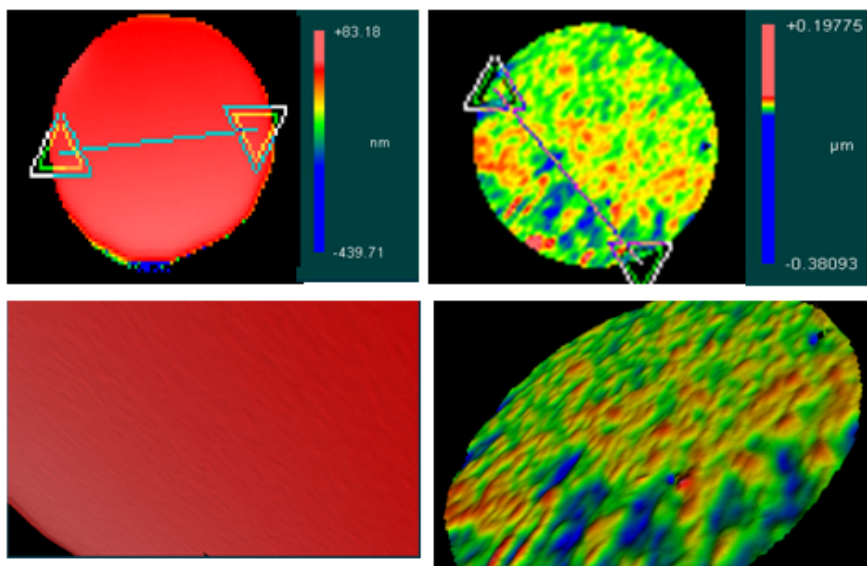


Figure 68. The superior surface finish of the Carnegie CVD diamond anvil (left) compared to the surface finish of a commercially-polished anvil.

along with enhanced toughness. The viability of such anvils is demonstrated in measurements on hydrogen at megabar pressures and high temperature.¹⁸

The CVD diamond laboratory at Carnegie has expanded its production and processing capacity to better serve and support the high pressure research community. Two Nd:YAG lasers are employed to shape anvils and produce windows. A ZYGO New View optical profilometer is used for analyzing the surface prior to and after diamond growth (Fig. 68). Two commercial-sized polishing wheels capable of producing professional finishes are now located in the diamond processing laboratory. A fine polishing wheel developed by CDAC Research Scientist **Chang-Sheng Zha** is able to produce a superior surface finish (0.48 nm RMS roughness, as compared to 8 nm RMS roughness obtained by a commercial polisher).

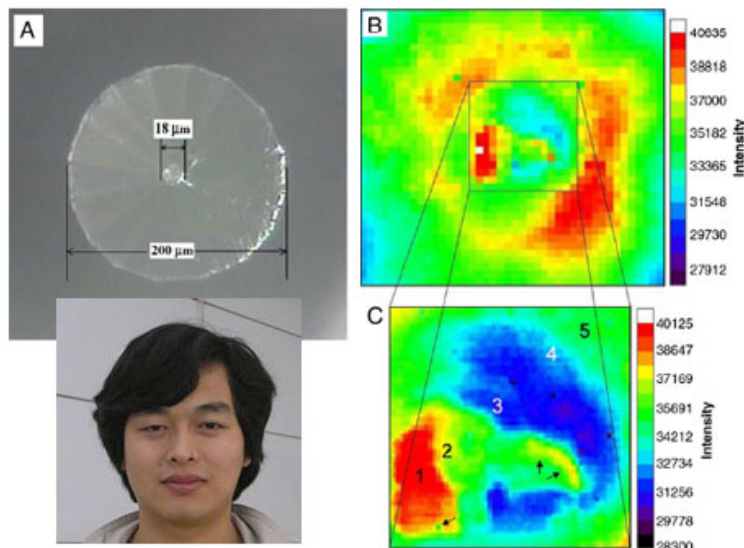


Figure 69. (A) Photomicrograph of the beveled diamond culet with the gasket and samples. (B) 2D transmission intensity map with a 1 $\mu\text{m}/\text{step}$ of the $40 \times 40 \mu\text{m}^2$ white-outlined square in A. (C) 250 nm/step map of the black-outlined square in B. The color scale indicates the transmitted x-ray intensity. Inset: **Lin Wang (HPSynC)**.

Nanoprobes at Megabars – The quality of measurements at extreme conditions is governed by the size of the analytical probe relative to the size of the samples. High energy synchrotron x-rays have been used in high-pressure studies for decades. However, at the existing dedicated high pressure facilities, these dimensions have been limited to 2-5 microns, which has become a key limitation to resolve properties of materials at megabar pressures where significant differences occur on the sub-micron scale.

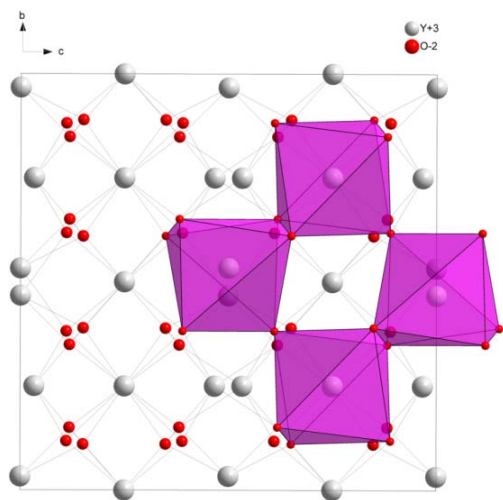


Figure 70. The cubic structure of Y_2O_3 viewed along the $[100]$ direction. Each octahedron shares two edges with four neighboring octahedra. The Y-Y distance across a shared edge is slightly shorter than the Y-Y distance across a shared corner.

A team led by **Lin Wang** and including scientists at **Carnegie**, the **Advanced Photon Source, Stanford University**, and **National Cheng Kung University (Taiwan)** has broken the micron barrier in these megabar pressure measurements by introducing nanoscale beams, an order of magnitude smaller than the existing high pressure x-ray beams, into high pressure studies. The work shows that the use of nanoscale x-ray probes overcomes several key limitations in the study of materials up to multimegabar pressures. Nanoscale probes readily resolve signals from individual materials, between sample and gasket, peak pressure and pressure gradient at a submicron length scale (Fig. 69). These beams also enable single-crystal x-ray diffraction studies in nominally polycrystalline samples at

ultrahigh pressure. These capabilities have potential for driving toward higher maximum pressures and further miniaturization of high-pressure devices.¹⁴⁶

At the Nanoscale, Size

Matters – With the availability of third-generation synchrotron x-ray facilities, the properties of nanoscale materials are now receiving increased attention. In particular, the high energy and brilliance coupled with the tight focus of the x-ray beams at **HPCAT** now make possible detailed structural studies of nanoscale solids. **Lin Wang (HPSynC)** and co-workers from **HPCAT, Argonne National Laboratory**, and **Stanford** have now shown that the compression behavior of nanoscale Y_2O_3 , an archetypal rare-earth oxide, differs in significant ways depending on the particle size of the material.

Using the microdiffraction capabilities of **HPCAT**, samples of Y_2O_3 with particle sizes of 16 nm, 21 nm, and 1000 nm (1 micron) were investigated to above 30 GPa. In each case, the ambient pressure structure is the cubic rare earth oxide (bixbyite) structure (Fig. 70). On compression, however, the 16 nm material becomes amorphous at 25 GPa, while the 21 nm material undergoes the well-known cubic-to-hexagonal phase transformation at 14 GPa. The micron-sized material, which is representative of the bulk solid, undergoes the same phase transition, but at a slightly lower pressure of 12 GPa. In addition, the 16 nm material remains amorphous on decompression, while the 21 nm material adopts a monoclinic structure on decompression rather than become amorphous like the 16 nm material, or revert to the cubic phase, as is the case with the bulk solid.

A pair distribution function analysis (Fig. 71), carried out with the 16 nm material, shows that the Y-O nearest neighbor distances do not change with pressure, suggesting that the YO_6 octahedra are essentially rigid and do not distort upon compression. The nearest-neighbor Y-Y

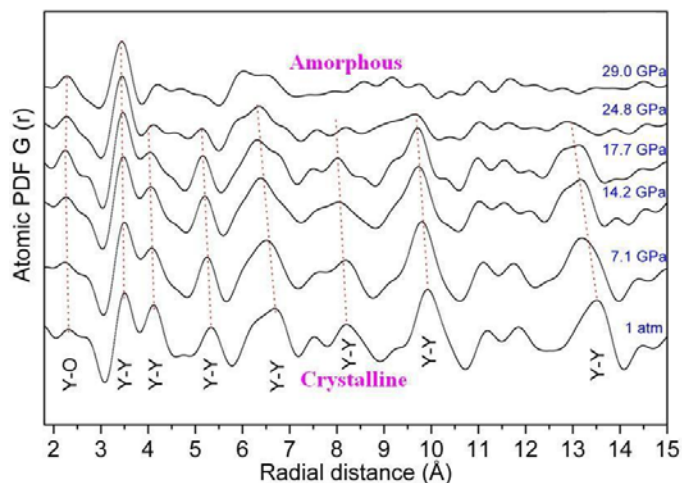


Figure 71. Pair distribution function of 16 nm Y_2O_3 with pressure. Y-O distances within the YO_6 octahedron and the distance between octahedra remain constant with pressure and intact through the crystalline-amorphous transition, while longer-range order disappears above 25 GPa.

distances across the shared edge also do not change and remain intact through amorphization. The onset of amorphization therefore appears to take place when the linkages between corner-shared octahedra reach a critical limit, at which point the longer-range order in the solid breaks down.

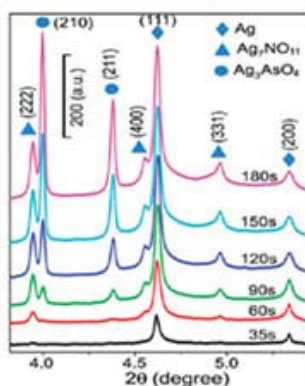
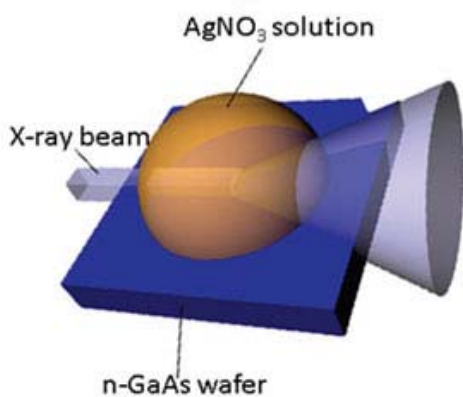


Figure 72. Left: Experimental design for monitoring the growth of Ag nanoparticles in real time. Ag nanoparticles are grown at a GaAs substrate- $AgNO_3$ solution interface. Right: X-ray diffraction patterns taken with 30 ns time resolution show the growth of the Ag nanoparticles in real time.

The work provides new insights into the behavior of nanoscale materials, in particular the point at which a collection

of atoms begins to behave like the bulk material, as well as the phenomenon of pressure-induced amorphization, which is observed in a number of important oxide materials.

Watching Nanocrystals Grow with X-rays –

For the first time, it is now possible to watch nanoparticles grow from the earliest stages of their formation. The breakthrough was made possible by high-brightness and high-energy synchrotron radiation techniques developed in part by **HPSynC**. The work should lead to new ways to control nanocrystal growth, a result that will affect applications ranging from making new energy materials such as solar cells to chemical and biological sensors important for national security.

Using high-energy x-rays from the APS, the group carried out diffraction studies as a function of time that provided information on crystal growth with high time resolution, and the high brilliance and high penetration of the x-ray source allowed a view on the growth of the crystals from their initial formation (Fig. 72). The atoms scatter very short wavelength x-rays and the resulting diffraction pattern reveals the structure of these unusual particles. Quite often the chemical reaction occurs in a very short time and then evolves. The study shows the promise of new techniques for probing crystal growth in real time (Fig. 73). The ultimate goal is to use these new methods to track chemical reactions as they occur under a variety of conditions, including variable pressures and temperatures, and to use that knowledge to design and make new materials for energy applications.²¹

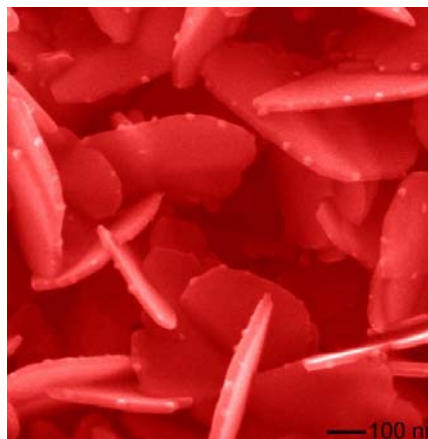


Figure 73. SEM images of the nanoparticles grown at the GaAs-wafer/ AgNO_3 -solution interface after 120 ns of growth time

5. MANAGEMENT AND OVERSIGHT

CDAC has a very horizontal management structure based at Carnegie. Active participation by oversight committees assists the management team and allows the maximum amount of resources to be allocated to our three main areas of focus for the Center.

5.1 CDAC Organization and Staff

CDAC is managed at Carnegie by a core staff comprised of the Director, Associate Director, Coordinator, Administrative Assistant and two Laboratory Managers (Fig. 74). Day-to-day operations of the Center are handled by the Director, Coordinator and Assistant, while CDAC laboratory facilities at Carnegie are supervised by the Laboratory Managers. The Associate Director serves as a liaison to the HPCAT/HPSynC groups at the APS.

Russell Hemley, Director, and **Ho-kwang Mao**, Associate Director are Staff Scientists at **Carnegie**. Other members of the Scientific Staff at **Carnegie** (Fig. 75) that are involved directly with CDAC are:

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

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

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

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

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

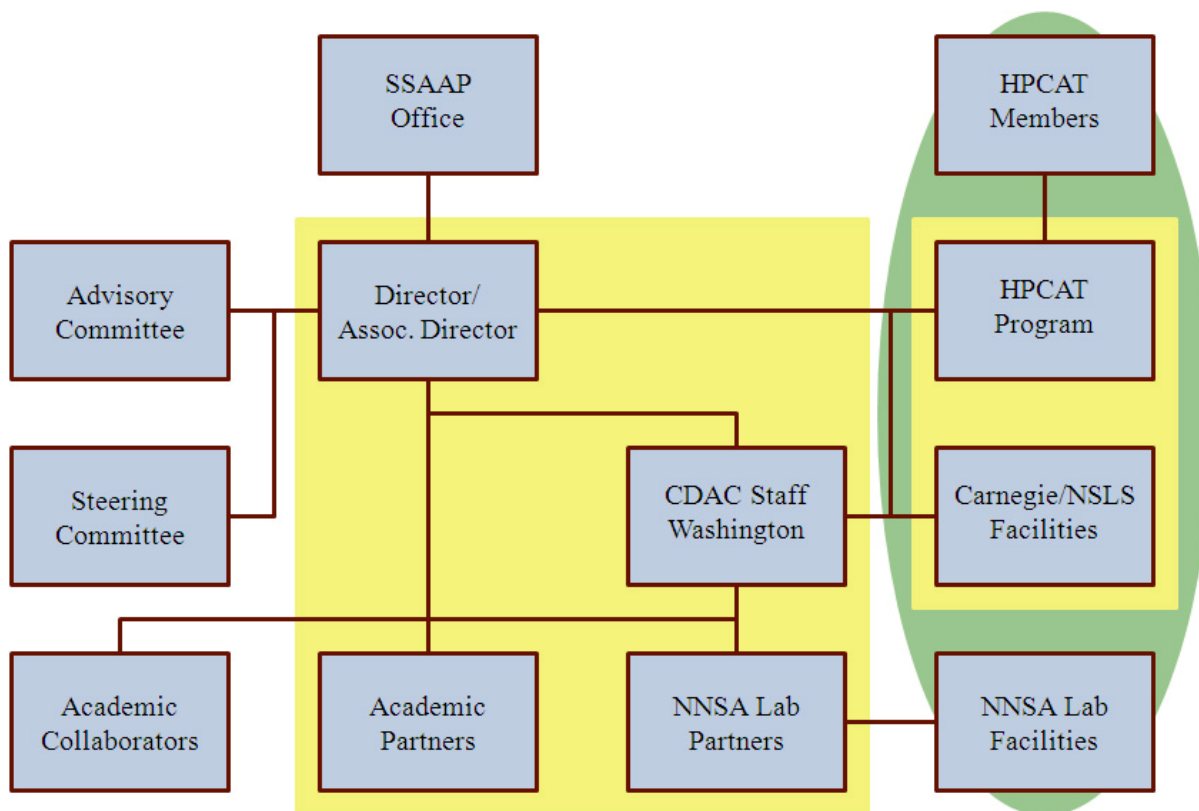


Figure 74. CDAC organizational chart. The yellow areas designate the principal components of CDAC. The oval area encompasses the three different groups of experimental facilities associated with CDAC.

A number of predoctoral and postdoctoral fellows at **Carnegie** supported by the Institution, other grants, or outside fellowships worked on CDAC tasks during Year 7. Their contributions also include training CDAC students, undergraduate summer scholars, and visitors in high-pressure experimental techniques:

- **Raja Chellappa** (former CDAC student from **Nevada-Reno**, now at LANL)
- **Douglas Allen Dalton**
- **Kadek Hemawan**
- **Daniel Hummer**
- **Joseph Lai**
- **Yufei Meng**
- **J. G. O. Ojwang**
- **Jerry Potter**

- **Luke Shulenberg** (now at SNL)
- **Tim Srobel**
- **Stewart McWilliams**

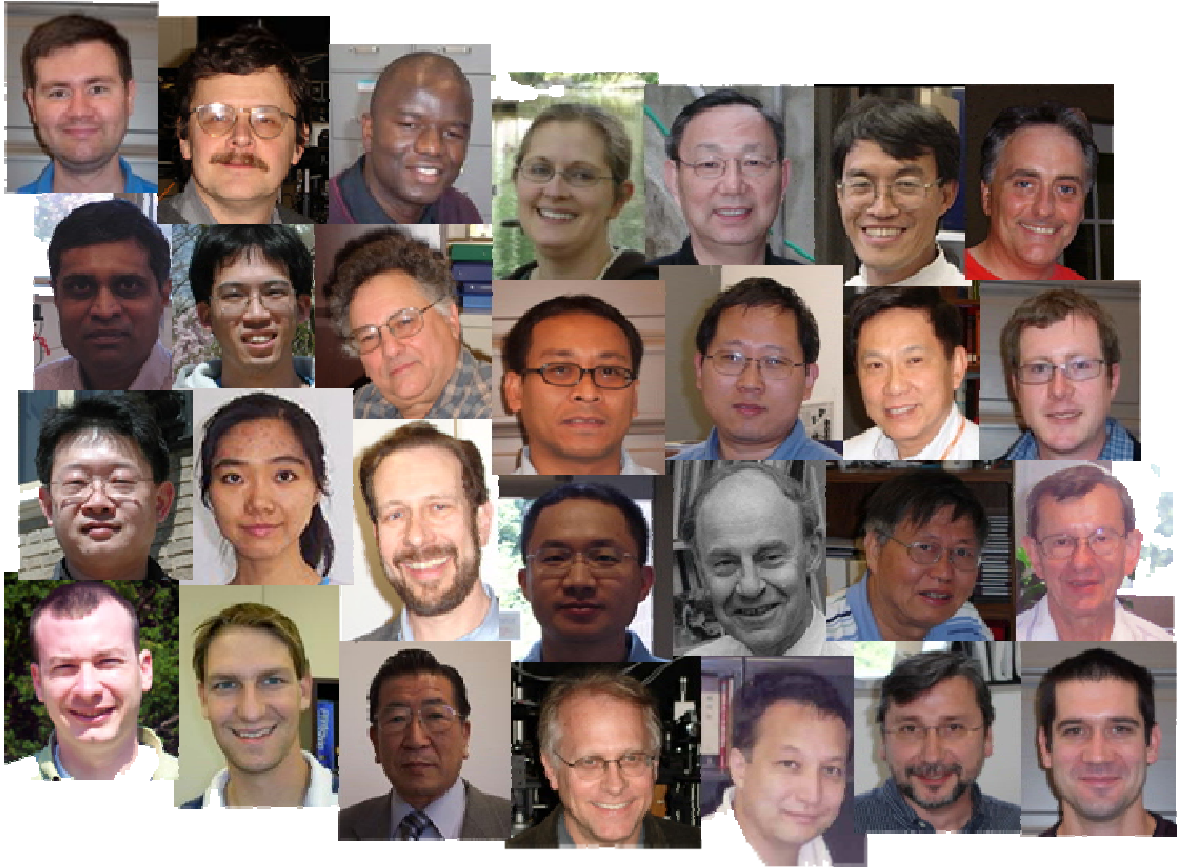


Figure 75. CDAC affiliated personnel at Carnegie.

5.2 CDAC Oversight

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

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

The Advisory Committee assists with long-term strategic planning, advises CDAC management on the scientific program, and provides points of contact between CDAC and the NNSA

Labs, other SSAA Centers, and the broader academic community. Current members of the CDAC Advisory Committee are

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

Members of both CDAC oversight committees are invited to attend regular HPCAT meetings and are invited to attend all CDAC functions. Committee members are updated regularly on progress in the scientific program, innovations in technique development, and plans for outreach. Each of the members of the two CDAC committees has agreed to continue serving through Year 8.

6. PLANS FOR YEAR 8 AND BEYOND

6.1 Dynamic Compression Initiatives

Berkeley-Carnegie Team to Carry Out Experiments at NIF – A combined team from **Berkeley** and **Carnegie** led by CDAC Academic Partner **Raymond Jeanloz** and CDAC Director **Russell Hemley**, and including **Paul Loubeyere** of the **CEA, France** and **G. W. (Rip) Collins** of **LLNL**, has been awarded time at the National Ignition Facility (NIF) for fundamental science experiments beginning in 2012. The Berkeley-Carnegie proposal, chosen from a group of 86 proposals initially under consideration, outlines work to be carried out on hydrogen and hydrogen-containing low-Z materials at the extreme conditions of pressure and temperature that can only be produced with NIF, such as the interiors of giant planets (Fig. 76). NIF houses the world's largest and most powerful laser and has been designed and built to carry out Inertial Confinement Fusion as part of the Laboratory's missions in national security and energy research. Apart from these programmatic goals, however, time at the facility is being made available through a competitive proposal process to academic institutions to carry out basic scientific research.

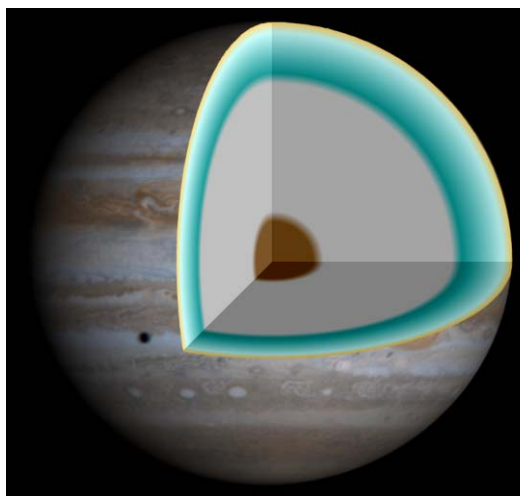


Figure 76. The technical capabilities of NIF will be used to produce states of matter to pressures above 100 Mbar, allowing investigation of the interiors of giant planets such as Jupiter.

The group has proposed to use NIF to dynamically compress hydrogen (H_2 and/or D_2) to the TPa regime – tens of Mbar – using two types of targets, cryogenic and pre-compressed, and temporally shaped pulses in order to achieve a wide range of pressure-temperature-density states that are accessible for the first time in controlled laboratory experiments. The proposed experiments would produce an invaluable new set of pressure-temperature-density-reflectivity measurements that would uniquely test current descriptions of the hydrogen plasma state over a wide range of thermodynamic conditions. A specific technical aim of the proposed experiments is to document, for the first time, that it is possible to perform quantitative multi-shock experiments on D_2 or H_2 and CH_4 (Fig. 77) pre-compressed to more than 1-5 GPa. Such pre-compression offers the only means currently known to experimentally access the very densest and coldest domains of the phase diagram, with pressure into the TPa range at temperatures below 0.3 eV, a regime in which new quantum many-body states of matter have

been predicted, Wigner crystallization of the dense hydrogen plasma should be observed, and, at the extreme 10 TPa range, pycno-nuclear processes might be detected.

The work will involve collaboration with scientists at NIF and will include postdoctoral fellows and graduate students from the above institutions.

6.2 New Academic Partners

Time-Domain

Thermoreflectance Measurements

at Extreme Conditions

Over the past several years, the research group of **David Cahill** at **Illinois** has worked to develop time-domain thermoreflectance (TDTR) as a robust and quantitative tool for the

measurement of thermal conductivity of almost any material that can be prepared with a smooth surface.¹⁴⁷⁻¹⁴⁸ Currently, the group is working to extend TDTR to extreme conditions of high temperature and high pressure as well as high magnetic fields. In the TDTR experiment, the output of a Ti:sapphire laser oscillator is split into pump and probe beams (Fig. 78). The pump beam are modulated at 10 MHz by an electro-optic modulator and passes through an optical delay line before being focused on the surface of the sample by a microscope objective. The probe beam is mechanically chopped and focused by the same objective. The reflected probe is re-collimated by the objective and focused onto a Si photodiode detector. Small changes in the reflected probe intensity are measured by an rf lock-in amplifier that is synchronized to the modulation frequency of the pump; the two output channels of the rf lockin are measured by two computer-based audio frequency lock-in amplifiers that are synchronized to the optical chopper. The noise level of the measurement is < 1 ppm/Hz. This TDTR approach has been thoroughly validated and extensively applied in to studies of the thermal properties of materials.

The next step in this development is to extend the measurements to high pressures. Recently, TDTR has been combined with DAC techniques to measure the thermal conductance of an Al/SiC interface to 10 GPa (using a SiC anvil cell) and the thermal conductivity of mica to 25 GPa (using a DAC, Fig. 79), the mica result having been obtained in collaboration with current CDAC partner **Jie Li**. These data provide new insights on the mechanisms of heat transport in layered materials with low thermal conductivity.

The studies of the conductance of the Al/SiC interface are ongoing but these initial data already show that the conventional models used to describe heat transport at interfaces is incomplete because the pressure dependence is much stronger than can be accounted for by the acoustic-mismatch diffuse-mismatch models. In the course of the initial experiments, it was discovered that the same physics that produces large thermoreflectance in Al also produces dramatic changes in the thermoreflectance as a function of pressure. Unfortunately, the thermoreflectance at $\lambda = 785$ nm passes through zero near 6 GPa. To obtain data in that pressure range, it is necessary to use a different set of optical filters and tune the Ti:sapphire laser to shorter wavelengths. The low melting point of Al limits measurements to $T < 400$ C because of surface roughening. Less obvious are the problems caused by the relatively low elastic modulus of Al. If Al is deposited on a material with a high modulus and placed under high pressure, the Al film will be placed under large biaxial tension and the film/substrate interface will eventually fail. Clear evidence of this phenomenon for

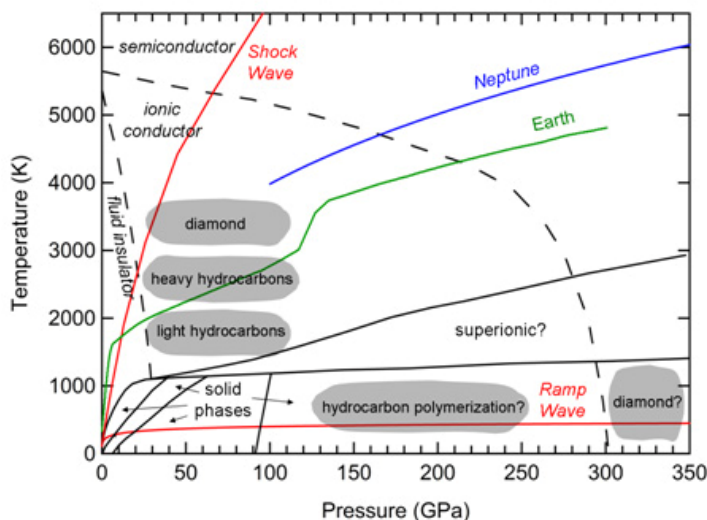


Figure 77. Generalized phase diagram for methane showing stability fields (grey areas) for possible products at various (P, T) conditions. The ramp and shock compression paths are also shown, along with the melt line (lower black curve) and isentropes for Earth and Neptune. Dashed black lines show proposed boundaries between states of different conductivity.

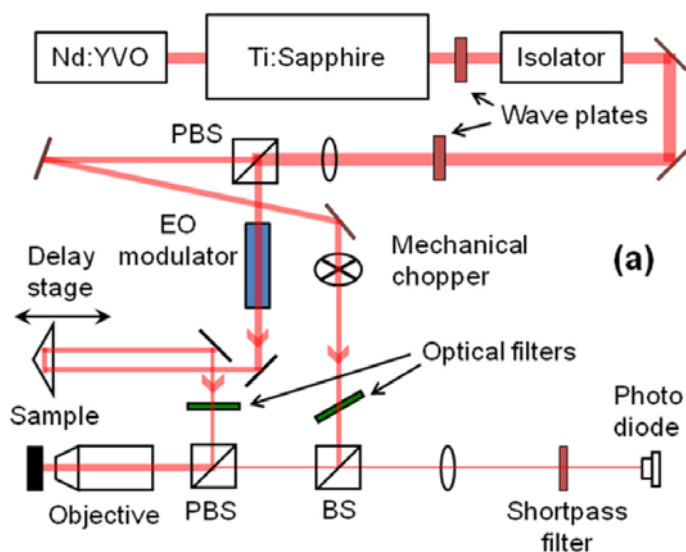


Figure 78 Schematic diagram of the time-domain thermoreflectance (TDTR) measurement system. Sharp-edged optical filters are used to create spectrally distinct pump and probe beams from the broad spectrum of the Ti:sapphire laser; a third optical filter blocks diffusely scattered pump light from reaching the Si photodiode detector.

absorption of Au nanoparticles.¹⁴⁹ In the proposed work, the changes in optical absorption and thermoreflectance created by alloying of Pd with Au, and the thermoreflectance of optimized dilute Au:Pd alloys as a function of pressure will be explored. Thin layers of Cr or Ti will be used to enhance the adhesion of the films to thinned silica substrates. A final objective will be to optimize metal film transducers to measure the thermal conductivity of MgO at high pressures, because MgO has emerged as an important testbed for both theory and experiment on the thermal conductivity of materials under extreme conditions.

Structural Transformations in Complex Oxides at High Pressure and Temperature –

In the research group of **Rod Ewing** at **Michigan**, high-pressure techniques will be combined with the use of swift heavy ion beams by injecting relativistic ions from, for example, the SIS heavy ion synchrotron of GSI in Darmstadt (Germany) through the diamond anvil of a high-pressure cell into a pressurized target, as shown schematically in Fig. 80. The first results showed that the application of high pressure simultaneously with the deposition of large energy densities by swift heavy ions triggers dramatic material modifications in a solid that are not observed with the application of only pressure or only ion irradiation.¹⁵⁰ This new technique provides for investigating a wide spectrum of applications from nanoscale simulations of fission-track formation under Earth's crustal conditions¹⁵¹ to phase transitions of radiation-damaged minerals resulting from meteorite impact.¹⁵² The extreme conditions induced by high pressure and high energy ion irradiation provide a new means for manipulating solids at the nanoscale and stabilizing novel materials to ambient conditions that otherwise could not be recovered upon the release of pressure.¹⁵³

The Ewing group proposes to investigate the high pressure irradiation of three classes of materials: (1) Important Earth materials, in order to simulate the effects of radioactive decay (simulated by the ions) in the Earth's interior (at elevated pressures and temperatures). These experiments will test the ability of charged particles to modify the phase relations of pressurized minerals and provide information on the occurrence of transformations within the Earth's interior at high pressure and temperature. (2) High-pressure materials with interesting physical and chemical properties to investigate their response to extreme environments. (3) Novel structures that contain actinides. This will provide important information about the interplay of ion-induced structural

Al films deposited on thin polymer layers grown on SiC has appeared in the early work. What are desired are metal transducer films that have a modulus that is well matched to the substrate.

In the proposed work, the deposition of tantalum, another metal with a large thermoreflectance at ambient conditions, on thinned silica glass will be evaluated and the adhesion and thermoreflectance will be studied as a function of pressure in the DAC. At ambient conditions, the thermoreflectance of Ta is close to a peak value at the $\lambda = 785$ nm wavelength of the Ti:sapphire laser. Vanadium and niobium also show strong peaks in their thermoreflectance at nearby wavelengths, so the thermoreflectance of these metals will also be evaluated at high pressure conditions.

Pd alloying of Au has been previously used to increase the transient

modifications at the nanoscale and high pressure.

The first experiments on zircon (ZrSiO_4) have shown that the energy deposition of swift heavy ions is able to induce phase transitions in pressurized materials at unexpectedly low pressures.¹⁵⁰ These studies will be extended to a number of other important minerals such as olivine ($\text{Mg,Fe}_2\text{SiO}_4$), TiO_2 polymorphs, SiO_2 polymorphs, and graphite.

There is also a wide spectrum of radiation effects in different materials at ambient conditions that involve interesting ion-induced modifications. Such investigations remain to be performed for non-quenchable high-pressure phases. It is of fundamental importance to understand how different materials cope with the large energy deposition of swift heavy ions. In particular, the plan will be to study the ability of radiation-induced formation of nanocrystals as a unique tool for *in situ* modifications (i.e., at high pressure) of phase transition pathways. As already demonstrated, this can lead to the stabilization of non-quenchable phases.¹⁵³ This approach will be applied to Ca-perovskite (CaSiO_3), among other materials, because Ca-perovskite has never been quenched to ambient conditions.

Natural brannerite (AB_2O_6) is a rather unique uranium containing phase, where U^{4+} or other actinide elements may occupy the A-site. B-site cations may be smaller transition elements, such as Ti and Fe. Brannerite is monoclinic with edge-shared BO_6 octahedra forming a layered structure. A-site cations occupy the voids between the layers. At high pressures, brannerite becomes amorphous just above 30 GPa. Infrared investigations have also confirmed the amorphous state. In order to understand the amorphization mechanism, systematic, high quality diffraction measurements are needed. ThTi_2O_6 with the brannerite-type structure will be investigated, as it has a very good Raman signal. Besides amorphization at high pressure, an additional phase transition has found at very low pressure (<5 GPa) by *in situ* Raman measurements. However, *in-situ* XRD experiments did not

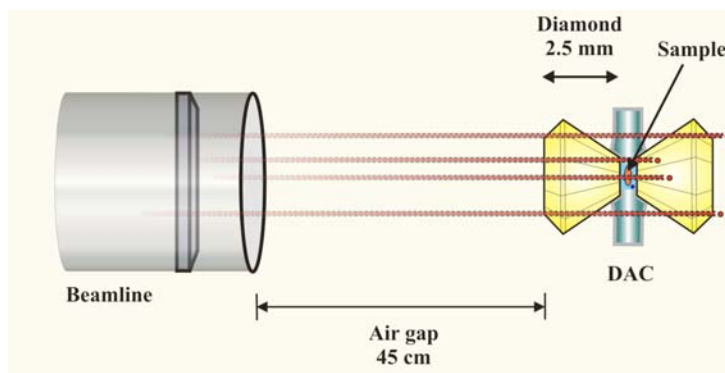


Figure 80. Experimental scheme for the irradiation of pressurized samples with relativistic heavy ions.

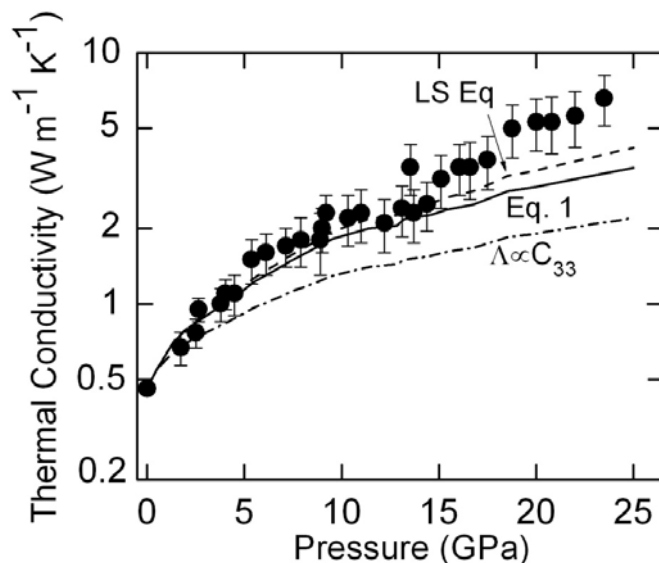


Figure 79. Thermal conductivity of mica as a function of pressure. Eq. 1 is the prediction of an anisotropic Debye model within the relaxation time approximation.¹⁵⁴ The elastic constant C_{33} was measured in the same set of experiments using picosecond acoustics; the lower solid line shows how the thermal conductivity would vary if the thermal conductivity was proportional to the modulus. The upper dashed line shows the scaling predicted by the Leibfried-Schlomann equation.

reveal any anomalous change at this pressure. Once the high-pressure studies have been completed, studies of the phase transitions under a combination of pressure and irradiation will be carried out.

Complex oxides, such as the pyrochlore materials ($\text{A}_2\text{B}_2\text{O}_7$), find application as inert matrix fuels for burning actinides, burnable neutron absorber materials to increase nuclear fuel burnup, nuclear waste forms, fast ionic conductors, catalysts

and metallic frustrated magnets. Due to their potential use as nuclear material, the behavior of pyrochlore in the presence of different types of radiation has been studied in great detail.¹⁵⁰⁻¹⁵¹ The chemical composition of the complex oxide has a strong effect on the character and energetics of the structural modifications that can be obtained under irradiation. During the past several years, pyrochlore oxides have been studied systematically at high pressures and the material response shows striking similarities to radiation-induced effects, such as order-disorder transitions and amorphization.¹⁵²⁻¹⁵³ In addition, new high-pressure phases have been produced during high pressure experiments. Up to now, the effect of temperature on pressure-induced structural transformations in pyrochlore has never been studied. The behavior of complex oxides to high pressure and high temperature are a unique opportunity to explore different phase-transition pathways in this important class of materials to better understand their performance under extreme conditions.

APPENDIX I: CDAC Publications and Presentations for Year 7

We list publications and presentations for 2009-2001, including all work supported fully or in part by CDAC. This list therefore includes work carried out at HPCAT by all of its members and users during this period.

A. CDAC Publications

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APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for Year 7

A. HPCAT (APS)

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

User Name	Affiliations	Project	Dates
C. Park G. Shen Qiang Mei D. Ikuta Olga Shebanova W. Yang	HPCAT HPSynC	Beamline development - Equipment optimization for PEC melt experiment	October 7-11, 2009
Patricia Kalita	University of Nevada - Las Vegas	High-pressure x-ray diffraction of hafnium hydride and titanium hydride	October 8-9, 2009
M. Somayazulu T. Strobel W. Yang P. Dera	Carnegie HPSynC GSECARS	Single crystal diffraction of xenon compounds at high pressure	October 9-10, 2009
Olga Shebanova	HPCAT	Beamline development - x-ray absorption and diffraction on Cs+Pt at high pressure	October 10-11, 2010
R. Kumar	University of Nevada - Las Vegas	Powder x-ray diffraction studies at high pressures on FeSe, TbPO ₄ and AgInTe ₂	October 11-12, 2009
T. Yu Y. Wang N. Hilairret C. Park W. Yang	GSECARS HPCAT HPSynC	Structure study of liquid gallium and liquid FeS at high pressure and high temperature	October 11-17, 2009
Olga Shebanova	HPCAT	Beamline development - x-ray absorption and diffraction on Cs+Pt at high pressure	October 12-13, 2009
H. K. Mao B. Li Pei-Lun Lee	Carnegie HPSynC National Chia-Yi University	High-pressure single crystal study on FeSe _{0.9} and FeSe _{0.5} Te _{0.5}	October 14-19, 2009
L. Wang H. K. Mao S. Sinogeikin Wendy Mao	HPSynC Carnegie HPCAT Stanford	High-pressure low-temperature crystallographic study of Ca	October 15-19, 2009
C. Park G. Shen Qiang Mei W. Yang	HPCAT HPSynC	Beamline development commission - Olivine Melt in PEC	October 17-19, 2009
H. K. Mao	Carnegie	Resonant inelastic scattering of hydrogen and helium	October 18-26, 2009
J. Jeffries N. Butch J. Hamlin	LLNL University of Maryland University of South Dakota	Probing the lattice response to hidden order and antiferromagnetism under pressure in UR ₂ Si ₂	October 21-23, 2009
Z. Jenei W. Evans	LLNL	Equation of state of Alloys	October 21-24, 2009

C. Park G. Shen Olga Shebanova T. Yu Y. Wang A. Yamada Y. Kono	HPCAT GSECARS Ehime University	Beamline development - <i>In-situ</i> ultrasonic measurement synchronized with x-ray scattering measurement for PEC application	October 21-27, 2009
H. Cynn M. Lipp B. Baer	LLNL	f-metal behavior at high temperature and high pressures using an external heating device	October 23-26, 2009
M. Aihaiti	Carnegie	Anomalous x-ray scattering of PbTiO_3	October 24-27, 2009
S. Gramsch	Carnegie	X-ray Raman spectrum of B_2O_3	October 26-29, 2009
Yu Lin Maaikie Kroon Wendy Mao	Stanford University	X-ray diffraction of hydrogen-rich molecular compounds at high pressures and low temperatures	October 26-30, 2009
Yun-yuan Chang C. Holl S. Jacobsen Sylvia-Monique Thomas	Northwestern University	High-Pressure micro-crystalline diffraction study of water-bearing magnesium silicates: Equation of state	October 28-30, 2009
B. Li	Seoul National University	Non-resonant inelastic x-ray scattering study of oxide glasses at 1 atm and high pressure: Fe- L-edge study and valence electron structure factor analysis	October 29- November 1, 2009
H. K. Mao B. Li Pei-Lun Lee	Carnegie HPSynC National Chia-Yi University	High-pressure single crystal study on $\text{FeSe}_{0.3}\text{Te}_{0.7}$	October 30- November 1, 2009
Johanna Nylen	Arizona State University	Structural investigation of ammonia borane, BH_3NH_3 , at high pressure and high temperature	October 30- November 1, 2009
T. Yu Y. Wang A. Yamada T. Inoue G. Shen	GSECARS Ehime University HPCAT	Structure investigation of silicate glasses and melts at high pressure	October 31- November 8, 2009
L. Wang W. Yang	HPSynC	High-pressure induced local structure transition in Y_2O_3	November 1-3, 2009
Y. Wang Y. Al-Khatatbeh	Yale University New Mexico State University	Determining the high-pressure behavior of transition metal oxides	November 1-3, 2009
H. K. Mao Y. Ding L. Wang Y. Xiao	Carnegie HPSynC HPCAT	High-pressure resonant XES of Ge K beta in GeO_2 glass	November 2-6, 2009
W. Yang	HPSynC	Beamline development - XRD of Nb powder in a DAC	November 4-5, 2009
B. Li Pei-Lun Lee	HPSynC National Chia-Yi University	High-pressure single crystal study on $\text{FeSe}_{0.3}\text{Te}_{0.7}$	November 4-5, 2009
M. Pravica M. Galley Y. Z. Feng S. Tkachev W. Pravica	University of Nevada - Las Vegas	X-ray diffraction study of melamine at high pressure	November 5-6, 2009

Y. Vohra N. Brady J. Montgomery W. Uhoya A. Stemshorn	University of Alabama – Birmingham	High-pressure studies on iron-based layered superconductors and heavy fermion systems	November 5-7, 2009
Z. Jenei	LLNL	Equation of state of alloys and metals	November 6-9, 2009
J. F. Lin M. Zhu	University of Texas – Austin	Electronic states of iron in lower-mantle minerals: An Fe K-edge RXES spectroscopic study at high pressures	November 6-10, 2009
H. Liu	Harbin Institute of Technology	Pair distribution function studies for FeS melt and FeSiB metallic glass at high pressure and high temperature conditions	November 7-9, 2009
W. Yang C. Park	HPSynC HPCAT	Beamline development commission - structure of Fe-based metallic glasses and melts at high pressures	November 8-13, 2009
M. Somayazulu D. A. Dalton	Carnegie	Micro diffraction of TMAB, olivine-calcite- H ₂ O system at high pressure	November 9-10, 2009
Olga Shebanova	HPCAT	Beamline development - x-ray absorption and diffraction on Cs+Pt at high pressure	November 11- 13, 2009
J. F. Lin C. Q. Jin	University of Texas – Austin Chinese Academy of Sciences	Pressure-induced transformation from spin density wave (SDW) to superconductivity in iron-based AFe ₂ As ₂ compounds: An Fe K- edge RXES spectroscopic study in a DAC	November 11- 13, 2009
M. Frank Elizabeth Aarestad A. Simon O. Tschauer	Northwestern University Northern Illinois University University of Nevada – Las Vegas	Quantifying trace element mass transfer of monazite at subduction zone conditions	November 13- 15, 2009
Wenge Yang	HPSynC	Beamline development - Fe-based amorphous metallic glasses and XRD of Nb powder in a DAC	November 13- 16, 2009
Pei-Lun Lee B. Li H. K. Mao	HPSynC Carnegie	Single crystal XRD of CH ₄ under high pressure	November 13- 16, 2009
Yue Meng L. Wang H. K. Mao W. Mao	HPCAT HPSynC Carnegie Stanford University	High-pressure crystallographic study of Ca	November 13- 16, 2009
Qiang Mei C. Park G. Shen	HPCAT	Beamline development commission - Amorphous phase transition in GeO ₂ Glass under pressure	November 13- 25, 2009
M. Lipp B. Baer K. Moore	LLNL	XES of f-metals at high pressure	November 15- 24, 2009
W. Yang	HPSynC	Beamline development - Anomalous x-ray scattering	November 18- 19, 2009
P. Dera Barbara Lavina	GSECARS University of Nevada – Las Vegas	High pressure study of ³ MgO ₄ SiO ₂ H ₂ O, Fe ₃ O ₄ , FeCO ₃ , FeO and ZnCO ₃ , XRD of SiO ₂ at high pressure	November 18- 20, 2009
J. H. Klepeis B. Baer Olga Shebanova	LLNL HPCAT	Strength measurement on TaW alloys	November 19- 22, 2009

S. Jacobsen Yun-yuan Chang Sylvia-Monique Thomas	Northwestern University	Effect of hydration on the compressibility of single-crystal wadsleyite, β -(Mg,Fe) ₂ SiO ₄	November 20-22, 2009
J. Baker A. Cornelius	University of Nevada – Las Vegas	AuX ₂ structural studies (X=Al, Ga, In)	November 22-23, 2009
T. Strobel	Carnegie	Single crystal diffraction study (silicon hydride)	November 22-23, 2009
H. K. Mao B. Li Pei-Lun Lee	Carnegie HPSynC National Chia-Yi University	High-pressure single crystal study on FeSe _{0.3} Te _{0.7}	November 23-25, 2009
M. Jacobsen A. Cornelius	University of Nevada – Las Vegas	High pressure studies of Ate compounds (A=Ga, In, GaIn)	November 24-25, 2009
V. Struzhkin Svetlana Kharlamova	Carnegie	X-ray emission spectroscopy of oxide compounds	November 24-30, 2009
D. Ikuta	HPCAT	Beamline development - Application of crystal structure analysis to rock thin section	November 25, 2009
J. Piggot Wendy Panero D. Reaman	Ohio State University	High pressure-temperature study of FeNi alloy, High pressure compression of hydrous gamma-Mg ₂ SiO ₄	November 27-29, 2009
Kanani Lee J. O'Rourke	Yale University	Determining the high-pressure melt behavior of potassium	November 27-29, 2009
M. Pravica E. Don Romano B. Yulga C. Park	University of Nevada – Las Vegas HPCAT	Beamline development commission - Phase transition in 1,3,5,7-cyclooctatetraene under pressure	November 27-29, 2009
Michelle Weinberger Jennifer Ciezak	Carnegie/US Army Research Laboratory	High pressure radial diffraction studies of GaON and AlON	November 29-December 1, 2009
M. Armentrout	University of California – Los Angeles	Phase stability and equation of state of iron silicate	November 29-December 1, 2009
Q. Zhou F. Li	Jilin University	High pressure behavior of Se and Te nanowire	December 2-4, 2009
M. Patten H. Bogac Poyraz M. Ghantasala D. Ravindra T. Kremenski S. Virkar M. Guthrie	Western Michigan University HPSynC	High pressure and temperature studies of silicon carbide	December 2-4, 2009
R. Kumar S. Veeramali D. Antonio	University of Nevada – Las Vegas	X-ray emission studies at high pressure on Fe based superconductors at ambient and low temperatures	December 2-6, 2009
R. Kumar S. Veeramali D. Antonio	University of Nevada – Las Vegas	High pressure powder diffraction studies on chalcogenides, titanates, and titanium alloys	December 4-7, 2009
Barbara Lavina	University of Nevada – Las Vegas	High pressure-temperature study of Fe ₂ VO ₄ , Fe ₃ O ₄ , FeO	December 4-5, 2009
M. Pravica S. Tkachev	University of Nevada – Las Vegas	X-ray induced decomposition of energetic materials	December 4-8, 2009
H. K. Mao Yue Meng W. Mao L. Wang	Carnegie HPCAT Stanford University HPSynC	High pressure-temperature study of Ca, mixture of olivine/Fe/S, sancalo olivine/H ₂ O	December 5-8, 2009

M. Pravica S. Tkachev	University of Nevada – Las Vegas	X-ray emission studies of gallium-containing compounds with pressure.	December 6-8, 2009
L. Wang	HPSynC	High-pressure stability and compressibility of APo_4 (A = La, Nd, Eu, Gd, Er, and Y) orthophosphates	December 9-11, 2009
M. Pravica S. Tkachev Y. Z. Feng B. Yulga E. Don Romano	University of Nevada – Las Vegas	X-ray diffraction studies of various compounds at high pressure (melamine, water, gallium, GaN, etc.)	December 9-14, 2009
H. K. Mao G. Shen M. Lerche L. Wang W. Yang M. Guthrie Y. Hwu Y. Chu J. Wang J. Yi S. T. Cheng C. I. Su	Carnegie HPCAT HPSynC Academia Sinica Chinese Academy of Sciences	3D tomography studies under high pressure with the TXM technique	December 9-15, 2009
R. Kumar J. Baker	University of Nevada – Las Vegas	High pressure powder diffraction studies on chalcogenides, skutterudites, and heavy fermions	December 11-13, 2009
S. MacLeod Z. Jenei	LLNL	Equation of state of Alloys	December 12-19, 2009
H. Cynn M. Lipp B. Baer	LLNL	f-metal behavior at high temperatures and high pressures using an external heating device	December 13-15, 2009
N. Velisavljevic G. Stevens G. Chesnut M. Bishop	LANL	High pressure x-ray diffraction of metals (group IV metals and cerium)	December 14-19, 2009
Dana Dattlebaum	LANL	Fe-Mg partitioning at ultra high pressure in perovskite and post-perovskite	December 16-18, 2009
Dana Dattlebaum N. Velisavljevic J. Yeager	LANL	High-pressure diffraction of explosives and related organic materials	December 16-18, 2009
P. Chow Y. Xiao G. Shen W. Yang M. Lerche L. Wang M. Guthrie H. K. Mao C. I. Su	HPCAT HPSynC Carnegie Chinese Academy of Sciences	3D tomography studies under high pressure with the TXM technique	December 16-22, 2009
E. Soignard	Arizona State University	Wavelength change	December 18-20, 2009
C. Park	HPCAT	Beamline development - Anomalous x-ray scattering	December 19, 2009
H. Cynn W. Evans S. MacLeod	LLNL	Phase stability and crystal structure analysis of Ti alloys using a high pressure micro-diffraction technique coupled with a DAC	December 19-21, 2009

W. Yang C. Park	HPSynC HPCAT	Beamline development – White beam Laue	December 19-22, 2009
Y. Song Z. Dong K. Zhuravlev	University of Western Ontario	Structural investigation of glycine lithium sulphate at high pressures	December 20-22, 2009
D. Ikuta	HPCAT	Beamline development - Application of crystal structure analysis to rock thin section	December 21-22, 2009
H. K. Mao J. Shu L. Bing Y. Ding	Carnegie Jilin University HPSynC	X-ray diffraction of U at high pressure and low temperature	February 4-6, 2010
W. Yang	HPSynC	Single crystal deformation study using x-ray Laue technique	February 4-6, 2010
H. K. Mao Li Zhang J. Shu Wendy Mao Y. Ding L. Wang Yue Meng L. Bing	Carnegie Stanford University HPSynC HPCAT Jilin University	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite and high-pressure crystallographic study of Ca	February 6-8, 2010
R. Kumar	University of Nevada – Las Vegas	Low temperature-high pressure NFS and nuclear resonant inelastic x-ray scattering	February 6-12, 2010
O. Tschauer Pamela Burnley	University of Nevada – Las Vegas	Laue diffraction	February 6-12, 2010
Barbara Lavina	University of Nevada – Las Vegas	Structural studies of high pressure phases	February 8-9, 2010
Yun-yuan Chang Steven Jacobsen Sylvia-Monique Thomas	Northwestern University	The pressure-volume equation of state of hydrous Fe-bearing wadsleyite in helium pressure medium	February 10-12, 2010
H. Sheng Q. Hu A. Cadien Yue Meng M. Xu	George Mason University HPCAT Johns Hopkins University	Probing liquid-liquid phase transitions in Ce and its alloys	February 10-12, 2010
M. Alevli Patricia Kalita Kristina Lipinska-Kalita	University of Nevada – Las Vegas	High pressure x-ray diffraction of a nanocrystalline composite material	February 12-13, 2010
V. Struzhkin A. Gavriluk	Carnegie Russian Academy of Science	Low temperature-high pressure NFS and nuclear resonant inelastic x-ray scattering	February 12-15, 2010
L. Bing J. Shu H. K. Mao S. Tozer	Jilin University Carnegie Florida State University	X-ray diffraction of U at high pressure and low temperature	February 12-16, 2010
T. Strobel Yue Meng	Carnegie HPCAT	Ca, C reaction at high pressure and temperature	February 13-14, 2010
M. Alevli Patricia Kalita Kristina Lipinska-Kalita	University of Nevada – Las Vegas	High pressure x-ray diffraction of a nanocrystalline composite material	February 14-15, 2010

M. Lang F. Zhang	University of Michigan	Phase transitions induced by simultaneous exposure to relativistic ion beams and high pressure	February 15-16, 2010
H. K. Mao P. Chow Y. Xiao W. Mao L. Bing Y. Ding	Carnegie HPCAT Stanford University Jilin University HPSynC	X-ray Mössbauer spectroscopy of Fe in (Fe,Mg)SiO ₃ post-perovskite	February 15-20, 2010
Kanani Lee J. O'Rourke Y. Wang	Yale University	High-pressure investigation of transition-metal oxides	February 17-19, 2010
M. Pravica M. Galley	University of Nevada – Las Vegas	High Pressure x-ray diffraction study of melamine	February 17-19, 2010
S. Gramsch C. Prewitt	Carnegie University of Arizona	High pressure structure and equation of state of FeAlO ₃	February 19-21, 2010
H. K. Mao J. Shu L. Bing Y. Ding	Carnegie Jilin University HPSynC	High-pressure low-temperature crystallographic study of Ca	February 20-22, 2010
Z. Jenei	LLNL	Equation of state of alloys and metals	February 20-23, 2010
M. Lucas Hillary Smith J. Munoz Lisa Mauger I. Halevy	Air Force Research Laboratory California Institute of Technology National Centre for Nuclear Research, Isreal	High temperature NRIXS in ⁵⁷ Fe and laves phase materials	February 20-March 1, 2010
Shibing Wang Maria Baldini	Stanford University	High pressure x-ray diffraction measurements on Boron polymorph	February 21-23, 2010
C. S. Yoo Amartya Sengupta M. Kim L. Dias	Washington State University	Novel extended nitrides at high pressures and temperatures	February 24-26, 2010
D. Reaman J. Piggot	Ohio State University	High temperature and pressure equation of state of rubidium hollandite	February 26-27, 2010
J. H. Klepeis Z. Jenei	LLNL	Strength measurements on Ta-W alloys	February 26-March 1, 2010
Dana Dattlebaum N. Velisavljevic	LANL	High pressure diffraction of metals and organics	February 27-March 1, 2010
M. Lipp	LLNL	X-ray scattering of liquid metals (bismuth, cerium) under high temperature and pressure	February 27-March 5, 2010
M. Pravica M. Galley	University of Nevada – Las Vegas	X-ray diffraction studies of cyclopentane, GaN, and AlN at high pressure	March 3-5, 2010
J. Montgomery A. Stemshorn	University of Alabama – Birmingham	High pressure studies on iron-based layered superconductors and heavy fermion systems	March 3-6, 2010
M. Lipp W. Evans K. Moore J. Jeffries	LLNL	XES of f-metals at high pressure	March 4-9, 2010
A. Kyono T. Yamanaka P. Dera D. Ikuta	Carnegie GSECARS HPCAT	High-pressure and high-temperature in situ x-ray diffraction study of magnetite–ulvospinel solid solution series to above 100 GPa	March 5-7, 2010

R. Kumar	University of Nevada – Las Vegas	High pressure powder diffraction studies on chalcogenides, superconductors and energetic materials	March 7-9, 2010
H. K. Mao Li Zhang J. Shu L. Bing Yue Meng	Carnegie Jilin University HPCAT	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite and high-pressure crystallographic study of Ca	March 7-9, 2010
Y. Ren J. Chen	ANL University of Texas – Austin	X-ray diffraction study of pressure-induced phase transition in (BaK)Fe ₂ As ₂ superconductors	March 10-12, 2010
Shibing Wang	Stanford University	XAS study of insulator-metal transition in LaMnO ₃ at high	March 10-13, 2010
W. Hu A. Cadien	George Mason University	Probing liquid-liquid phase transitions in Ce and its alloys	March 12-13, 2010
M. Frank Margaret Hasan H. Scott	Northern Illinois University Indiana University – South Bend	Carbon reactivity in the Earth's mantle	March 13-15, 2010
Y. Ding P. Chow Y. Xiao	HPSynC HPCAT	Study magnetic ordering of manganite using spin-selective fluorescent x-ray absorption spectroscopy at high pressure	March 13-18, 2010
Qiang Mei C. Park G. Shen	HPCAT	Study MgSiO ₃ glasses using PE cell and energy dispersive x-ray diffraction	March 13-20, 2010
D. Ikuta	HPCAT	Identification and crystal structure analysis for micro-diamond in garnet-bearing peridotite and its inclusions	March 14-16, 2010
Barbara Lavina	University of Nevada – Las Vegas	Structural studies of high pressure phases	March 17-18, 2010
Jennifer Ciezak Jennifer Gottfried	Carnegie/US Army Research Laboratory US Army Research Laboratory	Investigations of strength and deformation mechanisms of sapphire	March 17-19, 2010
M. Guthrie R. Winans	Carnegie APS	Pressure : a new route to organic polymerization	March 18-20, 2010
H. K. Mao Y. Xiao P. Chow Y. Ding L. Wang	Carnegie HPCAT HPSynC	RXES and EXAFS of Fe in Fe ₂ O ₃ and (Fe,Mg)SiO ₃ post-perovskite at high pressures	March 18-22, 2010
D. Ikuta	HPCAT	Application of crystal structure analysis to rock thin section	March 19-21, 2010
H. K. Mao L. Wang	Carnegie HPSynC	High-pressure low-temperature crystallographic study of Ca	March 20-23, 2010
Qiang Mei C. Park G. Shen	HPCAT	Study MgSiO ₃ glasses using PE cell and energy dispersive x-ray diffraction	March 20-29, 2010
V. Struzhkin	Carnegie	Pressure-dependent x-ray diffraction study of the LiCu ₂ O ₂ multiferroic cuprate	March 21-23, 2010
P. Chow S. Sinogeikin Y. Zhao R. Kumar	HPCAT University of Nevada – Las Vegas	X-ray emission studies at high pressure on Fe based superconductors at ambient and low temperatures	March 22-26, 2010
L. Wang	HPSynC	Size-dependent phase transitions in Y ₂ O ₃ nanocrystals	March 24-26, 2010

H. Cynn B. Baer S. Weir	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	March 24-27, 2010
R. Kumar	University of Nevada – Las Vegas	X-ray emission studies at high pressure on Fe based superconductors at ambient and low temperatures	March 26-27, 2010
J. H. Klepeis	LLNL	Strength studies on Ta-W alloys	March 26-29, 2010
H. K. Mao L. Wang	Carnegie HPSynC	High-pressure low-temperature crystallographic study of Ca	March 27-29, 2010
Svetlana Kharlamova V. Struzhkin	Carnegie	X-ray emission study of spinels with iron element (Fe_2SiO_4 and FeCr_2O_4) at high pressure and room temperature	March 27-April 2, 2010
Qiang Mei	HPCAT	Study MgSiO_3 glasses using PE cell and energy dispersive x-ray diffraction	March 31-April 2, 2010
F. Mark Elizabeth Aarestad	Northern Illinois University	Melting curve of ice VII made from 1.6 mole percent KCl- H_2O solution	April 1-2, 2010
W. Evans Z. Jenei	LLNL	Equation of state of alloys and compounds	April 1-4, 2010
J. H. Klepeis	LLNL	Equation of state studies on CaLi_2 and Ta-W alloys	April 2-3, 2010
Zhu Mao J. F. Lin	University of Texas – Austin	Spin states of iron in silicate perovskite and post-perovskite in the Earth's lower mantle	April 2-5, 2010
Y. Vohra W. Uhoya G. Tsoy	University of Alabama – Birmingham	High pressure studies on iron-based layered superconductors and heavy fermion systems	April 3-5, 2010
Barbara Lavina	University of Nevada – Las Vegas	Single crystal diffraction of magnetite	April 5-8, 2010
O. Tschauner Barbara Lavina N. Velisavljevic	University of Nevada – Las Vegas LANL	High pressure x-ray diffraction of metals	April 7-11, 2010
M. Lipp K. Moore Y. Xiao P. Chow	LLNL HPCAT	XES of f-metals at high pressure	April 7-11, 2010
Luana Caron E. Brück H. D. Nguyen	Delft University of Technology	Magnetoelastic properties of $\text{Mn}_{2-y}\text{Fe}_y\text{P}_{1-x}\text{Ge}_x$ compounds under pressure	April 11-13, 2010
Yu Lin	Stanford University	X-ray diffraction of hydrogen-rich molecular compounds	April 11-13, 2010
A. Simon O. Tschauner Elizabeth Tanis	University of Nevada – Las Vegas	Quantifying trace element mass transfer of monazite at subduction zone conditions	April 12-15, 2010
Jodie Bradby D. Sprouster Bianca Haberl M. Guthrie	Australian National University Carnegie	A new crystalline phase of silicon – Si-XIII	April 14-16, 2010
T. Strobel M. Ahart W. Wilson	Carnegie University of Nevada – Reno	General diffraction studies	April 14-17, 2010
H. Cynn B. Baer J. H. Klepeis Chantel Aracne	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	April 16-19, 2010

H. K. Mao Y. Ding L. Wang P. Chow Y. Xiao	Carnegie HPSynC HPCAT	RXES and EXAFS of Au in CsAuI ₃ in high pressures	April 16-19, 2010
L. Bing W. Yang H. K. Mao	Jilin University HPSynC Carnegie	High-pressure low-temperature crystallographic study of Ca	April 17-19, 2010
T. Yu	GSECARS	Structure study of alkali borate melt under high pressure	April 17-28, 2010
Patricia Kalita	University of Nevada – Las Vegas	High-pressure x-ray diffraction of aluminosilicate ceramics	April 19-20, 2010
C. Park C. Kenney-Benson P. Chow Y. Xiao	HPCAT	Development of surface/interface x-ray reflectivity technique at 16ID-D	April 19-22, 2010
Pei-Lun Lee	National Chia-Yi University	High-pressure structure study on compounds with MO ₄ structure	April 21-23, 2010
R. Kumar	University of Nevada – Las Vegas	Low temperature structural studies on iron arsenide compounds at high pressures	April 21-24, 2010
Y. Xiao P. Chow	HPCAT	Development of SWD emission spectrometer	April 22-28, 2010
N. Velisavljevic D. Preston G. Stevens	LANL National Securities Technologies	High pressure x-ray diffraction of metals	April 23-25, 2010
H. K. Mao L. Wang L. Bing S. Singeikin	Carnegie HPSynC HPCAT	High-pressure low-temperature crystallographic study of Ca	April 24-26, 2010
G. Shen Qiang Mei	HPCAT	SiO ₂	April 26, 2010
J. Zhao N. Souza-Neto	APS	EuO	April 26, 2010
H. Cynn Z. Jenei S. MacLeod	LLNL	Micro x-ray diffraction to study phase stability and phase diagram of 4f and 5f metal compounds and	April 26-28, 2010
B. Li	Jilin University	In-house test: Ca at high pressure, cryostat test	June 3-4, 2010
T. Yu	GSECARS	Structure study of alkali borate melt under high pressure	June 3-12, 2010
W. Yang	HPSynC	Ag Sample	June 4, 2010
H. K. Mao Wendy Mao L. Wang Y. Ding S. Sinogeikin B. Li S. Tozer	Carnegie Stanford University HPSynC HPCAT Jilin University Florida State University	High-pressure low-temperature crystallographic study of Ca	June 4-8, 2010
B. Li Y. Ding S. Tozer	Jilin University HPSynC Florida State University	X-ray diffraction of U at high pressure and low temperature	June 5-8, 2010
O. Delaire A. Moeira dos Santos M. Lucas	Oak Ridge National Laboratory Air Force Research Laboratory	Measurements of the ⁵⁷ Fe-partial phonon density of state in BiFeO ₃ as function of temperature and pressure	June 5-11, 2010

Y. Wang J. O'Rourke	Yale University	Determining the high-pressure melt behavior of potassium	June 9-11, 2010
H. Cynn M. Lipp S. Weir	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	June 9-12, 2010
V. Struzhkin A. Budzianowski	Carnegie Warsaw University	High pressure powder x-ray diffraction	June 11-12, 2010
Lisa Mauger Sally Tracy T. Lan J. Munoz H. Chu	Caltech Princeton University	High Pressure NRIXS on CeFe ₂ and PdFe	June 11-15, 2010
H. K. Mao Wendy Mao Y. Ding L. Wang S. Sinogeikin B. Li	Carnegie Stanford University HPSynC HPCAT Jilin University	High-pressure low-temperature superconductivity study of YH ₃	June 12-14, 2010
T. Sakamaki T. Yu Y. Wang	GSECARS	High temperature melt structure of Jadeite under pressure using a Paris-Edinburgh cell	June 12-20, 2010
M. Pravica	University of Nevada – Las Vegas	High pressure diffraction of explosives	June 13-15, 2010
H. Cynn B. Baer	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	June 16-17, 2010
J. F. Lin C. Jin	University of Texas – Austin Chinese Academy of Sciences	Electronic states of iron in mantle minerals: A high-pressure synchrotron Mossbauer study	June 16-22, 2010
S. Sinogeikin R. Kumar	HPCAT University of Nevada – Las Vegas	Low temperature structural studies on iron arsenide compounds at high pressures	June 20-22, 2010
H. Cynn J. H. Klepeis C. Park	LLNL HPCAT	Measurements of melting behavior of indium, polyethylene, and KBr using a Paris- Edinburgh cell at high temperature and high pressure	June 20-25, 2010
H. P. Liermann S. Petitgirard C. Nisr L. Miyagi S. Speziale Pamela Kaercher W. Kanitpanyacharoen	Deutsches Elektronen-Synchrotron (DESY) Universite des Sciences et Technologies de Lille Yale University GeoForschungsZentrum Potsdam University of California - Berkeley	Simultaneous high-pressure and – temperature investigation of texture development in polycrystalline MgSiO ₃ perovskite	June 23-25, 2010
R. Kumar	University of Nevada – Las Vegas	Nuclear resonant inelastic x-ray scattering experiments on FeSi, FeAs and related compounds	June 23-27, 2010
Patricia Kalita G. Harding	University of Nevada – Las Vegas	High-pressure x-ray diffraction of aluminosilicate ceramics and of titanium hydride	June 25-26, 2010
B. Li	Jilin University	CaH	June 25-28, 2010
T. Sakamaki	GSECARS	Commissioning high temperature melt structure of basalt minerals under pressure using a Paris-Edinburgh cell	June 25-July 8, 2010
M. Ahart C. DeVreugd	Carnegie Virginia Polytechnic Institute & State University	Pressure induced phase transitions in LiTaO ₃	June 26-28, 2010

Yu Lin	Stanford University	X-ray diffraction of hydrogen-rich molecular compounds at low temperatures and high pressures	June 26-28, 2010
Barbara Lavina	University of Nevada – Las Vegas	SMS studies of redox exchanges at high pressure	June 27-28
K. Loshkin V. Struzhkin	University of Tennessee, Knoxville Carnegie	Structure and electronic properties of Ni ₁₊ /Ni ₂₊ layered	June 30-July 1, 2010
O. Tschauner J. Howard N. Velisavljevic	University of Nevada – Las Vegas LANL	High Pressure-high temperature single crystal diffraction studies	July 1-3, 2010
B. Li	Jilin University	Superconductivity of Calcium Hydride (CaH ₂) under megabar pressure	July 3-5, 2010
J. Jeffries	LLNL	The consequences of crystalline environment on the pressure-induced antiferromagnetic ground state of URu ₂ Si ₂	July 6-8, 2010
M. Somayazulu	Carnegie	Micro diffraction studies on novel compounds - XeCl ₂ ; XeBr ₂ ; XeH ₂ at high pressures	July 6-8, 2010
Z. Jenai W. Evans	LLNL	X-ray Raman spectroscopy of boron compounds in DAC	July 7-11, 2010
Yuki Nakamoto	Carnegie	X-ray diffraction measurement of yttrium under high pressure	July 8-9, 2010
R. Kumar	University of Nevada – Las Vegas	Low temperature structural studies on iron arsenide compounds at high pressures	July 8-9, 2010
C. Park	HPCAT	MgGeO ₃ -H ₂ O	July 8-13, 2010
Luana Caron J. Vieira Leitao H. D. Nguyen	Delft Institute of Technology	Magnetoelastic properties of Mn _{2y} FeyP _{1-x} Ge _x compounds under pressure	July 9-11, 2010
H. Cynn B. Baer J. H. Klepeis	LLNL	f-metal behavior at high temperatures and high pressures using an external heating	July 9-12, 2010
Barbara Lavina	University of Nevada – Las Vegas	Single crystal diffraction of magnetite	July 11-15, 2010
Yu Lin Maria Baldini	Stanford University	Bonding changes in amorphous carbon at high pressure	July 11-16, 2010
Patricia Kalita	University of Nevada – Las Vegas	High-pressure x-ray diffraction of aluminosilicate type ceramics	July 12-13, 2010
W. Yang	HPSynC	EDXD and White beam diffraction study of Melting of SeTe with Paris Edinburg Cell	July 14-20, 2010
H. Zhu D. Hou	Texas Tech University	High pressure powder diffraction	July 15-17, 2010
H. K. Mao Li Zhang Wendy Mao Yue Meng	Carnegie Stanford University HPCAT	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	July 16-18, 2010
H. K. Mao Wendy Mao P. Chow Y. Xiao Y. Ding	Carnegie Stanford University HPCAT HPSynC	Inelastic scattering of sodium plasmons	July 16-19, 2010
D. Ikuta	HPCAT	Application of crystal structure analysis to rock thin section	July 17-19, 2010
T. Strobel Bethany Chidester	Carnegie University of Toledo	General diffraction studies of ammonia hydrogen and carbon systems	July 18-20, 2010
W. Yang	HPSynC	Powder diffraction of Sn and silicates under high pressure	June 19-21, 2010

B. Li Y. Ding	Jilin University HPSynC	X-ray diffraction of U at high pressure and low temperature	July 19-22, 2010
S. Gramsch Amanda Lindoo	Carnegie Augustana College	High pressure behavior of Norbergite	July 19-25, 2010
M. Ahart Yuki Nakamoto S. Gramsch	Carnegie	Pressure induced phase transitions in FeGa alloy	July 21-23, 2010
M. Pravica H. Ruiz M. Galley Jennifer Wojno N. Velisavljevic D. Hooks	University of Nevada – Las Vegas LANL	High pressure studies of organic compounds using a Paris-Edinburgh Cell	July 21-26, 2010
R. Kumar D. Wood Kristie Canaday	University of Nevada – Las Vegas	High pressure powder diffraction studies on chalcogenides and zirconium alloys	July 22-23, 2010
Barbara Lavina	University of Nevada – Las Vegas	Structural studies at high pressure and temperature	July 23-24, 2010
M. Frank Maggie Hanson	Northern Illinois University	Carbon reactivity in Earth's mantle	July 24-26, 2010
D. Ikuta G. Shen	HPCAT	Identification and crystal structure analysis for Pb-dominant feldspar	July 24-26, 2010
Barbara Lavina	University of Nevada – Las Vegas	Structural studies at high pressure and temperature	July 28-29, 2010
Z. Jenei W. Evans	LLNL	X-ray Raman spectroscopy of uranium and boron compounds in DAC	July 28-August 2, 2010
W. Evans B. Baer J. H. Klepeis M. Lipp Z. Jenei	LLNL	Equation of state of alloys and compounds	July 28-August 3, 2010
T. Sakamaki	GSECARS	High temperature melt structure of Jadeite under pressure using a Paris-Edinburgh cell	July 28-August 3, 2010
Susannah Dorfman T. Duffy B. Bennett C. Hull	Princeton University Northwestern University	Continuing study of Au, Pt, MgO, and NaCl to 300 GPa	July 30-August 1, 2010
D. Raeman M. Hawrylak	Ohio State University	Phase relations of FeNi alloys at high temperature and pressure and applications to Earth's inner core	August 1-3, 2010
V. Iota	University of Texas – Austin	Bonding transitions in carbon-oxygen compounds under pressure	August 2-6, 2010
J. Jeffries A. Schwartz Kerri Blobaum	LLNL	Thermal kinetics of the pressure-induced delta/alpha-prime transformation in retained delta-Pu	August 4-6, 2010
J. Montgomery G. Samudrala	University of Alabama – Birmingham	Structural, electrical, and magnetic studies on heavy rare earth metals at high pressures using designer diamond anvils	August 4-6, 2010
D. Ikuta	HPCAT	Application of crystal structure analysis to rock thin section	August 6-7, 2010
M. Kim J. Y. Chen D. Tomasino	Washington State University	Structural studies of halogen-containing compounds under extreme conditions	August 6-8, 2010

M. Pravica J. Robinson C. Callahan N. Bhattacharya M. Galley	University of Nevada – Las Vegas	X-ray Raman studies of nitrogen-containing compounds	August 6-13, 2010
T. Strobel	Carnegie	Single crystal and powder diffraction studies of a new hydrogen sulfur compound	August 7-8, 2010
B. Zou K. Wang B. Ling	Jilin University	High-pressure study of nano-materials	August 8-10, 2010
J. F. Lin G. Pradhan C. Lu J. Wu J. Liu	University of Texas – Austin	Phase stability and thermal equation of state of ferropicicase-(Mg,Fe)O in the Earth's lower mantle	August 8-10, 2010
Patricia Kalita Kristina Lipinska-Kalita	University of Nevada – Las Vegas	High-pressure x-ray diffraction of aluminosilicate type ceramics	August 11-12, 2010
D. Popov	HPCAT	Measurements on MgO	August 12-13, 2010
P. Zinn T. Acosta R. Jia	University of Hawai'i	High pressure phase transformations of the graphitic BCx compounds	August 12-14, 2010
Z. Jenei B. Baer	LLNL	Equation of state of compounds	August 13-15, 2010
O. Tschauner Pamela Burnley	University of Nevada – Las Vegas	Laue diffraction for strain measurements	August 13-16, 2010
H. K. Mao Wendy Mao Yu Lin P. Chow Y. Xiao Y. Ding	Carnegie Stanford University HPCAT HPSynC	Inelastic scattering of sodium plasmons	August 13-22, 2010
H. K. Mao Li Zhang Wendy Mao H. Ma Y. Wu	Carnegie Stanford University	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	August 14-16, 2010
Dana Dattlebaum R. Chellappa	LANL	High pressure phase behavior of organic compounds	August 16-18, 2010
B. Zou K. Wang B. Li	Jilin University	High-pressure study of nano-materials	August 18-20, 2010
H. K. Mao Li Zhang Wendy Mao Yue Meng	Carnegie Stanford University HPCAT	Fe-Mg partitioning at ultrahigh pressure in perovskite and post-perovskite	August 19-21, 2010
N. Velisavljevic B. Jensen D. Preston G. Stevens	LANL National Security Technologies	High-pressure x-ray diffraction of metals	August 20-24, 2010
S. Gramsch Yuki Nakamoto D. Ikuta	Carnegie	High-pressure in situ x-ray diffraction study of Fe ₂ SiO ₄ -FeFe ₂ O ₄ solid solution series up to 100 GPa	August 21-23, 2010
O. Tschauner	University of Nevada – Las Vegas	Laue diffraction for strain measurements	August 22-25, 2010

Kanani Lee Y. Wang	Yale University	Determining the high-pressure melt behavior of potassium	August 23-24, 2010
M. Galley	University of Nevada – Las Vegas	ADXRD studies of melamine and cyclopentane	August 24-25, 2010
Z. Levine	NIST	Development of standards for lung density as measured by medical CT	August 24-25, 2010

B. U2A Infrared Beamline (NSLS)

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

User Name	Affiliations	Project	Dates
S. Tkachev	University of Nevada – Las Vegas	Infrared studies of cyclooctatetraene at high pressure	September 10-11, 2009
Y. Wang	State University of New York – Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application	September 14-18, 2009
S. Tkachev	University of Nevada – Las Vegas	Infrared studies of cyclooctatetraene at high pressure	September 21-24, 2009
W. Han	Brookhaven	High-pressure IR Study gases storage in boron nitride nanotubes	September 25-26, Oct. 1-2, 2009
J. Smedley	Brookhaven	Characterization of impurities in diamond	October 5, 2009
D. Reaman J. Pigott	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals	October 8-9, 2009
Q. Cui	Jilin University	high pressure infrared studies on molybdenum trioxide hydrates $\text{MOO}_{3x}\text{H}_2\text{O}$ ($x= 1/3, 1/2, 1, 2$)	October 10-14, 2009
M. Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature	October 15-16, 2009
C. Seagle T. Strobel	Carnegie	Optical properties of tin at high pressures and temperatures	October 19-22, 2009
C. Lui	Columbia University	Probing the electronic structure of graphene nanoribbons by infrared photoconductivity	October 28-29, 2009
T. Tyson P. Gao	New Jersey Institute of Technology	Spin-driven local distortions in multiferroic hexagonal ReMnO_3 : IR measurements	November 1-6, 2009
G. Amulele K. Otsuka	Yale University	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements	November 8-9, 2009
G. Yang	Brookhaven	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe	November 10-12, 2009
K. Otsuka G. Amulele	Yale University	In situ measurements on hydrogen solubility and speciation in $(\text{Mg,Fe})\text{O}$ and olivine using synchrotron FTIR	November 12-14, 2009
G. Amulele K. Otsuka	Yale University	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements	November 15, 2009

M. Lang F. Zhang	University of Michigan	Phase transitions in minerals induced by ion beams and high-pressure: A novel approach in geosciences	November 16-20, 2009
Z. Liu	Carnegie	Coupling the new side station with the synchrotron source	January 5-25, 2010
Y. Wang	State University of New York – Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application	January 19-20, 2010
T. Strobel	Carnegie	Infrared spectroscopy of novel high-pressure low-temperature H ₂ O+H ₂ clathrate phases	January 26-29 2010
Jennifer Ciezak	Carnegie/Army Research Laboratory	Elastic-plastic transformation of ultrahard materials	January 31-February 1, 2010
Y. Lee D. Seoung M. Lee	Yonsei University	High-pressure powder diffraction studies of zeolites	February 2-5, 2010
G. Amulele K. Otsuka	Yale University	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements	February 16-20, 2010
W. Han	Brookhaven	High-pressure IR study gases storage in boron nitride nanotubes	February 24-27, 2010
Wendy Panero J. Pigott	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals	March 2-4, 2010
Y. Wang	State University of New York – Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application	March 8-10, 2010
K. Otsuka G. Amulele	Yale University	<i>In situ</i> measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR	March 15-19, 2009
M. Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature	March 24-25, 2010
B. Liu Q. Li	Jilin University	Pressure-induced amorphization and polyamorphism in TiO ₂ nanomaterials	March 29-31, 2010
G. Yang	Brookhaven	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe	April 6-9, 2010
T. Tyson P. Gao	New Jersey Institute of Technology	Spin-driven local distortions in multiferroic hexagonal ReMnO ₅ ; IR measurements	April 12-17, 2010
M. Lang F. Zhang	University of Michigan	Phase transitions in minerals induced by ion beams and high-pressure: A novel approach in geosciences	April 25-27, 2010
Y. Wang	State University of New York – Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application	May 27-29, 2010
M. Pravica M. Galley	University of Nevada – Las Vegas	Far- and mid- IR high pressure studies of detonation products	June 5-6, 2010
Janice Musfeldt	University of Tennessee	Pressure-induced switching of the Jahn-Teller axis in Cu(py ₂ z)F ₂ (H ₂ O) ₂ by synchrotron infrared spectroscopy	June 27-July 1, 2010
M. Lang F. Zhang	University of Michigan	Phase transitions in minerals induced by ion beams and high-pressure: A novel approach in geosciences	July 12-14, 2010
L. Wang	State University of New York – Stony Brook	Incorporation of water in nominally anhydrous mantle minerals	July 15-16, 2010

M. Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature	July 18-19, 2010
M. Pravica N. Velisavljevic	University of Nevada – Las Vegas LANL	Far- and mid- IR high pressure studies of detonation products	July 22-25, 2010
D. Reaman J. Pigott	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals	July 26-28, 2010
G. Yang	Brookhaven	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe	July. 29-31, 2010
H. Okamura	Kobe University	High pressure IR studies of strongly correlated electron materials	August 4-11, 2010
G. Amulele K. Otsuka	Yale University	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements	August 12-14, 2010
Y. Lee D. Liu D. Seoung M. Lee T. Kim	Yonsei University	High-pressure powder diffraction studies of zeolites	August 15-17, 2010
K. Otsuka G. Amulele	Yale University	<i>In situ</i> FTIR measurements on hydrogen solubility and speciation in olivine and magnesiowüstite at high pressures and temperatures	August 18-21, 2010
T. Tyson P. Gao	New Jersey Institute of Technology	Spin-driven local distortions in multiferroic hexagonal ReMnO ₃ : IR measurements	August 23-26, 2010
H. Feng	Montclair State University	Examination of organic contaminants (PAHs) in passaic river sediments using synchrotron-UV-FTIR techniques	August 27-29, 2010

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