



CDAC

CARNEGIE/DOE ALLIANCE CENTER

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

Year Four Annual Report

December 2007



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



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

YEAR FOUR ANNUAL REPORT

1. Overview	
1.1 Mission of CDAC	1
1.2 Highlights from Year 4	2
2. Scientific Progress	
2.1 High <i>P-T</i> Phase Relations and Structures	5
2.2 <i>P-V-T</i> EOS Measurements	12
2.3 Phonons, Vibrational Thermodynamics and Elasticity	15
2.4 Plasticity, Yield Strength and Deformation	20
2.5 Electronic and Magnetic Structure and Dynamics	23
2.6 High <i>P-T</i> Chemistry	28
3. Education, Training, and Outreach	
3.1 CDAC Graduate Students and Post-doctoral Fellows	36
3.2 CDAC Collaborators	41
3.3 Undergraduate Student Participation	47
3.4 DC Area High School Outreach	48
3.5 2007 Stewardship Science Academic Alliances (SSAA) Program Symposium	49
3.6 SMEC 2007: Study of Matter at Extreme Conditions	52
3.7 Pressure Calibration Workshop	54
3.8 Visitors to CDAC	55
3.9 High Pressure Seminars	57
4. Technology Development	
4.1 High <i>P-T</i> Experimental Techniques	59
4.2 Facilities at Brookhaven, LANSCE, and Carnegie	60
5. Interactions with NNSA/DP Laboratories	
5.1 Overview	64
5.2 Academic Alliance and Laboratory Collaborations	65
6. Management and Oversight	
6.1 CDAC Organization and Staff	66
6.2 CDAC Oversight	67
7. Plans for Year 5 and Beyond	
7.1 Scientific and Educational Focus	68
7.2 Implementation of CDAC Phase II	68
7.3 HPCAT Upgrade	72
Appendix I CDAC Publications and Presentations for Year 4	74
Appendix II CDAC Synchrotron Users/Experiments (APS and NSLS) for Year 4	101
References	116

1. OVERVIEW

1.1 Mission of CDAC

A thorough knowledge of material properties at high pressure and temperature is critical to the mission of the National Nuclear Security Administration in the support of science-based stockpile stewardship¹. This program covers a broad range of problems and materials at multiple scales – *d*- and *f*-electron elements and alloys, low-*Z* molecular compounds, energetic materials and detonation products, dense hydrogen, metal oxides and hydrides and bulk materials as well as composites and interfaces. Information on material behavior in crystalline, liquid, and amorphous phases, phase transitions, equations of state (EOS), phonon dynamics, elasticity and plasticity, electronic and magnetic structures, and chemical reactions likewise are key issues in the broad area of material properties under extreme conditions, as are accurate descriptions of matter in transient, ultra-high density states. In the long term, addressing these problems also requires the training of the next generation of scientists in academia and the national labs. The training of students in turn requires regular access to state-of-the-art facilities that are not readily accessible to research groups in the NNSA Labs or in academic groups. The Carnegie/DOE Alliance Center – CDAC – was created to address these critical needs.

New developments and opportunities on a broad range of fronts in science, technology, and training, as well as in the infrastructure within NNSA, require a Center-like approach. Having now completed its fourth year, CDAC continues to support the NNSA mission in these key areas of scientific research and training. The successes of our first three years allowed us to expand and bring a broader range of universities into the alliance, and these successes have continued with a group of 11 Academic Partners. CDAC is managed by **Russell Hemley** (Director), **Ho-kwang Mao** (Associate Director), and **Stephen Gramsch** (Coordinator). CDAC consists of six formal academic partners together with **Carnegie: Princeton University (Tom Duffy)**, **University of Chicago (Dion Heinz)**, **University of Illinois (Dana Dlott)**, **University of Alabama - Birmingham**

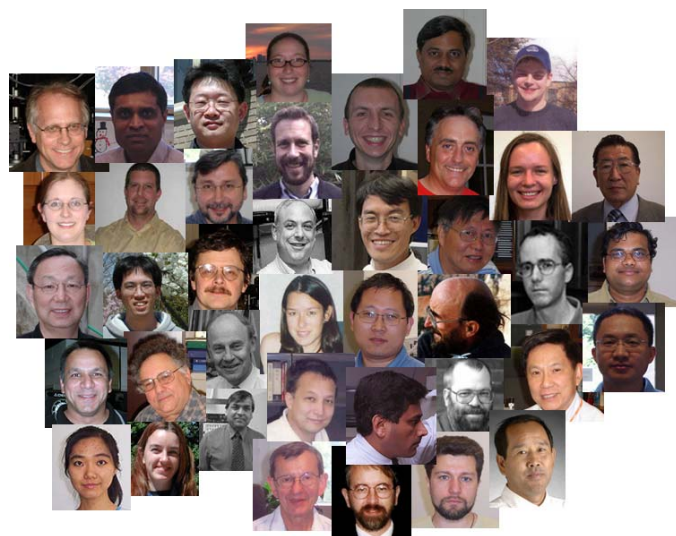


Figure 1. CDAC personnel from our Academic Partner institutions.

(Yogesh Vohra), **University of California - Berkeley (Hans-Rudolf Wenk)**, and **California Institute of Technology (Brent Fultz)**. At the beginning of Year 4, five new academic partners joined the CDAC effort: **New Mexico State University (Kanani Lee)**, **Florida International University (Surendra Saxena)**, **Texas Tech University (Yanzhang Ma)**, **University of Nevada - Reno (Dhanesh Chandra)**, and **Arizona State University (Jeffrey Yarger)**. Scientists at the national labs (CDAC Laboratory Partners) continue to benefit from the availability of beam time and technical training and the high *P-T* technique development taking place at **HPCAT**, the dedicated high-pressure synchrotron x-ray facility at the **Advanced Photon Source (APS)**, of which CDAC is a

member. Laboratory scientists are also able to take advantage of facilities at **Carnegie** and the **National Synchrotron Light Source, Brookhaven National Laboratory (NSLS)**. Active interactions also are in place with staff from the Lujan Center at **LANSCE (Los Alamos National Laboratory)** in the development of critically important high *P-T* neutron scattering capabilities. CDAC also has built an extensive list of collaborators from some 176 institutions worldwide.

The field of research on materials at extreme conditions continues to expand with the development of new methodologies, for example, in the overlap of static and dynamic compression experiments and the unprecedented accuracy needed for code validation. Despite the remarkable success of HPCAT, the full potential of the techniques it has pioneered is far from realized and requires a multi-beamline approach. Facilities developments within the NNSA/DP Labs such as NIF and Z_R are creating new challenges along with the need for input from the academic sector, and advances at neutron sources present new challenges and opportunities for NNSA/DP. CDAC continues to take the lead in enabling development of the next generation of high-pressure techniques, and CDAC personnel are carrying out systematic measurements of a full range of physical and chemical phenomena under extreme conditions. The centerpiece of the CDAC program from the beginning has been the HPCAT facility, which is led by **Ho-kwang Mao** (Director) and **Guoyin Shen** (Project Manager), and has been developed for high pressure physics, chemistry and materials science, providing technical developments and critical, state-of-the-art spectroscopic and diffraction tools. All four beamlines have been completed and are accepting general users through the General User Proposal (GUP) program at the APS. At this point, more than 360 different users (*i.e.*, from National Labs and academia) have conducted experiments at the facility to date. The original HPCAT vision of four independently operating experimental hutches has now been realized. High-pressure neutron facilities at LANSCE, synchrotron infrared spectroscopy at the NSLS, and specialized high-pressure facilities at **Carnegie** complement this effort. At **Carnegie**, developments continue in the area of high *P-T* spectroscopy and x-ray crystallography, new cell designs for a variety of experimental measurements, and advances in CVD diamond growth. Experimental work in high-pressure geoscience and planetary science is increasingly carried out with a materials science perspective and therefore provides excellent background for understanding problems in stewardship science and for future work in the NNSA/DP Labs. Interactions with theoretical groups in academia and the National Labs add significantly to the experimental work carried out within the CDAC program.

CDAC formally began operations on May 1, 2003 with the first funding year ending January 31, 2004. This report covers activities from the CDAC Academic Partners, Laboratory Partners, and University Collaborators from July 2006-July 2007. Research carried out by National Lab partners, but done outside of the CDAC facilities, is not included.

1.2 Highlights from Year 4

Outreach and Training

CDAC continues to make excellent progress in outreach and training, an important part of its mission. The following are highlights, in particular as they relate to student education and training:

- Through support of HPCAT, continued to promote the growth of the sector. To date, more than 360 users have carried out experimental work at HPCAT.
- Facilitated the growth of the high pressure research community in the US and worldwide through CDAC collaborations. Currently, there are approximately 420 outside collaborators from over 176 institutions in the US and around the world that have collaborated with us on stewardship science-related projects.
- Continued to support the Ph.D. thesis work of 18 graduate students at CDAC partner universities and **Carnegie**. Thus far, 11 graduate students from Academic Partner institutions have received the Ph.D. degree with CDAC support.
- Former CDAC graduate student **Wendy Mao**, following an Oppenhiemer Postdoctoral Fellow appointment at **LANL**, has just begun a faculty position at **Stanford University** and will continue to work on stewardship science-related projects.
- In partnership with **FIU**, sponsored the *Science of Matter at Extreme Conditions SMEC 2007* Conference in May 2007. The conference featured 41 presentations from groups affiliated with

CDAC. CDAC also supported the *Workshop on Pressure Calibration at High Temperature*, held at **Carnegie** in January 2007.

- Hosted numerous visitors to other CDAC facilities (e.g., **Carnegie** and **NSLS**) for training and technique development and continued to foster collaborations with high pressure programs at all the NNSA Labs.
- Hosted undergraduate and high school interns at **Carnegie**. This past year, four students (two high school students and two undergraduate interns), were working on CDAC-related research projects.

Scientific Breakthroughs

Since the inception of CDAC in May of 2003, some 491 papers based on CDAC research have been published as a result of the support from the grant. Papers describing work carried out by CDAC Academic Partners, Carnegie research supported by the CDAC grant, and research carried out at HPCAT and CDAC facilities at NSLS are included in this list. (This does not include the large amount of research performed by high-pressure groups within the National Labs not done at CDAC-supported facilities). Virtually all the papers represent student or post-doctoral training, and many describe important technique development, while a growing number involve active collaborations with NNSA/DP Lab scientists. Articles published in major high-impact journals include 30 in *Physical Review Letters*, 10 in *Science*, 20 in *Nature* magazines, and 23 in the *Proceedings of the National Academy of Sciences (PNAS)*. The following items represent just a portion of the scientific highlights from Year 4 of the CDAC program.

- *Pressure effects on the rate of β -capture in ^{40}K* : At **LANSCE**, a group from **New Mexico State** has made the first measurements of the effects of pressure on the rate of electron capture in ^{40}K .
- *New results in the high pressure behavior of iron-containing alloys*: The **Caltech** group used high-pressure nuclear resonant scattering techniques at HPCAT to uncover unusual pressure-induced Invar transitions in Pt_3Fe and Pd_3Fe^3 .
- *Melting of silicon at high pressures*: The **Princeton** group has measured the melting curve of elemental silicon up to 15 GPa using a miniaturized diamond anvil apparatus⁴.
- *Pressure induced phase transitions in PbTiO_3* : A team from **Carnegie** carried out theoretical calculations that predict colossal ferroelectricity in PbTiO_3 under pressure⁵; this was followed up with Raman and x-ray experiments, resulting in an updated *P-T* phase diagram⁶.
- *Polymers and their composites*: For the first time, EOS for a series of important polymers and composites were measured to above 10 GPa using light scattering techniques at **LANL** and **Carnegie**⁷⁻⁹.
- *Structural transitions in rare earth metals*: The **Alabama** group identified an unusual series of phase transformations in the heavy rare earth metal terbium, and uncovered evidence for *4f* shell localization.
- *Effects of vacancies in FeAl* : The **Caltech** group followed up last year's successful neutron work on FeAl with measurements of the partial phonon DOS of FeAl using nuclear resonant inelastic scattering at HPCAT.
- *Femtosecond measurement of interface dynamics*: At **Illinois**, the first vibrational spectrum of a monolayer at high pressure has been measured using newly-developed sum frequency generation techniques. The **Illinois** group continues the development of an ultrafast nonlinear vibrational spectroscopic technique to understand the dynamics of interfaces under laser-generated shock waves, and under high static pressures produced in an anvil apparatus¹⁰.

- Chemistry of hydrogen storage materials: A collaboration between the **Carnegie** group and Nevada-Reno on potential hydrogen storage materials led to new results on the phase transformations in LiAlH_4 and LiHH_2 ^{11, 12}.
- Synchrotron x-ray measurements of dynamic compression: Using beam time at HPCAT provided by CDAC and other members, a group from **WSU** led by CDAC advisory committee member **Yogendra Gupta** has for the first time monitored dynamic compression using synchrotron x-ray diffraction.

Technique Development

Supporting the development of enabling techniques for both routine and novel experimental measurements is a key aspect of the CDAC program. In Year 4, we have continued to make significant progress toward our program goal of advancing the state of the art in high *P-T* materials science research facilities and techniques, as illustrated by the following:

- Real-time synchrotron measurements of shock compression events: With CDAC support, a group from **SNL** was able to complete a feasibility study at **NSLS** showing that it is possible to use the pulse structure of the IR beam and conventional detectors to monitor dynamic compression in real time. Subsequently, a group from **WSU** carried out real-time x-ray diffraction measurements of shock compression on a variety of materials at **HPCAT**.
- Optical techniques for EOS measurements: The **Carnegie** group applied a classical optical reflectivity method for the measurement of the molecular polarizability of ice VII and ice X and showed that the pressure-volume relations give an EOS that is in excellent agreement with that obtained using diffraction methods¹³.
- Rapid EOS determination: At HPCAT, instrumentation has been developed to facilitate the changing of pressure in the DAC without removing the cell from the diffractometer. This will reduce the time necessary for high-resolution EOS measurements on materials of interest¹⁴. A dual-table configuration in the microdiffraction station has eliminated the downtime associated with changing from laser heating to ambient temperature experiments.
- Intensity increase at the HPCAT ID beamline: A second undulator for **HPCAT** is under consideration by the **APS**. Installation of a second undulator on the ID line would bring an increase of an order of magnitude or more in intensity, making new classes of high-resolution x-ray spectroscopy experiments possible, and increasing the efficiency of those techniques already available.
- Femtosecond laser spectroscopy at high pressure: A user-friendly but state-of-the-art third-generation femtosecond laser-based sum-frequency generation apparatus has been constructed at **Illinois** that will allow inexperienced users to start work early on the study of interfaces at high pressure. Diamond cells designed for these experiments have been built.
- Single crystal white-beam diffraction: A **Carnegie** group led by visiting investigator **Taksumitsu Yamanaka** has developed white-beam techniques at HPCAT station BM-B for structural refinements from high-pressure single crystal diffraction data.

2. SCIENTIFIC PROGRESS

Year 4 of the CDAC program has seen continued progress above and beyond the goals set out in the work plan of original three-year CDAC proposal. Our scientific program is divided into six areas of emphasis:

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

High P - T structural studies enabled by the unique capabilities available at HPCAT continue to be a forefront topic within CDAC. Improvements in laser heating and resistive heating techniques¹⁵, *in situ* high P - T Raman measurements with laser heating¹⁶, and improvements in refinement techniques have increased the variety of different types of systems being investigated by CDAC research groups. The following examples of studies of phase relations and structures at high pressure highlight ongoing work in this area.

Melting Curve of Silicon – Many aspects of the phase diagram of silicon are not known as few experiments have been carried out at simultaneous high pressure and temperature. There has also been much interest in melting curves at high pressures, but such studies suffer from well-known experimental limitations. The **Princeton** group has measured the melting curve of silicon up to 15 GPa using new techniques involving a miniaturized Kawai-type apparatus with second-stage cubic anvils made of x-ray transparent sintered diamond⁴. Melting is determined from the disappearance of x-ray peaks combined with the appearance of diffuse scattering background. Results are in good agreement with electrical resistivity measurements up to the phase I (diamond structure) – phase II (β -tin structure) – liquid triple point. The triple point of phase XI (orthorhombic, $Imma$) – phase V (simple hexagonal) – liquid has been constrained at 14.4(4) GPa and 1010(5) K. These results (see Fig. 2) demonstrate that the combination of x-ray transparent anvils and monochromatic diffraction with area detectors offers a reliable way to detect melting at high pressures in the multianvil press.

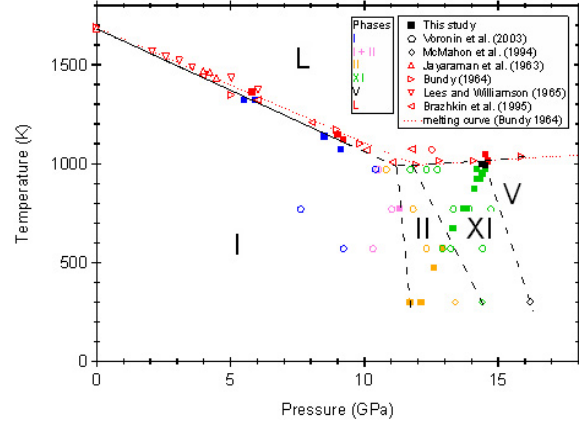


Figure 2. Melting curve of silicon to 15 GPa measured using synchrotron x-ray techniques. Results are in good agreement with earlier electrical resistivity measurements.

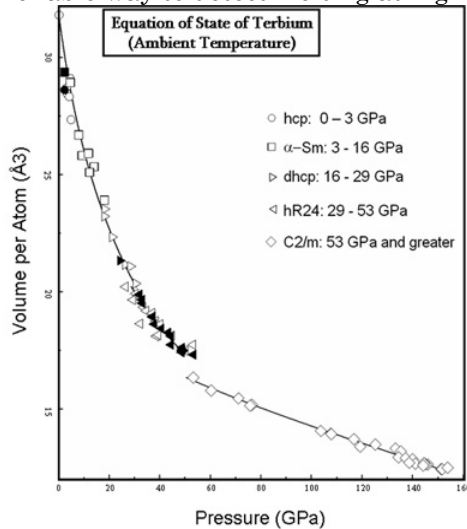


Figure 3. Volume per atom as a function of pressure for Tb metal; filled symbols are decompression data points. The equation of state has been measured to 154 GPa at room temperature. The complete regular trivalent rare earth structural sequence is observed with the exception of the fcc structure, which was not observed as a pure phase. Since these may have in fact been due to an emerging distorted fcc phase, the putative fcc points are neither displayed nor used in fits. At 51 ± 2 GPa a 5% volume collapse is observed as the structure transforms to the open, low symmetry C2/m phase. Note the sharp decrease in compressibility for this phase, indicating a change in the character of the metallic bonds, which is argued to be the onset of f -electron participation in bonding.

Structural evidence for f -shell delocalization in Terbium – The heavy rare earth metal terbium has been studied at synchrotron sources using both angular and energy dispersive x-ray diffraction to a maximum pressure of 154 GPa (volume fraction $V/V_0 = 0.39$). The complete regular trivalent rare earth structural sequence, $hcp \rightarrow \alpha\text{-Sm} \rightarrow dhcp \rightarrow fcc \rightarrow$ distorted-fcc ($hR24$), is observed at

low pressures except for the undistorted fcc structure. At 51 ± 2 GPa, Terbium (Tb) experiences a 5% collapse in volume per atom on compression, as illustrated in Fig. 3, and transforms to a low symmetry $C2/m$ monoclinic phase similar to the α'' phase of cerium (space group 12 with atoms at the $4(i)$ positions). The observation of additional peaks not predicted by body centered monoclinic (bcm) precludes that additional symmetry, and the $C2/m$ phase is assigned in accordance with data on Ce and more recent results on Gd. Despite this sudden drop in volume, it is not clear that full delocalization of the f -electrons occurs abruptly. Recent measurements on Gd show only a gradual loss of local magnetic ordering after the symmetry lowering transition, supporting the Kondo Volume Collapse model and screening of the correlated f -electron paramagnetic moments by the conduction electrons. Though the monoclinic $C2/m$ phase is observed to be stable to at least 154 GPa, the presence of the tetragonal bct phase at extreme compressions in both cerium, which has one $4f$ electron, and thorium, which has one $5f$ electron, indicates the possibility of observing a similar phase in terbium at ultrahigh pressures.

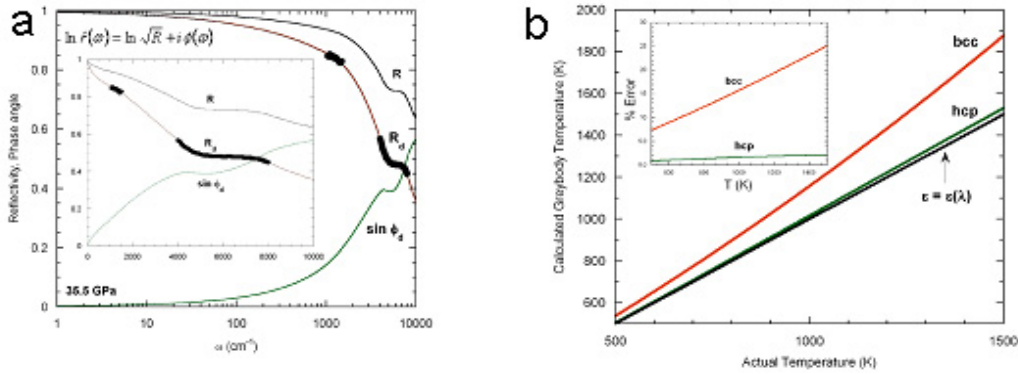


Figure 4. a) Measured reflectivity R_d of iron at 35.5 GPa along with the calculated phase change ϕ_d and the corresponding vacuum reflectivity on log and linear (inset) scales. b) Measured reflectivity R_d of iron at 35.5 GPa along with the calculated phase change ϕ_d and the corresponding vacuum reflectivity on log and linear (inset) scales.

High Pressure Melting of Iron – The **Heinz** group at **Chicago** has collected reflectivity data for iron at high pressure using the fourier transform infrared reflectivity technique at the CDAC-supported NSLS beamline U2A. One of the biggest sources of error for temperature measurement using the spectroradiometric method is the sample emissivity (both its magnitude and wavelength dependence). Reflectivity measurements of iron foil and powder have been collected up to 50 GPa at ambient temperature in an attempt to estimate the spectral emissivity of iron. This data was corrected for diamond absorption and the beam current – intensity relationship. The data was analyzed with the Kramers-Kronig relations to derive the phase change on reflection. This allowed a calculation of the pressure and wavelength dependence of the emissivity. The results show that at room temperature, hcp – Fe is a nearly perfect greybody, as the reflectivity has almost no dependence on wavelength. However, the reflectivity of bcc – Fe is strongly wavelength dependent and a sharp transition in both the magnitude and slope of the emissivity occurs at the bcc-hcp phase transition. Figure 4a shows one example of an analyzed reflectivity spectrum. The slope of the emissivity is nearly pressure independent within a single crystalline phase; therefore, the errors associated with the greybody assumption applied to iron were evaluated assuming a temperature-independent emissivity for hcp and bcc iron. This result is shown in Fig. 4b. Future plans include extending these measurements to high temperatures to determine the emissivity of fcc – Fe and to further evaluate the effects of phase transitions on the optical properties of iron.

Study of Ti₂₁βS to 70 GPa – High-pressure experiments initially performed in Year 3 on Ti₂₁βS were continued in Year 4 by **Nenad Velisavljevic, Neal Chesnut, and Liliana Sanchez at LANL**. Ti₂₁βS, which forms nanometer-sized particles at high pressure, is a new alloy important for NNSA programs. X-ray diffraction data were collected to above 70 GPa. In a second experiment, it was possible to again identify the bcc phase of Ti₂₁βS. Additional diffraction peaks were observed, however, and it was possible to assign these to the hcp phase. Ti₂₁βS is therefore a mixture of bcc and hcp phases. The *c/a* ratio of this material decreases from 1.60 at ambient conditions to 1.57 at 36 GPa, and then as pressure is increased to 44 GPa, the *c/a* ratio jumps back up to a value of 1.61 and remains in this range up to the highest pressure. The change in *c/a* ratio at 40 GPa is interpreted in terms of a change in electronic structure, leading to stiffening of the lattice in one direction. Separate EOS were fit for the bcc phase (Fig. 5a) and the hcp phase of Ti₂₁βS. In this pressure range (40 GPa), no structural phase change was observed. However, as the pressure is further increased, the peak intensities corresponding to the Ti₂₁βS hcp phase start to decrease at and above ~58 GPa. In the case of another alloy, Tiβ₂1S, experimental and theoretical work show that the ω phase can be suppressed altogether and a direct α → β, (Fig 5b), phase transition can be achieved^{17, 18}.

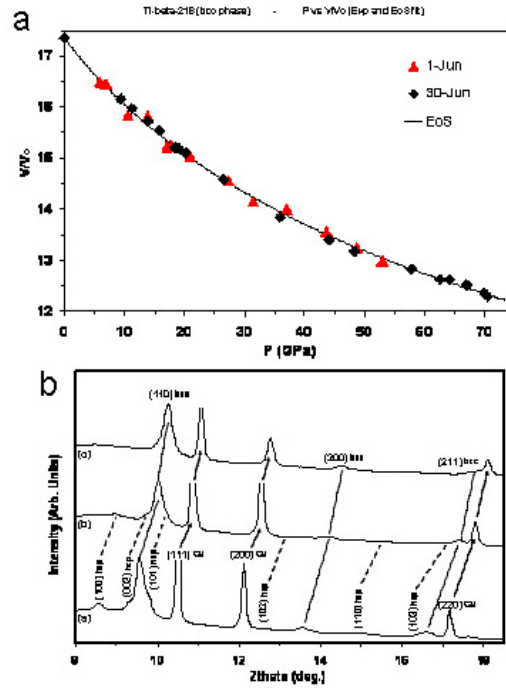


Figure 5. a) Ti₂₁β S bcc data from both experiments and the resulting EOS fit. b) Direct α → β structural phase transition in Tiβ₂1S.

Structural Transitions in Group IV Metals – Further work by the LANL group has concerned group IV metals Ti and Zr. Experiments performed at HPCAT in the last year have been focused on determining the influence of alloying, grain size, and impurities on structural phase stability and compressibility at high pressures. Previous studies performed on Ti and Zr indicate that at high pressures these metals undergo a series of structural phase transitions denoted α → ω → β. Impurities that may naturally be present in the sample or brought about by alloying can have a significant effect on the structural phase stability. Substitutional impurities like Al, V, and Mo change the d-band electron concentration in Ti and Zr. Experimental results show that when these impurities are present, the α → ω transition pressure can be increased from ~ 6 GPa in pure Ti up to ~ 27 GPa for Ti-6Al-4V alloy¹⁹. Interstitial impurities like O, N, and C, also play a significant role as they change the energy barrier of the α → ω transformation. In the Zr experiments, three different Zr samples with increasing impurity concentrations were investigated. Multiple experiments have been performed under both hydrostatic and non-hydrostatic conditions and show that as O, N, and C concentrations increased so also does the transition pressure needed for the α → ω transition to occur (Table 1)²⁰.

	α → ω (hydrostatic)	α → ω (nonhydrostatic)	ω → β
Zr	6.4	4.8	31.4
Zr I	7.5	6.9	*
Zr II	11.6	10.8	40.0

Table 1. Transition pressures for Zr samples with different impurity concentrations.

In addition to studying the influence of impurities, this group has also looked at the effect of grain size on the high-pressure behavior of Ti metal. In studying nano-crystalline Ti (nc-Ti), they have observed for example that the

compressibility on nc-Ti is greater than that of a coarse grained Ti (c-Ti) sample, as shown in Fig. 6²¹.

Continued Development of Isotopically Enriched ¹³C Diamond – The ¹³C pressure sensor developed by the Alabama group was calibrated to 156 GPa at room temperature under prior CDAC support. In Year 4, several additional isotopically enriched diamond anvils have been synthesized for future work. In a series of experiments, (100) oriented 0.3 carat brilliant cut diamonds were used as substrates in homoepitaxial growth experiments. All diamond anvil substrates had a flat (100) surface of

approximately 300 microns in diameter on which homoepitaxial diamond was deposited. The diamond anvil substrates were placed in a 1.2 kW microwave plasma chemical vapor deposition chamber. Homoepitaxial diamond deposition was carried out with isotopically enriched methane in hydrogen-oxygen plasma using microwave plasma chemical vapor deposition. The plasma was maintained with a gas flow rate of 390 standard cubic centimeters per minute (sccm) of H₂, 8 sccm of ¹³CH₄, and 0.8 sccm of O₂. The N₂ flow rate was varied for different experiments as 0, 0.2 sccm, 0.3 sccm, 0.4 sccm, 0.6 sccm, 1.0 sccm and 1.4 sccm. The diamond substrate temperature was maintained at 1212 ± 1 °C during the two hour deposition period. To keep the temperature constant at this value, the microwave power is adjusted using a computer controlled process. Future plans include investigation of the optical properties and ¹³C Raman mode pressure calibration for diamonds grown with varying amounts of substitutional nitrogen.

Pressure Induced Phase Transitions in PbTiO₃ – Raman scattering, x-ray diffraction, and first-principles electronic structure calculations have been used by Muhetaer Ahart and Ronald Cohen at Carnegie, along with collaborators from Argonne, Bayerisches Geoinstitut

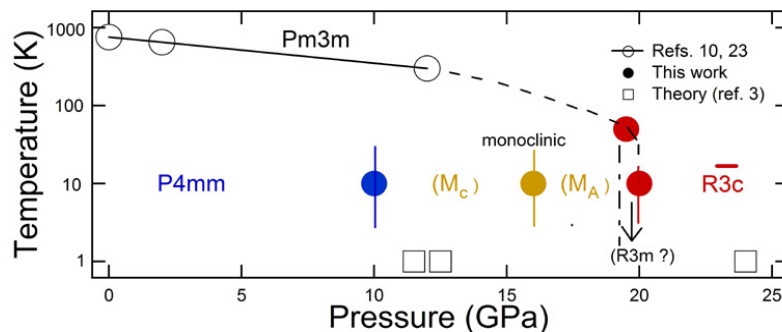


Figure 7. Phase diagram for lead titanate. Open circles are obtained from prior work from Ref²²; solid circles are experimental results from *n* work. Open squares are theoretical calculations from Ref²², which give tetragonal symmetry below 11 GPa, monoclinic symmetry between 11 and 12 GPa, and rhombohedral symmetry above 12 GPa. The solid and dashed lines (guides to the eye) indicate the boundaries between of different phases.

to obtain high coupling piezoelectricity. They also found that the transition in complex relaxor ferroelectrics or high performance ferroelectric solid solutions with lead titanate endmembers can be tuned down to ambient pressure by changing the composition. This opens the door to the possible

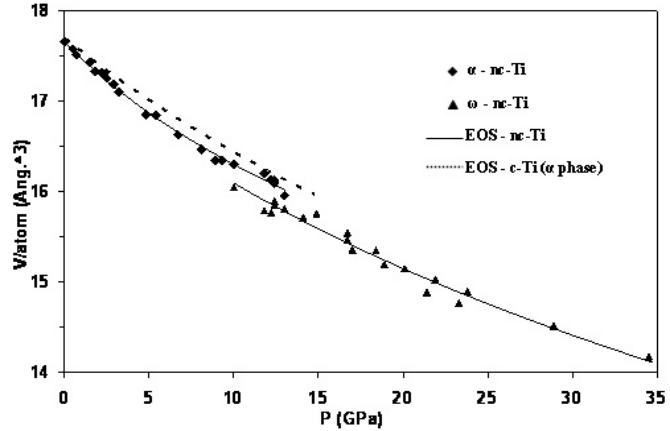


Figure 6. Comparison of change in volume/atom as a function of pressure for nc-Ti and c-Ti (dashed line).

(Bayreuth), and Berkeley to investigate the behavior of PbTiO₃ under pressure at low temperature (10 K). The results indicate that lead titanate undergoes successive phase transitions from tetragonal to monoclinic *Pm* at 10 GPa, monoclinic *Pm* to monoclinic *Cm* at 16 GPa, and monoclinic *Cm* to rhombohedral R-3c at 20 GPa, consistent with theoretical calculations. These experimental results provide a new phase diagram for PbTiO₃ (Fig. 7). Results reveal that complex microstructures or compositions are not necessary

discovery of high performance, pure compound electromechanical materials, which would greatly decrease costs and greatly expand the utility of ultrasonics used in medicine, sonar, hydrophones, and materials testing, as well as expand the range of actuators now available²².

Melting and Phase Relations in the Fe-FeO System – Over the past several years, the **Heinz group** at the **University of Chicago** has collected extensive data on the melting and phase relations in the Fe-FeO system from 18 to 136 GPa, spanning bulk compositions from 5 to 90 weight % FeO. Results show that the system is not a solid solution as some had predicted²³ up to at least the core – mantle boundary. Since the melting temperature of FeO at the Earth’s core-mantle boundary is significantly greater than the melting temperature of pure Fe^{23, 24}, a complete solid solution would be incompatible with the energy requirements of the geodynamo.

In the last year, the Chicago group, led by CDAC graduate student **Chris Seagle**, has studied melting in binary iron-light element systems at high pressure and the melting of end-member phases using x-ray diffraction techniques at the GSECARS beamline at APS. The nature of these binary iron–light element systems allows an evaluation of the likelihood and abundance of a particular light element to be incorporated into the Earth’s core. A manuscript on the thermal EOS of Fe₃S has been published²⁵, as has a paper detailing melting in the Fe-Fe₃S system²⁶. A manuscript detailing melting in the Fe – FeO system at pressures up to 93 GPa has been submitted for publication²⁷.

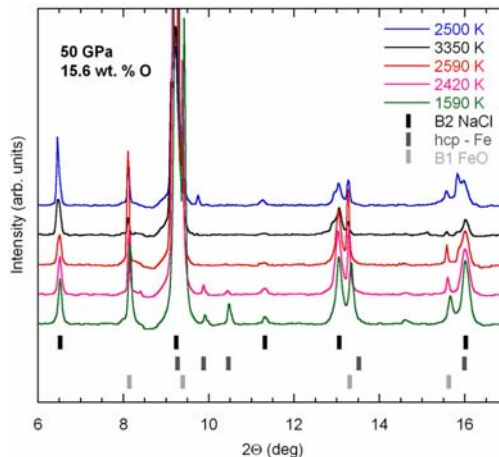


Figure 8. Partial melting in the Fe-FeO system at 50 GPa evidenced by x-ray diffraction. hcp-Fe peaks present in the 2420 K pattern disappear in the 2590 K pattern. An fcc-Fe peak reappears when the temperature was dropped to 2500 K indicating that partial melting and recrystallization had occurred.

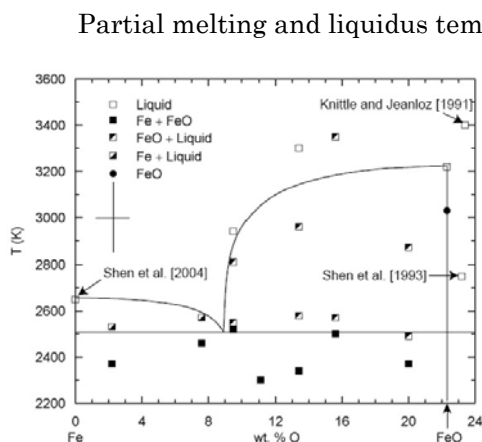


Figure 9. Phase diagram in the Fe – FeO system at 50 GPa based on the current experimental work. The melting temperature of pure Fe²⁹ and that of FeO^{23, 28} are shown for comparison.

Partial melting and liquidus temperatures were determined by x-ray diffraction and laser heating. Upon raising the temperature above the partial melting/liquidus temperature the Bragg reflections associated with a solid phase disappear; these peaks return when the temperature is dropped below the liquidus or solidus (Fig. 8). The group has been successful at cycling the temperature above and below the melting temperature several times in a single experiment to verify that the melting temperatures measured are accurate. In many cases, several samples were tested at the same pressure to verify consistency with the technique. In almost all cases, melting temperatures were reproducible to within 100 K. The characteristic of melting relations in iron – light element systems place important constraints on the composition and temperatures within Earth’s core. Recent experimental work has shown that the Fe – FeO system remains eutectic to at least 93 GPa, and the eutectic temperature has been measured up to this pressure.

Many samples were used to constrain the phase diagram at 50 GPa (Fig. 9). One important result of this study is that the two-liquid phase field in the Fe – FeO system observed at lower pressures³⁰⁻³² has disappeared by 50 GPa. There is no seismological evidence of a stratified liquid outer core; therefore, a two liquids phase field in the relevant phase diagram is not compatible. Work in the Chicago group has also shown that the eutectic temperature at 74 GPa is 500 K higher than the melting temperature of pure iron³³, suggesting that this melting curve is too low. Sub-solidus data allowed the constraint of the coefficient of thermal expansion for FeO which was previously only known to 3 GPa³⁴. The thermal expansion has a strong volume dependence which can be fit with a simple power law. Another important observation from this study is that FeO remains in the sodium chloride (B1) structure up to the highest pressures and temperatures reached. Much of this data was within the published stability field for the iB8 type structure of FeO^{35, 36}, which is likely only stable in an intermediate temperature range or possibly as a metastable phase^{27, 37}.

Studies on the Fe – Fe₃S system have continued and are now focused on measurement of the melting temperatures up to 155 GPa, well into the pressure range of Earth's core. Liquidus temperatures at a bulk composition of 10 wt. % S

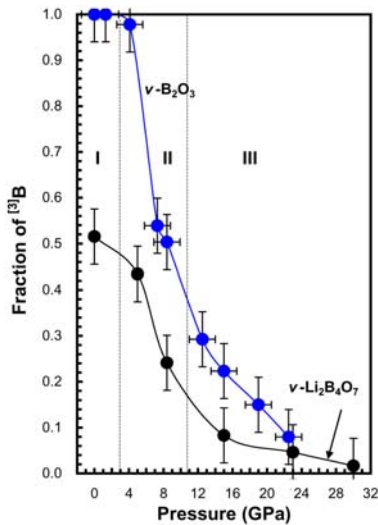


Figure 11. Pressure dependence of the percentage of three-coordinate boron in $\text{Li}_2\text{B}_4\text{O}_7$ glass (circles) and B_2O_3 glass (squares). Dashed lines are for ease of visualization. Labels I, II and III refer to distinct pressure ranges in which potentially different densification mechanisms may dominate the change in coordination.

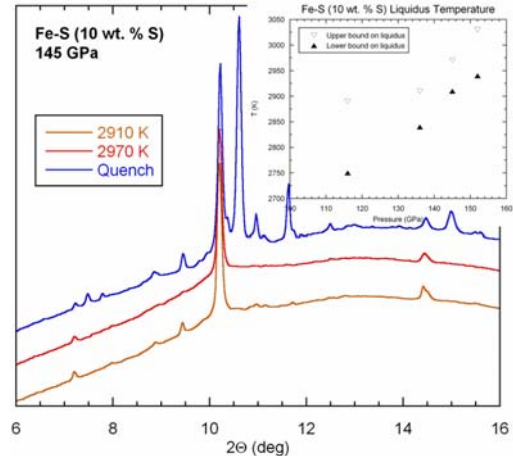


Figure 10. Integrated diffraction patterns detailing melting in the Fe-S system. In the 2970 K pattern, the only Bragg reflections present are those of the NaCl insulating medium. Below this temperature sample peaks are present at 2910 K; after quenching the sample, several peaks reappeared indicating melting and recrystallization. The inset shows the liquidus temperature for several different pressures up to 155 GPa.

were bound in several experiments. As is well known, phase transitions can significantly affect the melting curve. This can lead to large uncertainties when extrapolating data from pressures below the phase transition and illustrates the need for data in the megabar range. Figure 10 shows the result of this study. This data suggests a minimum temperature of 2800 K at the core-mantle boundary if the outer core contains 10 wt. % S. The melting of pure Fe₃S has also been studied from 25 up to 150 GPa. This data was collected very recently and is still being analyzed in detail, however it is apparent that Fe₃S continues to melt incongruently up to at least 55 GPa and remains tetragonal up to at least 150 GPa.

X-Ray Inelastic Scattering of Alkali Borate

Glasses – Led by former Carnegie postdoctoral fellow **Sung Keun Lee**, a group from **Seoul National University** and the **GSECARS** and **HPCAT** sectors at the APS reported the first *in situ* boron K-edge inelastic x-ray scattering (IXS) spectra for alkali borate glasses (with nominal composition $\text{Li}_2\text{B}_4\text{O}_7$) at high pressure. The glass was synthesized under pressure in a diamond anvil cell and taken to 30 GPa, where the glass undergoes a threefold to fourfold coordination change at boron. IXS spectra taken at the **HPCAT** beamline 16-

ID-D provide a local probe of the coordination environment with which the fraction of boron atoms in the glass having distinct coordination environments can be directly determined. Results show that the coordination transformation in the alkali borate glass begins at around 5 GPa, with the fraction of four-coordinated boron increasing with pressure from about 50% (at 1 atm) to more than 95% (at 30 GPa). The decrease in the fraction of three-coordinate boron with pressure (Fig. 11) shows three distinct pressure ranges, and points to the possibility of multiple densification mechanisms. The lithium K-edge IXS spectrum for lithium borate glasses at 5 GPa shows IXS features similar to those observed at 1 atm, suggesting that the Li environment does not change much with pressure up to 5 GPa. These results provide an improved understanding of the structure of low-Z glasses at high pressure, important both for glass technology and in relation to magmatic processes in the deep Earth³⁸.

Unique Structural Transformation in Vanadium Metal – HPCAT/HPSync staff scientist **Yang Ding** has observed a unique type of high-pressure phase

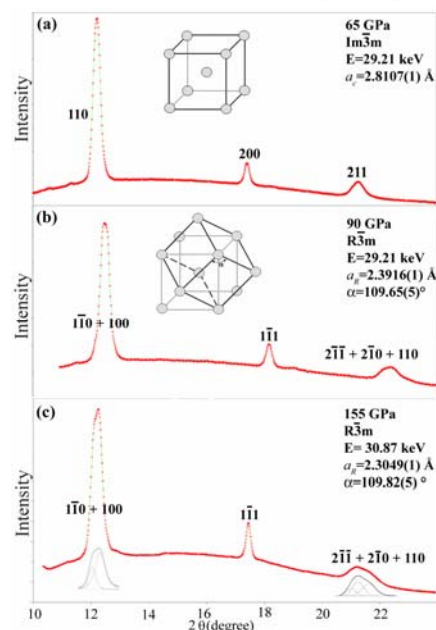


Figure 13. Non-hydrostatic x-ray diffraction patterns of vanadium metal at (a) 65 GPa, (b) 90 GPa and (c) 155 GPa. The insert in (b) illustrates the transformation of vanadium from a cubic to a rhombohedral structure. The inserts in (c) demonstrate the resolved splitting of peaks according to the refinement of the rhombohedral structure model. E denotes the energy of the x-ray photons used for the diffraction experiment.

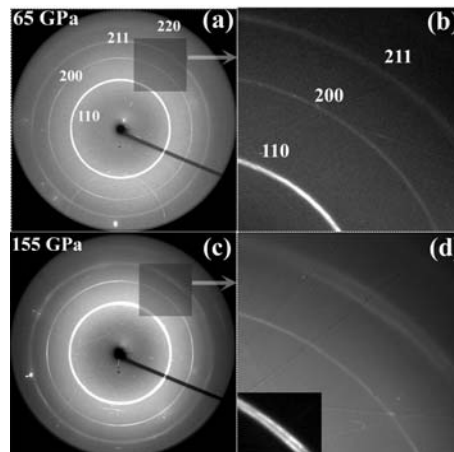


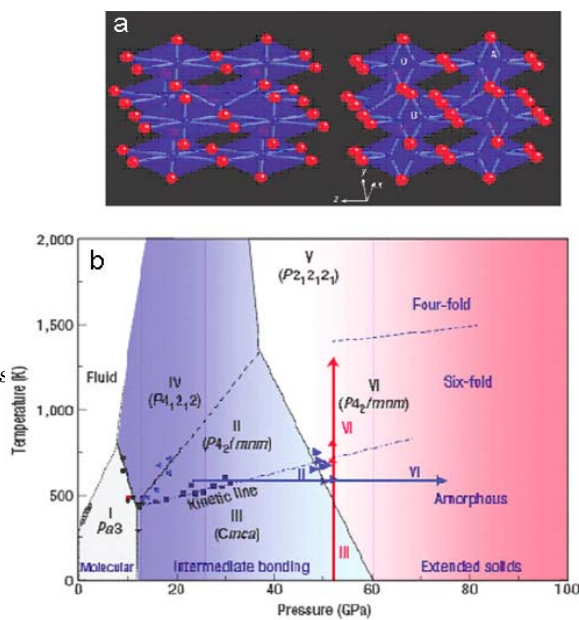
Figure 12. (a) Diffraction pattern of vanadium metal recorded on an image plate at 65 GPa under non-hydrostatic conditions. Indexing is based on a bcc lattice. (b) Enlarged image of the shadowed area in (a). (c) Diffraction pattern of vanadium metal at 155 GPa. (d) Enlarged image of the shadowed area in (c).

transition in vanadium that has not yet been documented for a pure element. At about 60 GPa, single crystal vanadium undergoes a cubic-to-rhombohedral transition in which the volume does not change at the transition. The displacive phase transformation is quite similar in nature to that observed in FeO at high pressure, where the paramagnetic-antiferromagnetic transition drives the second-order structural change. Theoretical work carried out by scientists from **Uppsala University** indicates that vanadium will show increased electronic and magnetic interactions at high pressure that would drive such a transition, this time in a pure element, without the benefit of metal-oxygen-metal contacts to mediate the magnetic interactions. In the case of vanadium, the electronic and magnetic interactions will be much more subtle in nature.

Working at the HPCAT's microdiffraction beamline 16-ID-B, Ding and co-workers used diamond anvil cell techniques to compress a single crystal of vanadium metal to 155 GPa. Above 65 GPa, the [110] and [220] diffraction peaks split, as illustrated in Fig. 12, indicating a transition from the bcc structure to a rhombohedrally strained variant, while the [200] peak does not undergo a similar splitting. The absence of splitting in the [200] peak confirms that the volume is conserved across the second-order transition. Figure 13 shows the non-hydrostatic x-ray diffraction patterns of vanadium at (a) 65 GPa, (b) 90 GPa and (c) 155 GPa.

New Findings in Simple Molecular Materials – It is well known that pressure can fundamentally alter the structural, physical and chemical properties of matter. In an extension of work reported early in the CDAC program, a group from LLNL led by **Choong-shik Yoo** has reported a novel

Figure 14. a) Structures of CO₂-II (left) and stishovite-type CO₂-VI with carbon in sixfold coordination by oxygen. b) Updated phase diagram for CO₂. Note that the transformation from CO₂-II to CO₂-VI links two separate phases with the same space group, but with two different but closely related structures.



stishovite-type structure for CO₂, following the earlier report of sixfold-coordinated carbon in CO₂-II (Fig. 14a)³⁹. Using microdiffraction techniques at HPCAT, the group was able to refine the new structure using powder diffraction data⁴⁰, and extend the phase diagram of the material (Fig 14b).

2.2 P-V-T EOS Measurements

P-V-T EOS provide crucial information for predicting material behavior and input for codes used in

numerous different stewardship science applications. Throughout CDAC, a wide variety of different methods are used for such experiments, including x-ray and neutron diffraction and sound velocity measurements using high-pressure Brillouin scattering and ultrasonic techniques. These static methods complement the data obtained from dynamic compression studies. EOS data for low-Z materials⁴¹⁻⁴⁴ provide key information on kinetics, thermal transport, and other important properties of detonation and other chemical processes^{41, 42, 44, 45}. Recent work in the computational area has shown that, even in simple systems, many-body effects can be crucially important⁴⁶.

High Pressure Studies of Nanocrystalline Tungsten and Tungsten Nitride – In the Texas Tech group, x-ray diffraction measurements have shown that a newly synthesized nanocrystalline W₂N has a substantially larger cell parameter than the bulk material, yet the lattice of nanocrystalline W remained unchanged from the bulk to the nanoscale. High-pressure x-ray diffraction measurements to 31 GPa resolved a much lower bulk modulus of 240 GPa for nanocrystalline W₂N, but the bulk modulus of 307 GPa for nanocrystalline W remained essentially unchanged compared to the bulk material (Fig. 15). The enlarged cell parameter and the relatively low bulk modulus of W₂N reflect the size effect of nanocrystalline W₂N.

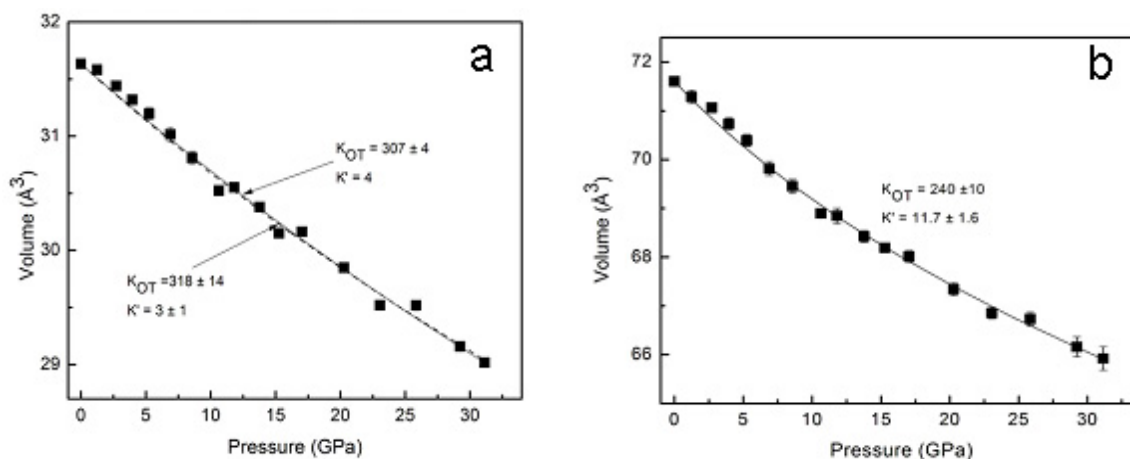


Figure 15. a) Volume reduction of tungsten at high pressures. b) Volume reduction of tungsten nitride at high pressures.

High-Pressure Behavior of Magnesium Germanate – The EOS of the perovskite and post-perovskite phases of MgGeO_3 were investigated by *in situ* x-ray diffraction experiments using the laser-heated diamond cell as well as by theoretical calculations^{47, 48}. The properties of the perovskite phase were compared to those of the MgGeO_3 post-perovskite phase near the observed phase transition pressure (~ 65 GPa). Across the transition, the density increased by 2.0(0.7)%. This is in excellent agreement with the theoretically determined density change of 1.9%; however both values are larger than those for the $(\text{Mg,Fe})\text{SiO}_3$ phase transition. The bulk sound velocity change across the transition is small and is likely to be negative (-0.5(1.6)% from experiment and -1.2% from theory). These results are similar to previous findings for the $(\text{Mg,Fe})\text{SiO}_3$ system. Magnesium germanate therefore appears to be a good analog system for studying the properties of the perovskite and post-perovskite phases in silicates.

Polymers – Dana Dattlebaum and colleagues at LANL, in collaboration with Muhetear Ahart and Russell Hemley at Carnegie are employing multiple approaches to the construction of EOS functions for polymer materials, including piston-cylinder measurements, Brillouin scattering, x-ray diffraction, vibrational spectroscopy, plate impact experiments, and positron annihilation lifetime spectroscopy. Following up on measurements carried out in Year 3, the acoustic properties and their pressure dependence have been determined for three polymer systems, Sylgard® 184, VCE, and Estane® 5703, using high-pressure Brillouin scattering. These results appear to be the first Brillouin scattering data on polymers to pressures exceeding 10 GPa. The elastic constant, mechanical property, and EOS analyses were performed for all three elastomers. Five commonly used isothermal EOS forms yielded a range of zero-pressure isothermal bulk moduli for Sylgard® 184, VCE, and Estane® 5703, with averages of 1.1, 2.0, and 3.2 GPa, respectively. The values of the bulk moduli reveal features of the polymer chemical and network structures influencing their compressibilities, namely, the flexible Si–O–Si backbone of the PDMS-based Sylgard® 184, and the organizing features, e.g., cross linking, and intermolecular interactions of crystallization and phase separation, in the C-, H-, and O- based polymers VCE and Estane® 5703⁴⁹.

In Year 3, the group also initiated new experiments on the high explosive material tri-amino-tri-nitrobenzene (TATB). Continuing on in this work, high pressure experiments, using diamond anvil cell and angle dispersive x-ray diffraction techniques (ADX), were carried out at HPCAT on polymers and high explosives. The goal of these high pressure experiments performed on polymers was to investigate whether the crystal structure of low-crystallinity polymers can be resolved at high pressures using ADXD techniques. The group was also interested in observing any indication of

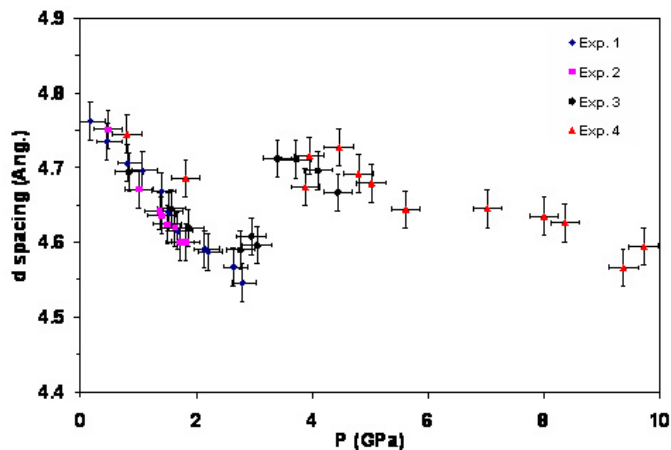


Figure 16. Change in *d* spacing for the most prominent THV peak with increasing pressure.

Sample	Start of Phase Transition (kbar)	Last Spectra Fit to Orthorhombic Phase (kbar)
PE2	14.95 – 45.25	14.95
PE3	47.81 – 54.14	47.81
PE4	38.29 – 41.47	41.47

Table 2. Observed transition pressure for three different polyethylene samples.

change in crystallinity and possible structural phase transitions, which could be correlated with other experiments performed on these samples, such as dynamic shock experiments, Raman spectroscopy, and Brillouin scattering measurements.

In the first set of experiments, two fluorinated co-polymers, poly(tetrafluoroethylene-co-vinylidene fluoride-co-hexafluoropropylene) (THV 500) and poly(chlorotrifluoroethylene-co-vinylidene fluoride) (Kel-F 800), were investigated. Due to their low crystallinity, only a few diffraction peaks were observed, but useful information was still extracted from the observed spectra. For example, by recording the shift in the most prominent diffraction peak of THV 500 with increasing pressure, it is possible to conclude that the sample crystallinity does not increase with pressure and also that there is some evidence of change in compressibility at ~ 4 GPa (Fig. 16). This is further supported by high pressure Raman spectroscopy measurements performed on this sample, which indicate that there is a measurable decrease in the shift of the measured Raman modes above 4 GPa⁵⁰.

In another study, the structural phase stability of three polyethylene samples with different crystallinity ratios was investigated. Initial analysis indicates that the structural phase stability is dependent on the initial crystallinity of the sample (Table 2); however additional experiments that will identify the transition pressures more accurately are in the planning stages.

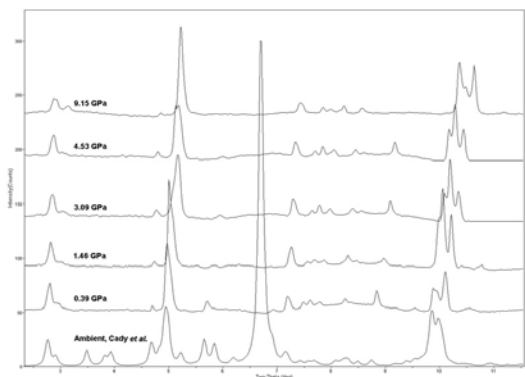


Figure 17. ADXD spectra collected for TATB with increasing pressure.

The HPCAT facility was also used to perform experiments on high explosive TATB. In this study the sample was investigated under hydrostatic conditions up to 13 GPa. Spectra collected during pressure increase are shown in Fig. 17. The collected spectra are currently being analyzed in order to extract P, V data and obtain the isothermal compression curve⁵¹.

EOS of Gelatin – At Carnegie, a team led by Muhetaer Ahart began a program in Year 3 to use Brillouin scattering techniques to obtain the EOS of gelatin. Figure 18a shows a typical Brillouin spectrum at 3.23 GPa at 25 °C. The Rayleigh scattering line (elastic scattering) at the zero frequency as well as the Brillouin scattering lines (inelastic scattering) at around 6 GHz for transverse acoustic mode and at around 14 GHz for longitudinal acoustic mode are observed (Fig. 18b).

In Year 4, the group determined the EOS for ballistic gelatin using Brillouin scattering spectroscopy with a diamond anvil cell by measuring the pressure dependence of the sound velocities

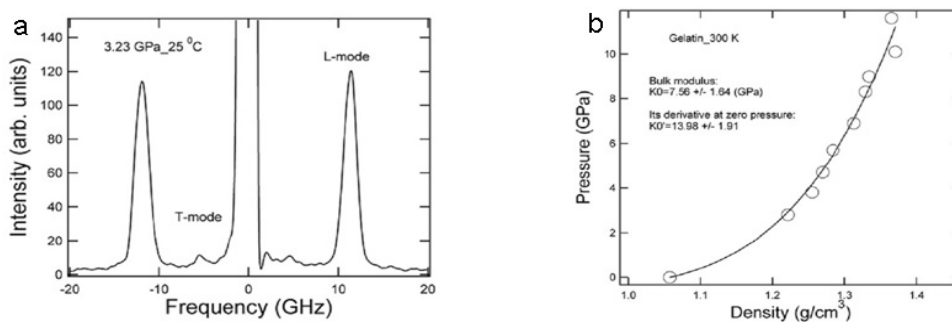
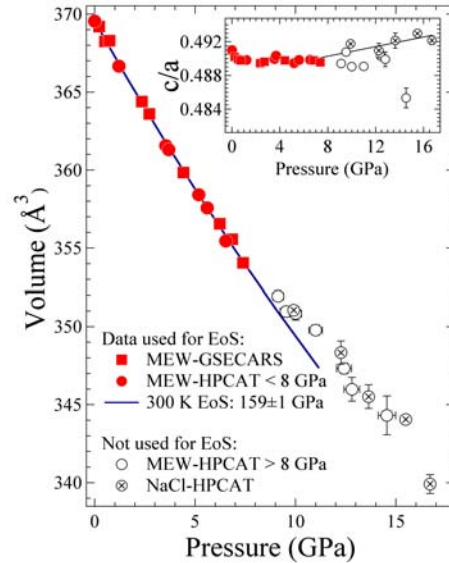


Figure 18. a) A representative Brillouin spectrum of gelatin at 3.23 GPa. The strong line at zero frequency is the Rayleigh scattering line, L- and T-modes represent the longitudinal and transverse acoustic modes, respectively. b) Pressure dependence of density of gelatin. The open circles represent the experimentally obtained density and the solid line represents the Vinet EOS fit ($K_0 = 7.6$ GPa and $K_0' = 13.98$).

from ambient pressure to 12 GPa at room temperature, and extended the previous measurements to a temperature range of 0 to 100 °C between ambient and 12 GPa. They analyzed the Brillouin data using a high temperature Vinet EOS (Fig. 18b) and obtained the bulk modulus, its pressure derivative, thermal expansion coefficient and the temperature derivative of the bulk modulus at ambient pressure. The Mie-Gruneisen method was also applied to the P, V, T data to obtain the

Figure 19. Pressure-volume data for Fe_3P . Only data below 8 GPa were used to determine the equation of state. $K_{0T} = 159(1)$ GPa, $dK/dT = 4.0$. A discontinuity in compressibility is observed above 8 GPa. Notably, two different data sets representing two pressure media used in the experiments (methanol-ethanol-water and NaCl) reflect this phenomenon. Inset: variation in the ratio of unit cell parameters as a function of pressure. The c/a ratio remains essentially constant up to 8 GPa, but a positive slope is observed above this pressure.



Gruneisen parameter, Debye temperature and thermal pressures for the gelatin⁵².

High P - T Structural Changes in Fe_3P —Laser heating of samples in the diamond anvil cell continues to be a crucial tool in the exploration of crystal structures at high temperatures and pressures. CDAC collaborator **Henry Scott of Indiana University – South Bend**, his student **Sabrina Huggins**, and scientists from **Northern Illinois University, SUNY**,

HPCAT, MIT, and UC-Santa Cruz have collected *in situ* x-ray diffraction patterns of end-member Fe_3P -schreibersite in a diamond anvil cell to pressures of 30 GPa at 300 K. Some samples of Fe_3P were also laser heated at high pressure to temperatures of ~ 2000 K and examined following thermal quench. Below 8 GPa, the variation in the schreibersite unit cell volume delineates a smooth P - V curve corresponding to a second order Birch-Murnaghan EOS with bulk modulus, K_{0T} , of 159(1) GPa (see Fig. 19). Above 8 GPa, however, the schreibersite structure shows substantial stiffening, and an unidentified structure develops between 17 and 30 GPa; upon decompression to ambient pressure the schreibersite structure returns. Therefore, although ubiquitous in iron rich meteorites, it is unlikely that schreibersite is the stable phosphorus-bearing phase in deep planetary cores⁵³.

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

Equations of state at high pressure can often be understood from the characteristics of the phonons in the material. Long-wavelength phonons are measures of the elastic constants, and phonons of higher frequency provide much of the heat capacity. The phonon density-of-states (DOS) can provide the phonon partition function, which gives key thermodynamic information.

The scattering of neutrons by nuclei gives immediate information on the energies and wavevectors of nuclear vibrations. Neutron scattering, especially inelastic neutron scattering, is well established, but it is weak, and requires large samples that are not easily subjected to high pressures. Synchrotron x-ray beams can be made quite small, however, and are much more compatible with diamond anvil cell methods. **HPCAT** and **LANL** have provided capabilities to advance the state of the art in phonon experiments. Brillouin spectroscopy also serves as an additional important tool for elucidating fundamental elastic properties of materials.

Pressure-Induced Invar Transitions in Ni-Fe, Pd-Fe and Pt-Fe Alloys – **Brent Fultz's** group at **Caltech**, led by CDAC graduate student **Mike Winterrose**, has recently found a pressure-driven Invar effect⁵⁴ in ordered and disordered samples of Pt_3Fe , Pd_3Fe (and Ni_3Fe , but this was known previously⁵⁴). The bulk modulus undergoes a significant change with pressure, as shown in Fig. 20a. Nuclear forward scattering measurements on ordered Pd_3Fe and disordered Pt_3Fe ,

completed in Year 4 at HPCAT, showed a total collapse of the hyperfine magnetic fields at 18.1 and 15.0 GPa, respectively (Fig. 20b).

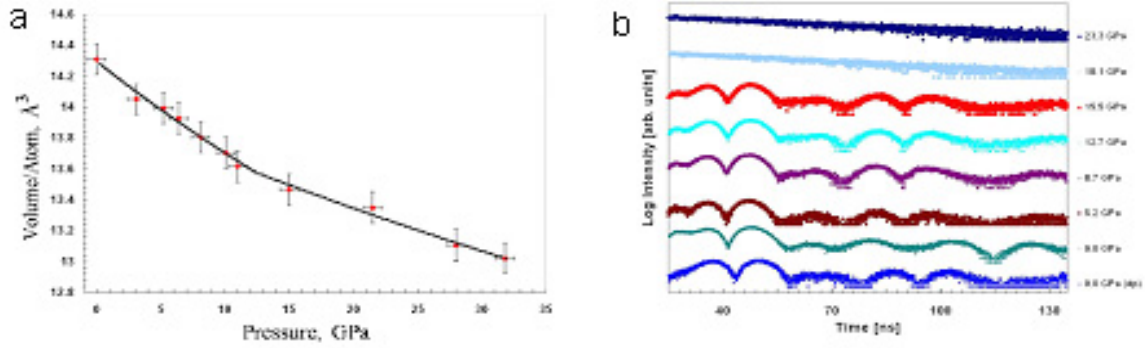


Figure 20. a) Volume versus pressure for ordered Pd_3Fe , showing two regions of behavior, with an approximate transition at 12 GPa to a state with a larger bulk modulus. The two regions were fit to a third-order Birch-Murnaghan equation of state. b) Nuclear forward scattering from Pd_3Fe , showing quantum beats from the hyperfine magnetic field at pressures of 15.5 GPa and below, and a paramagnetic behavior at higher pressures.

Curves showing the phonon partial DOS of ^{57}Fe in ordered Pd_3Fe , obtained from high-pressure nuclear resonant inelastic x-ray scattering measurements, are presented in Fig. 21. These ^{57}Fe partial DOS curves show a significant stiffening and change of shape at 18 GPa. Density functional theory calculations are underway to identify the relation between the changes in the phonon partial DOS under pressure and the collapse of magnetic order above 15 GPa.

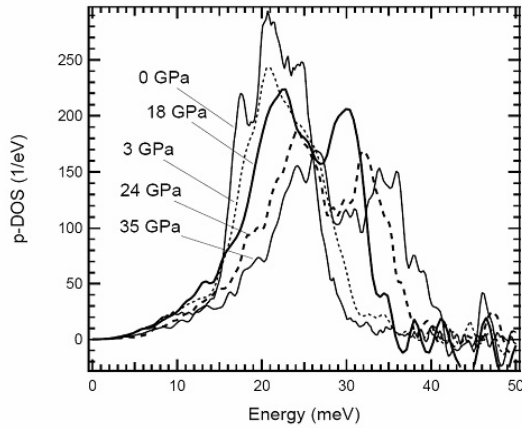


Figure 21. ^{57}Fe partial density of states curves from ordered Pd_3Fe .

At present, it appears that the large change in phonons shown in Fig. 21 at energies of 30 meV is caused by changes in the longitudinal force constant between first-neighbor Fe and Pd atoms. A manuscript describing this work is in preparation. In the next year, the group plans to perform similar measurements under pressure on Ni-Fe and Pt-Fe systems to better understand the pressure-induced Invar anomalies in these systems. Confirming a pressure-induced Invar effect will benefit from high-pressure x-ray diffraction measurements using isobaric heating to identify anomalies in the thermal expansion of these materials under pressure. These measurements will be performed between 300K and 600K and between 10 GPa and 30 GPa.

Effects of Defects on the Pressure Dependent Lattice Dynamics in FeAl – The Caltech group is also continuing their work on FeAl. Initial results, reported last year, were obtained from high pressure measurements on samples of FeAl that were quenched from high temperatures to preserve a vacancy concentration as high as 3%. Compared to the control sample, the sample with excess vacancies was known to have a broadening and stiffening of the phonon partial DOS of ^{57}Fe , which is consistent with prior inelastic neutron scattering experiments. The effect of vacancies becomes significantly larger at higher pressures (Fig. 22). The trend is clearly a systematic one, as are the stiffenings of the phonons in each material with increasing pressure. The vacancies in FeAl alter characteristic interatomic forces, changing the anharmonicity, expressed as a larger Grüneisen parameter. Further interpretations of the results are underway using a lattice dynamics inversion method, where the interatomic forces are tuned to match the measured scattering or phonon partial

DOS curves. The goal is to identify which force constants undergo the largest stiffening in the presence of vacancies.

In further work on FeAl, the **Caltech** group has recently completed experimental measurements on B2 FeAl with varying defect concentrations at high pressure using ^{57}Fe inelastic nuclear resonant scattering. The results from a first set of runs were so surprising that two other sets were performed, and show that the results shown in Fig. 22 are reliable. Two samples were prepared. One, annealed at 1273 K and quenched, has a vacancy concentration of approximately 3%. The other, annealed at 773 K and quenched, has a vacancy concentration of less than 1%. At ambient pressure, the ^{57}Fe phonon partial DOS curves of both materials are essentially the same, although there is some broadening of the features in the sample with more vacancies. Under pressure, the ^{57}Fe phonon partial DOS curves diverge. The 1273 K sample, rich in vacancies, shows the stronger stiffening of the DOS under pressure. It also has a higher bulk modulus, as confirmed by x-ray diffraction under pressure (Fig. 23). What is surprising is the size of these pressure-induced effects. Computational work using DFT codes for large unit cells with antisite defects do not show such a pressure-dependence of the phonon DOS. Although the origin of the effect shown in Fig. 22 is not well understood, the experimental result is believed to be correct.

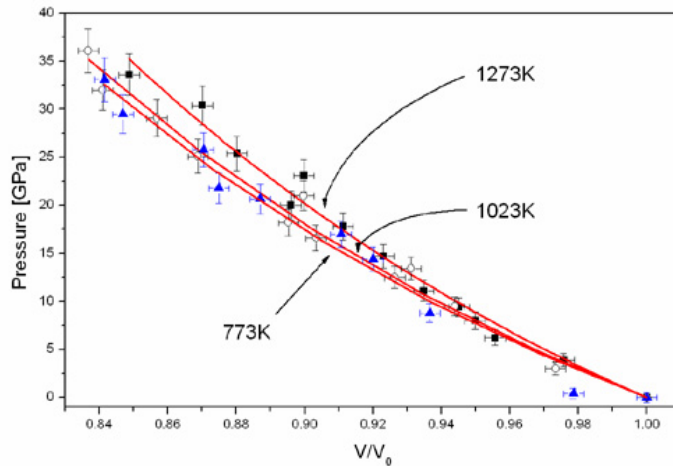


Figure 23. Pressure versus volume for B2 FeAl with different vacancy concentrations ranging from <1% (annealed at 773 K) to 3% (annealed at 1273 K).

product of an atomic correlation function for a localized atom cluster, and an interaction parameter to weight the importance of the cluster. An open question is how successful will be this cluster expansion method will be in accounting for the phonon entropy.

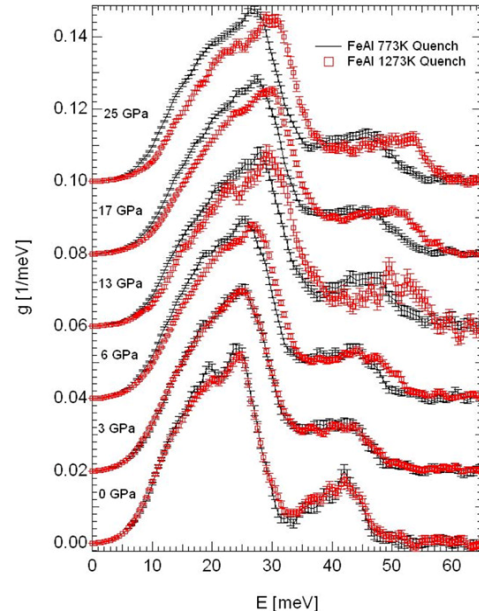


Figure 22. ^{57}Fe phonon partial DOS curves obtained by NRIXS. Two samples were used, one quenched from 1273 K containing an estimated 3% vacancies (red), and the other quenched from 773 K, containing less than 0.5% vacancies (black). Measurements were performed at a series of pressures matched to within approximately 0.3 GPa.

Cluster Expansions of Phonon

DOS in Fe-X – With alloying, it is expected that changes in the phonons will originate from the local arrangements of the different chemical species of atoms. To date, alloy free energies, phase diagrams and EOS have been successfully interpreted in terms of the thermodynamics of local atom configurations. Cluster expansion hierarchy can be performed systematically, and it is often found that most of the configurational thermodynamics depends on the statistical numbers of pairs of atoms of the different chemical species in an alloy. A cluster expansion is a systematic method for expressing a ground state function of an alloy as a sum of terms, each being the

^{57}Fe nuclear resonant inelastic x-ray scattering (NRIXS) spectra were measured by the **Caltech** group from disordered bcc alloys of Fe-Cr, and ^{57}Fe phonon partial DOS (pDOS) curves were obtained from them⁵⁵. These results were interpreted with a modification of the cluster expansion method, where interaction functions (instead of interaction parameters) were associated with the different local clusters. These "interaction pDOSs" were then used with surprising success to reconstruct the ^{57}Fe pDOSs of thin film multilayers reported by Ruckert, *et al.*⁵⁶.

These are particularly useful cluster expansion approaches for alloys under pressure. Cluster functions show the greatest differences if there is a large atomic size mismatch between atoms, coupled with a large difference in bond stiffness. This project has been started with a study on Fe-Os alloys under pressure. Osmium atoms are much larger than iron atoms, and Os-Os bonds are much stiffer than Fe-Fe bonds. It has been recently confirmed by high-pressure diffraction measurements at the NSLS that all Fe-Os alloys adopt an hcp structure under pressure. Unfortunately, Os absorbs 14.4 keV gamma rays enough to make the experiment very slow, although possible. Fortunately, Fe-Ru has a very similar phase diagram and is much less absorbing. During the next run cycle at the APS, inelastic nuclear resonant scattering measurements of the ^{57}Fe pDOS in Fe-Ru alloys at high pressure will be performed at HPCAT.

An example of the type of information that is possible from such work is presented in Fig. 24, which shows interaction phonon DOS curves from recent work on Fe-Cr. The goal of this experiment was to identify compositional trends in the phonons. The cluster functions in Fig. 24 have physical interpretations. The function $g_0(E)$ is for a disordered equiatomic alloy. (It is quite similar to the actual ^{57}Fe phonon partial DOS data that was measured on an alloy of nearly equiatomic composition.) The function $g_1(E)$ shows how $g_0(E)$ is modified by first-nearest-neighbor (1NN) Cr atoms. Extra Cr atoms tend to add intensity at high phonon frequencies, and subtract from the spectrum at lower frequencies. The triangle term, $g_2(E)$ in black, shows the effect of having like and unlike pairs of atoms within the 1NN and 2NN shells of the ^{57}Fe atom. These results will become part of the Ph.D. thesis of **Matt Lucas**.

Elastic Tensor of Stishovite – The full set of elastic constants of stishovite, an octahedrally coordinated form of SiO_2 , has been measured at high pressures for the first time⁵⁷ by **Tom Duffy's** group at **Princeton**. Brillouin scattering measurements (Fig. 25) to 12 GPa show that the shear modulus, C_{11} – C_{12} , exhibits softening behavior beginning from ambient pressure and it has decreased by 11% at 12 GPa. The acoustic softening is directly observed in the shear branch for one of the measured planes.

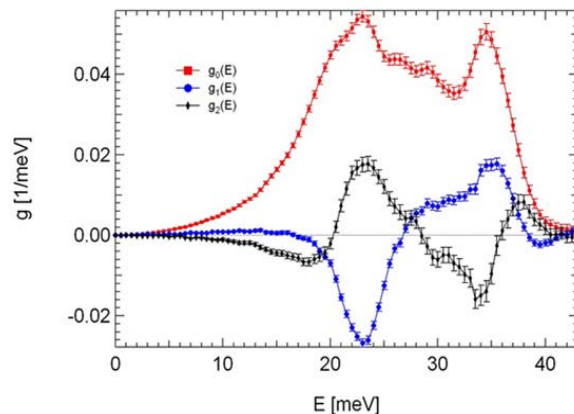


Figure 24. Interaction pDOS curves for ^{57}Fe in Fe-Cr. The red curve is the function $g_0(E)$. The blue function is $g_1(E)$, and the black function is the triangle term, $g_2(E)$. These functions have physical interpretations as explained in the text.

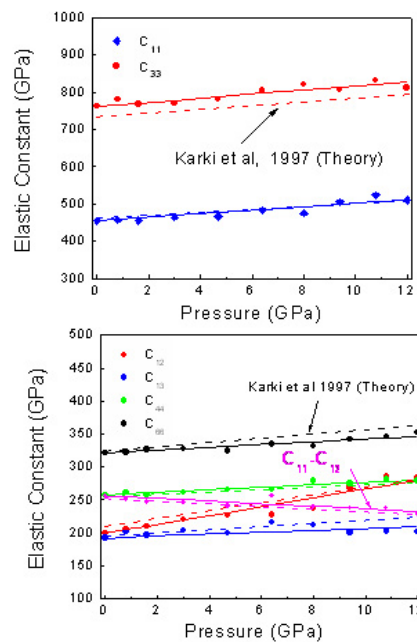


Figure 25. Elastic moduli of stishovite as a function of pressure to 12 GPa compared with theoretical calculations. The softening of C_{11} – C_{12} can be seen in the lower panel.

Experimental measurements show that previous theoretical calculations are in error by up to 10% for the individual elastic constants. The results will provide new constraints on models of the soft-mode driven transformation from stishovite to the CaCl_2 -type structure in SiO_2 .

Elasticity of Hydrous Silicates – The presence of hydrogen can profoundly affect many physical and chemical properties of oxides and silicates. The nominally anhydrous spinelloid mineral wadsleyite, $\beta\text{-Mg}_2\text{SiO}_4$, can accommodate up to several wt. % H_2O as defects. Wadsleyite is the major constituent of the Earth's transition zone, and hence this region could be an important component of the planet's H_2O budget. The first measurements of the single-crystal elastic constants of a suite of hydrous wadsleyites with water contents up to 1.7 wt. % has been made recently⁵⁸ by the **Princeton** group. The aggregate bulk and shear moduli decrease by 7% for each 1 wt. % H_2O . The results have implications for interpreting seismic velocities at 410-520 km depth and for interpreting the magnitude of the 410-km discontinuity. The first measurements of elastic constants of hydrous forsterite (0.9 wt. % H_2O)⁵⁹ have also been carried out.

Hydrous minerals in subduction zones are potential agents for transporting water to the deep Earth. Properties of these minerals, especially elastic moduli, are needed to model seismic wave speeds in subduction zones and hence place constraints on the cycling of H_2O through subduction zones. Zoisite is a metamorphic mineral of the epidote group containing 2 wt % water. It is likely to be one of the important phases in subduction zone environments. In this study, the single-crystal elastic constants of zoisite

$\text{Ca}_2\text{Al}_3\text{Si}_3\text{O}_{12}(\text{OH})$ were determined by CDAC graduate student **Zhu Mao (Princeton)** using Brillouin scattering at ambient conditions. Brillouin spectra were recorded in 37 directions for three separate crystal planes. The density of the sample and the orientation of each plane were determined by single-crystal diffraction using energy dispersive techniques at X17C of the NSLS. The complete elastic tensor was then obtained by an inversion of the acoustic velocity and orientation data⁶⁰. The aggregate bulk modulus, shear modulus, and Poisson's ratio are $K_{\text{VRH}} = 125.3(4)$ GPa, $G_0 = 72.9(2)$ GPa, and $\sigma_0 = 0.26(1)$ for the VRH (Voigt-Reuss-Hill) average,

respectively (Fig. 26). The maximum azimuthal anisotropy of zoisite is 22% for compressional velocity and 33% for shear velocity, and the maximum shear splitting is 21% along the [001] direction. The Voigt-Reuss-Hill averages of the aggregate bulk modulus, shear modulus and Poisson's ratio were determined. These results resolve discrepancies in previous static compression studies and provide the first determination of the shear modulus of zoisite.

Elastic Properties of Relaxor Ferroelectrics – **Muhetaer Ahart** and coworkers at **Carnegie** have obtained a full set of elastic and piezoelectric constants has been obtained for single-domain $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ (PMN) single crystals. An MD simulation has been carried out to calculate the elastic constants of PMN; experimental results are consistent with theoretical modeling⁶¹. The elastic constant measurements have been extended up to 10 GPa for a PMN single crystal. The results indicate that PMN may undergo a phase transition from a simple cubic to a antiferro-

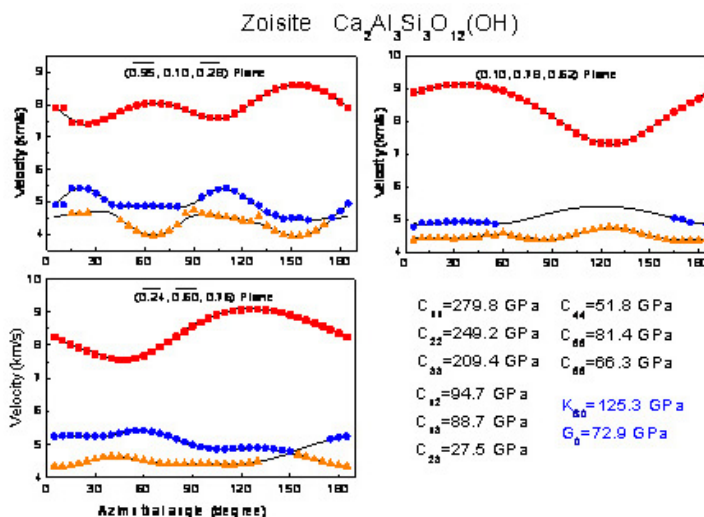


Figure 26. Measured compressional and shear wave speeds of the epidote-group mineral zoisite as a function of azimuthal angle for three separate crystals. Symbols show experimental velocities; solid lines are best-fit results. Elastic moduli derived from the least-squares fitting are listed at the right, together with aggregate bulk (K_{VRH}) and shear (G_0) moduli.

distortive structure⁶². X-ray diffraction techniques have been employed to investigate relaxor properties and pressure-induced phase transitions in PMN-32%PT. In addition, a microscopic imaging technique allowed an investigation of the domain structures as a function of pressure. The results indicate that PMN-32%PT undergoes a structural phase transition above 4 GPa. A manuscript describing these results is in preparation.

High energy single crystal x-ray diffraction experiments have been applied to investigate the pressure-induced phase transition in $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$ (PSN) single crystals. It is found that PSN undergoes a first order, rhombohedral-to-cubic phase transition at 2 GPa (300 K), and is consistent with earlier observations from dielectric spectroscopy. PSN undergoes quite different compression mechanisms above and below phase transition point. The temperature dependence of diffuse scattering around the (100) Bragg peak (Fig. 27)⁶² has also been obtained.

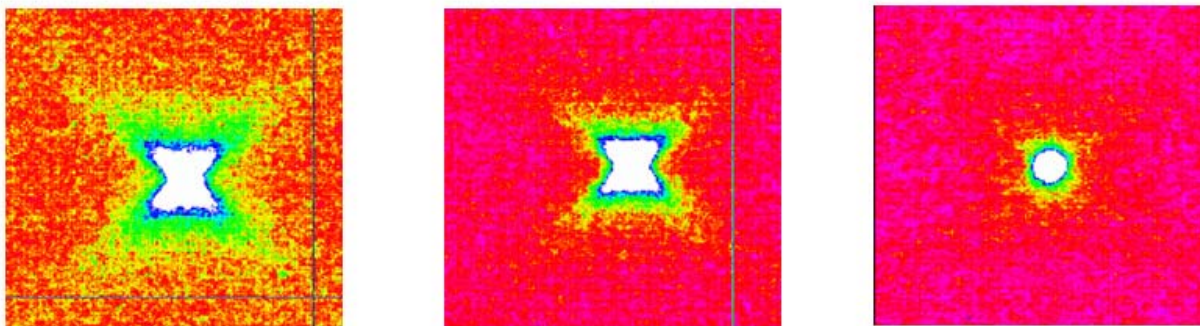


Figure 27. The diffuse scattering pattern around the (100) Bragg peak from a PSN single crystal at selected temperatures. In order to emphasize the diffuse scattering, the sample was oscillated from -6 to 6 degrees with respect to the incident beam in a horizontal plane. It is obvious that the diffuse scattering disappears with temperature.

2.4 Plasticity, Yield Strength, and Deformation

High plastic strain ($\epsilon_p > 100\%$), and high strain rates (up to 10^5) provide challenges to understanding material behavior at conditions relevant for stewardship science applications. Pressure- and temperature-induced phase transformations of materials produce systematic changes in texture patterns, which can allow a determination of transition mechanisms. During Year 4, work in various CDAC groups focused on the influence of non-hydrostatic stress on crystals and polycrystals, particularly at high and ultrahigh pressure. Anisotropy in polycrystals is also largely determined by preferred orientation (texture) considerations.

Static Strength of Materials to Megabar Pressures – Strength properties of materials under static and dynamic loading are essential quantities for characterizing mechanical behavior. Quantitative measurements of static strengths achieved in the diamond anvil cell can be made using x-ray diffraction in a radial geometry for samples under non-hydrostatic compression (Fig. 28a). This work provides a synthesis and summary of results for a range of materials including metals and strong ceramics⁶³. Results for several metals up to 68 GPa show that the ratio of yield strength to shear modulus ranges from 0.01-0.03 and increases weakly with compression. Trends at lower pressure for Re, W, and hcp-Fe are consistent with available data above 1 Mbar (Fig. 28b). Strong ceramics such as B_6O , c- Si_3N_4 , and TiB_2 achieve yield strengths as large at 10% of the shear modulus at pressures up to ~ 70 GPa. Strengths of materials used as pressure media can now be quantitatively compared and evaluated.

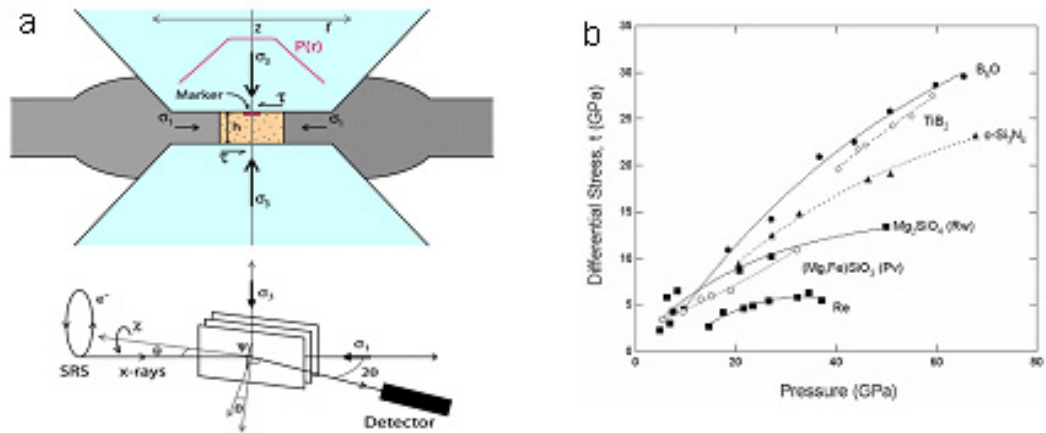


Figure 28. a) Schematic illustration of stress distribution and diffraction geometry in a radial x-ray experiment in the diamond anvil cell. b) Differential stresses in selected strong ceramics including oxides, borides, nitrides, and silicates. Differential stress values for Re metal are shown for comparison. Rw—ringwoodite; Pv—perovskite; c-Si₃N₄—cubic (spinel-type) silicon nitride.

High P-T Deformation of the CaIrO₃ Post-Perovskite Phase – At near ambient conditions, CaIrO₃ is isostructural with the high-pressure polymorph of MgSiO₃, “post-perovskite” (pPv). MgSiO₃ pPv is now thought to be a major phase in the earth’s lowermost mantle. CaIrO₃ can thus serve as a convenient analog for studying the deformation behavior of the pPv phase under conditions achievable with a multi-anvil deformation apparatus. The **Duffy** group has studied the rheologic behavior of CaIrO₃ pPv at a variety of pressure and temperature conditions from 2 GPa to 6 GPa and 300 K to 1300 K⁶⁴. Sintered, polycrystalline CaIrO₃ pPv was deformed in the D-DIA multi-anvil press in several shortening cycles up to 20% axial strain at each temperature and pressure. Shortening cycles were followed by lengthening back to 0% strain. Quantitative texture information was obtained using *in-situ* synchrotron x-ray diffraction and the Rietveld method to analyze images. In all cases the group found that (010) lattice planes align perpendicular to the compression direction upon shortening, and that there is little change in texture with temperature or pressure. This texture pattern (Fig. 29) is consistent with slip on (010)[100]. The texture observed here is different from that produced in room-temperature diamond anvil cell (DAC) measurements on MgGeO₃ and MgSiO₃ pPv, which both display textures of (100) and (110) lattice planes at high angles to the compression direction. This implies that CaIrO₃ post-perovskite may not be a good analog for the plastic behavior of MgSiO₃ pPv, or that post-perovskite textures in the DAC may be influenced by phase transformation or recrystallization.

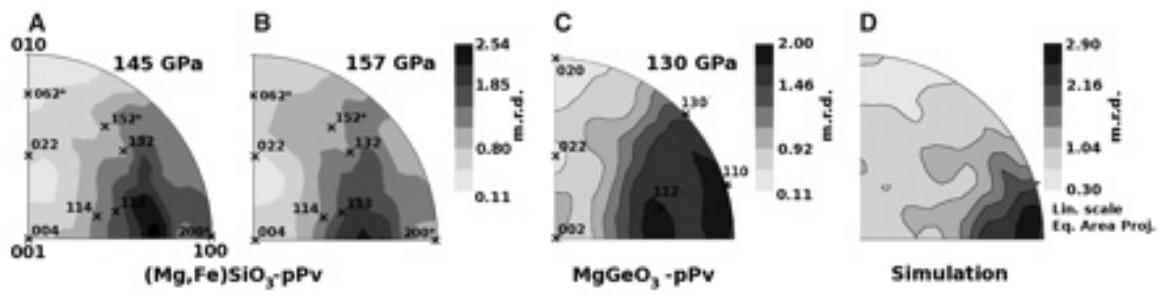


Figure 29. Comparison of experimentally determined inverse pole figures in $(\text{Mg,Fe})\text{SiO}_3$ and MgGeO_3 at high pressures with polycrystalline plasticity simulations assuming slip on (110) and (100).

Deformation of (Mg,Fe)SiO₃ Post-Perovskite – Polycrystalline (Mg_{0.9},Fe_{0.1})SiO₃ post-perovskite was plastically deformed in the diamond anvil cell between 145 and 157 GPa⁶⁵. The lattice-preferred orientations obtained in the sample suggest that slip on planes near (100) and (110) dominate plastic deformation under these conditions. Assuming similar behavior at lower mantle conditions, plastic strains and the contribution of post-perovskite to anisotropy in the D'' region at the Earth's core-mantle boundary was simulated using numerical convection and viscoplastic polycrystal plasticity models. The **Princeton** group found a significant depth dependence of the anisotropy that only develops near and beyond the turning point of a downwelling slab. Their calculated anisotropies are strongly dependent on the choice of elastic moduli and remain hard to reconcile with seismic observations.

Plastic Behavior of Post-Perovskite in the Earth's Deep Interior – Understanding texturing in minerals is important because it is a key parameter when modeling the development of seismic anisotropy with convection. As minerals deform plastically, they become anisotropic. This anisotropy strongly depends on the activated deformation mechanisms and can be observed with seismology—seismic waves passing through the material become distorted in a characteristic way. At the moment, there are numerous observations of anisotropy at the core-mantle boundary, the D'' layer. However, questions remain on whether this anisotropy is due to the orientation of silicate post-perovskite, partly due the lack of understanding on the plastic behavior of this phase at high pressure.

Sebastien Merkel (a Miller postdoctoral fellow at **Berkeley** in the group of CDAC partner **Hans-Rudolf Wenk**, and now at **CNRS** and the **University of Science and Technology of Lille, France**) and colleagues from **Berkeley**, **Princeton**, and **Carnegie** in Year 3 reported direct measurements of the plastic behavior of post-perovskite deep in the Earth's interior. From these measurements, it was discovered that (100) and (110) slip dominate the plastic deformation of post-perovskite. The CMB is a critical region for the Earth's dynamics and seismologists have long documented anisotropy at these depths. Seismic anisotropy is the expression of deformation dynamics and with the measurement capabilities developed as a result of this research, it can now be interpreted. Moreover, the application of this experimental technique is not limited to geophysics but can now be extended to improve understanding of the plastic behavior of a whole array of materials under extreme conditions of pressure, stress, and temperature⁶⁶.

In a continuation of this work, former Carnegie predoctoral fellow **Merkel** continued his collaboration with a group that included CDAC partners **Duffy (Princeton)**, CDAC student **Lowell Miyagi (Berkeley)** and scientists from **Arizona State University**, the **University of Chicago**,

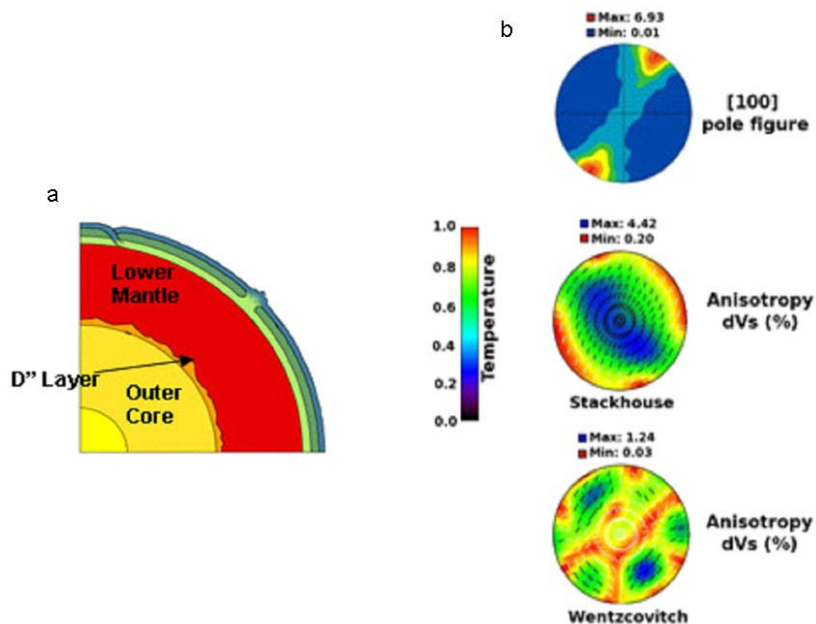


Figure 30. a) General model of the Earth's interior showing the location of the D'' layer at the base of the lower mantle. b) Top, a model of orientation and anisotropy in a polycrystal plastically deformed in D'', based on the x-ray measurements; middle and bottom, orientation and anisotropy of a polycrystal at step 5000 of a convection model calculated using the elastic moduli of Stackhouse et al.⁶⁶ and Wentcovitch et al.⁶⁷.

and HPCAT. The group conducted the first laboratory study of the deformation properties of high-pressure silicate post-perovskite⁶⁵.

In these experiments, the group studied how a polycrystal of post-perovskite can orient when plastically deformed under the pressures of the core-mantle boundary. Diffraction experiments showed that the orientation that was obtained is compatible with the activation of slip along the (100)-(110) planes. Using this result (Fig. 30), a convection model, and polycrystal plasticity, a simulation of the anisotropy induced by post-perovskite plastically deformed in D" gave poor agreement with seismic observations. These results are compatible with previous results obtained on an MgGeO₃ analogue last year⁶⁵. However, questions remain as to why this model does not reproduce seismic observations in D". Is this mechanism really active at the core-mantle boundary? Is post-perovskite really the source of the observed seismic anisotropy? Continued work is still necessary to unravel this fundamental problem.

2.5 Electronic and Magnetic Structure and Dynamics

The relationship between crystal structure and electronic and magnetic behavior is at the heart of material behavior at high pressures and temperatures, and an understanding of these complex interactions is necessary addressing many problems in stewardship science. CDAC continues to support both experimental and theoretical work in this area.

Effects of Pressure on Nuclear Electron Capture Processes – CDAC academic partner

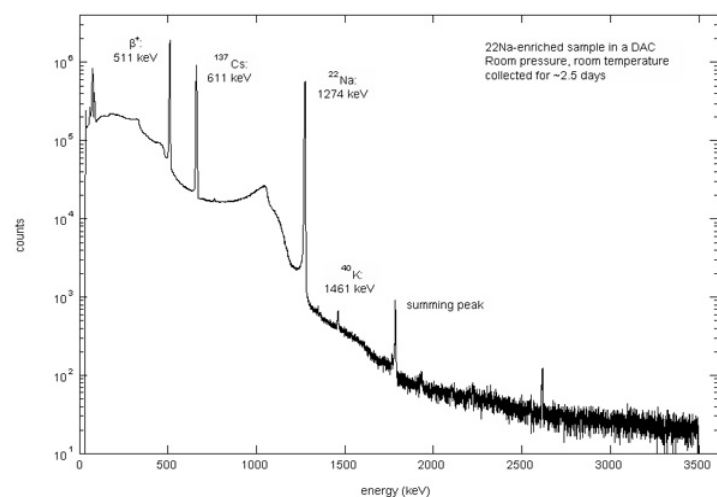


Figure 31. Gamma-ray measurements of a ²²Na-enriched sample within a DAC without pressure applied. Spectra are taken for ~2.5 days and will be used to benchmark high-pressure measurements. Major peaks are labeled and show significant positron (β^+) emission, both from the ²²Na sample as well from the background; calibrant ¹³⁷Cs; ²²Na sample peak; background ⁴⁰K peak and a summing peak from simultaneous β^+ and electron-capture decays (511 + 1275 keV).

Kanani Lee has begun experiments on how pressure affects the decay constant of electron capture isotope ²²Na at the LANSCE facility at LANL. A sample of ²²Na-enriched NaCl (activity ~ 10 μ Curie) is under pressure in a compact-cylinder diamond-anvil cell (DAC) within a Re gasket pre-compressed to a thickness of 10-15 μ m and a hole drilled with a diameter of ~120 μ m. Pressure has been determined by ruby fluorescence. Additionally, ¹³⁷CsCl (activity ~10 μ Curie) has been added into the DAC and used as an internal γ -ray standard as it does not decay by electron capture and so its decay constant should remain constant. To measure each ²²Na electron-capture decay and ¹³⁷Cs decay, two γ -ray detectors are arranged around the DAC to measure the characteristic γ -rays that are emitted with each decay: 1275 and 661 keV for ²²Na and ¹³⁷Cs respectively (Fig. 31). The decay rate at various pressures will be compared with the

decay rate measured without applied pressure. The experimental values will be compared with theoretical predictions calculated in a related project.

CaCu₃Ti₄O₁₂ at High Pressure – The mechanism of the unusual dielectric behavior of CaCu₃Ti₄O₁₂ (CCTO) has attracted much attention since the discovery of its dielectric constant of 10⁵ in a wide range of frequencies from DC to 10⁶ Hz, together with its outstanding high temperature performance between 100~600 K^{69, 70}. A large dielectric constant is usually the result of atomic displacements in a non-centrosymmetric structure. CCTO, however, adopts a cubic structure that necessarily has an inversion center. Investigations of crystal structure and spectroscopy under

ambient conditions find no structural or vibrational anomalies^{69, 71-73}. In addition, measurements reveal a much lower permittivity in a thin-film single crystal than in a polycrystal⁷⁴. These results have ruled out the possibility of attributing the unusual dielectric properties to perfectly crystalline CCTO. Thus far several mechanisms have been proposed: the creation of barrier layer capacitances, presumably at twin boundaries⁷⁰; the Maxwell-Wagner-type contribution at the interface between sample and contact, or at grain boundaries^{75, 76}; and the spatial heterogeneity of local dielectric responses. Very recently, current-voltage measurements revealed a large potential barrier at the grain boundary⁷⁷. A high-pressure measurement also found the unusual compressibility of CCTO powder, and the existence of an energy barrier from the exterior (surface or grain boundary) of the crystalline CCTO⁷⁸.

Synchrotron x-ray diffraction measurements of CdCu₃Ti₄O₁₂ (CDCTO) were performed to 55.5 GPa. There is no structural phase transformation in this pressure range. The irregular

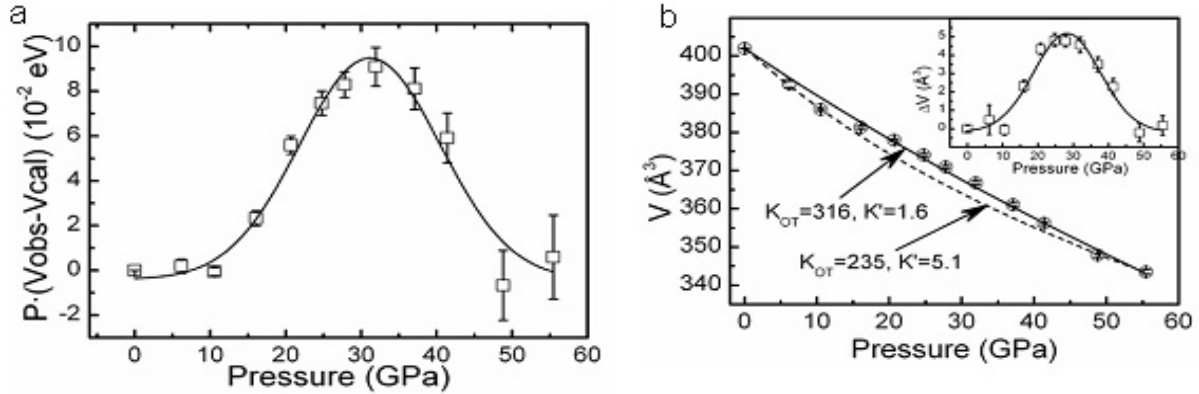


Figure 32. a) dielectric response of CDCTO as a function of pressure. b) The unit cell volume at high pressures. The solid line is the fitting curve of all the experimental data to a third-order Birch-Murnaghan equation of state. The dotted line is the fitting curve of the selected data points under hydrostatic pressure and after the second curvature drift. The error bars mark the error induced from the structure refinements. Inset: The difference in volume reduction under pressures between experimental measurements and the expected regular compression of the interior of the grain.

curvature shifts of the P - V curve (Fig. 32a) are attributed to the grain surface effect. Analysis indicates that the grain surface of CDCTO is stiffer than the grain interior at higher pressures. The atoms on the grain surfaces must be either densely packed or have strong correlations with the grain interior in order to have as high a high dielectric constant as observed in CaCu₃Ti₄O₁₂. The derived bulk modulus K_{OT} of CDCTO is approximately 235 ± 7 GPa with $K' = 5.1 \pm 0.4$ (Fig. 32b).

Antiferromagnetism in Chromium Metal – A new class of measurements on the high-pressure behavior of spin and charge density waves in single crystal metals has been carried out using high-resolution x-ray microdiffraction techniques at HPCAT. **Yejun Feng** from the **University of Chicago** and collaborators from **Argonne National Laboratory** and **University College, London** have shown that it is possible to drive the antiferromagnetic ordering temperature T_N in elemental Cr to zero with pressure. At the same time, the group has shown that both pressure and chemical doping have similar effects on the magnetic order at small dopant concentrations. At ambient pressure and a critical dopant concentration, the ordering temperature falls rapidly to zero. Combining the effects of doping and pressure should therefore allow a "tuning" of the ordering temperature.

These experiments are extremely challenging due to the very small signal levels (typically an order of magnitude smaller than Bragg diffraction peaks) and are the first of their kind to be performed.

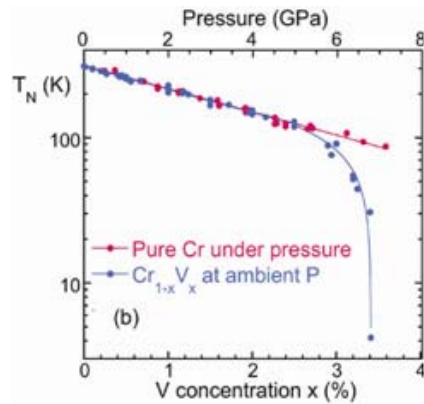


Figure 33. *P-T and x-T phase diagram for Cr and Cr_{1-x}V_x. The lower temperature ground state is an itinerant antiferromagnet spin-density wave, while the phase above the boundary is paramagnetic. The mapping between both doping and pressure is carried out by collapsing the exponential curve below $x = 2.5\%$ onto the pressure phase boundary.*

An entirely new technique was developed that allows analysis of the measurements of spin-density wave (SDW) and charge-density wave (CDW) diffraction peaks as a function of pressure at liquid He temperatures. The HPCAT facility as a whole was designed and built to allow a variety of such demanding experiments. Using a two-band model of a nested SDW gives the ordered moment as a function of pressure. Assuming BCS-type superconductivity, the linear relationship between the energy gap and T_N gives the ordering temperature as a function of pressure, as shown in Fig. 33. Doping pure chromium with vanadium also has the effect of reducing T_N in a manner analogous to pressure below about 2.5 atomic percent vanadium. As disorder sets in, however, the system is moved away from typical BCS-type behavior and the ordering temperature decreases to zero at a level of 3.4 at.% vanadium in the alloy. These experiments now open up the possibility of investigating SDW and CDW phenomena in a host of other materials, such as high T_c superconductors and dilute alloys both as a function of temperature and pressure⁷⁹.

Pressure Induced Spin Transitions in Simple Oxides

The investigation of mineral properties at the pressure and temperature conditions of the deep mantle represents a key step in understanding the structure and evolution of the Earth's deep interior. With recent

developments in diamond anvil cell techniques, particularly the application on of laser heating at near-megabar pressures, a more accurate picture of the behavior of important mineral phases at relevant conditions is now possible.

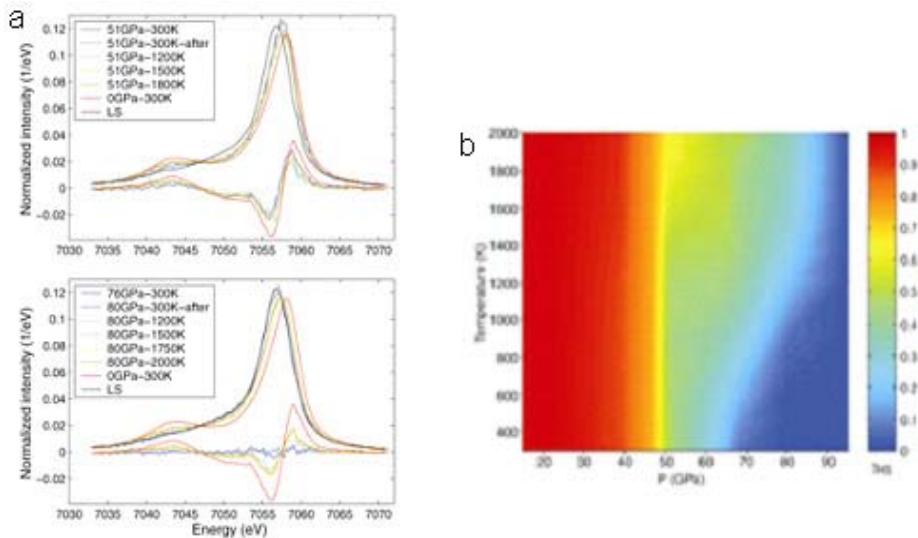


Figure 34. *a) X-ray emission spectra for (Mg,Fe)O at high pressure and temperature. Top, 51 GPa and high temperature. Bottom, 80 GPa and high temperature. Differences in the line shape are used to derive the ratio of high-spin to low-spin Fe²⁺ in the sample. b) Phase diagram illustrating the fraction of Fe²⁺ in the high-spin state as a function of P and T. Colors in the panel at the right indicate the fraction of high-spin Fe²⁺: red, all high-spin; blue, all low-spin.*

Former CDAC Research Scientist **Jung-Fu Lin**, now a Lawrence Fellow at LLNL, has recently shown that divalent iron in the ferroperricite structure (Fe,Mg)O gradually undergoes a transition from a high-spin state to a low-spin state from approximately 1000 km depth and 1900 K in temperature to 2200 km and 2300 K. Lin and co-workers from **Carnegie**, LLNL and the **ESRF**, working at the **GSECARS** sector at the APS, used x-ray emission spectroscopy to monitor the spin

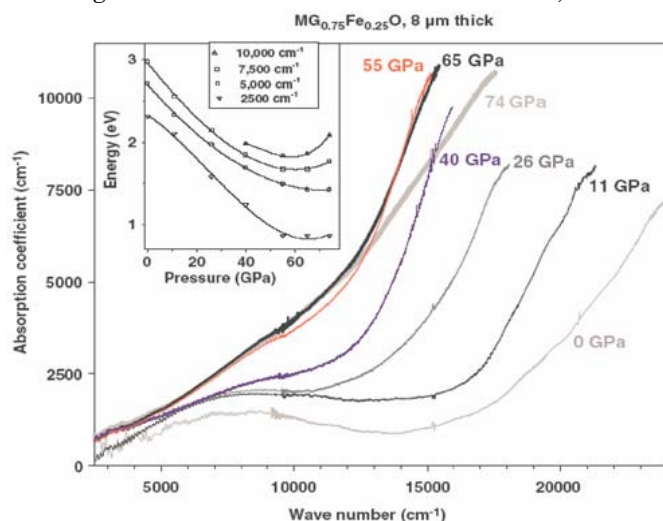


Figure 35. Infrared absorption of (Mg,Fe)O as a function of frequency at various pressures.

state of iron in $\text{Mg}_{0.75}\text{Fe}_{0.25}\text{O}$. As shown in Fig. 34a, the satellite emission peak at 7043 keV, representative of the high-spin state of Fe^{2+} , decreases in intensity with pressure beginning at approximately 50 GPa, where the high- to low-spin transition begins to take place. Between 50 and 95 GPa, elevated temperatures can reverse the formation of low-spin Fe^{2+} , causing the P - T space of the transition to become broader at high pressure and temperature (Fig. 34b). This effect is minimal above 95 GPa, however, after the transition to a low-spin state is complete. Diffraction measurements taken before, during and after laser heating at various pressures show clearly that the change in spin state takes place completely within the B2 structure, with no evidence of a phase transition.

The spin state of iron in the lower mantle as well as the structure of ferroperricite has important implications for a number of lower mantle properties, among them the density, sound velocities, and thermal conductivity, as well as element partitioning. The presence of such a "spin-transition" zone in the lower mantle would appear seismically as a region with a unusually steep density gradient⁸⁰.

The proposed spin transition zone in the lower mantle has important implications for heat transfer, which may also be hindered by the collapse of magnetism in Fe^{2+} . **Alexander Goncharov** and colleagues at **Carnegie**, including undergraduate summer scholar **Benjamin Haugen** found that the spin transition in (Mg,Fe)O to the low-spin state increased infrared absorption of the material, as shown in Fig. 35. This would therefore reduce radiative heat transfer; this result leads to alternative models of plume stabilization and convection dynamics in the deep mantle⁸¹.

Pressure-Induced Metallization – Understanding how the application of pressure results in metallic behavior in condensed matter is one of the signature problems in current solid state physics. With state-of-the-art spectroscopy facilities now on-line at HPCAT, it is now possible to probe valence band structure with new x-ray emission spectroscopy techniques. A group from **Carnegie** led by **Viktor Struzhkin**, along with colleagues from LLNL, the **National Research Council of Canada**, NSLS and HPCAT investigated the metallization of Ge at pressures up to 31 GPa. The emission from Ge 4p states to the 1s core state at 11.1 keV is investigated as a function of pressure, as shown in Fig. 36a. Up to 10 GPa, the valence band width of elemental Ge in the diamond structure shows no pressure dependence, but in the β -Sn structure above 12 GPa, the valence band width broadens significantly⁸². When compared with the results from current density functional calculations (Fig. 36b), the experimental measurements show that the theoretical methods for treating such complex interactions are lacking; at the same time, it is possible for this interplay between theory and experiment to guide the development of future theoretical models for electron-electron interactions.

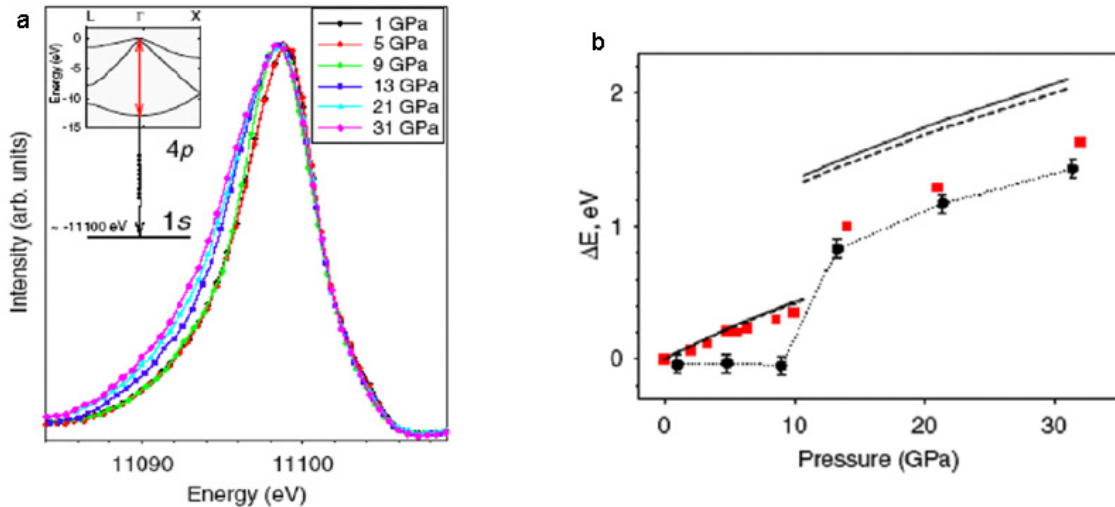


Figure 36. a) Valence band emission spectra of Ge at selected pressures. The inset shows schematically the transition from the 4p states to the 1s state. At sufficiently high pressure, the 4p states broaden and merge into a single band, giving a single emission line. b) Comparison of experimental measurements of the valence band width calculated values. The theoretical determinations are shown by the solid and dashed lines; symbols show the experimental measurements. Lines through the experimental points are guides to the eye.

Oxygen Isotope Effects in Cuprate Superconductors – High-temperature superconductivity in cuprate superconductors was discovered almost exactly 20 years ago, but a satisfactory theoretical explanation for this phenomenon is still lacking. Observations of the isotope effect in conventional superconductors (Nb₃Ge for example) have played an important role in establishing the electron–phonon interaction as the dominant contribution to the mechanism of superconductivity in these materials. Up to the present, however, conflicting experimental and theoretical results have not allowed a confirmation of the role of electron-phonon coupling in high-temperature, cuprate superconductors.

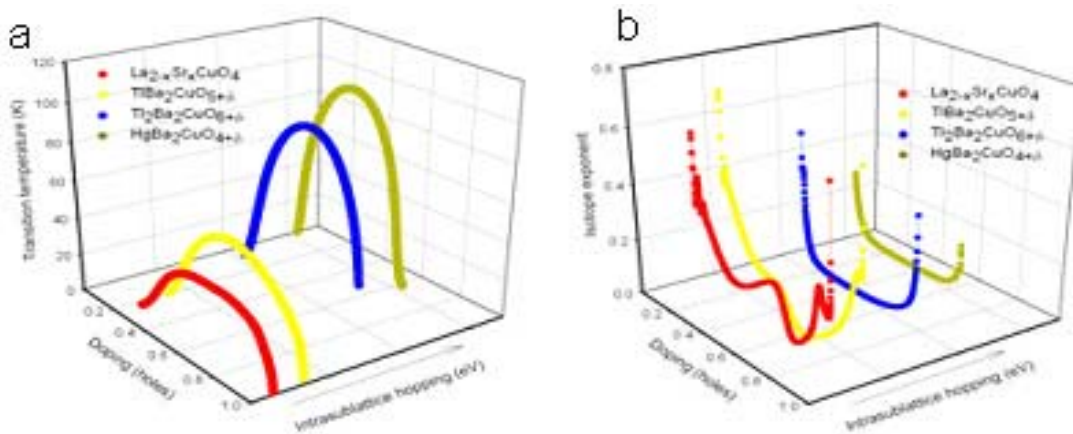


Figure 37. a) Theoretical results for the superconducting transition temperature as a function of hole concentration and intralattice hopping for various cuprate superconductors. Intrasublattice hopping is not hindered by antiferromagnetic order, leading to a free motion for the hole carriers. b) Isotope effect in cuprate superconductors as a function of hole concentration and intrasublattice hopping.

In recent work, **Xiao-Jia Chen** and colleagues at **Carnegie** have calculated the oxygen isotope exponents and transition numbers for a number of optimally doped cuprates using a

theoretical model that incorporates a phonon-mediated d-wave pairing potential. As shown in Fig. 37a, the calculated superconducting transition temperature peaks at different hole concentrations for different families of compounds, and is a straightforward function of the intrasublattice hopping; this result agrees well with experiment. Figure 37b reveals, however, that the oxygen isotope effect does not follow the same trend as a function of hole concentration, indicating that superconductivity in the cuprates is mediated by additional processes.

Using diamond anvil cell techniques, the group also investigated the behavior of the superconducting transition temperature and Raman spectrum with pressure, and found that the isotope effect and pressure effect on the transition temperature are closely related. In correlating results from experiment and theory, the work shows that the oxygen isotope effect is controlled by next nearest neighbor (Cu-O-Cu) interactions, and indicates that phonon-mediated processes are likely important in the mechanism of high-temperature superconductivity⁸³.

2.6 High *P-T* Chemistry

Ongoing studies in the area of high *P-T* chemistry are taking on an increasingly central role in CDAC research as the compositional basis of materials behavior is more fully appreciated and understood. CDAC supports a wide range of research, including investigations of novel phase transformations, high-pressure, high temperature synthesis of new materials, and the development of advanced analytical capabilities for evaluating chemical reactions in the bulk and at interfaces.

Lithium Hydrides at High Pressure – The high pressure studies at the **University of Nevada, Reno** led by CDAC graduate student **Raja Chellappa** in the group of **Dhanesh**

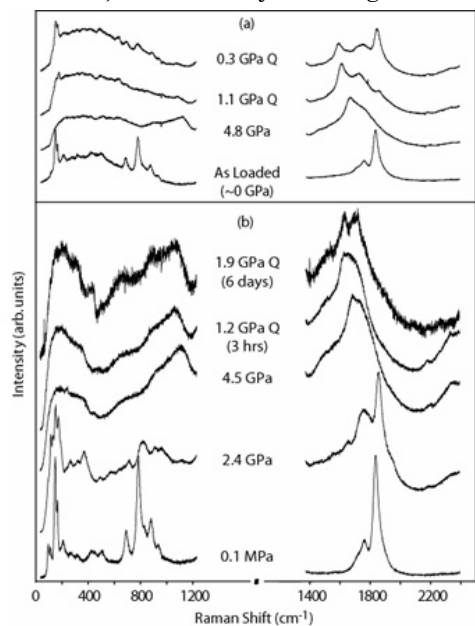


Figure 38. Raman spectra of two quenching experiments performed on LiAlH_4 . (a) A step wise increase to 4.5 GPa, then quenched to ~ 1.2 GPa (spectra taken after 3 hours), and held at constant load for 6 days. (b) A rapid increase of the as-loaded sample to ~ 4.8 GPa and quenched in two steps to 1.1 GPa and finally to 0.3 GPa.

Chandra, focus on determining the pressure-induced transformations in light metal complex hydrides, using *in situ* Raman spectroscopy and synchrotron x-ray diffraction. The Nevada group has continued studies on LiAlH_4 ¹², and has initiated Raman spectroscopy and synchrotron x-ray diffraction studies on LiNH_2 . Specifically, new results on the metastable recovery of the high pressure phase of LiAlH_4 ⁸⁴ and phase transitions in LiNH_2 ¹¹ were reported. *In situ* high-pressure Raman spectroscopy studies on LiNH_2 (lithium amide) have been performed at pressures up to 25 GPa. The pressure-induced changes in the Raman spectra of LiNH_2 indicates a phase transition that begins at ~ 12 GPa is complete at ~ 14 GPa from ambient-pressure α - LiNH_2 (tetragonal, *I*-4) to a high-pressure phase denoted here as β - LiNH_2 . New results on the metastable recovery of the high pressure β - LiAlH_4 phase are also presented. An examination of the lattice translational and librational modes reveals that the high pressure β - LiAlH_4 phase is disordered while there is evidence of orientational ordering in the high pressure β - LiNH_2 phase. High pressure work has also been initiated on the orientationally disordered plastic crystals and preliminary synchrotron x-ray diffraction data for tris-aminomethane (TRIS) has been obtained.

The catalyzed Li-based aluminohydrides (LiAlH_4), amides (LiNH_2), borohydrides (LiBH_4), and others are potential candidates for on-board hydrogen storage applications. The preferred method of catalyst

addition through solid-state ball milling; a dynamic, non-equilibrium process during which the samples can experience instantaneous pressures of up to 6 GPa⁸⁵. The formation of metastable high-

pressure phases and pressure-induced instabilities during ball milling is a distinct possibility. A deeper understanding of the pressure-induced transformations in these complex hydrides can provide insights into effects of pressure on the Al-H, N-H, and B-H bonding and its implications for hydrogen desorption/adsorption. In their previous study¹² on LiAlH_4 , a high-pressure phase transition ($\alpha\text{-LiAlH}_4$ transforms to $\beta\text{-LiAlH}_4$ at ~ 3 GPa) was confirmed (Fig 38). In addition, it was also suggested that pressure-induced weakening of Al-H bonds and the emergence of disorder can be related to the facilitation of hydrogen desorption.

New quenching experiments on LiAlH_4 were conducted to determine if the high pressure $\beta\text{-LiAlH}_4$ phase can be retained metastably at lower pressures. These experiments differ from previously reported¹² quenching experiments and were aimed to see if a quick pressurization and quenching would be enough to retain the high pressure phase metastability. As shown in Fig 38, the pressure was increased to ~ 4.8 GPa and then held for about 30 minutes and then quenched to 1.1 GPa, spectra collected, and quenched to 0.3 GPa. It can be clearly seen that in both quenched samples, the lattice and bending modes are not well defined; however, the Al-H stretching vibrations can be seen although lowered in relative intensity. The behavior of the stretching vibrations during the rapid increase and quenching experiment is not the same as the previously reported. It appears that the disorder in the lattice can be recovered metastably however probably a longer time in compression is required for retaining the weakened Al-H bonding characteristic of the high pressure $\beta\text{-LiAlH}_4$. It is also possible that a combination of pressure-temperature treatment may also be useful in the metastable retention of the high pressure phases which may have enhanced hydriding/dehydriding properties.

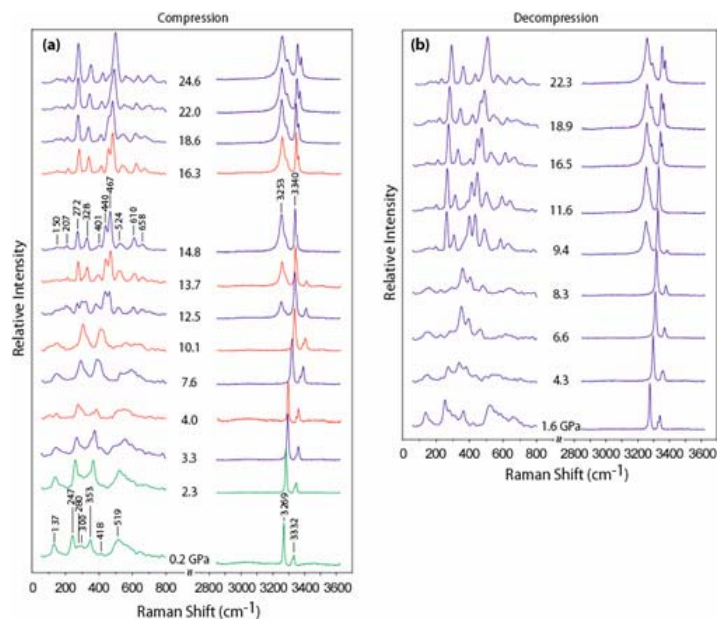


Figure 39. Raman spectra of LiNH_2 as a function of pressure are shown for (a) compression, and (b) decompression. During compression, the phase transition from $\alpha\text{-LiNH}_2$ (tetragonal) to $\beta\text{-LiNH}_2$ (unknown structure) begins at ~ 12 GPa and is complete at ~ 14 GPa. During decompression, the reverse phase transition occurs between 9.4 and 8.3 GPa. The three runs are color coded; Run 1 (Green), Run 2 (Blue), and Run 3 (Red).

In situ high-pressure Raman spectroscopy of LiNH_2 ¹¹ reveal a structural phase transition from ambient-pressure $\alpha\text{-LiNH}_2$ (tetragonal) to a phase referred to here as $\beta\text{-LiNH}_2$, at 298 K. A large hysteresis is observed with the onset of this phase transition at ~ 12 GPa (complete by ~ 14 GPa) and ~ 9.4 GPa (complete by 8.3 GPa), on decompression. In the low-pressure $\alpha\text{-LiNH}_2$ phase, the presence of broad overlapped peaks due to librations of the $[\text{NH}_2]^-$ ion, low-intensity lattice modes, and apparent lack of crystal field effects on the vibrational modes is attributed to the presence of orientational disorder. The high-pressure phase is characterized by multiple mode splitting (external and internal) and the sharpened lattice modes suggest an orientational ordering of $[\text{NH}_2]^-$ ions in the lattice (Fig. 39). High-pressure diffraction studies will be useful in identifying the crystal structure of $\beta\text{-LiNH}_2$ and to confirm the existence of pressure-induced ordering.

In the area of technique development, a microdiffraction cell for kinetic analyses using synchrotron radiation (Fig. 40) is in the design stage. The idea is to have synthetic diamonds or sapphire plates compressing the sample disk and to allow hydrogen to pass circumferentially. Intermediate products formed at the edge of the disk are evaluated by either scanning or performing spot analyses from the edge inwards. In many cases metastable phases form during the hydrogen loading and can be detected by structural analyses.

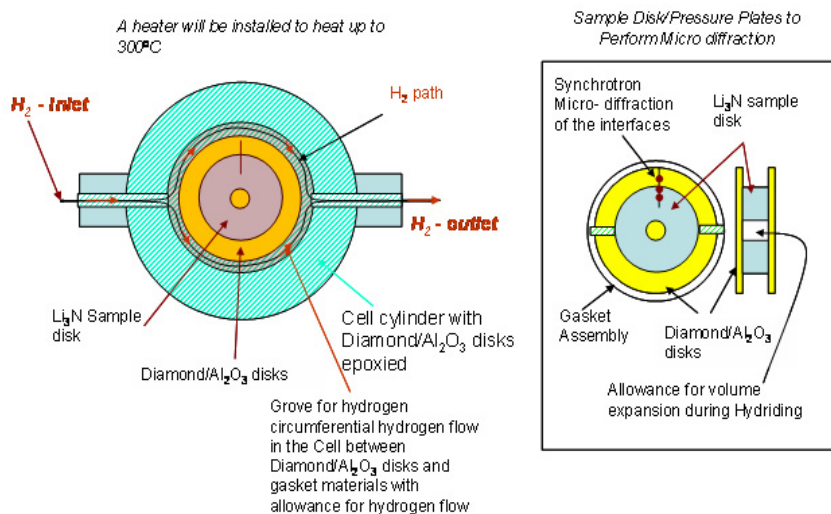


Figure 40. A schematic of the micro-diffraction cell for in-situ hydriding.

Ammonia-Water System at High Pressure – Vivek Venkakataraman, an undergraduate student in physics, at **Chicago**, completed his senior thesis project with CDAC academic partner **Dion Heinz** the pressure – composition phase diagram of the ammonia-water system. Water and ammonia are composed of volatile elements thought to be important in the interiors of the satellites of the outer planets. A knowledge of the effect of ammonia on the phase diagram of pure water is important for interior structure models and compositional models of the icy satellites of the gas giant planets. X-ray diffraction data at high pressure have been collected for a number of compositions in this system. Ammonia has the effect of increasing the freezing pressure of ice at room temperature, which implies that a deep liquid layer could exist on Titan or other icy satellites with ammonia present. Surprisingly, at high ammonia concentrations (>25 wt. %) ice IV is the first phase to crystallize. Figure 41a shows a series of integrated diffraction patterns taken with increasing pressure to illustrate the phase transitions and Fig. 41b shows the *P-x* phase diagram obtained from the data.

Metallic Glasses under Pressure – Pure substances that form glasses are quite common, but up to now the formation of a bulk glass formed through vitrification of a pure monatomic elemental liquid has been elusive. When crystal nucleation times are long compared to the time for assembly of amorphous forms, then the glassy state can be observed. A key requirement is the lowering of the freezing point of the liquid sufficiently so as to increase the competition between crystals and a stabilized liquid. Recently a group from **Arizona State University**, led by **M. H. Bhat** and including CDAC academic partner **Jeff Yarger**, has used pressure to stabilize the metallic liquid state of elemental germanium, subsequently temperature quenching the liquid to create for the first time a bulk metallic glass of a monoatomic element⁸⁶. In the process, the group has also observed an unusual transition from this high density amorphous, metallic (HDA) phase to a low density amorphous, non-metallic (LDA) phase.

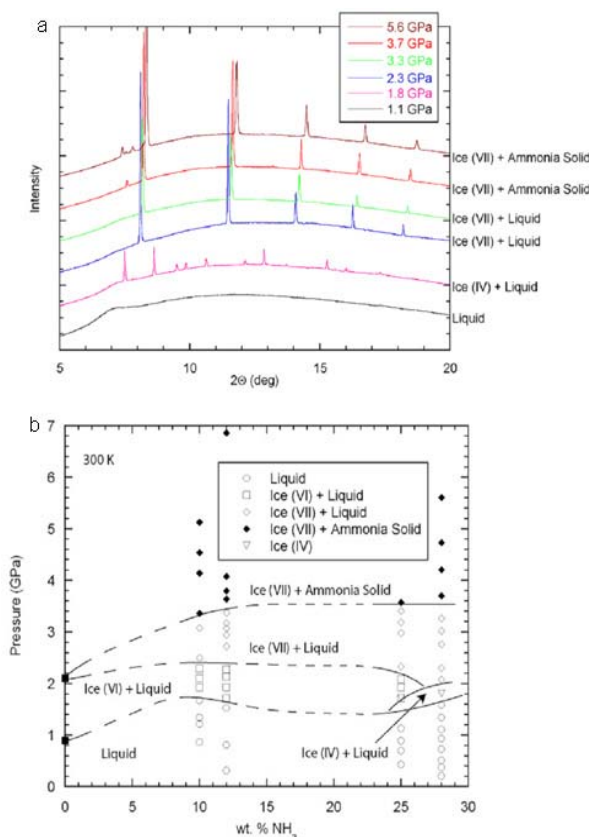


Figure 41. a) Integrated diffraction patterns of a 28 wt. % NH_3 solution showing the series of phase transitions observed. b) Updated phase diagram of the $\text{H}_2\text{O} - \text{NH}_3$ system at room temperature.

the amorphous solid formed on temperature quench of the metallic liquid at 7.9 GPa (metallic HDA) is quite different than the phase present after the release of pressure (LDA), and that the pressure quench from 7.9 GPa to ambient conditions has resulted in an unusual HDA-LDA transition.

The group is currently working to show that the vitrification of Ge is not unique to this system, but rather that many materials can be ‘pressure-tuned’ to quench new glasses. Starting with materials that have melting point minima and binary eutectic materials where the melting point falls at high pressure. Current systems under investigation include Si, Ba, $\text{Ca}(\text{OH})_2$ and $\text{BeH}_2 \cdot \text{LiH}$. Also, under study is of viscosity increasing/decreasing

Single crystals of elemental Ge approximately 20 microns in diameter were loaded into a diamond anvil cell. Melting of the Ge was then achieved by pulsed laser heating of the Ge crystals held at 5-11 GPa. The material was then quenched from high temperature. Above 7.9 GPa, the Raman band characteristic of crystalline Ge is replaced by a broadened fluorescence signal, indicating the amorphization of the quenched liquid. Samples were then removed from the pressure cell for electron and optical microscopy analysis. Figure 42 shows an electron micrograph of the quenched sample. Globules of the quenched material (Fig. 42a) are partially amorphous and partly crystalline, as illustrated by the electron diffraction patterns taken from two separate parts of the same globule (Fig. 42b, 42c). The boundary between crystalline and glassy domains is clearly seen in the micrograph in Fig. 42d.

Structure factors derived from the electron diffraction patterns confirm that the quenched sample is essentially identical to amorphous, non-metallic Ge derived from vapor deposition, but very different from liquid Ge (Fig. 43a). Molecular dynamics simulations (Fig. 43b) of liquid Ge at ambient conditions give excellent agreement with experiment, but the simulation of liquid Ge at 7.9 GPa shows significant differences from the quenched samples in Fig. 43a. This result indicates that

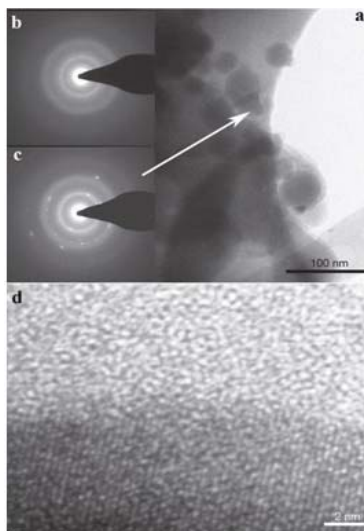


Figure 42. TEM and electron diffraction patterns of globules formed by temperature and pressure quenching of metallic liquid Ge at 7.9 GPa. (a) Electron micrograph of globules indicating the position of a crystalline-amorphous boundary. Scale bar, 100 nm. (b) and (c) Electron diffraction patterns taken from amorphous and crystalline portions of the same globule. (d) Electron micrograph showing the boundary between crystalline and amorphous regions of a globule. Scale bar, 2 nm.

with pressure versus fusion temperature increasing/decreasing with pressure to help predict systems that may become better glass-formers at high pressure.

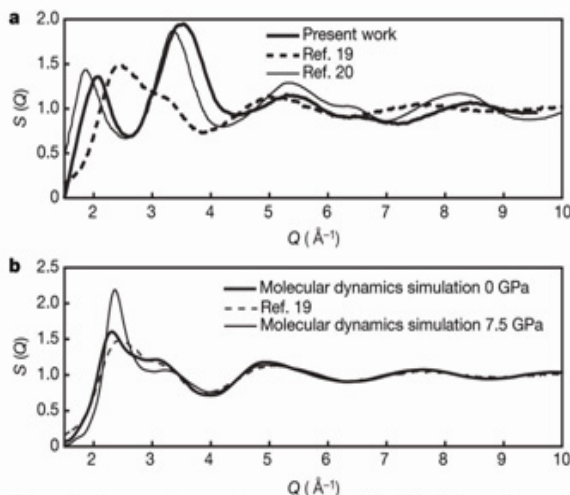


Figure 43. Structure factors of various Ge samples. (a) Thick solid line, amorphous region of Ge globule from Figure 42; thin solid line, vapor-deposited amorphous metallic Ge; dashed line, liquid Ge. (b) Calculated structure factors from molecular dynamics simulations compared with experimental results for liquid Ge. Thick solid line, liquid Ge at 0 GPa; thin solid line, liquid Ge at 7.9 GPa; dashed line, liquid Ge at 0 GPa from experiment.

Yarger's group has started to look into amorphous-amorphous and polyamorphic transitions at high-pressure and have just finished a complete study of As_2O_3 at high pressure. Figure 44 shows the visual evidence of continuous amorphous-amorphous transition in glassy As_2O_3 at high pressure. These results are preliminary and are currently being written up for publication. The 'red' phase is a high-density phase with high coordination arsenic and the 'clear' phase has is the low-density, standard three-coordinated arsenic glass. Results show that the same transition and high-density amorphous material can be produced from crystalline As_2O_3 , which undergoes a crystal-amorphous transition at 15-20 GPa. In collaboration with ANL, HPCAT and **Chris Benmore's** group, an *in-situ* x-ray study of amorphous As_2O_3 at high pressure has been completed, which will allow quantification of the coordination change and densification at high pressure.

The group at ASU has preliminary results on several new amorphous-amorphous transitions in systems such as PbGeO_3 , BeF_2 , GeSe_4 and Ab/NTS. **Erin Oelker**, a graduate student at ASU, is performing the research on PbGeO_3 and BeF_2 .

Postdoctoral fellows **Emmanuel Soignard** and **Samrat Amin** are exploring polyamorphic transitions in BeH_2 , GeSe_4 , TPP, ZnCl_2 and AlCl_3 .

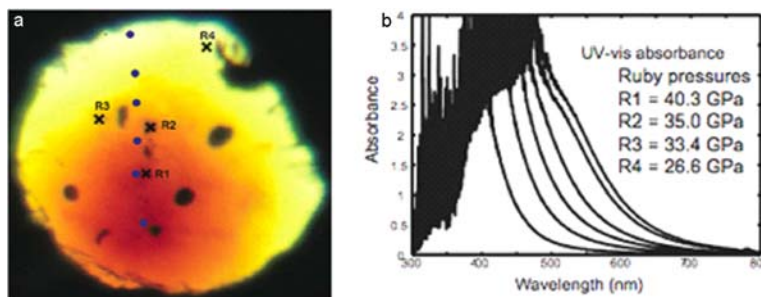


Figure 44. a) Photo of As_2O_3 sample in a diamond anvil cell. b) UV/Vis line scan that follows the blue dots from 26 to 40 GPa.

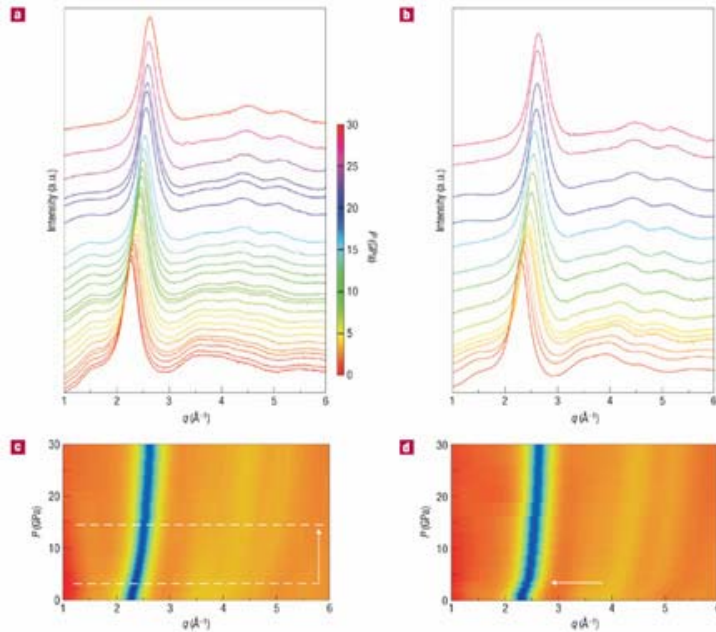


Figure 45. X-ray diffraction patterns of the $Ce_{55}Al_{45}$ metallic glass in a diamond anvil cell. a) Patterns obtained during the compression experiments; b) Decompression experiments. Pressures are given by the color scale at the right of each panel. c) and d) Behavior of diffraction peak intensity shift with pressure during compression and decompression, respectively. The arrow in (c) illustrates a gradual movement during compression between 2.0 and 13.5 GPa (marked with dashed lines), whereas the arrow in (d) marks the abrupt shift towards lower q , at around 2 GPa during compression.

Polyamorphism in a Metallic Glass – Metals and alloys often exist in more than one crystal structure, the fcc and bcc structures of iron being a familiar example of such polymorphism. When metallic materials exist in an amorphous form, a parallel ‘polyamorphism’ should be possible as discussed above. So far, polyamorphic phase transitions in the glassy state have been observed only in glasses involving directional and open, coordination environments such as tetrahedral (4,5). A group composed of researchers from **Johns Hopkins**, **HPCAT**, **Harbin Institute of Technology**, the **Chinese Academy of Sciences**, and **APS** now report the observation of a pressure-induced transition between two distinct amorphous polymorphs in a $Ce_{55}Al_{45}$ metallic glass⁸⁷ by *in-situ* x-ray diffraction (Fig. 45). The large density difference observed between the two polymorphs is attributed to their different electronic and atomic structures, in particular the bond shortening revealed by *ab initio* modeling of the effects of f -electron delocalization. This discovery offers a new perspective on the amorphous state of metals, and has implications for understanding the structure, evolution and properties of metallic glasses and related liquids. The work also opens a new avenue towards technologically useful amorphous alloys that are compositionally identical but with different thermodynamic, functional and rheological properties due to different bonding and structural characteristics.

Chemistry of Energetic

Materials – At Illinois, in the group of **Dana Dlott**, work on surface spectroscopy of energetic materials using vibrational sum-frequency spectroscopy (SFG) has continued, led by postdoctoral fellow **S. Eric Surber** and second year graduate student **Aaron Lozano**. A surprising finding was that the surfaces of β -HMX crystals obtained from national laboratories or grown in their own labs contain significant microscopic deposits of δ -HMX impurities which had not been detected before. Since δ -HMX is much more sensitive than β -HMX, this could be a serious safety concern. Because the

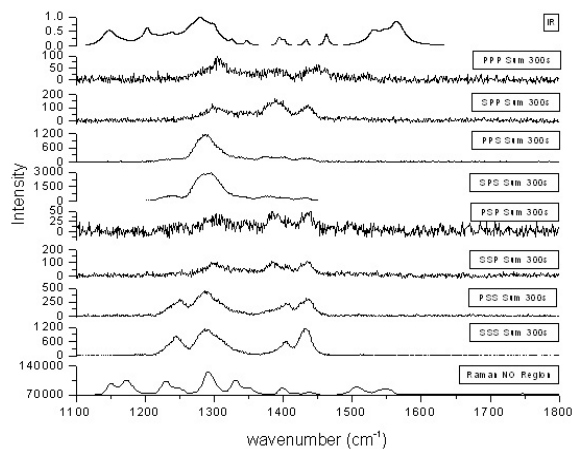


Figure 46. SFG spectra of HMX crystal surfaces in the NO_2 region, compared to ordinary IR and Raman spectra.

existence of these deposits was not previously known, processing and fabrication techniques were not developed to reduce their abundance. Now that these surface deposits have been identified, it is possible to produce HMX surfaces with much greater purity and homogeneity, and the spectra of surface methylene (CH_2) and nitro (NO_2) groups may be understood in great detail. SFG spectra (Fig. 46) have been obtained using the eight possible polarization conditions, which will allow an understanding of the frequency shifts, splittings and symmetries of the surface vibrations and in comparison with them to bulk vibrations.

A third-generation SFG apparatus has been constructed (Fig. 47), which produces high quality spectra and is very user friendly. The original apparatus used in the group could be used only



Figure 47. Third-generation SFG apparatus.

by a trained laser professional. This new apparatus can be used by an inexperienced user, which will allow more young scientists to participate in the project. Due to the difficulty of combining diamond anvil cell technology with femtosecond laser methods, it has been difficult to train researchers to a high level of proficiency in both types of expertise. With this new laser the learning curve for SFG laser operation is much less steep.

Eric Surber and Kathryn Brown, a first year graduate student at **Illinois**, are studying surfaces and interfaces at high pressure. Photonic substrates have been fabricated that amplify the Raman spectra of adsorbed

molecules by a factor of $\sim 10^5$. In other words, a monolayer ~ 1 nm thick gives the same Raman spectrum as a layer $100 \mu\text{m}$ thick, making the signal from the nanometer-scale monolayer very easy to detect. The group has also finished building a diamond anvil cell Raman system that allows the measurement of ruby fluorescence and Raman spectra simultaneously. They have measured the surface plasmon spectra of the photonic substrates and the pressure-dependent Raman spectrum of a

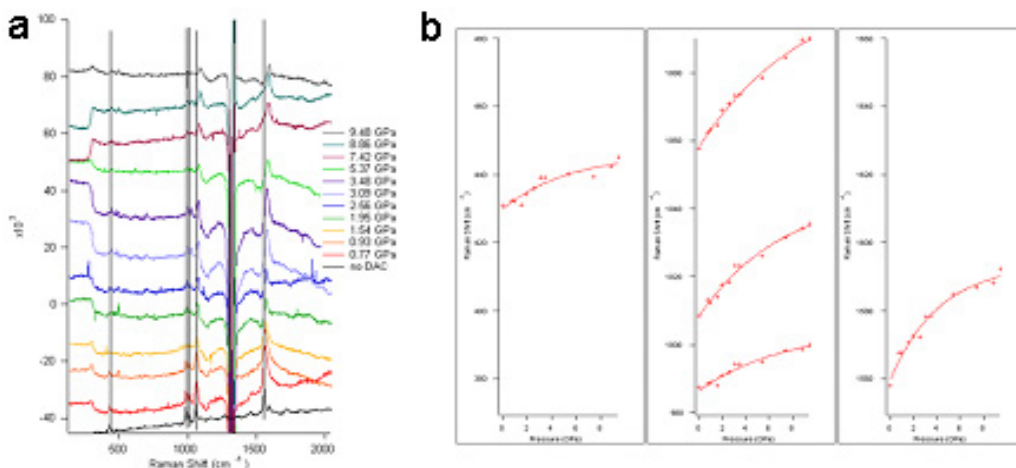


Figure 48. Left: Pressure-dependent Raman spectra of a benzene thiolate ($\text{C}_6\text{H}_5\text{S}$) monolayer bound to a silver nanostructured photonic substrate which amplifies the Raman spectrum by $\sim 10^5$. Right: Pressure-dependent frequency shifts for a benzene-thiolate monolayer.

monolayer of benzenethiolate inside a diamond cell (Fig. 48). This appears to be the first vibrational spectrum of a monolayer at high pressure.

The **Diott** group plans to use SFG techniques to study the vibrational spectra of molecules absorbed on an electrode during an electrochemical oxidation of CO to CO₂. The group has studied the oxidation of CO on a polycrystalline Pt electrode and on a single crystal Pt (111) electrode

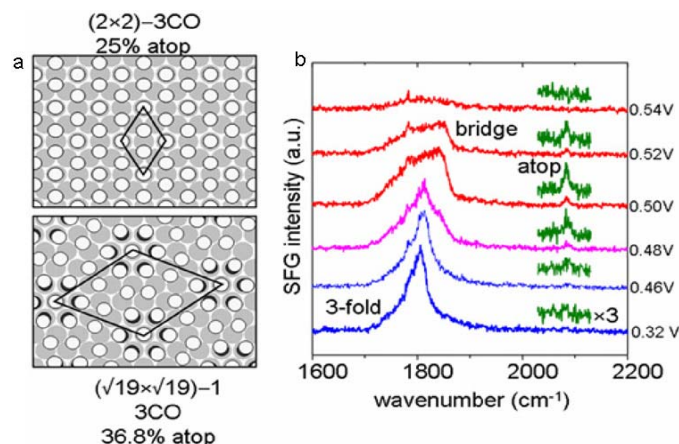


Figure 49. a) Structures of the two phases of a CO adlayer on a Pt(111) single crystal. b) SFG spectra showing how the 3-fold CO transitions to bridge-bonded CO when the potential is stepped through 0.48V.

previously. On Pt (111) there is an interesting phase transition of the CO adlayer prior to the onset of oxidation (Fig. 49). This work is done in conjunction with **A. Wieckowski** and his second year graduate student **Rachel Behrens**. Ultimately, the long-term objective will be to extend this expertise to study electroadsorbed CO with static methods and dynamic shock compression. The motivation for the static experiments is a better fundamental understanding of electrochemistry, since there are no high-pressure spectroscopy experiments known at this point. The motivation for the shock compression experiments stems from earlier measurements of self-assembled monolayers (SAMs). The SAMs were very relevant, but the long-chain molecules have a complicated response. CO should have a much simpler

response that can be better understood, and CO produces a giant SFG signal. This work is leading up to using shock compression as the ultimate probe of shock front structure.

New Results on High-Pressure Phases of Nitrogen – McMahan and LeSar⁸⁸ predicted the formation of a 'polymeric' network structure of nitrogen in 1985 at LANL. This work was extended by Mailhiot⁸⁹ and colleagues at LLNL in 1992. In a recent paper, former CDAC research scientist **Eugene Gregoryanz** (now at the **University of Edinburgh**) and colleagues from **Carnegie**, the **Université Pierre et Marie Curie**, and the **Institut de Physique du Globe du Paris** reported x-ray diffraction and Raman spectroscopic measurements on nitrogen compressed to 170 GPa and heated to 2500 K (Fig. 50a). Diffraction data show that ϵ -N₂ undergoes two successive structural changes, one to the complex molecular ζ phase at 62 GPa and another to the newly

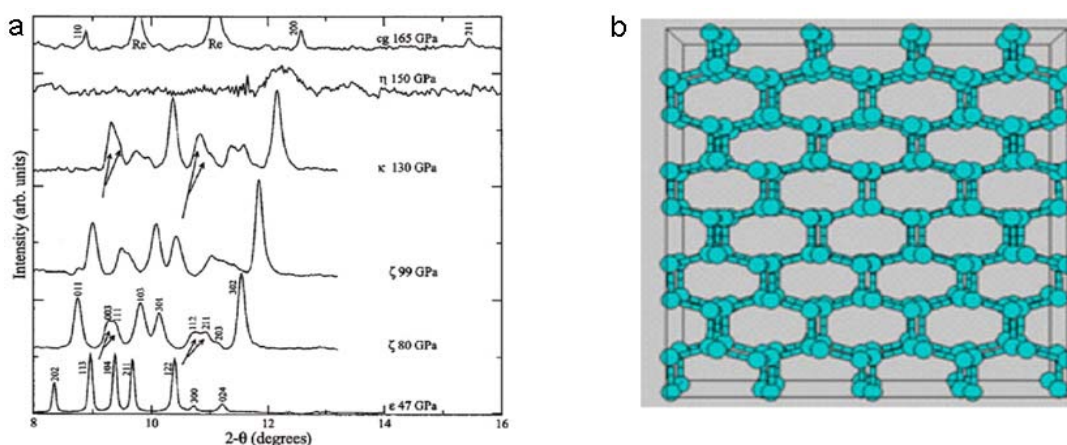


Figure 50. a) X-ray diffraction patterns of ϵ , ζ , κ , amorphous and cubic gauche phases measured at different pressures. Arrows point to the two split peaks in the patterns for the ζ and κ phases. b) structure of the cubic gauche phase of nitrogen (cg-N).

discovered κ phase at 110 GPa. κ -N₂ becomes an amorphous, narrow-gap semiconductor on further compression, while the crystalline cubic gauche structure (cg-N) (Fig. 50b) is observed at temperatures above 2000 K and pressures above 150 GPa. The diffraction data show that the transition to cg-N is accompanied by a 15% volume reduction⁹⁰.

In addition, former Carnegie scientist **Mikhail Eremets** (now at the **Max Planck Institute für Chemie**), along with scientists from the Max Planck Institute and the **Russian Academy of Sciences** synthesized single-crystal polymeric nitrogen at pressures above 110 GPa with laser heating above 2000 K. A report of this work has appeared recently⁹¹.

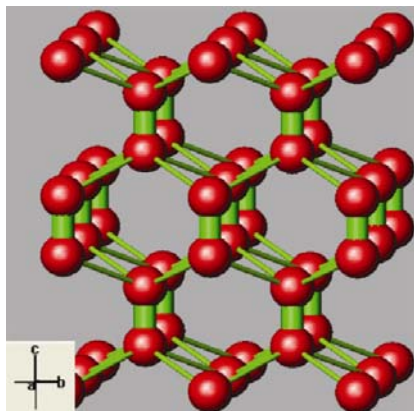


Figure 51. Crystal structure (space group *Immm*) of a theoretically predicted body-centered tetragonal phase of nitrogen

The existence of new polyatomic structures of nitrogen at high density has also been examined using first-principles density-functional theory. Former **Carnegie** postdoctoral fellow **Razvan Caracas** (now at the **Bayerisches Geoinstitut, Bayreuth**) and **Russell Hemley (Carnegie)** report that a structure with *Immm* symmetry (Fig. 51) and two molecules per unit cell is found to be stable relative to the known high density diatomic and polymeric phases of nitrogen⁹². The structure is dynamically stable from ambient pressure to at least 90 GPa and thus may represent a new class of observable polynitrogen phases at high pressures and temperatures. Other newly predicted structures may be observed experimentally as stable or metastable phases in different *P-T* ranges.

3. EDUCATION, TRAINING, AND OUTREACH

3.1 CDAC Graduate Students and Post-doctoral Fellows

The education, training and outreach mission of CDAC continues to focus on the support of graduate student preparation in the areas of high pressure research important to stewardship science. In Year 4 of the CDAC program, our 11 academic partners supported a total of 18 graduate students and three postdoctoral fellows.

Princeton:	Susannah Dorfman Fuming Jiang (Postdoctoral Fellow) Zhu Mao
Caltech:	Matt Lucas Michael Winterrose
Chicago:	Chris Seagle
Berkeley:	Lowell Miyagi
Alabama:	Nicholas Cunningham Gopi Samudrala Andrew Stemshorn
Illinois:	Kathryn Brown Aaron Lozano Eric Surber (Postdoctoral Fellow)
Arizona State:	Erin Oelker Janelle Jenkins Samrat Amin
New Mexico State:	Stefanie Japel (Postdoctoral Fellow)

Texas Tech: **Resul Aksoy**
 Emre Selvi
 Florida International: **Srinivas Kulkarni**
 Nishad Phatak
 Nevada – Reno: **Raja Chellappa (now at Carnegie)**



Figure 52. CDAC graduate students Lowell Miyagi (Berkeley) and Emri Selvi and Resul Aksoy (Texas Tech).

In addition, two graduate students supported by the National Labs, **Zsolt Jenei (LLNL, University of Stockholm)**, and **Amy Lazicki (LLNL, University of California, Davis, now at Carnegie)**, were working directly with the high-pressure groups. Postdoctoral associate **Kirill Zhuravlev (Washington State University)** is also working with high pressure groups at LANL. Texas Tech also supported two undergraduate students, **Jeff Aycock and Russell Knudson**.

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

- James Devine (Chicago, 2004)**
- James Patterson (Illinois, 2004)**
- Wendy Mao (Chicago, 2005)**
- Jenny Pehl (Berkeley, 2005)**
- Sergio Speziale (Princeton, 2005)**
- Tabitha Swan-Wood (Caltech, 2005)**
- Raja Chellappa (Nevada-Reno, 2004)**
- Joanna Dodd (Caltech, 2007)**
- Joel Griffith (Alabama-Birmingham, 2006)**
- Alexander Papandrew (Caltech, 2006)**
- Nenad Velisavljevic (Alabama-Birmingham, 2006)**

CDAC graduate students continue their work on a wide variety of problems in experimental high pressure research relevant to stewardship science, spanning the fields of materials science,

physics, chemistry and high-pressure mineral physics and geophysics. In addition, **Carnegie** has a well-established post-doctoral program, and a competitive predoctoral program as well as internships for college undergraduates and high school students. The close integration of computational theory within CDAC provides an environment in which graduate students in this area become intimately familiar with advanced experimental techniques and results, in addition to receiving exposure to state-of-the-art computational methods (e.g., Refs.⁹³⁻⁹⁵).

Publications and presentations involving CDAC-supported students and postdoctoral fellows in Year 4 are listed below.

Student Publications

- Aksoy, R., Y. Ma, E. Selvi, M. C. Chyu, A. Ertas, and A. White, Equation of state measurements of molybdenum disulfide, *J. Phys. Chem. Solids*, **67**, 1914-1917 (2006).
- Aksoy, R., E. Selvi, R. Knudson, and Y. Ma, High pressure x-ray diffraction studies of titanium disulfide, *J. Phys. Chem. Solids*, submitted.
- Aksoy, R., E. Selvi, and Y. Ma, X-ray diffraction study of molybdenum diselenide to 35.9 GPa, *J. Phys. Chem. Solid*, submitted.
- Campbell, A. J., C. T. Seagle, D. L. Heinz, G. Y. Shen, and V. Prakapenka, Partial melting in the iron-sulfur system at high pressure: A synchrotron x-ray diffraction study, *Phys. Earth Planet. Inter.*, **162**, 119-128 (2007).
- Cunningham, N., W. Qiu, K. M. Hope, H. P. Liermann, and Y. K. Vohra, Symmetry lowering under high pressure: structural evidence for *f*-shell delocalization in heavy rare Earth metal terbium, *Phys. Rev. Lett.*, in press.
- Cunningham, N., W. Qiu, and Y. K. Vohra, Observation of complete trivalent rare earth sequence in heavy lanthanide metal holmium under high pressure, *High Press. Res.*, **26**, 43 (2006).
- Jiang, F., J. Majzlan, S. Speziale, D. He, and T. S. Duffy, Single-crystal elasticity of diaspore, AlOOH, to 12 GPa by Brillouin scattering, *Phys. Earth Planet. Inter.*, submitted.
- Jiang, F., S. Speziale, and T. S. Duffy, Single-crystal elasticity of brucite, Mg(OH)₂, to 15 GPa by Brillouin scattering, *Am. Mineral.*, **91**, 1893-1900 (2006).
- Kunz, M. C., W. A., L. Miyagi, and H. R. Wenk, In situ laser heating and radial synchrotron diffraction in a diamond anvil cell, *Rev. Sci. Instrum.*, **78**, 063907 (2007).
- Lucas, M. S., A. B. Papandrew, B. Fultz, and M. Y. Hu, Partial phonon densities of states of ⁵⁷Fe in Fe-Cr: analysis by a local-order cluster expansion, *Phys. Rev. B*, **75**, 054307 (2007).
- Ma, Y. and R. Aksoy, Compression of CdCu₃Ti₄O₁₂ perovskite to 55 GPa, *Solid State Comm.*, in press.
- Mao, Z., S. D. Jacobsen, F. Jiang, J. R. Smyth, C. Holl, D. J. Frost, and T. Duffy, Single-crystal elasticity of wadsleyites, β-Mg₂SiO₄, containing 0.37-1.66 wt % H₂O, *Earth Planet. Sci. Lett.*, submitted.
- Mao, Z., F. Jiang, and T. Duffy, Single-crystal elasticity of zoisite, Ca₂Al₃Si₃O₁₂(OH), by Brillouin scattering, *Am. Mineral.*, **92**, 570-576 (2007).
- Mei, Q., C. J. Benmore, S. Sampath, J. K. R. Weber, K. Leinenweber, S. Amin, P. Johnston, and J. L. Yarger, The structure of permanently densified CaAl₂O₄ glass, *J. Phys. Chem. Solids*, **67**, 2106-2110 (2006).
- Mei, Q., C. J. Benmore, E. Soignard, S. Amin, and J. Yarger, Analysis of high-energy x-ray diffraction data at high pressure: The case of vitreous As₂O₃ at 32 GPa, *J. Phys. Chem. Solids*, in press.
- Mei, Q., R. T. Hart, C. J. Benmore, S. Amin, K. Leinenweber, and J. L. Yarger, The structure of densified As₂O₃ glasses, *J. Non-Crystalline Solids*, **353**, 1755-1758 (2007).
- Merkel, S., A. Kubo, L. Miyagi, S. Speziale, T. S. Duffy, H. K. Mao, and H. R. Wenk, Plastic deformation of MgGeO₃ post-perovskite at lower mantle pressures, *Science*, **311**, 644-646 (2006).
- Merkel, S., A. K. McNamera, A. Kubo, S. Speziale, L. Miyagi, Y. Meng, T. S. Duffy, and H. R. Wenk, Deformation of (Mg,Fe)SiO₃ post-perovskite and D" anisotropy, *Science*, **316**, 1729-1732 (2007).
- Miyagi, L., S. Merkel, T. Yagi, N. Sata, Y. Ohishi, and H. R. Wenk, Diamond anvil cell deformation of CaSiO₃ perovskite up to 49 GPa, *Phys. Earth Planet. Inter.*, submitted.
- Miyagi, L., S. Merkel, T. Yagi, N. Sata, Y. Ohishi, and H. R. Wenk, Quantitative Reitveld texture analysis of CaSiO₃ perovskite deformed in a diamond anvil cell, *J. Phys. Cond. Matt.*, **18**, S995-1005 (2006).
- Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. Duffy, and H. R. Wenk, Deformation of the CaIrO₃ post-perovskite phase to 5 GPa and 1300 K, *Earth Planet. Sci. Lett.*, submitted.
- Papandrew, A. B., M. S. Lucas, R. Stevens, B. Fultz, M. Y. Hu, I. Halevy, R. E. Cohen, and M. Somayazulu, Absence of magnetism in hcp iron-nickel at 11 K, *Phys. Rev. Lett.*, **97**, 087202 (2006).
- Selvi, E., Y. Ma, R. Aksoy, A. Ertas, A. White, and S. Jagdev-Singh, High pressure x-ray diffraction study of tungsten disulfide, *J. Phys. Chem. Solids*, **67**, 2183-2186 (2006).

- Surber, E., A. Lozano, A. Lagutchev, H. Kim, and D. D. Dlott, Surface nonlinear vibrational spectroscopy of energetic materials: HMX, *J. Phys. Chem. C*, **111**, 2235-2241 (2007).
- Surber, E., A. Lozano, A. Lagutchev, H. Kim, and D. D. Dlott, Surface vibrational spectroscopy of energetic materials: HMX, *J. Phys. Chem.*, **111**, 2235-2241 (2007).
- Wenk, H. R., I. Lonardelli, S. Merkel, L. Miyagi, J. Pehl, S. Speziale, and C. Tommaseo, Deformation textures produced in diamond anvil experiments, analyzed in radial diffraction geometry, *J. Phys. Cond. Matt.*, **18**, S933-947 (2006).

Student Presentations

- Aksoy, R., X-ray diffraction study of molybdenum diselenide to 35.88 GPa, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Aksoy, R., High pressure x-ray diffraction studies of titanium disulfide, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Aksoy, R., E. Selvi, and Y. Ma, High pressure x-ray diffraction studies of nickel disulfide, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Aksoy, R., E. Selvi, and Y. Ma, X-ray diffraction study of niobium diselenide to 45.1 GPa, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cunningham, N., High pressure structural phase transformations in heavy rare earth metal terbium to 154 GPa: Evidence for f-shell delocalization, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Cunningham, N. C., W. Qiu, K. M. Hope, and Y. K. Vohra, Structural trends in heavy rare earth metals at high pressure - possible f-delocalization mechanisms, *Gordon Conference on Research at High Pressure* (Biddeford, ME, June 25-30, 2006).
- Delaire, O., M. Kresch, M. Lucas, R. Stevens, J. Munoz, and B. Fultz, Anharmonic phonons in vanadium alloys and compounds, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Dorfman, S. M., F. Jiang, Z. Mao, A. Kubo, V. Prakapenka, and T. S. Duffy, Phase transitions and equations of state of alkaline earth fluorides CaF₂ and SrF₂ to 95 GPa, *Eos Trans. AGU Fall Meet., Suppl.*, **88**(2007).
- Duffy, T. S. and Z. Mao, Elasticity of the olivine (Mg,Fe)₂SiO₄ polymorphs: Current understanding and implications for mantle composition, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Duffy, T. S., Z. Mao, S. D. Jacobsen, F. Jiang, J. R. Smyth, C. M. Holl, and D. J. Frost, Elasticity of hydrous olivine polymorphs: implications for seismic structure of the transition zone, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Heinz, D. L., C. T. Seagle, A. J. Campbell, N. Miller, V. Prakapenka, and G. Shen, Thermal equations of state in the Fe-FeS, Fe-FeO, and ammonia-water systems, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Jacobsen, S. D., F. Jiang, J. R. Smyth, T. S. Duffy, Z. Mao, C. M. Holl, and D. J. Frost, Sound velocities of hydrous olivine and the effects of water on the equation of state of nominally anhydrous minerals, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Japel, S. and B. Keifer, Iron phosphide (Fep) to 60 GPa: Equation of state and phase transition, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Jiang, F., G. D. Gwanmesia, and T. S. Duffy, Elasticity of stishovite and acoustic mode softening under high pressure by Brillouin scattering, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Jiang, F., G. D. Gwanmesia, and T. S. Duffy, Elasticity of stishovite and acoustic mode softening under high pressure by brillouin scattering, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Kulkarni, S., Ternary layered carbides - MAX phases, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Liermann, H., S. Merkel, L. Miyagi, H. R. Wenk, G. Shen, H. Cynn, and W. J. Evans, New experimental method for in situ determination of material textures at simultaneous high-pressure and -temperature by means of radial diffraction in the diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Lucas, M., O. Delaire, M. Winterrose, I. Halevy, B. Fultz, M. Y. Hu, and J. Hu, Effect of vacancies on the pressure dependence of lattice dynamics in B₂FeAl, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Mao, Z., S. Jacobsen, F. Jiang, C. Holl, J. R. Smyth, and T. S. Duffy, Effect of water on the elastic properties of wadsleyite, B-Mg₂SiO₄, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Mao, Z., S. D. Jacobsen, F. Jiang, J. R. Smyth, C. M. Holl, D. J. Frost, and T. S. Duffy, Single-crystal elasticity of hydrous wadsleyite to 12 GPa, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Mao, Z., F. Jiang, S. D. Jacobsen, J. R. Smyth, C. Holl, T. S. Duffy, and D. J. Frost, Single-crystal elasticity of hydrous wadsleyite by Brillouin scattering, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).

- Miyagi, L., M. Kunz, M. Voltolini, and H. R. Wenk, In-situ laser heating and pressure change with radial diffraction to investigate deformation of deep Earth relevant minerals, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. S. Duffy, and H. R. Wenk, Deformation of the CaIrO₃ post-perovskite phase to 5 GPa and 1300 K in the multi-anvil press, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. S. Duffy, and H. R. Wenk, Texture development in the CaIrO₃ post-perovskite phase deformed in the multi-anvil press up to 5 GPa and 1300 K, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Miyagi, L. and H. R. Wenk, Deformation of Earth materials at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Oelker, E., Pressure-induced amorphization of PbGeO₃ crystal, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, N. Miller, and V. Prakapenka, Liquidus temperatures in the iron - sulfur system and melting of Fe₃S at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, and V. Prakapenka, Melting in the Fe-FeO system at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, V. B. Prakapenka, and G. Shen, Experimental determination of binary phase diagrams at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Seagle, C. T., D. L. Heinz, Z. Liu, and R. J. Hemley, Synchrotron infrared reflectivity of iron at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Soignard, E., J. Yarger, S. Amin, and Q. Mei, Pushing new boundaries in high pressure x-ray diffraction within supercooled liquids and amorphous solids: exploration of phase transformations, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Speziale, S., F. Jiang, Z. Mao, P. J. Monteiro, H. R. Wenk, T. S. Duffy, and F. Schilling, Single-crystal elasticity of ettringite at ambient conditions, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Surber, E., Surfaces and interfaces of high explosives probed by nonlinear spectroscopy, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Surber, E., Surfaces and interfaces of explosives probed by nonlinear optical spectroscopy, *American Chemical Society* (Chicago, IL, March, 2007).
- Surber, S. E., Surfaces and interfaces of explosives probed by nonlinear optical spectroscopy, *Ohio State University International Symposium on Molecular Spectroscopy* (Columbus OH, June 18-22, 2007).
- Surber, S. E., Sum frequency generation characterization of the surface structure of HMX, *Joint Army Research Office MURI on Insensitive Munitions* (Aberdeen, MD, July 11-13, 2007).

3.2 CDAC Collaborators

As discussed above, CDAC also has established active collaborations with high-pressure groups throughout the country and around the world. These collaborations play an important role fulfilling the mission of the center, specifically by training new students and researchers in high-pressure materials science and exposing them to problems of importance to the NNSA Labs. Some other collaborations are just starting and still others that are in the preliminary planning stages, but in all cases the infrastructure made possible by CDAC has given leverage to work on a number of exciting new research directions. The CDAC collaborators to date include faculty and students from the following institutions:

Aarhus University, Denmark

A. N. Christensen

Abdus Salam International Center for

Theoretical Physics, Trieste, Italy

S. Scandolo

Argonne National Laboratory

C. J. Benmore

J. A. Cowan

P. L. Lee

S. D. Shastri

W. Sturhahn

J. Urquidi

R. Yang

J. Zhao

Arizona State University

K. Leinenweber

A. K. McNamara

J. Yarger

Auburn University

Y. C. Chen

J. Dong

T. Tzeng

Bayerisches Geoinstitut, Bayreuth, Germany

Tiziana Boffa Ballaran

R. Caracas

L. S. Dubrovinsky

D. J. Frost

Anastasia P. Kantor

I. Y. Kantor

Catherine A. McCammon

Brookhaven National Laboratory

G. L. Carr

O. Gang

W. Q. Han

J. Hanson

C. C. Kao

Laura Lewis

M. M. Maye

Lisa Miller

W. Wen

D. Yi

Bulgarian Academy of Sciences

I. K. Bonev

I. Mitov

Daniela Paneva

Rossitsa D. Vassileva

California Institute of Technology

O. Delaire

S. Kung

H. Su

California State University at Channel

Islands

Tabitha Swan-Wood

Carleton College

Frances R. Reid

Case Western Reserve University

J. Van Orman

Chinese Academy of Science

T. D. Hu

J. Liu

J. Wen

Chinese University of Hong Kong

H. Q. Lin

Cleveland State University

J. Vitali

Colby College

Elizabeth Littlefield

Colorado College

T. D. Atkinson

P. Cervantes

Katie M. Chynoweth

Colorado School of Mines

Carolyn A. Koh

E. D. Sloan

Columbia University

D. Walker

E. Cottrell

Cornell University

W. Bassett

Dalhousie University, Canada

S. A. Bonev

Democritos National Simulation Center,

Trieste Italy

A. F. Young

DTC Research Centre, United Kingdom

D. Fisher

Drexel University

M. W. Barsoum

Euskal Herriko Unibertsitatea, Spain

A. Bergara

M. Martínez Canales

European Synchrotron Radiation Facility, France

F. Berberich

T. Le Bihan

Nicola Guignot

M. Mezouar

J. Serrano

F.E.E. GmbH, Germany

D. Rytz

Florida State University

A. El-Azab

Friedrich-Schiller-University, Germany

F. Langenhorst

Geoforschungszentrum, Potsdam, Germany

Monika Koch-Müller

H. J. Reichmann

George Washington University

Lauren Borkowski

C. Cahill

M. Frisch

Georgia Institute of Technology

X. Wang

Z. L. Wang

GSECARS, APS

P. J. Eng

M. Newville

M. Rivers

S. Sutton

Ecole Normale Supérieure, Lyon, France

P. Beck

P. Gillet

EPFL, Switzerland

H. Berger

L. Forro

G. Margaritondo

**European Synchrotron Radiation Facility,
France**

G. Aquilanti

P. Bouvier

Florida A&M University

R. Little

Florida International University

S. K. Saxena

H. P. Liermann

H. Yang

Harvard University

D. R. Herschbach

S. Rekh

Sarah T. Stewart-Mukhopadhyay

Indiana University – South Bend

Sabrina Huggins

H. P. Scott

Institut für Geowissenschaften, Germany

K. Knorr

Institut für Mineralogie, Germany

B. Winkler

Institut für Physik, Germany

A. Krimmel

**Institute de Ciencia de Materials de
Barcelona, Spain**

E. R. Hernandez

**Institute for Earth Sciences, Acad. Sinica,
Taiwan**

E. Huang

Institute of Crystallography, Moscow

V. V. Artemov

**Institute of Geochemistry, Chinese
Academy of Sciences**

M. Chen

X. Xie

Institute of Metal Physics, Russia

Y. S. Ponomov

S. V. Streltsov

**Institute for High Pressure Physics,
Troitsk, Russia**

V. Denisov

A. G. Gavriluk

I. S. Lyubutin

M. Yu. Popov

I. A. Trojan

**Institute for Problems of Chemical
Physics, Chernogolovka, Russia**

E. B. Gordon

**Institute for Solid State Physics,
Chernogolovka, Russia**

Valentina F. Degtyareva

N. I. Novokhatskaya

M. K. Sakharov

**Institute für Mineralogie and
Petrographie, Switzerland**

W. van Westrenen

Institutio di Gioscienze e

Georisorse, Italy

L. Ottolini

**Instituto Potosino de Investigación
Científica y Tecnológica, Mexico**

T. Terrence

Iowa State University

K. A. Gschneider, Jr.

Y. Mudryk

V. K. Pecharsky

**James Franck Institute, University of
Chicago**

Y. Feng

E. D. Isaacs

R. Jaramillo

T. N. Rosenbaum

**Japanese Synchrotron Radiation
Research Institute**

K. Funakoshi

Japan Marine Science Center

S. Nagayoshi

N. Sata

Japan National Defense Academy, Tokyo

Y. Yoshimura

Jilin University, Changchun, China

G. Zou

Johns Hopkins University

Y. Q. Cheng
Y. Ding
W. K. Luo
E. Ma
H. W. Sheng
D. R. Veblen

Karl-Franzens-Universität Graz, Austria

J. K. Dewhurst
S. Sharma

Kent State University

C. C. Almasan

KFKI Research Institute for Particle and Nuclear Physics, Hungary

G. Vankó

Kirensky Institute of Physics, Russia

S. G. Ovchinnikov
Y. S. Orlov

Laboratoire Leon Brillouin, France

I. N. Goncharenko

Lawrence Berkeley National

Laboratory

J. F. Banfield
B. Gilbert

LENS, Florence

M. Santoro

London Centre of Nanotechnology, United Kingdom

G. Aeppli

Massachusetts Institute of Technology

J. Santillan

Max Planck Institut für Chemie, Mainz, Germany

R. Boehler
D. A. Dzivenko
M. I. Eremets

Max Planck Institut für Festkörperforschung, Stuttgart, Germany

G. Gu
H. U. Habermeier
B. Liang
C. T. Lin
K. Syassen
C. Ulrich
H. Zhang

Moscow State University, Russia

B. N. Feygelson

Nagoya University, Japan

T. Okuchi

National Aerospace Laboratories, India

A. K. Singh

National Cheng-Kung University, Taiwan

J. Kung

National Institute for Materials Science, Japan

S. Nakano
T. Sekine

National Institute of Standards and Technology

T. Jenkins

J. Leão

S. Prosandeev

National Laboratory of Superhard Materials, Jilin, China

C. Gao

National Research Council, Ottawa

D. J. Klug

J. S. Tse

National Synchrotron Radiation Research Center, Taiwan

Y. Q. Cai

C. C. Chen

C. T. Chen

P. Chow

E. P. Huang

H. Ishii

I. P. Jarringe

C. Kendziora

Naval Research Laboratory

S. J. Charles

J. E. Butler

New Jersey Institute of Technology

J. P. Carlo

C. Cui

Y. Qin

T. Tyson

Z. Zhong

New Mexico State University

B. Kiefer

Northern Illinois University

D. E. Brown

M. R. Frank

S. J. Maglio

Northwestern University

K. Brister

S. Jacobsen

Y. C. Tseng

Nuclear Research Center-Negev, Israel

I. Halevy

Oak Ridge National Laboratory

M. Guthrie

G. E. Ice

B. C. Larson

C. A. Tulk

J. Z. Tischler

Okayama University, Japan

H. Fuki

Physikalisches Institut, Germany

K. J. Choi

G. Guentherodt

Purdue University

P. C. Doerschuk

Rensselaer Polytechnic Institute

A. Sharma
E. B. Watson
Heather Watson

Rutgers University

Martha Greenblatt
M. V. Lobanov

Royal Institution, London, United Kingdom

P. McMillan
E. Soignard

Royal Institution of Technology, Sweden

A. Delin
B. Johansson
V. Kachana
G. Vaitheeswarn

Rutherford Appleton University, United Kingdom

W. G. Marshall

St. John Fisher College

Kristina M. Lantzky

School of Physics & Astronomy, Tel Aviv, Israel

A. Milner
M. P. Pasternak

Scripps Oceanographic Institute

I. Gan
I. Gertsman
J. E. Johnson
T. Lin

Seoul National University, Korea

S. K. Lee

Soliel, France

R. Fourme

Spring-8, Japan

A. Q. R. Baron
S. Tsutsui

Steacie Institute for Molecular Science, Canada

S. Patchkovskii

Stanford University

G. E. Brown
Tanja Cuk

SUNY-Stony Brook

J. Chen
Jennifer King
B. Li
L. Li
C. D. Martin
J. B. Parise
L. Wang
D. J. Weidner

Technological Institute for Superhard and Novel Carbon Materials, Russia

N. R. Serebryanaya

Texas Christian University

R. Senter

Texas Tech University

Y. Ma
V. Levitas
J. Sandhu
E. Selvi
J. Rasty
A. White

Tohoku University, Japan

K. D. Litasov
E. Ohtani

Tokyo Institute of Technology, Japan

K. Hirose
T. Komyayashi

Universidad Complutense de Madrid, Spain

J. Santamaria
M. Varela

Universidad de La Laguna, Spain

J. Lopez-Solano

A. Mujica
A. Muños
S. Radescu

P. Rodriguez-Hernandez

Università di Roma Tre, Italy

G. Della Ventura

Università di Trento, Italy

L. Lutterotti

G. Mariotto

Università G. D'Annunzio, Italy

Gianluca Iezzi

Universität Bonn, Germany

Winfried Kockelmann

N. Zotov

Universitat de Valencia, Italy

D. Errandonea

C. Ferrer-Roca

N. Garro

J. Pellicer-Poers

A. Segura

Universitat Politècnica de València, Spain

F. J. Manjòn

Université Catholique de Louvain, Belgium

X. Gonze

Université Parisé, France

P. Cartigny

University College London, United Kingdom

D. Dobson

University of Aarhus, Denmark

A. Svane

University of Alaska

T. Trainor

University of Arizona

R. T. Downs
W. B. Hubbard
D. Krishnamoorthy
A. Krishnamurthy
M. Origlieri
C. Prewitt
Kimberly Tait

University of Arkansas

A. Khanna

University of Bristol, United Kingdom

H. Darwish

A. E. Mora

J. W. Steeds

University of California, Berkeley

A. A. Correa
G. Ischina
R. Jeanloz
S. Merkel
W. B. Montgomery
D. Prendergast
S. Speziale
Caterina E. Tommaseo
Z. Wu

University of California, Davis

D. M. Krol
Brian Maddox
W. E. Pickett
R. T. Scalettar

University of California, Los Angeles

Abby Kavner
Anat Shahar
Sarah Tolbert
Michelle Weinberger

University of California, Riverside

H. Green, II
Larissa Dobrzhinetskaya
J. Zhang

University of California, Santa Cruz

Q. Williams

University of Chicago

X. Hong
A. Kuznetsov
J. J. Pluth
V. B. Prakapenka
M. L. Rivers
W. Schildkamp
S. R. Sutton

University of Colorado

B. D. Haugen
C. M. Holl
J. R. Smyth
H. Spetzler

University of Connecticut

P. D. Mannheim

University of Edinburgh, United Kingdom

Olga Degtyareva
E. Gregoryanz
J. Loveday

R. J. Nelmes

University Firenze, Italy

R. Bini
M. Ceppatelli
D. Chelazzi
M. Santoro
V. Schettino

University of Guelph, Canada

D. T. Jiang

University of Hawaii

G. M. Amulele
M. H. Manghnani
L. Ming
S. Sharma
S. Tkachev

University of Hyogo, Japan

Y. Akahama
H. Kawamura

University of Illinois

J. D. Bass
B. Chen
H. Hellwig
W. Huang
A. S. Lagutchev
D. L. Lakshtanov
J. Li

Jennifer M. Jackson

Y. Pang

J. P. Perrillat

Carmen Sanches-Valle

J. Wang

University of Kaiserlautern, Germany

H. J. Jodl
J. Kreuzt

University of Kentucky

G. Cao

University of Louisville

G. A. Lager

University of Manitoba, Canada

F. Hawthorne

University of Maryland

A. J. Campbell

B. Liang

University of Michigan

Wendy Panero

L. Stixrude

University of Minnesota

S. Demouchy

University of Missouri, Kansas City

B. Chen

E. P. Gogol

M. B. Kruger

J. Murowchick

University of Nebraska at Omaha

J. Liu

W. N. Mei

University of Nevada-Las Vegas

C. Chen

A. L. Cornelius

M. Daniel

H. Giefers

C. L. Gobin

T. Hartmann

D. Hartnet

O. A. Hemmers

X. Ke

E. Kim

R. S. Kumar

M. K. Jacobsen

Kristina Lipinska-Kalita

Patricia E. Kalita

J. McClure

M. Nicol

T. Pang

Z. Quine

E. Romano

Y. Shen

W. Stanberry

Elizabeth A. Tanis

I. Tran

O. Tschauner

University of Nevada-Reno

D. Chandra

S. Chandra

R. Chellappa

University of New Mexico

C. Agee

University of Northern Florida

L. V. Gasparov

D. Arenas

University of Ottawa, Canada

S. Desgreniers

R. R. Flacau

J. S. Smith

University of Paris VI, France

J. Badro

G. Calas

G. Fiquet

Chrysteal Sanloup

University of Saskatchewan, Canada

N. Chen

University of Tennessee

M. Anand

L. A. Taylor

University of Texas, Arlington

S. Sharma

University of Tokyo, Japan

S. Merkel

M. Takigawa

T. Yagi

University of Toronto, Canada

M. Fujihashi

University of Tsukuba, Japan

K. Matsuishi

University of Warsaw, Poland

W. Grochala

University of Warwick, United Kingdom

D. L. Carroll

M. L. Newton

University of Washington

J. M. Brown

University of Western Ontario, Canada

S. R. Shieh

Y. Song

University of Wyoming

S. Sampath

Uppsala University, Sweden

R. Ahuja

W. Luo

Verkin Institute, Kharkov, Ukraine

Y. A. Freiman

M. A. Strzhemechny

S. M. Tret'yak

Vernadsky Institute, Moscow

Delia Tchkheta

M. A. Nazarov

Virginia Polytechnic Institute

R. J. Angel

B. E. Hanson

Carla Slebodnick

Nancy L. Ross

J. Zhao

Waseda University, Tokyo, Japan

Y. Ohki

Washington State University

J. E. Patterson

Washington University, St. Louis

S. Deemyad

J. J. Hamlin

J. S. Schilling

Wilbur Wright College

W. Pravica

Woods Hole Oceanographic Institution

N. Shimizu

Zhejiang University, China

C. M. Feng

J. Z. Jiang

Q. S. Zeng

3.3 Undergraduate Student Scholars

A number of university undergraduate students participating in the highly successful Carnegie Summer Intern Program (Fig. 53) have worked on projects directly related to CDAC goals during the past year. This NSF-funded program, which is run by CDAC coordinator **Stephen Gramsch**, seeks to identify students at smaller institutions who may not have the opportunity for front-line research during the academic year, or students without a significant research background. At **Carnegie**, such students experience a rigorous an introduction to scientific research, and within the structure of CDAC, are learning about the important problems in the field of high-pressure research. During the summers of 2006-2007, the following students participated in this program.

2006:

Cheng Chin, Columbia University

*Optical Emission Spectroscopy of Simulated Microwave Plasma Enhanced CVD
Diamond Growing Process*

Benjamin Haugen, University of Colorado

*Optical Absorption Spectra of Iron-Bearing Magnesium Silicate Perovskite at Lower
Mantle Pressures*

Seth Jacobsen, Cornell University

A Genetic Algorithm for Predicting High-Pressure Phases of Water Ice

Frances Reid, Carleton College

High-Pressure Synchrotron Infrared Studies of OH in Silicate Perovskite

Robert Thomas, University of Maryland

Platinum Group Element Partitioning in the Iron-Sulfur-Ruthenium System

2007:

Seth King, Purdue University

Investigation of the High P-T Phase Diagrams in the H₂-He System

Zachary Newman, Case Western Reserve University

Melting of Silicon at High Pressures



Figure 53. 2007 Carnegie Summer Scholars.

Former CDAC summer undergraduate intern **Andrea F. Young** was the first author on two papers in 2006. The first, published in *Physical Review Letters*, was on the discovery of new metal nitrides. This work was done in collaboration with former CDAC Scientist **Eugene Gregoryanz**

(currently at the **University of Edinburgh**), **Crystele Sanloup** (**Universit e Pierre et Marie Curie**), **Sandro Scandolo** (**Democritos National Simulation Center** in Trieste), **Russell Hemley**, and **Ho-kwang Mao** (**Carnegie**)⁹⁶. The second paper was on a theoretical study of PtN₂ and appeared in *Physical Review B*⁹⁷. He carried out the latter work during a 2005 internship summer in Trieste at the **Democritos National Simulation Center**. He has finished studies at **Columbia University** has started graduate school in physics.

3.4 DC Area High School Outreach

Every year at **Carnegie**, several local high school students are hosted and offered guidance in their science fair projects and in other areas of research. In 2006, three students from Washington, DC worked on various projects with **Carnegie** scientists. **Alexander Levedahl**, who worked with **Maddury Somayazulu**, used the research he completed on the preparation and characterization of a hydrogen clathrate hydrates to enter the 2006 Intel Science Talent Search. **Andrew Kung** worked with **Chang-Sheng Zha** on the development of resistive heating methods for hydrogen at high pressure. Kung measured the frequency of the H₂ vibron at 20 GPa, from 300 to 500 K. Both students continuing their work at **Carnegie** over the course of the 2006-2007 school year. **Kung** and **Levedahl** also returned in the summer of 2007 to continue their research (Fig. 54).

2006:

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

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

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

2007:

Andrew Kung, Winston Churchill High School, Potomac, MD
Temporal and Compressional Behavior of X-Ray Induced Dissociated Water

Alexander Levedahl, St. Anselm's Abbey School, Washington, DC
Stability of a H₂-H₂O Clathrate at High Pressures

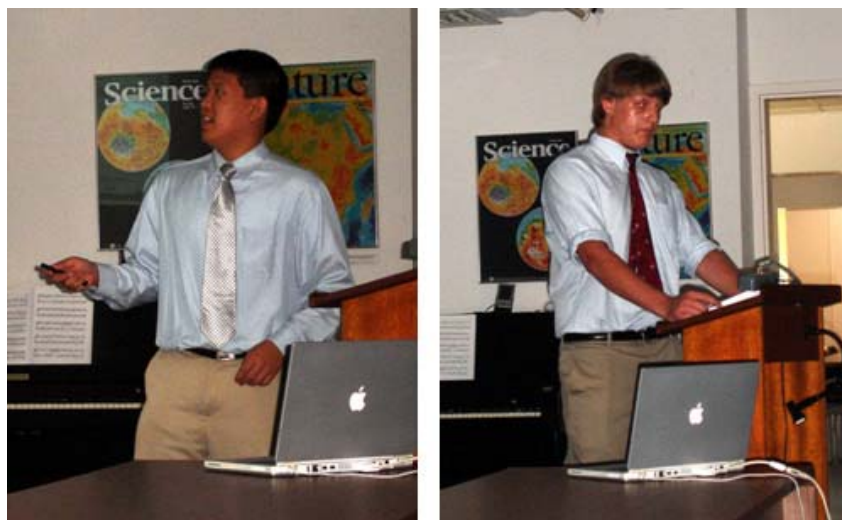


Figure 54. 2007 High School summer scholars, **Andrew Kung** (left) and **Alexander Levedahl** (right), presenting their research at the Summer Scholar Seminar.

3.5 2007 Stewardship Science Academic Alliances (SSAA) Program Symposium

The third annual SSAAP symposium was hosted by **Carnegie** at its historic administration building on February 5-7 in downtown Washington, DC (Fig. 55). Center directors and individual grant recipients 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 program, and CDAC laboratory partner **Dana Dattlebaum (LANL)** gave a keynote address outlining the high pressure materials science activities at **Los Alamos**. University of Nevada-Reno student **Raja Chellappa** (now a postdoctoral fellow at **Carnegie**) gave a talk about high pressure research on complex hydrides and energy storage materials.



Figure 55. The Carnegie Institution of Washington's administration building, site of the 2007 Stewardship Sciences Academic Alliances Program symposium.

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

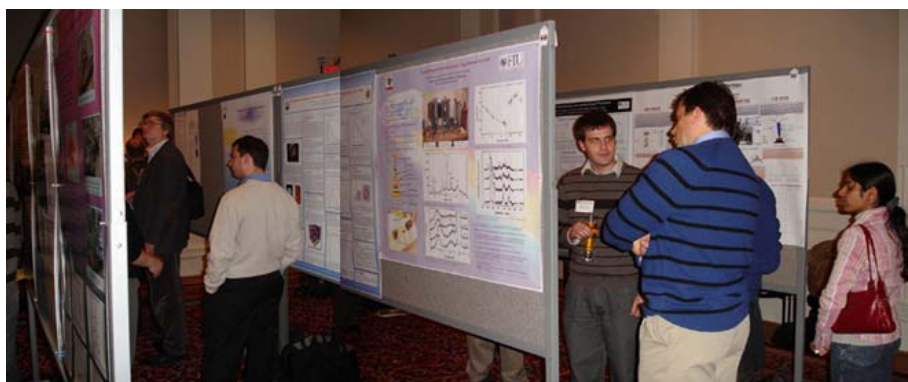


Figure 56. Poster session during the 2007 SSAA symposium in Washington, DC.

At the student poster session (Fig. 56), CDAC graduate students were well represented, with 14 of the 19 students currently supported giving poster presentations. In all, 30 posters were presented by CDAC students, postdoctoral fellows, collaborators and partners. The following is a list of CDAC related talks and posters:

Aihaiti, M., Novel phase transitions in perovskite ferroelectrics under pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).

Aksoy, R., X-ray diffraction study of molybdenum diselenide to 35.88 GPa, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).

- Aksoy, R., High pressure x-ray diffraction studies of titanium disulfide, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Beck, P., A. F. Goncharov, V. Struzhkin, B. Militzer, and R. J. Hemley, Measurements of thermal diffusivities under planetary interiors pressure temperature conditions, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chellappa, R., Pressure-induced transformations and order-disorder phenomena in Li-based complex hydrides: Implications to hydrogen storage, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chellappa, R., D. Chandra, S. Gramsch, M. Somayazulu, and R. J. Hemley, High pressure research on complex hydrides and energy storage materials, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chen, X. J., Optical evidence for the metallization of solid silane under pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chen, X. J., Superconductivity and lattice effects in mercury-based superconductors, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chen, X. J., On the oxygen isotope effect in high-Tc superconductors, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Cunningham, N., High pressure structural phase transformations in heavy rare earth metal terbium to 154 GPa: Evidence for f-shell delocalization, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Esler, K., Computational prediction of material properties under extreme pressure: The equation of state of cubic boron nitride, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Goncharov, A. F. and J. Crowhurst, Simple molecular materials under conditions of high pressure and temperature, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Gupta, Y. M., Institute for Shock Physics: Research objectives, activities, and capabilities, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Hemley, R. J., New developments at CDAC - The Carnegie/DOE Alliance Center: A center of excellence for high pressure science and technology (invited), *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Japel, S. and B. Keifer, Iron phosphide (Fep) to 60 GPa: Equation of state and phase transition, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Jenkins, T., W. Mao, H. K. Mao, V. Struzhkin, B. Militzer, and R. J. Hemley, High pressure hydrogen clathrate research using inelastic neutron scattering and x-ray diffraction, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Jiang, F., G. D. Gwanmesia, and T. S. Duffy, Elasticity of stishovite and acoustic mode softening under high pressure by Brillouin scattering, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Kollias, A., Ab initio study of the pressure-induced spin transition in $Mg_{1-x}Fe_xO$, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Krasnicki, S., C. S. Yan, J. Lai, H. Y. Shu, T. Yu, S. S. Ho, Y. Meng, H. K. Mao, and R. J. Hemley, Fabrication and properties of large CVD diamond single crystals, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Kulkarni, S., Ternary layered carbides - MAX phases, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Lee, K. and G. Steinle-Neumann, Pressure and chemistry-dependent electron-capture radioactive decay: ${}^7\text{Be}$, ${}^{22}\text{Na}$, and ${}^{40}\text{K}$ in crystalline materials, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Liu, Z., Synchrotron far-infrared spectroscopy and ab initio study of phonon density of states in ice VII at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Lucas, M., O. Delaire, M. Winterrose, I. Halevy, B. Fultz, M. Y. Hu, and J. Hu, Effect of vacancies on the pressure dependence of lattice dynamics in B_2FeAl , *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Mao, W. L., H. K. Mao, Y. Meng, P. Eng, M. Y. Hu, P. Chow, Y. Cai, J. Shu, and R. J. Hemley, X-ray induced dissociation of H_2O and formation of O_2-H_2 compound at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).

- Mao, W. L., H. K. Mao, W. Sturhahn, J. Zhao, V. B. Prakapenka, Y. Meng, J. Shu, Y. Fei, and R. J. Hemley, Iron-rich silicates at the Earth's core-mantle boundary, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Mao, Z., S. Jacobsen, F. Jiang, C. Holl, J. R. Smyth, and T. S. Duffy, Effect of water on the elastic properties of wadsleyite, B-Mg₂SiO₄, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., M. Y. Hu, P. Chow, E. Rod, A. Bommannavar, and G. Shen, X-ray spectroscopy beamline at HPCAT, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., H. P. Liermann, W. Wang, Y. Ding, E. Rod, A. Bommannavar, and G. Shen, Micro focus x-ray diffraction at high-pressure and low/high temperature at 16BMD (HPCAT): Present and future capabilities, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., S. Sinogeikin, H. Liu, E. Rod, A. Bommannavar, and G. Shen, Micro-focused angle dispersive undulator beamline for x-ray diffraction studies under extreme P-T condition, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., S. V. Sinogeikin, H. P. Liermann, P. Chow, E. Rod, and G. Shen, Online systems at Sector 16 (HPCAT): Efforts to improve beamtime efficiency, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., W. Wang, H. P. Liermann, Y. Ding, E. Rod, A. Bommannavar, and G. Shen, High energy x-ray diffraction at high-pressure and -temperature at 16BMB (HPCAT): Amorphous and melting studies, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Miyagi, L. and H. R. Wenk, Deformation of Earth materials at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Oelker, E., Pressure-induced amorphization of PbGeO₃ crystal, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Runge, C., A. Kubo, B. Kiefer, V. B. Prakapenka, G. Shen, and T. S. Duffy, Equation of state of MgGeO₃ post perovskite to 65 GPa: Comparison with perovskite phase, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, V. B. Prakapenka, and G. Shen, Experimental determination of binary phase diagrams at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Sha, X. and R. Cohen, Multiscale modeling of iron at high temperatures and pressures, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Somayazulu, M., S. Gramsch, H. K. Mao, and R. J. Hemley, High pressure-high temperature studies on Xe-Cl₂, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Surber, E., Surfaces and interfaces of high explosives probed by nonlinear spectroscopy, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Vohra, Y. K. and S. T. Weir, Development of designer diamond technology for high pressure high temperature experiments in support of stockpile stewardship program, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Vorberger, J., I. Tamblyn, S. A. Boney, and B. Militzer, Dense fluid hydrogen and helium in the interior of giant planets, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Zha, C. S., R. J. Hemley, S. A. Gramsch, H. K. Mao, and W. A. Bassett, Optical study of H₂O ice to 120 GPa: Dielectric function, molecular polarizability, and the equation of state, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Zha, C. S., R. J. Hemley, S. A. Gramsch, H. K. Mao, W. A. Bassett, and K. Mebe, New internal resistive heating DAC extends the thermal equation of state of platinum to 80 Pa and 1900 K, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).

3.6 SMEC 2007: Study of Matter at Extreme Conditions

The 2007 meeting for the Study of Matter at Extreme Conditions (SMEC) from April 15-20 in Miami was a great success. The conference was sponsored by CeSMEC and CDAC, and featured 46 scientific presentations from CDAC affiliated scientists (including 42 abstracts and 5 Symposia Panel Talks). Graduate students and postdoctoral fellows at CDAC institutions included **Resul Aksoy** (Texas Tech), **Emre Selvi** (Texas Tech), **Lowell Miyagi** (Berkeley), **Wendy Mao** (LANL), **Michelle Weinberger** (Carnegie), **Matt Schrenk** (Carnegie), **Muhetaer Ahart** (Carnegie), along with new CDAC-Affiliated Staff Member **Takamitsu Yamanaka** and former CDAC students and post-docs **Jennifer Jackson** (Caltech), **Sebastien Merkel** (Universite des Sciences et Technologies de Lille), **Sung Keun Lee** (Seoul National University), **Eugene Gregoryanz** (University of Edinburgh) and **Kristina-Lipinska Kalita** (UNLV). Symposia Panel talks were presented by Carnegie staff members **Alexander Goncharov**, **Yingwei Fei**, and **Ronald Cohen**, as well as HPCAT scientists Haozhe Liu (with **Martin Kunz** from ALS) and **Hanns-Peter Liermann** (with **Hyunchae Cynn** from LLNL).

- Ahart, M., M. Somayazulu, R. E. Cohen, and R. J. Hemley, Morphotropic phase boundary in a pure material: Pressure induced phase transitions in PbTiO_3 , *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Aksoy, R., E. Selvi, and Y. Ma, High pressure x-ray diffraction studies of nickel disulfide, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Aksoy, R., E. Selvi, and Y. Ma, X-ray diffraction study of niobium diselenide to 45.1 GPa, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Benmore, C. J., Q. Mei, J. L. Yarger, S. Sen, and J. Parise, The first and second sharp diffraction peaks in network and molecular glasses, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cohen, R. E., Theory of minerals at high pressure beyond band theory, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cohen, R. E., Theory and experiments on ferroelectrics and other active materials, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cohen, R. E. and Z. Wu, Prediction of pressure induced morphotropic phase boundary in PbTiO_3 and the origin of giant electromechanical coupling via polarization rotation, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cynn, H. and H. P. Liermann, Mechanical properties under extreme conditions, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Drozd, V., S. K. Saxena, A. Durygin, and S. V. Garimella, Chemical reactions for hydrogen storage and generation, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Fei, Y., Chemistry and physics of the Earth's deep interior, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Gao, C., Y. Ma, Y. Han, M. Li, and G. Zou, In-situ conductivity measurement of matter under extreme conditions by film fabrication of diamond anvil cell, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Gao, C., Y. Ma, J. He, D. Yu, and Y. Tian, In-situ x-ray diffraction of BCN compound under pressure up to 30 GPa, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Goncharov, A., Simple molecular systems under high pressure and temperature, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Goncharov, A., Molecular systems under high compression, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- He, C., C. Gao, and Y. Ma, In-situ electrical property study of CdSe under pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- He, C., C. Gao, and Y. Ma, Electrical impedance spectrum study of CdS under high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Jackson, J. M. and L. Wagner, Elasticity of orthopyroxene at high-temperature: Novel phase transitions and applications to geophysics, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Jung, H., Y. Fei, P. S. Silver, and H. W. Green, Detecting acoustic emissions at high pressure and high temperature using multianvil press: Application to deep seismicity, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).

- Kharlamova, S. A., A. G. Gavriiliuk, S. Sinogeiken, V. V. Struzhkin, I. S. Lyubutin, W. Sturhahn, and S. G. Ovchinnikov, Phase transitions in $\text{GdFe}_3(\text{BO}_3)_4$ under high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Kubo, A., B. Keifer, S. H. Shim, G. Shen, V. B. Prakapenka, R. J. Cava, and T. S. Duffy, Rietveld structure refinement of MgGeO_3 post perovskite (ppv) phase to 1 Mbar, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Kumar, R. S., A. L. Cornelius, M. F. Nicol, M. Y. Hu, P. Chow, E. D. Bauer, and J. L. Sarrao, Valences changes in YbCu_2Si_2 and YbAgCu_4 studied by high pressure x-ray absorption and resonant inelastic x-ray scattering, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Lazor, P., H. K. Mao, W. L. Mao, J. Shu, M. Y. Hu, P. Chow, M. Somayazulu, and R. J. Hemley, X-ray induced dissociation of NH_3 at high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Lerche, M., W. Sturhahn, G. Shen, V. B. Prakapenka, A. Ryder, and K. S. Suslick, Synchrotron mossbauer spectroscopy of amorphous iron at pressures up to 30 GPa, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Liermann, H. P., W. Yang, S. Sinogeiken, G. Shen, H. Cynn, S. Merkel, H. R. Wenk, M. Somayazulu, and P. Dera, Measurement of mechanical properties of materials at high-pressure and temperatures in the diamond anvil cell, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Lipinska-Kalita, K. E., O. A. Hemmers, P. E. Kalita, G. Mariotto, Y. Ohki, S. A. Gramsch, R. J. Hemley, T. Hartmann, and L. Ma, Amorphous matrix-based composite materials: Fabrication, high-pressure structural integrity and structural transformations, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Liu, H., X-ray scattering studies for materials under high pressure: From powder to amorphous samples, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Liu, H. and M. Kunz, High-pressure materials science: Synchrotron x-ray scattering studies *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, H. K. and W. L. Mao, Hydrogen storage in molecular compounds, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, H. K., G. Shen, and R. J. Hemley, High-Pressure Synergetic Center (HPSynC) - The APS-wide approach to high-pressure synchrotron research, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, W. L., H. K. Mao, Y. Meng, P. Eng, M. Y. Hu, P. Chow, Y. Q. Cai, J. Shu, and R. J. Hemley, X-ray induced dissociation of H_2O and formation of an $\text{O}_2\text{-H}_2$ compound at high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, W. L., V. V. Struzhkin, A. Baron, C. Tommaseo, H. R. Wenk, M. Y. Hu, P. Chow, J. Shu, R. J. Hemley, D. L. Heinz, and H. K. Mao, Experimental determination of elasticity of iron at high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Merkel, S., H. R. Wenk, and C. Tomé, Evaluation of stress in high pressure radial diffraction experiments: Application to Co, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. S. Duffy, and H. R. Wenk, Texture development in the CaIrO_3 post-perovskite phase deformed in the multi-anvil press up to 5 GPa and 1300 K, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Oganov, A. R., Y. Ma, J. Chen, Y. Ma, and C. W. Glass, Light elements under pressure: Insights into unusual structures and bonding, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Palasyuk, T., M. Tkacz, L. Dubrovinsky, A. Durygin, and S. K. Saxena, Raman studies of REH_3 under pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Prakapenka, V. B., A. Kunznetsov, S. V. Sinogeiken, M. L. Rivers, and S. R. Sutton, Pressure-assisted synthesis of nano-sized materials in a diamond anvil cell, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Pravica, M., H. Giefers, Z. Quine, E. Romano, B. Yulga, S. Bajar, W. Yang, and H. P. Liermann, Radiation-induced decomposition of energetic materials, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Schrenk, M. O. and R. J. Hemley, Physiological adaptations of microorganisms to the environmental changes of the deep biosphere, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Singh, A. K., H. P. Liermann, Y. Akahama, and S. K. Saxena, The pressure and grain-size dependence of strength of platinum to 330 GPa from the x-ray diffraction data, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).

- Soignard, E., J. Yarger, S. Amin, and Q. Mei, Pushing new boundaries in high pressure x-ray diffraction within supercooled liquids and amorphous solids: exploration of phase transformations, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Struzhkin, V. V., A. G. Gavriluk, and I. S. Lyubutin, Pressure-induced spin transition in multiferroics and related compounds, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Vennila, S., A. Durygin, M. Merlini, and S. K. Saxena, High pressure - high temperature study on TiH₂ up to 823 K, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Vennila, S., L. George, V. Drozd, and S. K. Saxena, In situ x-ray diffraction and Raman study on the phase transformation in LiAlH₄ under high pressure - A comparison, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Wang, L., H. Liu, J. S. Tse, and H. K. Mao, Experimental and first-principles calculation studies for several NIST x-ray powder diffraction standards under high pressure conditions, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Weinberger, M., J. Levine, H. Y. Chung, R. Kaner, A. Kavner, and S. Tolbert, In situ studies of osmium and transition metal diborides under high stress conditions, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Yang, W., W. Liu, B. C. Larson, G. E. Ice, H. P. Liermann, and G. Shen, Deviatoric and dilation strain measurements with x-ray micro-diffraction, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).

3.7 Pressure Calibration Workshop

CDAC-affiliated Carnegie staff member **Alexander Goncharov** and an organizing committee including CDAC academic partner **Thomas Duffy** (Princeton), **Yingwei Fei** (Carnegie), **Kurt Leinenweber** (Arizona State) and **Russell Hemley** (Carnegie) recently convened a workshop on "Current Status and Prospects for Establishing Precise and Accurate Pressure Scales at High Temperature." Held at Carnegie's Broad Branch Road campus in Washington, DC, January 26-28, 2007 the workshop featured 13 scientific talks by leaders in the science and technology of pressure calibration. Keynote presentations were given by **Wilfried Holzapfel** (Paderborn, Germany), **William Nellis** (Harvard University), **Ho-kwang Mao** (Geophysical Laboratory, Carnegie), **Agnes Dewaele** (CEA, France), **Kenichi Takemura** (NIMS, Japan), **Jay Bass** (Illinois), **Baosheng Li** (Stony Brook) and **Renata Wentzcovich** (Minnesota).



Figure 57. Attendees of the workshop on "Current Status and Prospects for Establishing Precise and Accurate Pressure Scales at High Temperature."

The proceedings from the meeting will be published in an upcoming special issue of the journal *High Pressure Research*.

Figure 58. William Nellis (Harvard University) delivers a lecture entitled, "Reduced-Adiabatic Isotherms of Metals" at the workshop.



Lecturers – Talks were given by thirteen presenters who are leaders in the field of pressure calibration. Lecturers supported by CDAC funds (staff, partners, post-doc, etc.) are designated by an asterisk (*)

Scientific Session I (Discussion Leader: Russell Hemley)

Wilfried Holzapfel (University of Paderborn, Germany), *EOS simple solids for wide ranges in pressure and temperature*

William Nellis (Harvard University, Fig. 58), *Reduced-adiabat isotherms of metals*

Ho-kwang Mao* (Geophysical Laboratory), *Three challenges of pressure calibration – 1% accuracies in 0.1-1 GPa, 100-300 GPa, and 1000-5000 K*

Alexander Goncharov* (Geophysical Laboratory), *High pressure calibration at high temperature using cBN and fluorescence standards*

Agnes Dewaele (CEA), *Isotherms of metals by static compression pressurizing conditions and consequences on pressure calibration*

Peter Dorogokupets (Institute of the Earth's Crust SB RAS), *Pressure measurements at high temperature: open issues and solutions*

Scientific Session II (Discussion Leader: Yingwei Fei)

Jay Bass (University of Illinois), *Redundant measurements in MgO, NaCl at high temperatures*

Renata Wentzcovitch (University of Minnesota), *PVT relations in MgO: an ultra-high PT scale for planetary sciences application*

Baosheng Li (Mineral Physics Institute, Stony Brook), *Elasticity*

Neil C. Holmes (Lawrence Livermore National Laboratory), *Platinum sensor*

Scientific Session III (Discussion Leader: Jay Bass)

Frederic Datchi (University of Paris), *Optical sensors for high temperature studies in DAC: the case of cubic BN, diamond and Sm-doped SrBO*

Takemura Kenichi (NIMS), *Pressure scales and hydrostaticity*

Yuichi Akahama (University of Hyogo), *Diamond Anvil Raman Gauge as a practical pressure determination method in Multimegabar pressure Range*

3.8 Visitors to CDAC

As part of CDAC's outreach program, **Carnegie** receives many visiting scientists each year. These scientists utilize the **Carnegie** laboratory facilities to prepare and perform experiments that would be impossible to do at their home institutions. Scientists from around the country and the world have visited **Carnegie** to take advantage of this program.

C. Tulk S. Chae J. Molaison	Oak Ridge National Laboratory	SNAP update	September 12, 2006
P. Lazor	University of Uppsala	Gas loading ammonia	September 21-22, 2006
H. P. Liermann	HPCAT	Gas loading	September 26-27, 2006
A. Martinez	Opticut, Inc	Diamond cutting	September 29-October 2, 2006
Svetlana Kharlamov	Argonne National Laboratory	Sample preparation in DAC for synchrotron experiments	October 2-October 4, 2006
W. Sturhahn	Argonne National Laboratory	Talk on sound velocities of iron-bearing Earth materials under extreme conditions	October 9-October 10, 2006
P. Liu	OMAX	STTR grant	October 16, 2006
R. Jaramillo	University of Chicago	Pulsed laser for cutting Cr single xals	October 25, 2006

R. Jaramillo	University of Chicago	Cutting Cr single crystals using pulsed laser	October 30, 2006
G. Chesnut	LANL	Preparing a resistive heating cell for expts at HPCAT	October 30-November 1, 2006
Wendy Mao	LANL	Sample preparation	October 30-November 6, 2006
A. Gavrilyuk	Institute for High Pressure Physics, Russian Academy of Sciences	Work with Viktor Struzhkin	November 16-December 21, 2006
R. Chellappa	University of Nevada – Reno	Sample loading	December 11-17, 2006
Y. Ma	Texas Tech University	Work with Ho-kwang Mao	December 15, 2006 – January 7, 2007
R. Chellappa	University of Nevada – Reno	Sample loading	February 1-March 1, 2007
D. Kurzdrowski	University of Warsaw, Poland	Work with Viktor Struzhkin	February 5-25, 2007
Svetlana Kharlamova	Argonne National Laboratory	Sample preparation in DAC for synchrotron experiments	February 22-25, 2007
R. Chellappa	University of Nevada – Reno	Sample loading	March 30-April 4, 2007
C. R. Rotundu	University of Maryland	Work with Viktor Struzhkin	April 5, 2007-ongoing
T. Yamanaka	Osaka University	Visiting investigator	April 5, 2007-ongoing
Y. Wu	China University of Geoscience	Origin of the ultra-high pressure metamorphic rocks discovered in Dabie Mt., China	April 11, 2007- ongoing
A. Gavriliuk	Institute for High Pressure Physics, Russian Academy of Sciences	Work with Viktor Struzhkin	April 13-May 16, 2007
C. Grant	LLNL	Work with Alexander Goncharov	June 13-14, 2007
C. Tulk	Oak Ridge National Laboratory	SNAP update	June 15, 2007
D. Spaulding	University of California – Berkeley	Sample loading	June 19, 2007
H. Jahn	Morgan Lewis	Diamond analysis	June 25, 2007
M. Strzhemechny		Work with Alexander Goncharov	July 2-3, 2007
S. Wax	SRI International	Diamond analysis	July 5, 2007
K. Landskron	Lehigh University	Work with Yingwei Fei	July 9-13, 2007
M. Lucas	California Institute of Technology	Sample loading	July 12, 2007
Anat Shahar	UCLA	Work with Yingwei Fei	July 16-27, 2007
E. Young	UCLA	Work with Yingwei Fei	July 16-19, 2007
T. Kuribayashi	Tohoku University	Work with Ho-kwang Mao	July 16-27, 2007
H. Liu	HPCAT	Discussions with CDAC staf	July 20, 2007
Jing Liu	Chinese Academy of Sciences	He gas loading	July 23-26, 2007
Lingyun Tang			
S. Richardson	University of Capetown	Diamond laser cutting	August 15-September 15, 2007
W. Xiao	Institute of Geochemistry, Chinese Academy of Sciences	Gas loading	August 6-30, 2007

Y. Bi	Institute of Fluid Physics, Chinese Academy of Engineering Physics	Gas Loading	August 6-September 10, 2007
J. Xu	Institute of Fluid Physics, Chinese Academy of Engineering Physics	Gas Loading	August 6-30, 2007; September 4-10, 2007
F. Peng	Sichuan University	Visiting with Ho-kwang Mao	August 24-September 6, 2007
Michelle Minnitti	Arizona State University	Visiting Investigator with Yingwei Fei	August 27, 2007-ongoing
G. Crabtree Michelle Buchanan	Argonne National Laboratory OLRN	DOE-BRN Workshop NNSA presentation	August 28, 2007
Kim Cone	George Mason University	Visiting Investigator with Robert Hazen	August 30-ongoing

3.9 High Pressure Seminars

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

P. Lazor	University of Uppsala	High pressure developments in uppsala	September 22, 2006
Q. Liang	University of Alabama-Birmingham	Applications of nanocrystalline diamond	September 29, 2006
M. Ahart	Carnegie	Spectroscopic studies of ferroelectrics, polymers and gelatin	October 12, 2006
P. Beck	Carnegie	Continuous and time-resolved Raman spectroscopy and radiometry in the DAC	October 19, 2006
C. Alexander	Carnegie	What the microscopic can tell us about the evolution of the solar system and galaxy	October 26, 2006
P. Griffin	Carnegie	Function complexity and artificial life	November 2, 2006
N. Romero	US Army Research Laboratory	First-principles calculations of shock compressed diamond and superconductivity in fullerene-based solids	November 9, 2006
M. Schrenk	Carnegie	Microbes at the bottom of the Marianas Trench grow at atmospheric pressures - Justifying a need for more high-pressure experimental microbiology	November 14, 2006
T. Jenkins	Carnegie	Low temperature, high pressure hydrogen clathrate an ice VIII analog	December 7, 2006
A. Sokolov	University of Akron	New kinds of optical spectroscopy with nano-size resolution	December 19, 2006

Y. Ma	Texas Tech University	High pressure in the panhandle	January 4, 2007
S. A. Khairallah	University of Illinois at Urbana-Champaign	Theory of para-hydrogen clusters: magic numbers and superfluid sizes	January 11, 2007
L. Yonggang	Geochemistry Institute, Guiyang, China	Challenges in Ultrasonic Measurements at High Pressure	January 26, 2007
Kanani Lee	New Mexico State University	Pressure- and chemistry-dependent electron-capture radioactivity	February 2, 2007
Jennifer Ciezak	Carnegie/ARL	New physics and chemistry of energetic materials at high pressure	February 22, 2007
Michelle Weinberger	Carnegie	Materials under high pressure and nonhydrostatic stress	March 16, 2007
Liwei Deng	Carnegie	Shock loading of MgSiO ₃ perovskite and implications for the lower mantle	March 22, 2007
D. Foustoukos	Carnegie	Formation of metastable carbon phases under hydrothermal conditions	March 30, 2007
P. Ganesh	Carnegie Mellon	Geometrical frustration in liquid Fe and Fe-based metallic glass	April 24, 2007
J. Vorberger	Carnegie	Melting of sodium under pressure (and a little bit about hydrogen-xenon)	May 2, 2007
Barbara Lavin	UNLV	The ion size constraint on the cation distribution determination in spinel	May 10, 2007
J. Cleaves	Carnegie	Geochromatography and the origins of life	June 7, 2007
P. Griffin	Carnegie	A survey of E. coli at high pressure	July 5, 2007
T. Komabayashi	Carnegie	Phase transition in CaSiO ₃ perovskite: Detecting subducted oceanic crust in the Earth's lower mantle	July 12, 2007
T. Kuribayashi	Tohoku University, Japan	Structure variation of humite minerals and Phase A under high-pressures	July 19, 2007
H. Liu	HPCAT	Synchrotron x-ray scattering studies of materials under pressure: From A to Z	July 20, 2007
Anat Shahar	University of California – Los Angeles	High-temperature iron isotopic fractionation - An experimental approach	July 24, 2007
Kai Landskron	Lehigh University	Phosphorus(V)-nitrides with high framework densities and their mesoporous forms	July 30, 2007
J. Janik	Florida State University	Understanding hidden order in URu ₂ Si ₂ : Inelastic neutron scattering studies of itinerant spin excitations	August 1, 2007
C. Rotundu	University of Maryland – College Park	PrOs ₄ Sb ₁₂ : High magnetic fields and La-alloying studies	August 3, 2007

W. Zhu	Simon Fraser University	Synthesis, structure, and properties of perovskite materials for multiferroism and piezoelectricity	August 30, 2007
K. Driver	Ohio State University	Pushing the envelope of accuracy and cost in high-pressure electronic structure theory: Application to elasticity of silica	August 30, 2007
Svetlana Kharlamova	Argonne National Laboratory	Pressure-induced phase transition in $\text{GdFe}_3(\text{BO}_3)_4$	September 27, 2007
J. Dick	University of California – Berkeley	Geochemical forces in protein evolution	September 28, 2007

4. TECHNOLOGY DEVELOPMENT

4.1 High P - T Experimental Techniques

High P - T Methods – **Carnegie** continues to perfect the fabrication of single crystal diamond by CVD with **LANL**⁹⁸. CDAC graduate student Wendy Mao, while a postdoctoral fellow at **LANL**, showed that the diamond can be used to generate multimegabar pressures⁹⁹. Additional studies of the strength and annealing effects were also carried out this year by undergraduate interns¹⁰⁰. Large single-crystal diamonds, transparent from the UV to IR, have been fabricated^{101, 102}. To enhance sample sizes in DACs for neutron diffraction in the megabar range, diamond single crystals greater than 10 carats have been produced¹⁰³. The **Carnegie** CVD diamond synthesis has broad applications for NNSA/DP; single crystals have been produced for both static and dynamic compression in collaboration with teams at **SNL** and **LANL**¹⁰³.

New DACs were developed for integration of multiple probes and for reaching higher P - T conditions. P - V - T calibrations using both optical and x-ray methods were extended through **LLNL** collaborations¹⁰⁴. Advances in GHz interferometry provide an important complement to existing techniques for high pressure elasticity studies¹⁰⁵, creating another tool for stewardship science. An isotopically enriched ^{13}C homoepitaxial diamond layer grown on brilliant cut diamond anvil by CVD provides a new calibration to megabar pressure¹⁰⁶. New developments in rotational DACs (RDACs) allow controlled shear stress and strain to be generated and controlled for comparison with dynamic and quasi-static strength measurements at ambient pressure¹⁰⁷. Pulsed heating/Raman spectroscopy in DACs was developed¹⁰⁸. New electrical methods have been developed using FIB technology with a **Stanford** student¹⁰⁹. Building on the success of laser-shock molecular interface studies¹¹⁰, grazing incidence cells for SFG measurements have been constructed and tested, and the surface plasmon spectra of the photonic substrates and Raman spectra of monolayers inside a DAC have been measured.

New Classes of Synchrotron and Neutron Techniques – Synchrotron x-ray methods for measuring electron and phonon band structures at high P - T conditions were developed at HPCAT. Single crystal diffraction to higher pressure was extended, including work done in collaboration with **UNLV**¹¹¹. Neutron diffraction measured above 30 GPa¹¹² and the combination of large anvil and Kirkpatrick-Baez (K-B) focusing will make megabar studies possible in the next phase of CDAC. Pulsed laser heating and time-resolved measurements of IR reflectivity, electrical conductivity, and x-ray diffraction were developed^{81, 113}. As discussed above, *in situ* high P - T x-ray diffraction has been extended to above to above 9000 K¹¹⁴. **SNL** and **Carnegie** have tested time-resolved synchrotron IR techniques in dynamic compression experiments. At **LANL**, the team initially investigated texture changes associated with phase transformations in hexagonal metals^{115, 116} at LANSCE. Extending the thesis work of CDAC graduate student **Jenny Pehl**,¹¹⁷ current **Berkeley** graduate student

Lowell Miyagi is continuing this work, and is addressing phase transformations under applied as well as residual stress at LANSCE. The **NMSU** group is using LANSCE to investigate the effects of pressure on rates of radioactive decay. Techniques for obtaining quantitative texture information from single diffraction images were extended¹¹⁷. Methods have been developed to use 50 carat SiC crystals for pressurizing very large single crystals for neutron diffraction¹¹².

Coupling Dynamic Compression and Synchrotron Radiation – A key goal in the next phase of CDAC is to bridge the gap between static and dynamic compression measurements. There are great new opportunities for coupling lasers and synchrotron radiation for problems in stewardship science. An important recent milestone was successful installation, testing, and measurements with a gas gun at a synchrotron source; specifically with the **SNL** group made the first real-time IR measurements during dynamic compression¹¹⁸. This work will be extended to include other drivers, including larger gas guns and lasers with the **LLNL**, **WSU** and **LANL** groups. To test the feasibility of shock wave experiments using synchrotron x-rays, the **WSU** group performed preliminary experiments in April 2007 at HPCAT on both single crystal (LiF, Si) and polycrystalline (Ta) samples with single-bunch x-rays¹¹⁹. The first shock-wave experiments probed by synchrotron x-rays took place at HPCAT in August, 2007.

4.2 Facilities at ANS, BNL, and LANSCE

4.2.1 Technical Advances at HPCAT

Four simultaneously operating beamlines (now all available for general user access) having very different capabilities allow the flexibility for HPCAT to optimize various x-ray experiments and to



Figure 59. *Experimental setup in the spectroscopy station 16-ID-D at HPCAT.*

integrate them with optical, transport, and other measurements on the same samples at extreme *P-T* conditions. Currently commissioned x-ray diffraction techniques at HPCAT include angle- and energy-dispersive x-ray diffraction (ADX and EDXD). Single crystals, polycrystalline, amorphous and liquid samples can be routinely examined in the DAC. Thermal diffuse scattering (TDS) is now also a routine technique, as is radial diffraction. Two types of nuclear resonant scattering spectroscopy, nuclear forward scattering (NFS, also known as synchrotron Mössbauer spectroscopy) and nuclear resonant inelastic x-ray scattering (NRIXS) are available. X-ray emission spectroscopy (XES) is also performed in resonant mode (RXES); inelastic x-ray scattering (IXS) techniques also include the capability to do resonant inelastic x-ray scattering (RIXS), phonon inelastic x-ray scattering (PIXS) and

x-ray Raman spectroscopy (XRS). The beamlines have been designed so that x-ray absorption spectroscopy (EXAFS and XANES) can be implemented in the future if the demand is sufficient.

Spectroscopy Station – The ID-D station (Fig. 59) is dedicated to x-ray spectroscopy of materials under high pressure, with a typical beam size at the sample position is 20(v)x50(h) μm^2 . The sample stack can accommodate heavy devices such as cryostats and external heaters. An on-line spectrometer system is now available for Raman and pressure measurements. At present ID-D has a dedicated backscattering spectrometer with about 1 eV energy resolution. A 17-element backscattering analyzer array was commissioned late in 2007. Capabilities for higher resolution spectroscopy are being developed.

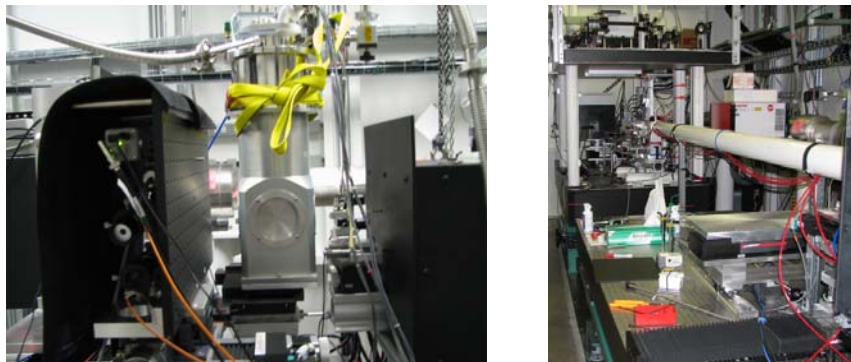


Figure 60. Configuration inside the 16-ID-B hutch. Left: cryostat on the general purpose table for high-pressure and low-temperature x-ray diffraction, with on-line spectroscopic system (at left) for pressure and Raman signal measurements. Right: two-table layout with general purpose table in the foreground and laser heating table in the background. Laser heating optics are set up on a table above the laser heating table.

Micro-diffraction station – The ID-B station has been recently re-configured into two major setups, one for general purpose micro-diffraction, and the other dedicated for laser heating experiments (Fig. 60). This two-table configuration in ID-B provides the necessary space and stability for a wide variety of different micro-diffraction applications. The general purpose table is designed for angle dispersive diffraction measurements with a monochromatic beam, and is capable of holding bulky and heavy equipment (e.g. cryostat, graphite resistive heating assembly, large high-pressure cells) and with minimum space restrictions. The open structure and flexibility of the general purpose table allows easy modifications for performing especially demanding experiments (e.g. single crystal measurements) and the development of new techniques (e.g. high-resolution diffraction with point detectors).

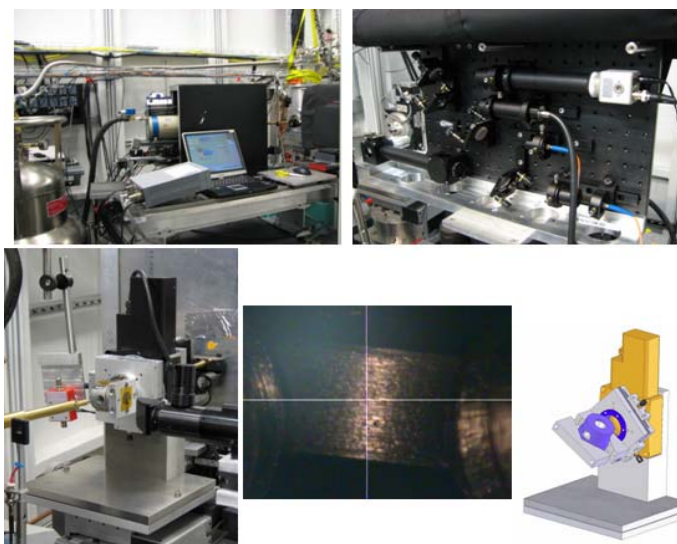


Figure 61. Features of the 16-BM-D beamline. Top left: detector setup. Top right: on-line pressure measurement system. Bottom left: radial diffraction setup at BM-D using a symmetric DAC. Bottom center: image of the centered Be gasket as seen by the online microscope. Bottom right: technical drawing of the membrane-driven DAC for symmetric cell and radial EDXD.

Micro-Diffraction with Both Polychromatic and Monochromatic Beams – Construction and commissioning of instrumentation on station BM-D is now complete. The station is now fully operational for white beam diffraction (Fig. 61). Significant improvements over other white beam diffraction stations are the small beam focus ($\sim 5 \mu\text{m}$) and the large flexibility in positioning and adjusting the collimation, (e.g. the angular resolution and collimation can be easily adjusted to optimize the experimental setup and to match the energy resolution of the detector). A new monochromator has been installed and is now available. This is therefore the only station that is

capable of doing both white beam, energy dispersive (EDXD) and monochromatic, angle dispersive (ADX) diffraction on powders and single crystals at extreme pressures and temperatures. Available techniques are:

- EDXD and ADXD (summer 2007) in the DAC at simultaneous high pressure and high temperature.
- EDXD and ADXD (spring 2007) in the DAC at high pressure and low temperature
- Single crystal EDXD diffraction for full structure refinements at high P in the DAC.
- Radial EDXD and ADXD for stress-corrected cell parameters, texture and strength of materials at high-pressure in the DAC that has been adapted with a membrane drive.

Micro-Diffraction with Polychromatic Beams – The BM-B station is dedicated for white beam diffraction. With the low divergence and broad energy spectrum of the APS source, a small focus spot has been obtained at the sample position with a broad white beam spectrum (to above 100 keV). The instrument allows changing the distance between the focusing optics and sample, with flexible focused beam sizes from 5 μm to 15 μm or larger depending on experimental requirements. The EDXD technique is now fully operational and open to general users. The sample stack can handle bulky devices such as a cryostat, resistive heating device, or Paris-Edinburgh cell. New capabilities under development or already in commissioning for use in this station include the scanning angle EDXD technique (Fig. 62), the combination white beam-Laue diffraction technique, the x-ray anomalous scattering technique, and x-ray absorption spectroscopy.

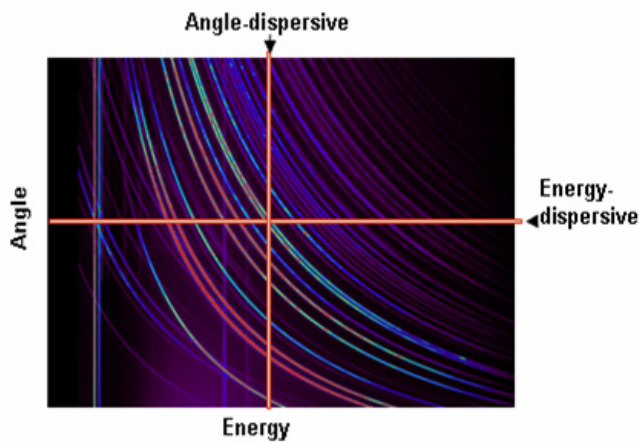


Figure 62. Two-dimensional image of intensity as a function of angle and energy from a Fe_2O_3 sample in a DAC. The plot yields data suitable for single crystal refinement and solves problems associated with the limited angular range imposed by the DAC

4.2.2 Developments at NSLS-U2A

Vibrational infrared (IR) spectroscopy provides unique, detailed information on the bonding properties of materials, thereby yielding a microscopic description of thermochemical properties. Use of synchrotron radiation for infrared studies substantially improves our ability to probe microscopic samples including *in situ* measurements under extreme conditions, due to its high brightness and broad-spectrum distribution. Beamline U2A on the VUV ring of the National Synchrotron Light Source is the first, and still the only, dedicated high-pressure synchrotron IR beamline in the world, with many unique capabilities compared to high-pressure x-ray beamlines. During the past four years, the beamline operation has been supported by CDAC and NSF-COMPRES (CONsortium for Materials Properties Research in Earth Sciences). In return, the IR beamline gives all CDAC and COMPRES users access to this world-class facility and makes available frontier high-pressure spectroscopic measurements as well as a diversity of other microspectroscopy experiments. A number of important scientific and technical challenges are being addressed at the facility, making it a highly attractive complement to x-ray sources.

During the past year, an exciting opportunity has arisen to create a side station on the beamline as a result of new space that has been created next to the U2 port. Part of the new configuration includes the vacuum pipe for beam delivery that was installed for the gas-gun shock wave experiments. The distance from the synchrotron source to the IR system will then be only about 3 meters (Fig. 63). This will remove the problem of beam divergence and image distortion. Ray-tracing calculations have indicated a significant improvement in spatial resolution. The new

facility will allow measurements on high-pressure samples with the highest spatial resolution possible at a synchrotron source while also having the highest broadband IR brightness. With a new microscope coupling a newly developed IR FPA detector and FTIR instrument, the facility will be ideal for mapping heterogeneous charges from high-pressure experiments, as well as laser heated samples *in situ* at very high pressure in diamond or moissanite anvil cells. Therefore, the side station facility will complement the main beamline, with its general-purpose microscopes, vacuum capability, far-IR features, and laser spectroscopy systems. Optical components are available to split the beam and allow the option of operating both the existing and the new station alternately.

In addition, this side station combined with the FTIR spectrometer, vacuum bench and custom IR microscope will provide new capabilities for studies in the THz region routinely. One of the important applications of THz spectroscopy is to investigate phase mixing and demixing in complex materials such as explosives, binders and foams. Current studies indicate that high-pressure far-IR spectroscopy is a powerful tool for resolving interactions between molecular species and surfaces in a variety of applications.

4.2.3 CDAC at LANSCE

At LANL, the team initially investigated texture changes associated with phase transformations in hexagonal metals^{115, 116} at LANSCE. **Berkeley** graduate student Lowell Miyagi is continuing work at the HIPPO diffractometer on texture development at high pressure in silicate perovskite and related materials, under applied as well as residual stress at LANSCE. The α - β quartz transformation was originally used as a model system, but the method has now also been applied to metals such as iron, and important Earth materials such as magnesio-wüstite and silicate perovskites. The NMSU group has made the first measurements at LANSCE on the effects of pressure on rates of radioactive decay. Techniques for obtaining quantitative texture information from single diffraction images were extended¹¹⁷. Methods have been developed to use 50 carat SiC crystals for pressurizing very large single crystals for neutron diffraction¹¹².

Phase II of the High-Resolution Chopper Spectrometer (PHAROS) led by CDAC academic partner Brent Fultz (**Caltech**) has been completed and is suitable for scattering angles between -10° and 140° . Yusheng Zhao (LANL) has designed a 500 ton TAP-98 device enabling neutron diffraction of large-volume samples to 20 GPa. Hemley and Mao are participants in the new Edinburgh center (CSEC) which is currently the leading group in high-pressure neutron research. Hemley is also a Co-PI of the high-pressure instrument (SNAP) at the Spallation Neutron Source (SNS). This facility is scheduled to receive its first neutron beams in mid-2007. CDAC is helping to bring the U.S. high-pressure neutron capability on a par with Europe, and is helping to build the U.S. high- P neutron community through workshops and collaborations. Results at moderate P have provided an accurate baseline for higher-pressure studies with other probes used within CDAC. Ultimately CDAC will advance neutron science to megabar pressures with the development of large volume DACs. With the proposed 3-4 orders of magnitude increase in DAC sample size and similar improvements in the neutron sources, optics, and detectors, the intensity deficit between x-ray and neutron diffraction methods eventually will be bridged. Neutron diffraction measured above 30 GPa¹¹² and the combination of large anvil and Kirkpatrick-Baez (K-B) focusing will make megabar studies possible in the next phase of CDAC.

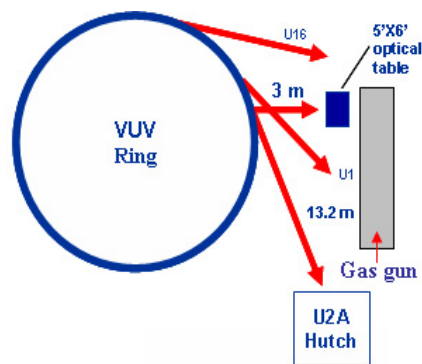


Figure 63. Arrangement of optical paths at the U2A beamline with the addition of a new side station. This configuration will improve spatial resolution for a variety of high pressure experiments as well as shock compression measurements.

5. INTERACTIONS WITH NNSA/DP LABORATORIES

5.1 Overview

As a primary part of its mission, CDAC seeks to provide access to all of the facilities maintained by our academic partner groups, as well as synchrotron beamlines and the CDAC high-pressure labs at Carnegie. Laboratory partners are also welcome to attend the regularly scheduled HPCAT meetings at the APS. We promote visits to the National Labs, university nodes, or **Carnegie** for experimental work and coordination of results. In all cases, travel support for graduate students has been provided from the core CDAC budget. The *CDAC Summer School* in 2005, and the *SSAAP Symposia* in Albuquerque (2004) and Las Vegas (2005) and Washington (2007), the *Synergy of 21st Century High-Pressure Science and Technology Workshop* in 2006 and the SMEC meeting in 2007 (Section 3.6) have all been highly successful ventures in terms of promoting interaction between CDAC students and scientists from the NNSA Labs. In addition, we have made other opportunities available to enhance collaboration and interaction:

- **Beam time for experiments at HPCAT.** Each year, groups from LLNL and LANL take advantage of discretionary beam time provided by CDAC to carry out experimental work in one or more of the sectors now on-line at HPCAT. Records of visits by NNSA Lab scientists, CDAC academic partners, CDAC collaborators, and other users are listed below in Appendix II. In the past year, we have made available beam time for groups from SNL and WSU to carry out the first synchrotron measurements of dynamic compression events at NSLS and HPCAT, respectively.
- **Carnegie high-pressure facilities.** During Year 4, we have interacted on a continuing basis with the high-pressure groups from LLNL and LANL, from hosting individuals and groups for specialized experimental procedures and sample preparation to arranging loans of specialized high-pressure cells for experiments at HPCAT and NSLS. In Year 4, 44 different people visited Carnegie for work at CDAC facilities.

The screenshot displays the CDAC website interface. At the top, there are logos for CDAC, Carnegie Mellon University, and the DOE/NSA Academic Alliance Program. The main content area features a research article titled "Spins under Pressure: Antiferromagnetism in Chromium". The article includes a graph of ordering temperature T_N (K) versus vanadium concentration x (%). The graph shows two data series: "Pure Cr under pressure" (red circles) and " $Cr_{1-x}V_x$ at ambient P" (blue squares). The T_N for pure Cr increases with pressure, while for the doped samples, it decreases with increasing vanadium concentration. The article text discusses the experimental challenges and the discovery of a new class of measurements on spin and charge density waves in single crystal metals. A "People Highlights" section on the right features a portrait of Ho-kwang Mao, who has been awarded the Inge Lehmann Medal of the American Geophysical Union for 2007. The website also includes a navigation menu on the left with options like Home, About CDAC, People, Facilities, Publications, Abstracts, and Contact Us.

Figure 64. Screen shot of the CDAC website, <http://cdac.gl.ciw.edu>

located at <http://cdac.gl.ciw.edu>, serves as a primary source of information to the CDAC community and the public (Fig. 64). The site presents an array of scientific and technical developments, meeting announcements and links, beam time updates, the site serves as gateway to high-pressure research not only at CDAC, but throughout the US and around the world. Publication records and abstracts for the CDAC community are updated regularly. Research highlights detailing information on new papers or research breakthroughs that have been supported by CDAC are also featured and updated on monthly basis.

5.2 HPCAT Membership and Beam Time Allocation

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

CDAC beam time is allocated based on the membership shares of each of the contributing members. For each beamline, the available shifts (three per day) during a beam time run period are totaled. After subtracting shifts for the General User Proposal (GUP) program of the APS (25% of beam time) and HPCAT time for technique development, beamline upgrades and staff research (25%), the available shifts are distributed among the HPCAT partners: **Carnegie** (25% of remaining time), CDAC (30%), LLNL H-Division (20%), and **University of Nevada-Las Vegas** (25%). At this point, that means approximately 30-35 shifts per beamline in a typical run period (about 200 shifts total) will go to CDAC academic partners, their students, and National Laboratory partners. During Year 4, 22 proposals were submitted for beam time through CDAC (14 from National Lab scientists and 8 from Academic Partners). Some of these proposals were granted beam time through the GUP process, allowing other users from within CDAC to benefit from the extra time allotted. In all cases, however, CDAC users who requested beam time were able to receive it. A detail of those who obtained beam time at HPCAT and the experiments they performed is given in Appendix II. In the future, it may become necessary to award beam time to those proposals not awarded GUP time on a competitive basis, but this has not happened as yet. Having three experimental stations with diffraction capabilities of various types ensures continued availability of beam time for the CDAC community.

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

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

6. MANAGEMENT AND OVERSIGHT

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

6.1 CDAC Organization and Staff

The Center is managed at **Carnegie**. The group leaders from each academic node of CDAC together with representatives from directorates (or divisions) at NNSA/DP Labs form an Executive Committee to direct and coordinate research, development, and access to facilities. The organizational structure of CDAC is shown in Fig. 65. CDAC directly supports the HPCAT facility and graduate students in the groups of the Academic Partners. Beam time at HPCAT and NSLS is awarded to the academic partners, laboratory partners and university collaborators. Coupled with beam time at **Carnegie**-managed facilities at the NSLS and interactions with National Lab Partners at its unique NNSA Lab facilities, CDAC has put in place a proven structure that promotes collaboration and interaction and a sharing of a broad range of unique experimental and theoretical capabilities.

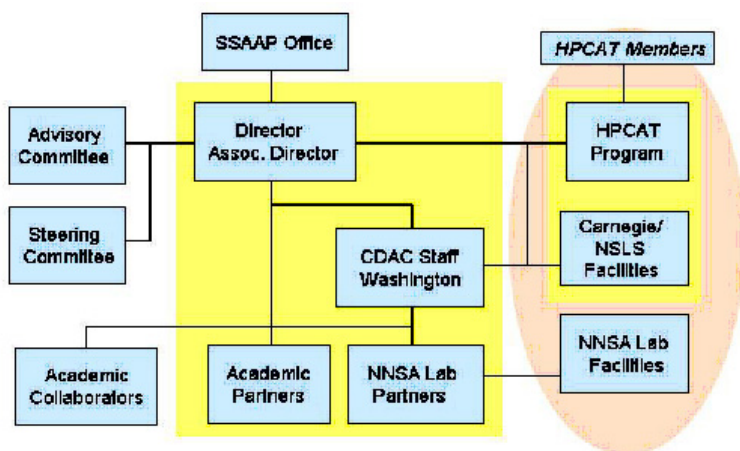


Figure 65. CDAC organizational chart. The yellow area designates the principal components of CDAC. The oval area encompasses the three different groups of experimental facilities associated with CDAC.

At **Carnegie** the CDAC staff includes **Russell Hemley**, Director, and **Ho-kwang Mao**, Associate Director. Members of the scientific staff at **Carnegie** that are involved directly with CDAC are

- **Ronald Cohen** Computational Theory
- **Premyslaw Dera** Crystallography (now at **CARS, APS**)
- **Yingwei Fei** Geochemistry and Petrology
- **Joe Feldman** Senior Visiting Fellow
- **Alexander Goncharov** Optical Spectroscopy
- **Dudley Herschbach** Senior Visiting Fellow
- **Burkhard Militzer** Computational Theory (now at **UC – Berkeley**)
- **Viktor Struzhkin** Electronic and Magnetic Properties
- **Takamitsu Yamanaka** Senior Visiting Investigator

Takamitsu Yamanaka came to **Carnegie** in April of 2007 from **Osaka University** as a Visiting Investigator. He is collaborating with CDAC researchers on high pressure crystal chemistry and working on improving methods for laboratory-based single crystal diffraction at high pressure.

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:

- **Xiao-Jia Chen** (Low-Z compounds)
- **Szczesny Krasnicki** (CVD diamond)
- **Qi Liang** (CVD diamond)
- **Jinfu Shu** (sample preparation and powder diffraction)
- **Chih-shiue Yan** (CVD diamond)

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

A number of predoctoral and postdoctoral fellows at **Carnegie** supported by the Institution, other grants, or outside fellowships worked on CDAC tasks during Year 4. Their contributions also include training CDAC students, undergraduate summer scholars, and visitors in high-pressure experimental techniques:

- **Muhetaer Ahart (Aihaiti)**
- **Pierre Beck** (now at **Laboratoire de Planétologie de Grenoble**)
- **Raja Chellappa** (former CDAC student from **University of Nevada – Reno**)
- **Jennifer Ciezak**
- **Yang Ding** (now at **HPSynC**)
- **Patrick Griffin**
- **Jennifer Jackson** (now at the **California Institute of Technology**)
- **Tim Jenkins** (now at the **National Institute of Standards and Technology**)
- **Joseph Lai**
- **Amy Lazicki**
- **Yufei Meng**

6.2 CDAC Oversight

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

- **Gilbert W. (Rip) Collins** (LLNL)
- **Dana Dattelbaum** (LANL)
- **Daniel Dolan** (SNL)
- **Jon H. Eggert** (LLNL)
- **Daniel Farber** (LLNL)
- **David Funk** (LANL)
- **Choong-shik Yoo** (WSU)
- **Joe M. Zaug** (LLNL)
- **Yusheng Zhao** (LANL)

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

- **Neil W. Ashcroft** (Cornell)
- **Robert Cauble** (LLNL)

- **Yogendra M. Gupta** (WSU)
- **Alan J. Hurd** (LANL)
- **Chi-chang Kao** (Brookhaven)
- **Marcus Knudson** (SNL)
- **Christian Mailhot** (LLNL)

Members of the committees are invited to attend the monthly CDAC/HPCAT meeting and many interact frequently with the Director and Associate Director. Each of the members of the two CDAC committees has renewed their commitment to serving through Year 5 of the CDAC program.

7. PLANS FOR YEAR 5 AND BEYOND

7.1 Scientific and Educational Focus

Support of graduate students continues to be a primary goal of the CDAC program, and has expanded to include a total of 18-20 students in the whole of the Center in Year 4, and an equivalent number is anticipated for Year 5. We continue to sponsor student travel (not just for those in CDAC, but also for our collaborators and other students active in the field), to meetings of direct interest to the high pressure materials science community. For example, CDAC cosponsored SMEC2007, held in Miami, by supporting student travel and helping to organize the program (more information on SMEC2007 can be found at <http://www.cesmec.fiu.edu>). We are also well poised continue advances in our six areas of scientific focus as outlined in Section 2. Finally, we will continue to support beamline operations and upgrades at HPCAT (for information on upgrade plans at HPCAT, see the upgrade proposal submitted to DOE-BES in Section 7.3 below). The planned upgrade will enhance our ability to meet our goal of keeping this facility available to our academic and laboratory partners.

7.2 Major New Initiatives

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

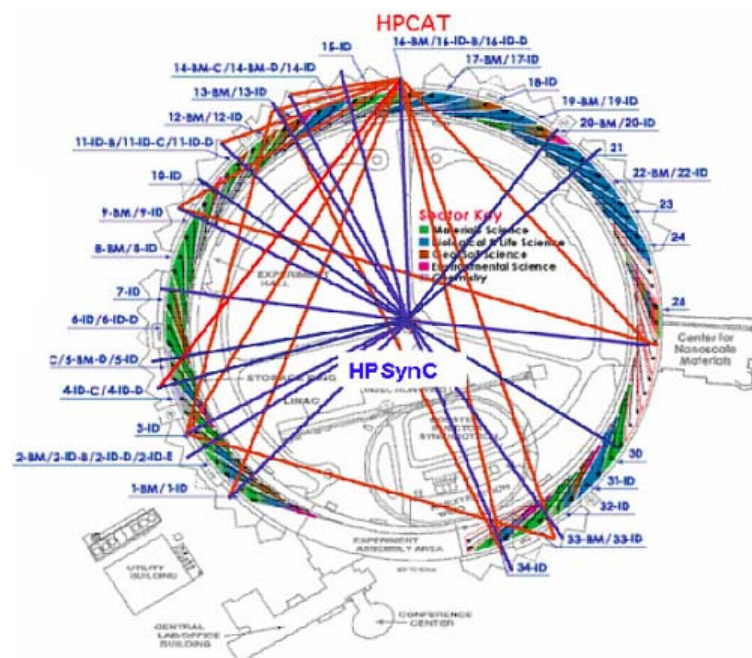


Figure 66. Coordination among sectors of APS enabled by HPSynC for high-pressure experiments.

From HPCAT to HPSynC – Since its completion in 2004, HPCAT has emerged as the most productive beamline, quantitatively and qualitatively (in terms of high scientific impact publications), among the 30 beamlines at APS. The success demonstrates the power of the three-way alliance: *i.e.*, APS provides the high-brilliance x-ray source, HPCAT staff develop, optimize, and operate dedicated high-pressure synchrotron radiation instrumentation at the beamline, and CDAC provides infrastructure and expert users who explore broad scientific and technical frontiers. The high-pressure revolution, however, has only started; as a single beamline with multiple purposes, HPCAT is limited to mutually compatible synchrotron techniques. Meanwhile APS pushes the envelope at highly specialized, single-purpose beamlines, and synchrotron technology is progressing at an astonishing rate. These specialized beamlines are uniquely configured for very high energy resolution, high photon energy, and small focused beams. Sophisticated instrumentation, methodology, and software are then developed for novel synchrotron techniques. The next surge of breakthroughs will be assured if we can utilize these novel synchrotron techniques for high-pressure applications.

Integration of high-pressure instruments with specialized beamlines has become increasingly demanding. Learning from past experience, our team has launched a new infrastructure program – the **High Pressure Synergetic Center (HPSynC)** – to fill this need. The aim is to build a ten-staff team with moderate operation funds similar to that of an APS beamline team, but with access to all APS beamlines. High pressure synchrotron scientists, engineers, and postdocs at HPSynC will advance scientific goals presented by users through the development of novel high pressure synchrotron techniques at specialized APS beamlines. HPSynC staff will facilitate modifications of the beamline optics, sample stages, detector geometries, etc. to enable high pressure studies while preserving superior x-ray diffraction, spectroscopic and imaging capabilities at the specialized beamline. They will also modify and optimize the high pressure instruments, including a variety of anvils^{99, 120, 121}, seats, gaskets, cell geometries and mechanisms, portable high temperature and cryogenic devices, and allied optical, electrical, and magnetic accessories, to accommodate the specific synchrotron techniques. Harnessing the full capabilities of the APS will then open many new areas in high-pressure research; examples important for stewardship science are as follows:

High-Pressure Phonon Dynamics – The lattice dynamics of *5f*-metals are key to understanding their complex high *P-T* behavior. In the past, lattice dynamics could only be determined by inelastic neutron scattering (*e.g.*, U¹²²) with large single crystals often unavailable for *5f*-metals. Pioneering studies of phonon dispersion have been carried out successfully on ambient-pressure Pu-Ga alloy (at the ESRF)^{123, 124}, the localized soliton of U^{125, 126}, and high-pressure single crystal Mo¹²⁷. With the unprecedented high resolution (1.2 meV) at the new APS HRIXS beamline (ID30), HPSynC will provide a mechanism for developing an optimized high pressure IXS program for efficient experiments variable *P-T* conditions, thereby establishing this important technical capability at a U.S. facility. Phonon dispersion measurements can also be obtained from x-ray transmission studies using single-crystal thermal diffuse scattering (TDS)¹²⁸⁻¹³⁰. Ultrahigh energy beamlines, such as ID11 which delivers 60-200 keV photons over a very large *q*-range, are useful for such studies. HPSynC will extend the application of these techniques to extreme conditions.

Time-Resolved Dynamic Compression – With accurate control of the 25-65 ps electron bunch length and 2.84-1590 ns spacing between bunches, APS offers many possible operational modes ideally suited for probing dynamical processes under extreme conditions, including dynamic compression. The latter studies would complement shock-wave studies with fourth-generation free-electron lasers (*e.g.*, LCLS) which offer a very short and brilliant pulse at a very low repetition rate. WSU has pioneered a pilot time-resolved shock study that was completed at HPCAT in August 2007. HPSynC will expand such projects to other APS beamlines optimized for time-resolved, (*e.g.*, XOR-7ID) x-ray diffraction, EXAFS, and ultrafast, high-intensity diagnostic lasers.

Nanoprobes at High Pressure – The smallest focused x-ray beam used at HPCAT is 3-5 μm, which leads other high-pressure beamlines at the ESRF and SPring-8, but is far larger than the typical beam size (< 100 nm with 3D resolution^{131, 132}) at nanoscience beamlines. With anvil tips of tens of microns and optical and x-ray probes, major breakthroughs were achieved in the 1970s and

'80s to advance the sustainable pressure from 50 to 350 GPa¹³³⁻¹³⁶. With new prospects for nanofabrication of diamond anvils and new beamlines to probe high-pressure samples with tens of nanometers resolution, we can expect to reach the TPa pressures that will open new areas for discovery of novel materials and nanoscale phenomena. HPSynC will be the interface for developing a high pressure nanoscale research program. The capabilities of x-ray diffraction, x-ray spectroscopy, x-ray imaging, and x-ray coherent scattering with nanoscale resolution will impact NNSA science issues ranging from material dynamics to aging.

High-Pressure X-ray Spectroscopy for Strongly Correlated Electronic Systems – Compression dramatically affects electronic and magnetic interactions among *d*- and *f*-electrons in strongly correlated systems. The development of high-pressure x-ray spectroscopy has been highly successful and productive in exploring the rich pressure-induced physics and chemistry in these materials (*e.g.* Refs.^{82, 137-142}). These techniques, however, are often element-specific; for example, entirely different instrumentation is required for nuclear resonant x-ray spectroscopy of different Mössbauer elements, and different analyzers are needed for resonant or non-resonant x-ray emission spectroscopy of various emission lines. As a single sector, HPCAT can only efficiently support the instrumentation required for high-demand elements (among HPCAT users), while instruments for other elements can be found at other specialized beamlines at APS. Moreover, some powerful techniques such as x-ray magnetic circular dichroism (XMCD)¹⁴³ and x-ray absorption spectroscopy (XAS)¹⁴⁴ are incompatible with the current HPCAT setup. HPSynC will ensure the availability of the full range of instrumentation needed for NNSA/DP-related x-ray spectroscopy at the APS.

The above examples provide a glimpse of the immense potential of new high *P-T* materials science capabilities under the next phase of CDAC. Many other research directions will be initiated at HPSynC to develop novel high pressure synchrotron science at APS. HPSynC will not replace the crucial role of dedicated high pressure beamlines, such as HPCAT and proposed beamlines (*e.g.*, a dedicated dynamic pressure facility, “DPCAT”). Instead, it complements these more focused projects by exploring new directions, conducting pilot studies, and helping to facilitate new projects at APS. In effect, HPSynC will make the whole APS a high-pressure-ready facility. Initial funding from DOE-BES, NSF, APS, and **Carnegie** has been secured, and CDAC will also provide seed funding.

High *P-T* Neutron Scattering – Neutron-based probes in the study of materials of importance for stewardship science are complementary to synchrotron x-ray and laser optical experiments. A key part of the CDAC program from the beginning has been to support the development of high-pressure neutron scattering at LANSCE. Since that time, the **Berkeley** and **Carnegie** groups have developed procedures for measurement and analysis of synchrotron diffraction data¹⁴⁵⁻¹⁴⁷. These emerging techniques can now be extended to neutron methods at much higher pressures. Members of CDAC helped to plan and build the dedicated high-pressure instrument (SNAP) and the ARCS instrument at the SNS, which will be ready in 2008. During the first phase, the Lujan Center played a major role in helping to develop and test instrumentation for SNAP. In the second phase of CDAC, SNAP will be a testbed for next generation scattering experiments at LANSCE, including proposed major upgrades¹⁴⁸. CDAC will support the development of new classes of instrumentation and state-of-the-art high-pressure devices, advance the pressure range of neutron studies into the megabar range, and improve sample size by orders of magnitude. The goal is to put high *P-T* neutron scattering on a par with x-ray methods and for the U.S. to regain the lead in this important area.

NSLS, NSLS-II, and Future Light Sources – High-pressure IR measurements have become an increasingly important part of the CDAC research effort, and one of the techniques with which CDAC is growing the high-pressure material science community. The **Carnegie** group developed the field of high-pressure synchrotron IR micro-spectroscopy, which takes advantage of the flux advantage of synchrotron radiation at long wavelengths.¹⁴⁹ The recently upgraded U2A beamline at the NSLS features a custom-built, long working distance IR microscope for diffraction-limited high *P-T* studies, and an optical/Raman spectrometer system. Under CDAC, NNSA/DP Labs are 20% members of the U2A facility beamline, thereby insuring access. As needs arise, experiments can be carried out at beamlines X17C, X17B3, and other x-ray beamlines. Finally, CDAC

management is involved in planning next-generation x-ray/IR synchrotron facilities (*e.g.*, NLSLS-II) and are emphasizing NNSA/DP needs.

NIF and Z_R – CDAC will take advantage of new scientific opportunities at NIF (**LLNL**) and Z_R (**SNL**). As part of the program to sponsor academic use of NIF, CDAC is a major part of the campaign for the first ultrahigh *P-T* materials studies at the facility. This proposal was spearheaded by G.W. Collins, and involves a partnership with CDAC collaborators **Raymond Jeanloz (UC Berkeley)** and **Yogendra Gupta (WSU)**, CDAC partner **Tom Duffy (Princeton)**, and other academic scientists, as well as **Paul Loubeyre of CEA France**. The team regularly meets to address major technical challenges and develop new diagnostics. CDAC will also work closely with **Marcus Knudson** at Z_R in complementary pulsed power experiments. Both programs will involve extending the range of high *P-T* studies with a new generation of targets based on precompressed diamond cell samples¹⁵⁰, including the use of the large CVD diamond windows that will be needed. CDAC is uniquely poised to help lead this effort with its established program in advancing static high-pressure technology development, infrastructure, and collaborating groups with major student involvement.

This new generation of large facilities provides capabilities to address scientific questions related to the behavior of condensed matter to above 1000 GPa. Shock compression studies will significantly advance the field of materials studies into the warm dense matter regime. New types of ramp loading experiments access a pressure regime that overlaps static experiments to allow very precise cross checking of results. VISAR and other diagnostics will allow the study of phase transitions, EOS, and dynamic strength¹⁵¹. Examples include studies of Fe alloys above 200 GPa^{152, 153}. Direct experimental studies of transitions in Au at 200-300 GPa^{154, 155} and phase stability of bcc Mo to 700 GPa are needed to resolve discrepancies in the literature¹⁵⁶⁻¹⁵⁹, and Cu and Al are particularly important to testing strength models¹⁶⁰⁻¹⁶³. Phase transitions in oxides and silicates can also be addressed^{164, 165}. We will directly engage students in the projects at these facilities as part of our education and training goals.

Static High-Pressure Technology – CDAC will continue to advance high *P-T* techniques by bringing together the technical strengths from academia and the NNSA/DP Labs. Advances in laser driven shocks^{166, 167}, gas-guns¹⁶⁸, and magnetic compression methods¹⁶⁹ and continued refinements of DAC techniques at the NNSA/DP Labs^{170, 171} complement activities within CDAC¹⁷². New links between static and dynamic compression experiments will be established through pulsed laser studies building on laser techniques developed in CDAC^{15, 173}, which have become routine in a number of NNSA/DP Labs and calibrated by NRIXS¹⁷⁴. CDAC scientists will continue to lead the development of new cell designs^{175, 176}.

CDAC will also continue to work with the NNSA/DP Labs to develop and apply new non-linear optical methods for high *P-T* materials science^{113, 177}. The non-linear optical studies set the stage and provide valuable training for work with free-electron lasers and combined static/laser shock methods. New SFG techniques can now be applied to investigate the structure, chemistry and aging properties of interfaces and crack propagation relevant to stewardship science. The growth in high *P-T* Brillouin spectroscopy under CDAC is leading to applications to a broad range of problems as well as at higher *P-T* conditions for NNSA/DP needs (*e.g.*, polymers, foams, and energetic materials).

Not anticipated when the project was started, the **Carnegie** CVD diamond effort is now clearly of great interest for a broad range of problems important to NNSA/DP, including use of diamond as a window and impactor in dynamic compression experiments (explored in an LDRD at **SNL**) and for targets at NIF. Other applications include its use as particle detectors, x-ray monochromators, and as an injector for tokomaks (explored with General Atomics). This unique development is the only large single crystal diamond project in this country. **UAB** continues to develop complementary designer anvil technology. In the next phase, CDAC will work to make designer anvils produced by **UAB/LLNL** and the large diamonds produced with the **Carnegie** process available to the wider community, including NNSA/DP Lab scientists, through its user programs at its facilities. All of these developments will set the stage for the next generation of still

higher pressure under static conditions (*i.e.* toward the TPa range) needed to address numerous important problems in stewardship science^{178, 179}.

7.3 HPCAT Upgrade

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

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

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

7.3.1 Second Undulator at HPCAT and the APS Ring Upgrade

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

In the long term (in a decade), APS is planning new storage ring lattice and whole facility upgrade. Several options are being seriously considered as we prepare for this upgrade. Foremost amongst these is the energy-recovery LINAC (ERL) which may offer a revolutionary upgrade path that brings fourth-generation capabilities to the APS while preserving all that we have today and

involving less user disruption than would a storage ring lattice upgrade. Having the second undulator together with the new APS innovative developments in the accelerator lattice and insertion devices, we anticipate an increase in x-ray radiation brilliance by more than an order of magnitude at HPCAT. The present HPCAT high heat load optics upgrade will also prepare us for the anticipated higher brilliance.

7.3.2 Supplementary Material Available

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

APPENDIX I: CDAC Publications and Presentations for Year 4*

A. CDAC Publications

- Aberg, D., B. Sadigh, J. C. Crowhurst, and A. F. Goncharov, Thermodynamic ground states of platinum metal nitrides, *Phys. Rev. Lett.*, submitted.
- Ahart, M., A. Asthagiri, R. E. Cohen, J. L. Yarger, H. K. Mao, and R. J. Hemley, Brillouin spectroscopy of relaxor ferroelectrics and metal hydrides, *J. Mat. Sci. and Engineering A*, **442**, 519-522 (2006).
- Ahart, M., A. Asthagiri, P. Dera, H. K. Mao, R. E. Cohen, and R. J. Hemley, Single-domain electromechanical constants for $\text{Pb}(\text{Zn}_{1/3}\text{Nb}_{2/3})\text{O}_3$ -4.5% PbTiO_3 from micro-brillouin scattering, *Appl. Phys. Lett.*, **88**, 042908 (2006).
- Ahart, M., A. Asthagiri, Z. G. Ye, P. Dera, H. K. Mao, R. E. Cohen, and R. J. Hemley, Brillouin scattering study of $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$, *Phys. Rev. B*, **75**, 144410 (2007).
- Ahart, M., M. Somayazulu, P. Dera, H. K. Mao, R. E. Cohen, R. J. Hemley, R. Yang, H. P. Liermann, and Z. Wu, Origin of morphotropic phase boundaries in ferroelectrics, *Nature*, in press.
- Ahart, M., J. L. Yarger, K. M. Lantzky, S. Nakano, H. K. Mao, and R. J. Hemley, High-pressure Brillouin scattering of amorphous BeH_2 , *J. Chem. Phys.*, **124**, 14502 (2006).
- Aksoy, R., Y. Ma, E. Selvi, M. C. Chyu, A. Ertas, and A. White, Equation of state measurements of molybdenum disulfide, *J. Phys. Chem. Solids*, **67**, 1914-1917 (2006).
- Aksoy, R., E. Selvi, R. Knudson, and Y. Ma, High pressure x-ray diffraction studies of titanium disulfide, *J. Phys. Chem. Solids*, submitted.
- Aksoy, R., E. Selvi, and Y. Ma, X-ray diffraction study of molybdenum diselenide to 35.9 GPa, *J. Phys. Chem. Solid*, submitted.
- Angel, R., M. Bijak, J. Zhao, G. D. Gatta, and S. D. Jacobsen, Static and ultrasonic observations on the effective hydrostatic limits of pressure media for high-pressure studies, *J. Appl. Cryst.*, submitted.
- Atkinson, T. D., K. M. Chynoweth, and P. Cervantes, Electronic band gap of SrSe at high pressure, *Solid State Comm.*, **139**, 215 (2006).
- Atkinson, T. D., K. M. Chynoweth, V. Sarkar, and P. Cervantes, Electronic band gap of FeS_2 under pressure, *Phys. Rev. B*, submitted.
- Barton, N. and H. R. Wenk, Dauphine twinning in polycrystalline quartz, *Modeling Simul. Mater. Sci. Eng.*, **15**, 369-384 (2007).
- Beck, P., A. F. Goncharov, V. V. Struzhkin, B. Militzer, H. K. Mao, and R. J. Hemley, Flash heating high-pressure measurement of thermal diffusivity of materials in diamond cells, *Appl. Phys. Lett.*, in press.
- Beck, P., A. F. Goncharov, V. V. Struzhkin, B. Militzer, H. K. Mao, and R. J. Hemley, Measurement of thermal diffusivity at high pressure using a transient heating technique, *Appl. Phys. Lett.*, **91**, 181914 (2007).
- Bhat, M. H., V. Molinero, E. Soignard, V. C. Solomon, J. L. Yarger, and C. A. Angell, Vitrification of a monatomic metallic liquid, *Nature*, **448**, 787-791 (2007).
- Brglez, F., X. Y. Li, M. F. Stallmann, and B. Militzer, Evolutionary and alternative algorithms: reliable cost predictions for finding optimal solutions to the LABS problem, *Inform. Sci.*, in press.
- Brown, G. E., G. Calas, and R. J. Hemley, Role of user facilities in Earth sciences research, *Elements*, **2**, 23-30 (2006).
- Campbell, A. J., C. T. Seagle, D. L. Heinz, G. Y. Shen, and V. Prakapenka, Partial melting in the iron-sulfur system at high pressure: A synchrotron x-ray diffraction study, *Phys. Earth Planet. Inter.*, **162**, 119-128 (2007).
- Caracas, R. and R. J. Hemley, New structures of dense nitrogen: pathways to the polymeric phase, *Chem. Phys. Lett.*, **442**, 65-70 (2007).
- Chellappa, R., D. Chandra, M. Somayazulu, S. A. Gramsch, and R. J. Hemley, Pressure induced phase transformation in LiNH_2 , *J. Phys. Chem. B*, **111**, 10785-10789 (2007).
- Chellappa, R. S., D. Chandra, S. A. Gramsch, R. J. Hemley, J. F. Lin, and Y. Song, Pressure induced phase transformation in LiAlH_4 , *J. Phys. Chem. B*, **110**, 11088-11097 (2006).
- Chellappa, R. S., D. Chandra, S. A. Gramsch, M. Somayazulu, and R. J. Hemley, Pressure-induced phase transformations in Li-based complex hydrides, in *Materials Research at High Pressure* (eds. M. R.

* We list publications and presentations for 2006-2007, 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.

- Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 133-138 (Materials Research Society, Warrendale, Pennsylvania, 2007).
- Chen, J., Y. Wang, T. S. Duffy, G. Shen, and L. Dobrzhinetskaya, ed. *Advances in High-Pressure Technology for Geophysical Applications*, (Elsevier, Amsterdam, in press).
- Chen, X. J., B. Liang, Z. Wu, C. Ulrich, C. T. Lin, V. V. Struzhkin, R. J. Hemley, H. K. Mao, and H. Q. Lin, Oxygen isotope effect in $\text{Bi}_2\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{2n+4+\square}$ ($n=1, 2, 3$) Single Crystal, *Phys. Rev. B*, **76**, 140502 (2007).
- Chen, X. J., V. V. Struzhkin, A. F. Goncharov, R. J. Hemley, and H. K. Mao, Oxygen isotope effect in a high-temperature superconductor under high pressure, *J. Phys.: Cond. Matt.*, **19**, 425236 (2007).
- Chen, X. J., V. V. Struzhkin, Y. Song, A. F. Goncharov, M. Ahart, Z. Liu, H. K. Mao, and R. J. Hemley, Pressure-induced metallization of solid silane, *Proc. Nat. Acad. Sci.*, in press.
- Chen, X. J., V. V. Struzhkin, Z. G. Wu, R. J. Hemley, H. K. Mao, and H. Q. Lin, Phonon-mediated superconducting transitions in layered cuprate superconductors, *Phys. Rev. B*, **75**, 734504 (2007).
- Chen, X. J., V. V. Struzhkin, Z. G. Wu, H. Q. Lin, R. J. Hemley, and H. K. Mao, Unified picture of the oxygen isotope effect in cuprate superconductors, *Proc. Nat. Acad. Sci.*, **104**, 3732-3735 (2007).
- Chesnut, G. N., N. Velisavljevic, and L. Sanchez, Static high pressure x-ray diffraction of Ti-6Al-4V, in *Shock Compression of Condensed Matter - 2007* (eds. M. D. Furnish, Elert, M. L., Russell, T. P. and White, C. T.), (AIP, New York, 2007).
- Ciezak, J. A., T. A. Jenkins, Z. Liu, and R. J. Hemley, High-pressure vibrational spectroscopy of energetic materials: Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), *J. Phys. Chem.*, **111**, 59-63 (2007).
- Correa, A. A., S. A. Bonev, and G. Galli, Carbon under extreme conditions: phase boundaries and electronic properties from first principles calculations, *Proc. Nat. Acad. Sci.*, **103**, 1204-1208 (2006).
- Crowhurst, J. C., J. M. Brown, A. F. Goncharov, and S. D. Jacobsen, Elasticity of (Mg,Fe)O through the spin transition of iron in the lower mantle, *Science*, submitted.
- Crowhurst, J. C., A. F. Goncharov, B. Sadigh, C. L. Evans, P. G. Morrall, J. L. Ferreira, and A. J. Nelson, Synthesis and characterization of the nitrides of platinum and iridium, *Science*, **311**, 1275-1278 (2006).
- Crowhurst, J. C., A. F. Goncharov, B. Sadigh, J. M. Zaug, Y. Meng, and V. Prakapenka, Synthesis and characterization of nitrides of iridium and palladium, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 3-10 (Materials Research Society, Warrendale, Pennsylvania, 2007).
- Cumalioglu, I., A. Ertas, Y. Ma, and T. T. Maxwell, State of the art: Hydrogen storage, *Transaction of the ASME: Journal of Fuel Cell Science and Technology*, in press.
- Cumalioglu, I., Y. Ma, A. Ertas, and T. T. Maxwell, High pressure hydrogen storage tank: A parametric design study, *ASMA Journal of Pressure Vessel Technology*, **129**, 216 (2007).
- Cunningham, N., W. Qiu, K. M. Hope, H. P. Liermann, and Y. K. Vohra, Symmetry lowering under high pressure: structural evidence for *f*-shell delocalization in heavy rare Earth metal terbium, *Phys. Rev. Lett.*, in press.
- Cunningham, N., W. Qiu, and Y. K. Vohra, Observation of complete trivalent rare earth sequence in heavy lanthanide metal holmium under high pressure, *High Press. Res.*, **26**, 43 (2006).
- Dattlebaum, D. M., L. L. Stevens, E. B. Orler, M. Ahart, and R. J. Hemley, Brillouin-scattering determination of the acoustic properties of polymers at high pressure, in *Shock Compression of Condensed Matter -- 2007* (American Institute of Physics, Melville, NY).
- Degtyareva, O., E. R. Hernandez, J. Serrano, M. Somayazulu, H. K. Mao, E. Gregoryanz, and R. J. Hemley, Vibrational dynamics and stability of the high-pressure chain and ring phases in S and Se, *J. Chem. Phys.*, **126**, 084503 (2007).
- Degtyareva, O., M. Martinez Canales, A. Bergara, X. J. Chen, V. V. Struzhkin, H. K. Mao, and R. J. Hemley, Crystal structure of SiH_4 at high pressure, *Phys. Rev. B*, **76**, 064123 (2007).
- Degtyareva, O., V. V. Struzhkin, and R. J. Hemley, High-pressure Raman spectroscopy of antimony: As-type, incommensurate host-guest, and bcc phases, *Solid State Comm.*, **141**, 164-167 (2007).
- Degtyareva, V. F., O. Degtyareva, H. K. Mao, and R. J. Hemley, High-pressure behavior of CdSb: compound decomposition, new phase formation and amorphization, *Phys. Rev. B*, **73**, 214108 (2006).
- Ding, Y., R. Ahuja, J. Shu, P. Chow, W. Luo, and H. K. Mao, Structural phase transition of vanadium at 69 GPa, *Phys. Rev. Lett.*, **98**, 085502 (2007).
- Ding, Y., P. Chow, and H. K. Mao, Determining thermal diffuse scattering of vanadium with x-ray transmission scattering, *Appl. Phys. Lett.*, **88**, 061903 (2006).
- Ding, Y., D. Haskel, S. G. Ovchinnikov, Y. C. Tseng, Y. Orlov, and H. K. Mao, A novel magnetic transition in magnetite (Fe_3O_4) between 12-16 GPa, *Phys. Rev. Lett.*, submitted.

- Dobrzhinetskaya, L. F., Z. Liu, P. Cartigny, J. Zhang, D. Tchkhetaia, R. J. Hemley, and H. W. Green II, Synchrotron infrared and Raman spectroscopy of microdiamonds from Erzgebirge, Germany, *Earth Planet. Sci. Lett.*, **248**, 325-334 (2006).
- Duffy, T. S., Strength of materials under static loading in the diamond anvil cell, in *Shock Compression of Condensed Matter - 2007* (eds. M. D. Furnish, Elert, M. L., Russell, T. P. and White, C. T.), submitted (AIP, New York, 2007).
- Emmons, E. D., N. Velisavljevic, J. R. Schoonover, and D. M. Dattelbaum, High-pressure Raman spectroscopy and x-ray diffraction studies of a terpolymer of tetrafluoroethylene-hexafluoropropylene-vinylidene fluoride: THV-500, *Appl. Spectr.*, in press.
- Errandonea, D., Landau theory applied to phase transitions in calcium orthotungstate and isostructural compounds, *Euro. Phys. Lett.*, **77**, 56001 (2007).
- Evans, W. J., M. J. Lipp, C. S. Yoo, H. Cynn, J. L. Herberg, R. S. Maxwell, and M. F. Nicol, Pressure-induced polymerization of carbon monoxide: Disproportionation and synthesis of an energetic lactonic polymer, *Chem. Materials*, **18**, 2520-2531 (2006).
- Evans, W. J., C. S. Yoo, G. W. Lee, H. Cynn, M. J. Lipp, and K. Visbeck, Dynamic diamond anvil cell (dDAC): A novel device for studying the dynamic-pressure properties of materials, *Rev. Sci. Instrum.*, **78**, 073904 (2007).
- Fei, Y., A. Ricolleau, M. Frank, K. Mibe, G. Shen, and V. Prakapenka, Toward an internally consistent pressure scale, *Proc. Nat. Acad. Sci.*, **104**, 9182-9186 (2007).
- Fei, Y., L. Zhang, A. Corgne, H. Watson, A. Ricolleau, Y. Meng, and V. Prakapenka, Spin transition and equation of state of (Mg,Fe)O solid solutions, *Geophys. Res. Lett.*, **34**, 17307 (2007).
- Feng, Y., R. Jaramillo, G. Srajer, J. C. Lang, Z. Islam, M. S. Somayazulu, O. G. Shpyrko, J. J. Pluth, H. K. Mao, E. D. Isaacs, G. Aeppli, and T. F. Rosenbaum, Pressure-tuned spin and charge ordering in an itinerant antiferromagnet, *Phys. Rev. Lett.*, **2007** (2007).
- Gao, C., Y. Ma, Y. Han, M. Li, and G. Zou, In-situ conductivity measurement of matter under extreme conditions by film fabrication on diamond anvil cell, *J. Phys. Chem. Solids*, submitted.
- Gavriliuk, A. G., V. V. Struzhkin, I. S. Lyubutin, M. I. Erements, I. A. Trojan, and V. V. Artemov, Equation of state and high pressure irreversible amorphization in $Y_3Fe_5O_{12}$, *JETP Lett.*, **83**, 41-45 (2006).
- Gavriliuk, A. G., V. V. Struzhkin, I. S. Lyubutin, S. G. Ovchinnikov, M. Y. Hu, and P. Chow, Reversible insulator-metal transition in $BiFeO_3$ at high pressure, *Phys. Rev. Lett.*, submitted.
- Gavriliuk, A. G., V. V. Struzhkin, I. S. Lyubutin, I. A. Trojan, M. Y. Hu, and P. Chow, Phase transition in multiferroic $BiFeO_3$, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 147-152 (Materials Research Society, Warrendale, Pennsylvania, 2007).
- Giefers, H., E. A. Tanis, S. P. Rudin, C. Greeff, X. Ke, C. Chen, M. F. Nicol, M. G. Pravica, W. Pravica, J. Zhao, A. Alatas, M. Lerche, W. Sturhahn, and E. Alp, Phonon density of states of metallic Sn at high pressures, *Phys. Rev. Lett.*, **98**, 245502 (2007).
- Goncharov, A. F., P. Beck, V. V. Struzhkin, B. Haugen, and S. D. Jacobsen, Thermal conductivity of lower mantle minerals, *Phys. Earth Planet. Inter.*, submitted.
- Goncharov, A. F., P. Beck, V. V. Struzhkin, R. J. Hemley, and J. C. Crowhurst, Laser heating diamond anvil cell studies of simple molecular systems at high pressures and temperatures, *J. Phys. Chem. Solids*, submitted.
- Goncharov, A. F. and J. C. Crowhurst, Raman spectroscopy of hot compressed hydrogen and nitrogen: implications for the intramolecular potential, *Phys. Rev. Lett.*, **96**, 055504 (2006).
- Goncharov, A. F. and J. C. Crowhurst, Proton delocalization under extreme conditions of high pressure and temperatures, *Phase Trans.*, **80**, 1051-1072 (2007).
- Goncharov, A. F., J. C. Crowhurst, J. K. Dewhurst, S. Sharma, C. Sanloup, E. Gregoryanz, N. Guignot, and M. Mezouar, Thermal equation of state of cubic boron nitride. Implications for a high-temperature pressure scale, *Phys. Rev. B*, **75**, 224114 (2007).
- Goncharov, A. F. and R. J. Hemley, Probing hydrogen-rich molecular systems at high pressures and temperatures, *Chem. Soc. Rev.*, **35**, 899-907 (2006).
- Goncharov, A. F., S. D. Jacobsen, V. V. Struzhkin, and P. Beck, Optical properties of minerals in the deep-earth, in *McGraw Hill 2008 Yearbook of Science & Technology* (McGraw Hill).
- Goncharov, A. F., C. Sanloup, N. Goldman, J. C. Crowhurst, S. Bastea, L. E. Fried, N. Guignot, M. Mezouar, and Y. Meng, Dissociative melting of ice at high pressure, *Proc. Nat. Acad. Sci.*, submitted.
- Goncharov, A. F., C. Sanloup, N. Goldman, J. C. Crowhurst, L. E. Fried, N. Guignot, M. Mezouar, and R. L. Meng, Probing of structure factor of water to 57 GPa and 1500 K, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 121-126 (Materials Research Society, Warrendale, Pennsylvania, 2007).

- Goncharov, A. F., S. V. Sinogeiken, J. C. Crowhurst, M. Ahart, D. L. Lakshtanov, V. Prakapenka, J. D. Bass, P. Beck, S. N. Tkachev, J. M. Zaug, and Y. Fei, Cubic boron nitride as a primary calibrant for a high temperature pressure scale, *High Press. Res.*, **27**, 409-417 (2007).
- Goncharov, A. F., V. V. Struzhkin, and S. D. Jacobsen, Reduced radiative conductivity of low-spin (Mg, Fe)O in the lower mantle, *Science*, **312**, 1205-1208 (2006).
- Gregoryanz, E., A. F. Goncharov, C. Sanloup, M. Somayazulu, H. K. Mao, and R. J. Hemley, High P-T behavior of nitrogen to 170 GPa, *J. Chem. Phys.*, **126**, 184505 (2007).
- Gregoryanz, E., C. Sanloup, R. Bini, J. Kreutz, H. J. Jodl, M. Somayazulu, H. K. Mao, and R. J. Hemley, On the ϵ - ζ transition of nitrogen, *J. Chem. Phys.*, **124**, 116102 (2006).
- Griffith, J. D., Structural and magnetic measurements on Au₄V under high pressures to 60 GPa, *Masters Thesis in Physics, University of Alabama at Birmingham*, (2006).
- Hamlin, J. J., S. Deemyad, J. S. Schilling, M. K. Jacobsen, R. S. Kumar, A. L. Cornelius, G. Cao, and J. J. Neumeier, ac susceptibility studies of the weak itinerant ferromagnet SrRuO₃ under high pressure to 34 GPa, *Phys. Rev. B*, **76**, 014432 (2007).
- Han, W. Q., W. Wen, D. Yi, Z. Liu, M. M. Maye, L. Lewis, J. Hanson, and O. Gang, Fe-doped trititanate nanotubes: Formation, optical and magnetic properties, and catalytic applications, *J. Phys. Chem. C*, **111**, 14339-14342 (2007).
- Haskel, D., Y. C. Tseng, J. C. Lang, and S. V. Sinogeiken, Instrument for x-ray magnetic circular dichroism measurements at high pressures, *Rev. Sci. Instrum.*, **78**, 083904 (2007).
- He, D. W. and T. S. Duffy, X-ray diffraction study of the static strength of tungsten to 69 GPa, *Phys. Rev. B*, **73**, 134106 (2006).
- Hemley, R. J., Erskine Williamson, extreme conditions, and the birth of mineral physics, *Phys. Today*, **59**, 50-56 (2006).
- Hemley, R. J., A pressing matter, *Phys. World*, **19**, 26-30 (2006).
- Hemley, R. J., V. V. Struzhkin, and R. E. Cohen, Measuring high-pressure electronic and magnetic properties, in *Treatise on Geophysics* (ed. G. D. Price), **2**, 293-337 (Elsevier, Amsterdam, 2007).
- Ho, S. S., C. S. Yan, Z. Liu, H. K. Mao, and R. J. Hemley, Prospects for large single crystal CVD diamonds, *Industrial Diamond Review*, **66**, 28-32 (2006).
- Hong, X., G. Shen, V. B. Prakapenka, M. Newville, M. L. Rivers, and S. R. Sutton, Intermediate states of GeO₂ glass under pressures up to 35 GPa, *Phys. Rev. B*, **75**, 104201 (2007).
- Hong, X., G. Shen, V. B. Prakapenka, M. L. Rivers, and S. Sutton, Density measurements of noncrystalline materials at high pressure with diamond anvil cell, *Rev. Sci. Instrum.*, **78**, 103905 (2007).
- Hu, J. Z., H. K. Mao, J. F. Shu, Q. Z. Guo, and H. Liu, Diamond anvil cell radial x-ray diffraction program at the National Synchrotron Light Source, *J. Phys. Cond. Matt.*, **18**, S1091-1096 (2006).
- Huang, W., J. E. Patterson, A. S. Lagutchev, and D. D. Dlott, Shock compression spectroscopy with high time and space resolution, *AIP Confer. Proc.*, **845**, 1265-1270 (2006).
- Iezzi, G., Z. Liu, and G. Della Ventura, Synchrotron infrared spectroscopy of synthetic Na(NaMg)Mg₅Si₈O₂₂(OH)₂ up to 30 GPa: Insights on a new amphibole high pressure polymorph, *Am. Mineral*, **91**, 479-482 (2006).
- Iota, V., C. S. Yoo, J. H. P. Klepeis, Z. Jenei, W. Evans, and H. Cynn, Six-fold coordinated carbon dioxide VI, *Nature Materials*, **6**, 34-38 (2006).
- Jacobsen, S. D., Effect of water on the equation of state of nominally anhydrous minerals, in *Water in Nominally Anhydrous Minerals* (eds. H. Keppler and Smyth, J. R.), in press (Rev. Min. Geochem.).
- Jacobsen, S. D. and J. R. Smyth, Effect of water on the sound velocities of ringwoodite in the transition zone, in *Earth's Deep Water Cycle* (eds. S. D. Jacobsen and van der Lee, S.), in press (Am. Geophys. Union Washington DC).
- Jeanloz, R., P. M. Celliers, G. W. Collins, J. H. Eggert, K. K. M. Lee, R. S. McWilliams, S. Brygoo, and P. Loubeyre, Achieving high-density states through shock-wave loading of precompressed samples, *Proc. Nat. Acad. Sci.*, **104**, 9172-9177 (2007).
- Jenkins, T., V. V. Struzhkin, J. Leão, H. K. Mao, and R. J. Hemley, Inelastic neutron scattering spectroscopy of tetrahydrofuran, hydrogen clathrate, *Chem. Phys. Lett.*, submitted.
- Jiang, F., J. Majzlan, S. Speziale, D. He, and T. S. Duffy, Single-crystal elasticity of diaspore, AlOOH, to 12 GPa by Brillouin scattering, *Phys. Earth Planet. Inter.*, submitted.
- Jiang, F., S. Speziale, and T. S. Duffy, Single-crystal elasticity of brucite, Mg(OH)₂, to 15 GPa by Brillouin scattering, *Am. Mineral.*, **91**, 1893-1900 (2006).
- Kaminskii, A. A., R. J. Hemley, J. Lai, C. S. Yan, H. K. Mao, V. G. Ralchenko, H. J. Eichler, and H. Rhee, High-order stimulated Raman scattering in CVD single crystal diamond, *Laser Phys. Lett.*, **4**, 350-353 (2007).
- Kim, H., A. Lagutchev, and D. D. Dlott, Surface and interface spectroscopy of energetic materials: HMX and Estane, *Propellants, Explosives, Pyrotechnics*, **31**, 116-123 (2006).

- Klug, D. D., J. S. Tse, Z. Liu, and R. J. Hemley, Hydrogen-bonded dynamics and Fermi resonance in high-pressure methane-filled ice, *J. Chem. Phys.*, **125**, 154509 (2006).
- Kubo, A., B. Kiefer, G. Shen, V. Prakapenka, R. J. Cava, and T. S. Duffy, Stability and equation of state of the post-perovskite phase of MgGeO₃ to 2 Mbar, *Geophys. Res. Lett.*, **33**, L12S12 (2006).
- Kubo, A., B. Kiefer, S. H. Shim, G. Shen, V. B. Prakapenka, R. J. Cava, and T. S. Duffy, Rietveld structure refinements of MgGeO₃ post-perovskite phase to 1 Mbar, *Am. Mineral.*, submitted.
- Kubo, A., Y. Wang, C. E. Runge, T. Uchida, B. Kiefer, N. Nishiyama, and T. S. Duffy, Melting curve of silicon to 15 GPa determined by angle-dispersive x-ray diffraction using a Kawai-type apparatus, *J. Phys. Chem. Solids*, submitted.
- Kumar, R. S., A. L. Cornelius, and M. Nicol, Structure of nanocrystalline ZnO up to 85 GPa, *Curr. Appl. Phys.*, **7**, 135-138 (2007).
- Kumar, R. S., A. L. Cornelius, and M. F. Nicol, Equation of state of nanocrystalline BaTiO₃ up to 52 GPa at room temperature, *Phys. Stat. Sol.*, **244**, 290-294 (2007).
- Kumar, R. S., A. L. Cornelius, M. G. Pravica, M. F. Nicol, M. Y. Hu, and P. C. Chow, Bonding changes in single wall carbon nanotubes (SWCNT) on Ti and TiH₂ addition probed by x-ray Raman scattering, *Diamond Relat. Mater.*, **16**, 1136-1139 (2007).
- Kumar, R. S., A. L. Cornelius, M. Somayazulu, D. Errandonea, M. F. Nicol, and J. S. Gardner, High pressure structure of Tb₂Ti₂O₇ pyrochlore at cryogenic temperatures, *Phys. Stat. Sol. (b)*, **244**, 266-269 (2007).
- Kumar, R. S., E. Kim, O. Tschauer, A. L. Cornelius, M. P. Sulic, and C. M. Jensen, Pressure-induced structural phase transition in NaAlH₄, *Phys. Rev. B*, **75**, 174110 (2007).
- Kumar, R. S., M. G. Pravica, A. L. Cornelius, M. F. Nicol, M. Y. Hu, and P. C. Chow, X-ray Raman scattering studies on C₆₀ fullerenes and multi-walled carbon nanotubes under pressure, *Diamond Relat. Mater.*, **16**, 1250-1253 (2007).
- Kunz, M. C., W. A., L. Miyagi, and H. R. Wenk, In situ laser heating and radial synchrotron diffraction in a diamond anvil cell, *Rev. Sci. Instrum.*, **78**, 063907 (2007).
- Lakshmanov, D. L., S. V. Sinogeiken, K. D. Litasov, V. B. Prakapenka, H. Hellwig, J. Wang, C. Sanches-Valle, J. P. Perrillat, B. Chen, M. Somayazulu, J. Li, E. Ohtani, and J. D. Bass, The post-stishovite phase transition in hydrous alumina-bearing SiO₂ in the Earth's lower mantle, *Proc. Nat. Acad. Sci.*, **104**, 13588-13590 (2007).
- Larson, B. C., A. El-Azab, W. Yang, J. Z. Tischler, W. Liu, and G. E. Ice, Experimental characterization of the mesoscale dislocation density tensor, *Phil. Mag.*, **87**, 11-21 (2007).
- Lazicki, A. K., C. S. Yoo, W. J. Evans, W. E. Pickett, and R. T. Scalettar, Pressure-induced antifluorite-to-anticoinnite phase transition in lithium oxide, *Phys. Rev. B*, **73**, 184120 (2006).
- Lee, S. K., Microscopic origins of macroscopic properties of silicate melts and glasses at ambient and high pressure: Implications for melt generation and dynamic, *Geochim. Cosmochim. Acta*, submitted.
- Lee, S. K., P. J. Eng, H. K. Mao, Y. Meng, and J. Shu, Structure of alkali borate glasses at high pressure: B and Li K-edge inelastic x-ray scattering study, *Phys. Rev. Lett.*, **98**, 105502 (2007).
- Lee, S. K., Y. Fei, G. D. Cody, and B. O. Mysen, Structures of non-crystalline silicates at high pressure: 17O and 27Al solid-state (3QMAS) NMR study, in *Frontiers in High Pressure Research* (eds. J. Chen, Wang, Y., Duffy, T., Shen, G. and Dobrzhinetskaya, L.), in press (AGU).
- Levine, L. E., B. C. Larson, W. Yang, M. E. Kassner, J. Z. Tischler, M. A. Delos-Reyes, R. J. Fields, and W. Liu, X-ray microbeam measurements of individual dislocation cell elastic strains in deformed single-crystal copper, *Nature Materials*, **5**, 619-622 (2006).
- Li, J., Electronic transitions and spin states in perovskite and post-perovskite, in *The Last Phase Transition* (eds. J. P. Brodholt, Lay, T., Yuen, D. A. and Hirose, K.), (American Geophysical Union, 2007).
- Li, J. and Y. Fei, Experimental constraints on core composition, in *Treatise on Geochemistry, Vol. 2: The Mantle and Core* (ed. R. W. Carlson), **2**, 1-31 (Elsevier Science, 2007).
- Liermann, H. P., A. K. Singh, M. Somayazulu, and S. K. Saxena, Compression behavior of NbC under nonhydrostatic conditions to 57 GPa, *J. Ref. Met. Hard Mat.*, **25**, 386-391 (2007).
- Lin, J. F., H. Fukui, D. Prendergast, T. Okuchi, Y. Q. Cai, N. Hiraoka, C. S. Yoo, A. Trave, P. Eng, M. Y. Hu, and P. Chow, Electronic bonding transition in compressed SiO₂ glass, *Phys. Rev. B*, **75**, 012201 (2007).
- Lin, J. F., A. G. Gavriluk, V. V. Struzhkin, S. D. Jacobsen, W. Sturhahn, M. Y. Hu, P. Chow, and C. S. Yoo, Pressure-induced electronic spin transition of iron in magnesiowustite-(Mg,Fe)O, *Phys. Rev. B*, **73**, 113107 (2006).
- Lin, J. F., S. D. Jacobsen, and R. M. Wentzcovitch, Electronic spin transition of iron in the Earth's deep mantle, *Eos*, **88**, 13-24 (2007).
- Lin, J. F., V. V. Struzhkin, A. G. Gavriluk, and I. S. Lyubutin, Comment on "Spin crossover in (Mg,Fe)O: A Mossbauer effect study with an alternative interpretation of x-ray emission spectroscopy data, *Phys. Rev. B*, **75**, 177102 (2007).

- Lin, J. F., G. Vankó, S. D. Jacobsen, V. Iota, V. V. Struzhkin, V. Prakapenka, A. Kuznetsov, and C. S. Yoo, Spin transition zone in Earth's lower mantle, *Science*, **317**, 1740.
- Lipinska-Kalita, K., O. A. Hemmers, P. E. Kalita, G. Mariotto, S. A. Gramsch, R. J. Hemley, and T. Hartmann, High-pressure structural integrity and structural transformations of glass-derived nanocomposites: A review, *J. Phys. Chem. Solids*, submitted.
- Lipinska-Kalita, K. E., P. E. Kalita, and R. J. Hemley, α - to β - Ga_2O_3 phase transition in a nanocomposite material: In situ high pressure synchrotron x-ray diffraction investigations, *Phys. Rev. B*, submitted.
- Lipinska-Kalita, K. E., P. E. Kalita, D. M. Krol, R. J. Hemley, C. L. Gobin, and Y. Ohki, Spectroscopic properties of Cr^{3+} ions in nanocrystalline glass-ceramic composites, *J. Non-Crystalline Solids*, **352**, 524-527 (2006).
- Lipp, M. J., J. H. P. Klepeis, B. Baer, H. Cynn, W. J. Evans, V. Iota, and C. S. Yoo, Transformation of molecular nitrogen to nonmolecular phases at megabar pressures by direct laser heating, *Phys. Rev. B*, **76**, 014113 (2007).
- Liu, H., H. R. Wenk, and T. S. Duffy, Rheology and elasticity studies at ultra-high pressures and temperatures, *J. Phys. Cond. Matt.*, **18**, S921-1103 (2006).
- Lonardelli, I., N. Gey, H. R. Wenk, S. Vogel, and M. Humbert, In situ texture evolution during phase transformation in titanium alloys, *Acta Mater.*, submitted.
- Lopez-Solano, J., P. Rodriguez-Hernandez, S. Radescu, A. Mujica, A. Munoz, D. Errandonea, and F. J. Majon, Crystal stability and pressure-induced phase transitions in scheelite AWO_4 (A = Ca, Sr, Ba, Pb, Eu) binary oxides. I: A review of recent ab initio calculations, ADXRD, XANES, and Raman studies, *Phys. Stat. Sol. B*, **244**, 325-330 (2007).
- Lucas, M. S., A. B. Papandrew, B. Fultz, and M. Y. Hu, Partial phonon densities of states of ^{57}Fe in Fe-Cr: analysis by a local-order cluster expansion, *Phys. Rev. B*, **75**, 054307 (2007).
- Luo, W., R. Ahuja, Y. Ding, and H. K. Mao, Unusual lattice dynamics of vanadium under high pressure, *Proc. Nat. Acad. Sci.*, **104**, 16428-16431 (2007).
- Lyubutin, I. S., A. G. Gavriluk, and V. V. Struzhkin, Magnetic collapse and insulator-metal transitions in some 3D metal oxides under high pressure, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 167-178 (Warrendale, Pennsylvania, Warrendale, Pennsylvania, 2007).
- Ma, Y. and R. Aksoy, Compression of $\text{CdCu}_3\text{Ti}_4\text{O}_{12}$ perovskite to 55 GPa, *Solid State Comm.*, in press.
- Ma, Y., Q. Cui, and H. Shen, X-ray diffraction study of nanocrystalline tungsten nitride and tungsten, *J. Appl. Phys.*, **102**, 013525 (2007).
- Ma, Y., V. I. Levitas, and J. Hashemi, X-ray diffraction measurements in a rotational diamond anvil cell, *J. Phys. Chem. Solids*, **67**, 2083-2090 (2006).
- Ma, Y., J. Liu, C. Gao, A. D. White, W. N. Mei, and J. Rasty, High-pressure x-ray diffraction study of the giant dielectric constant material $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$: Evidence of stiff grain surface, *Appl. Phys. Lett.*, **88**, 191903 (2006).
- Ma, Y., E. Selvi, V. I. Levitas, and J. Hashemi, Effect of shear strain on the α - ϵ phase transition of iron: a new approach in the rotational diamond anvil cell, *J. Phys. Cond. Matt.*, **18**, S1075-S1082 (2006).
- Maddox, B. R., A. Lazicki, C. S. Yoo, V. Iota, M. Chen, A. K. McMahan, M. Hu, P. Chow, R. T. Scalettar, and W. E. Pickett, 4f delocalization in Gd: Inelastic x-ray scattering at ultrahigh pressure, *Phys. Rev. Lett.*, **96**, 215701 (2006).
- Majon, F. J., D. Errandonea, J. Lopez-Solano, P. Rodriguez-Hernandez, S. Radescu, A. Mujica, A. Munoz, N. Garro, J. Pellicer-Poers, A. Segura, C. Ferrer-Roca, R. S. Kumar, O. Tschauer, and G. Aquilanti, Crystal stability and pressure-induced phase transitions in scheelite AWO_4 (A=Ca, Sr, Ba, Pb, Eu) binary oxides. II: Towards a systematic understanding, *Phys. Stat. Sol. (b)*, **244** (2007).
- Majzlan, J., S. Speziale, T. S. Duffy, and P. C. Burns, Single-crystal elastic properties of Alunite, $\text{KAl}_2(\text{SO}_4)_2(\text{OH})_6$, *Phys. Chem. Minerals*, DOI:10.1007/s00269-00006-00104-z (2006).
- Mao, H. K., J. Badro, J. Shu, R. J. Hemley, and A. K. Singh, Strength, anisotropy, and preferred orientation of solid argon at high pressures, *J. Phys. Cond. Matt.*, **8**, S963-S968 (2006).
- Mao, H. K. and R. J. Hemley, The high-pressure dimension in earth and planetary science, *Proc. Nat. Acad. Sci.*, **104**, 9114-9115 (2007).
- Mao, H. K. and W. L. Mao, Diamond-anvil cells and probes for high P-T mineral physics studies, in *Treatise on Geophysics* (ed. G. D. Price), **2**, 231-268 (Elsevier, Amsterdam, 2007).
- Mao, W. L., A. J. Campbell, D. L. Heinz, and G. Shen, Phase relations of Fe-Ni alloys at high pressure and temperature, *Phys. Earth Planet. Inter.*, **155**, 146-151 (2006).
- Mao, W. L., C. A. Koh, and E. D. Sloan, Clathrate hydrates under pressure, *Phys. Today*, submitted.
- Mao, W. L. and H. K. Mao, Ultrahigh-pressure experiment with a motor-driven diamond anvil cell, *J. Phys. Cond. Matt.*, **18**, S1069-S1103 (2006).

- Mao, W. L., H. K. Mao, Y. Meng, P. Eng, M. Y. Hu, P. Chow, Y. Q. Cai, J. Shu, and R. J. Hemley, X-ray dissociation of H₂O and formation of an O₂-H₂ alloy at high pressure, *Science*, **314**, 636-638 (2006).
- Mao, W. L., H. K. Mao, V. B. Prakapenka, J. Shu, and R. J. Hemley, The effect of pressure on the structure and volume of ferromagnesian post-perovskite, *Geophys. Res. Lett.*, **33**, L12S02 (2006).
- Mao, W. L., H. K. Mao, W. Sturhahn, J. Zhao, V. B. Prakapenka, Y. Meng, Y. Fei, and R. J. Hemley, Iron-rich post-perovskite and the origin of ultralow-velocity zones, *Science*, **312**, 564-565 (2006).
- Mao, W. L., V. V. Struzhkin, A. Q. R. Baron, S. Tsutsui, C. E. Tommaseo, H. R. Wenk, M. Y. Hu, P. Chow, W. Sturhahn, J. Shu, R. J. Hemley, D. L. Heinz, and H. K. Mao, Experimental determination of the elasticity of iron at high pressure, *J. Geophys. Res.*, submitted.
- Mao, Z., S. D. Jacobsen, F. Jiang, J. R. Smyth, C. Holl, D. J. Frost, and T. Duffy, Single-crystal elasticity of wadsleyites, β -Mg₂SiO₄, containing 0.37-1.66 wt % H₂O, *Earth Planet. Sci. Lett.*, in press.
- Mao, Z., F. Jiang, and T. Duffy, Single-crystal elasticity of zoisite, Ca₂Al₃Si₃O₁₂(OH), by Brillouin scattering, *Am. Mineral.*, **92**, 570-576 (2007).
- Mei, Q., C. J. Benmore, S. Sampath, J. K. R. Weber, K. Leinenweber, S. Amin, P. Johnston, and J. L. Yarger, The structure of permanently densified CaAl₂O₄ glass, *J. Phys. Chem. Solids*, **67**, 2106-2110 (2006).
- Mei, Q., C. J. Benmore, E. Soignard, S. Amin, and J. Yarger, Analysis of high-energy x-ray diffraction data at high pressure: The case of vitreous As₂O₃ at 32 GPa, *J. Phys. Chem. Solids*, in press.
- Mei, Q., R. T. Hart, C. J. Benmore, S. Amin, K. Leinenweber, and J. L. Yarger, The structure of densified As₂O₃ glasses, *J. Non-Crystalline Solids*, **353**, 1755-1758 (2007).
- Meng, Y., P. J. Eng, M. Y. Hu, J. Shu, C. C. Kao, R. J. Hemley, and H. K. Mao, Inelastic x-ray scattering of high-pressure phases of oxygen: evidence for intermolecular π -bonding, *Phys. Rev. Lett.*, submitted.
- Meng, Y., G. Shen, and H. K. Mao, Double-sided laser heating system at HPCAT for in situ x-ray diffraction at high pressure and high temperatures, *J. Phys. Cond. Matt.*, **18**, S1097-S1103 (2006).
- Meng, Y., R. B. Von Dreele, B. H. Toby, P. Chow, M. Y. Hu, G. Shen, and H. K. Mao, Hard x-ray radiation induced dissociation of N₂ and O₂ molecules and the formation of ionic nitrogen oxide phases under pressure, *Phys. Rev. B*, **74**, 214107 (2006).
- Merkel, S., A. Kubo, L. Miyagi, S. Speziale, T. S. Duffy, H. K. Mao, and H. R. Wenk, Plastic deformation of MgGeO₃ post-perovskite at lower mantle pressures, *Science*, **311**, 644-646 (2006).
- Merkel, S., A. K. McNamera, A. Kubo, S. Speziale, L. Miyagi, Y. Meng, T. S. Duffy, and H. R. Wenk, Deformation of (Mg,Fe)SiO₃ post-perovskite and D" anisotropy, *Science*, **316**, 1729-1732 (2007).
- Militzer, B., First principles calculations of shock compressed fluid helium, *Phys. Rev. Lett.*, **97**, 175501 (2006).
- Militzer, B. and R. L. Graham, Simulations of dense atomic hydrogen in the Wigner crystal phase, *J. Phys. Chem. Solids*, **67**, 2136-2149 (2006).
- Militzer, B. and R. J. Hemley, Solid oxygen takes shape, *Nature*, **443**, 150-151 (2006).
- Militzer, B. and W. B. Hubbard, Implications of shock wave experiments with precompressed materials for giant planet interiors, in *Shock Compression of Condensed Matter -- 2007* (American Institute of Physics, Melville, NY).
- Militzer, B., E. L. Pollock, and D. Ceperley, Path integral Monte Carlo calculation of the momentum distribution of the homogeneous electron gas at finite temperature, *Phys. Rev. B*, submitted.
- Miyagi, L., S. Merkel, T. Yagi, N. Sata, Y. Ohishi, and H. R. Wenk, Diamond anvil cell deformation of CaSiO₃ perovskite up to 49 GPa, *Phys. Earth Planet. Inter.*, submitted.
- Miyagi, L., S. Merkel, T. Yagi, N. Sata, Y. Ohishi, and H. R. Wenk, Quantitative Reitveld texture analysis of CaSiO₃ perovskite deformed in a diamond anvil cell, *J. Phys. Cond. Matt.*, **18**, S995-1005 (2006).
- Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. Duffy, and H. R. Wenk, Deformation of the CaIrO₃ post-perovskite phase to 5 GPa and 1300 K, *Earth Planet. Sci. Lett.*, submitted.
- Murakami, M., S. V. Sinogeiken, H. Hellwig, J. D. Bass, and J. Li, Sound velocity of MgSiO₃ perovskite to Mbar pressure, *Earth Planet. Sci. Lett.*, **256**, 47-54 (2007).
- Okuchi, T., M. Takigawa, J. Shu, H. K. Mao, R. J. Hemley, and T. Yagi, Fast molecular transport in hydrogen hydrates by high-pressure diamond anvil cell NMR, *Phys. Rev. B*, **75**, 144104 (2007).
- Papandrew, A. B., M. S. Lucas, R. Stevens, B. Fultz, M. Y. Hu, I. Halevy, R. E. Cohen, and M. Somayazulu, Absence of magnetism in hcp iron-nickel at 11 K, *Phys. Rev. Lett.*, **97**, 087202 (2006).
- Ponsov, Y. S., V. V. Struzhkin, S. V. Streltsov, and A. F. Goncharov, Pressure-induced effect on electronic excitations in osmium, *2007 AIRAPT Proceedings*, submitted.
- Pravica, M. G., Y. Shen, Z. Quine, E. Romano, and D. Hartnett, High-pressure studies of cyclohexane to 40 GPa, *J. Phys. Chem. B*, **111**, 4103-4108 (2007).
- Qiu, W., P. A. Baker, N. Velisavljevic, Y. K. Vohra, and S. T. Weir, Calibration of an isotopically enriched carbon-13 layer pressure sensor to 156 GPa in a diamond anvil cell, *J. Appl. Phys.*, **99**, 046906 (2006).
- Reichmann, H. J. and S. D. Jacobsen, Sound velocities and elastic constants of ZnAl₂O₄ spinel and implications for spinel-elasticity systematics, *Am. Mineral.*, **91**, 1049-1054 (2006).

- Runge, C. E., A. Kubo, B. Kiefer, Y. Meng, V. Prakapenka, G. Shen, R. J. Cava, and T. S. Duffy, Equation of state of MgGeO₃ perovskite to 65 GPa: Comparison with the post-perovskite phase, *Phys. Chem. Minerals*, **33**, 699-709 (2006).
- Santoro, M., E. Gregoryanz, H. K. Mao, and R. J. Hemley, Anomalous optical emission in hot dense oxygen, *Solid State Comm.*, doi:10.1016/j.scc.2007.1008.1032 (2007).
- Scott, H. P., S. Huggins, M. R. Frank, S. J. Maglio, C. D. Martin, Y. Meng, J. Santillan, and Q. Williams, Equation of state and high-pressure stability of Fe₃P-Schreibersite: Implications for phosphorus storage in planetary cores, *Geophys. Res. Lett.*, **34**, L06302 (2007).
- Scott, H. P., Z. Liu, R. J. Hemley, and Q. Williams, High pressure infrared spectra of talc and lawsonite, *Am. Mineral.*, **92**, 1814-1820 (2007).
- Seager, S., M. Kuchner, C. A. Hier-Majumder, and B. Militzer, Mass-radius relationships for solid exoplanets, *Astrophys. Lett.*, submitted.
- Seagle, C. T., A. J. Campbell, D. L. Heinz, G. Shen, and V. B. Prakapenka, Thermal equation of state in Fe₃S and implications for sulfur in Earth's core, *J. Geophys. Res. - Solid Earth*, **111**, B06209 (2006).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, V. Prakapenka, and S. T. Wanless, Melting and thermal expansion in the Fe-FeO system at high pressure, *Earth Planet Sci. Lett.*, in press.
- Selvi, E., Y. Ma, R. Aksoy, A. Ertas, A. White, and S. Jagdev-Singh, High pressure x-ray diffraction study of tungsten disulfide, *J. Phys. Chem. Solids*, **67**, 2183-2186 (2006).
- Sha, X. and R. E. Cohen, Lattice dynamics and thermodynamics of bcc vanadium at high pressures, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 185-195 (Materials Research Society, Warrendale, Pennsylvania, 2007).
- Shen, G., H. P. Liermann, S. V. Sinogeiken, W. Yang, X. Hong, C. S. Yoo, and H. Cynn, Distinct thermal behavior of GeO₂ glass in tetrahedral, intermediate and octahedral forms, *Nature*, **104**, 14576-14579 (2007).
- Shen, Y. R., R. S. Kumar, A. L. Cornelius, and M. F. Nicol, High-pressure structural studies of dysprosium using angle-dispersive x-ray diffraction, *Phys. Rev. B*, **57**, 064109 (2007).
- Sheng, H. W., H. Z. Liu, Y. Q. Cheng, J. Wen, P. L. Lee, W. K. Luo, S. D. Shastri, and E. Ma, Polymorphism in a metallic glass, *Nature Materials*, **6**, 192-197 (2007).
- Shieh, S. R., T. S. Duffy, A. Kubo, G. Shen, V. B. Prakapenka, N. Sata, K. Hirose, and Y. Ohishi, Equation of state of the post-perovskite phase synthesized from a natural (Mg,Fe)SiO₃ orthopyroxene, *Proc. Nat. Acad. Sci.*, **103**, 644-646 (2006).
- Shieh, S. R., A. Kubo, T. S. Duffy, V. B. Prakapenka, and G. Shen, High-pressure phases in SnO₂ to 117 GPa, *Phys. Rev. B*, **73**, 014105 (2006).
- Shim, S. H., A. Kubo, and T. S. Duffy, Raman spectroscopy of perovskite and post-perovskite phases of MgGeO₃ to 123 GPa, *Earth Planet. Sci. Lett.*, **260**, 130-178 (2007).
- Shu, J., W. L. Mao, R. J. Hemley, and H. K. Mao, Pressure-induced distortive phase transition in chromite-spinel at 29 GPa, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 179-184 (Materials Research Society, Warrendale, Pennsylvania, 2007).
- Singh, A. K., H. P. Liermann, Y. Akahama, and M. Nishimura, Aluminum as a pressure-transmitting medium cum pressure standard for x-ray diffraction experiments to 200 GPa with diamond anvil cells, *J. Appl. Phys.*, **101**, 123526 (2007).
- Singh, A. K., H. P. Liermann, and A. Jain, Compression of high-purity silver to 40 GPa in a diamond anvil cell: pressure dependence of strength and grain size from x-ray diffraction data, *Int. J. Plasticity*, submitted.
- Singh, A. K., H. P. Liermann, S. K. Saxena, and H. K. Mao, Compressive strength of gold crystallites under pressure up to 60 GPa: observation of crystallite size effect, *J. Appl. Phys.*, submitted.
- Singh, A. K., H. P. Liermann, S. K. Saxena, H. K. Mao, and S. U. Devi, Nonhydrostatic compression of gold powder to 60 GPa in a diamond anvil cell: estimation of compressive strength from x-ray diffraction data, *J. Phys. Cond. Matt.*, **18**, S969-S978 (2006).
- Smedley, J., I. Ben-Zvi, A. Burril, X. Chang, J. Grimes, T. Rao, Z. Segalov, and Q. Wu, Electron amplification in diamond, in *2006 Workshop on Advanced Accelerator Concepts* **887**, 672-674 (2006).
- Smyth, J. R. and S. D. Jacobsen, Nominally anhydrous minerals and Earth's deep water cycle, in *Earth's Deep Water Cycle* (eds. S. D. Jacobsen and S. van der Lee), in press (Am. Geophys. Union).
- Somayazulu, M., S. A. Gramsch, H. K. Mao, and R. J. Hemley, High pressure-high temperature reactions in xenon-chlorine system, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 127-132 (Materials Research Society, Warrendale, Pennsylvania, 2007).
- Somayazulu, M., J. Shu, C. S. Zha, A. F. Goncharov, O. Tschauer, H. K. Mao, and R. J. Hemley, In-situ high-pressure x-ray diffraction study of H₂O ice in VII, *J. Chem. Phys.*, submitted.

- Speziale, S., V. E. Lee, S. M. Clark, J. F. Lin, M. P. Pasternak, and R. Jeanloz, Effects of Fe spin transition on the elasticity of (Mg,Fe)O magnesiowustites and implications for theseismological properties of the Earth's lower mantle, *J. Geophys. Res.*, **112**, B10212 (2007).
- Speziale, S., S. R. Shieh, and T. S. Duffy, High-pressure elasticity of calcium oxide: A comparison between Brillouin scattering and radial x-ray diffraction, *J. Geophys. Res.*, **111**, B02203 (2006).
- Stevens, L. L., E. B. Orler, D. M. Dattelbaum, M. Ahart, and R. J. Hemley, A Brillouin-scattering determination of the acoustic properties and their pressure dependence for three polymeric elastomers, *J. Chem. Phys.*, **127**, 104906 (2007).
- Struzhkin, V. V., M. I. Erements, I. M. Erements, J. F. Lin, W. Sturhahn, J. Zhao, and M. Y. Hu, Synchrotron mossbauer spectroscopy and resistivity studies of iron oxide under high pressure, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 161-166 (Materials Research Society, Warrendale, Pennsylvania, 2007).
- Struzhkin, V. V., A. F. Goncharov, R. Caracas, H. K. Mao, and R. J. Hemley, Synchrotron infrared spectroscopy of the pressure induced insulator-metal transitions in glassy As₂S₃ and As₂Se₃, *Phys. Rev. B*, submitted.
- Struzhkin, V. V., H. K. Mao, J. F. Lin, R. J. Hemley, J. S. Tse, Y. Ma, M. Hu, P. Chow, and C. C. Kao, Valence band x-ray emission spectra of compressed germanium, *Phys. Rev. Lett.*, **96**, 137402 (2006).
- Struzhkin, V. V., B. Militzer, W. L. Mao, H. K. Mao, and R. J. Hemley, Hydrogen storage in molecular clathrates, *Chem. Rev.*, **107**, 4133-4151 (2007).
- Strzhemechny, M. A., Anisotropic interactions between HD molecules, *Phys. Rev. B*, **73**, 174301 (2006).
- Surber, E., A. Lozano, A. Lagutchev, H. Kim, and D. D. Dlott, Surface nonlinear vibrational spectroscopy of energetic materials: HMX, *J. Phys. Chem. C*, **111**, 2235-2241 (2007).
- Surber, E., A. Lozano, A. Lagutchev, H. Kim, and D. D. Dlott, Surface vibrational spectroscopy of energetic materials: HMX, *J. Phys. Chem.*, **111**, 2235-2241 (2007).
- Tommaseo, C., S. Speziale, S. Merkel, H. R. Wenk, and J. Devine, DAC investigations of plasticity and elasticity in the MgO-FeO series, *Phys. Chem. Minerals*, **33**, 84-87 (2006).
- Tse, J., D. D. Klug, S. Desgreniers, J. Smith, R. R. Flacau, Z. Liu, J. Hu, N. Chen, and D. T. Jiang, Structural phase transition in CaH₂ at high pressures, *Phys. Rev. B*, **75**, 134108 (2007).
- Tseng, Y. C., D. Haskel, J. C. Lang, S. V. Sinogeiken, Y. Mudryk, V. K. Pecharsky, and K. A. Gschneider Jr., Effect of hydrostatic pressure upon the magnetic transition in the Gd₅(Si_xGe_{1-x})₄ giant magnetocaloric compounds: X-ray magnetic circular dichroism study, *Phys. Rev. B*, **2007**, 014411 (2007).
- Vaitheeswaran, G., V. Kanchana, R. S. Kumar, A. L. Cornelius, M. F. Nicol, A. Svane, A. Delin, and B. Johansson, High-pressure structural, elastic, and electronic properties of the scintillator host material KMgF₃, *Phys. Rev. B*, **76**, 014107 (2007).
- van Westrenen, W., J. Li, Y. Fei, W. Minarik, J. V. Orman, T. Komabayashi, and K. Funakoshi, In situ determination of magnesiowustite thermal equation of state to 25 GPa and 2073 K, *Phys. Chem. Minerals*, submitted.
- Velisavljevic, N. and G. N. Chesnut, Direct hcp --> bcc structural phase transition observed in titanium alloy at high pressure, *Appl. Phys. Lett.*, **91**, 101906 (2007).
- Vorberger, J., I. Tamblyn, B. Militzer, and S. A. Bonev, Hydrogen-helium mixtures in the interiors of giant planets, *Phys. Rev. B*, **75**, 024206 (2007).
- Wan, J. T. K., T. S. Duffy, S. Scandolo, and R. Car, First principles study of density, viscosity, and diffusion coefficients of liquid MgSiO₃ at conditions of the Earth's deep mantle, *J. Geophys. Res.*, **112**, B03208 (2007).
- Wang, Z., Y. Pang, and D. D. Dlott, Hydrogen-bond disruption by vibrational excitations in water, *J. Phys. Chem. A*, **111**, 3196-3208 (2007).
- Wenk, H. R., ed. *Neutron Scattering in Earth Sciences.*, Reviews in Mineralogy, (Amer. Mineral. Soc., 2006).
- Wenk, H. R., M. Bortolotti, N. Barton, E. Oliver, and D. Brown, Dauphine twinning and texture memory in polycrystalline quartz. Part 2: In situ neutron diffraction compression experiments, *Phys. Chem. Minerals*, **34**, 599-607 (2007).
- Wenk, H. R., I. Huensche, and L. Kestens, In-situ observation of texture changes during the bcc-fcc phase transformation in ultralow carbon steel, *Metall. Trans.*, **38A**, 261-267 (2007).
- Wenk, H. R., I. Lonardelli, S. Merkel, L. Miyagi, J. Pehl, S. Speziale, and C. Tommaseo, Deformation textures produced in diamond anvil experiments, analyzed in radial diffraction geometry, *J. Phys. Cond. Matt.*, **18**, S933-947 (2006).
- Wenk, H. R., I. Lonardelli, E. Rybacki, G. Dresen, N. Barton, H. Franz, and G. Gonzalez, Dauphine twinning and texture memory in polycrystalline quartz. Part 1: Experimental deformation of novaculite, *Phys. Chem. Minerals*, **33**, 667-676 (2006).
- Wenk, H. R., L. Lutterotti, and M. Bortolotti, Neutron texture analysis with HIPPO at your fingertips, *Los Alamos National Laboratory Report LA*, in press.

- Wenk, H. R., S. Speziale, A. K. McNamera, and E. J. Garnero, Modeling anisotropy development in the lower mantle, *Earth Planet. Sci. Lett.*, **245**, 302-314 (2006).
- Yarger, J. and C. A. Agnell, Vitrification of a monatomic metallic liquid, *Nature*, submitted.
- Yoshimura, Y., H. K. Mao, and R. J. Hemley, Relaxation of low-density amorphous ice at high pressures: In-situ Raman study, *J. Phys. Chem.*, submitted.
- Yoshimura, Y., H. K. Mao, and R. J. Hemley, Direct transformation of ice VII' to low-density amorphous ice, *Chem. Phys. Lett.*, **420**, 503-506 (2006).
- Yoshimura, Y., H. K. Mao, and R. J. Hemley, In situ Raman spectroscopic study on the reversible transition between low-density and high-density amorphous ices at 135 K, *J. Phys.: Cond. Matt.*, **19**, 425214 (2007).
- Yoshimura, Y., S. T. Stewart, H. K. Mao, and R. J. Hemley, In situ Raman spectroscopy of low temperature high pressure transformations of H₂O, *J. Chem. Phys.*, **126**, 174505 (2007).
- Yoshimura, Y., S. T. Stewart, M. Somayazulu, H. K. Mao, and R. J. Hemley, High-pressure x-ray diffraction and Raman spectroscopy of ice VIII, *J. Chem. Phys.*, **124**, 024502 (2006).
- Young, A. F., C. Sanloup, E. Gregoryanz, S. Scandolo, R. J. Hemley, and H. K. Mao, Synthesis of novel transition metal nitrides IrN₂ and OsN₂, *Phys. Rev. Lett.*, **96**, 155501 (2006).
- Zeng, Q., Y. C. Li, C. M. Feng, H. P. Liermann, M. Somayazulu, G. Y. Shen, and H. K. Mao, Anomalous compression behavior in lanthanum/cerium-based metallic glass under high pressure, *Proc. Nat. Acad. Sci.*, **34**, 13565-13568 (2007).
- Zha, C. S., R. J. Hemley, S. A. Gramsch, H. K. Mao, and W. A. Bassett, Optical study of H₂O ice to 120 GPa: dielectric function, molecular polarizability, and equation of state, *J. Chem. Phys.*, **126**, 074506 (2007).
- Zha, C. S., K. Mibe, W. A. Bassett, O. Tschauner, H. K. Mao, and R. J. Hemley, The P-V-T equation of state of platinum to 80 GPa and 1900 K using new internal resistive heating diamond-anvil cell techniques, *J. Appl. Phys.*, submitted.
- Zhang, H., B. Chen, B. Gilbert, and J. F. Banfield, Kinetically controlled formation of a novel nanoparticulate ZnS with mixed cubic and hexagonal stacking, *J. Mater. Chem.*, **16**, 249-254 (2006).
- Zhao, Y., H. Xu, L. L. Daemen, K. A. Lokshin, K. T. Tait, W. L. Mao, J. Luo, R. P. Currier, and D. D. Hickmott, High-pressure/low-temperature neutron scattering of gas inclusion compounds: progress and prospects, *Proc. Nat. Acad. Sci.*, **104**, 5727-5737 (2007).

B. CDAC Presentations

- Ahart, M., P. Dera, R. E. Cohen, and R. J. Hemley, Pressure-induced phase transitions in PbTiO_3 , *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Ahart, M., P. Dera, R. J. Hemley, and R. E. Cohen, Pressure induced phase transitions in PbTiO_3 , *Fundamental Physics of Ferroelectrics 2006* (Williamsburg, VA, February 12-15, 2006).
- Ahart, M., M. Somayazulu, R. E. Cohen, and R. J. Hemley, High-pressure x-ray diffraction of PbTiO_3 at low temperature, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Ahart, M., M. Somayazulu, R. E. Cohen, and R. J. Hemley, Morphotropic phase boundary in a pure material: Pressure induced phase transitions in PbTiO_3 , *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Ahart, M., M. S. Somayazulu, H. K. Mao, R. J. Hemley, and R. E. Cohen, Pressure induced phase transitions in PbTiO_3 , *Workshop on Fundamental Physics of Ferroelectrics* (Williamsburg, VA, February 11-14, 2007).
- Aihaiti, M., Novel phase transitions in perovskite ferroelectrics under pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Aksoy, R., X-ray diffraction study of molybdenum diselenide to 35.88 GPa, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Aksoy, R., High pressure x-ray diffraction studies of titanium disulfide, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Aksoy, R., E. Selvi, and Y. Ma, High pressure x-ray diffraction studies of nickel disulfide, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Aksoy, R., E. Selvi, and Y. Ma, X-ray diffraction study of niobium diselenide to 45.1 GPa, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Al Katatbeh, Y. M., K. K. Lee, and B. Kiefer, High-pressure phase diagram of TiO_2 as determined by experiment and theory, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Al-Khatatbeh, Y., K. Lee, and B. Kiefer, Phase diagrams of titanium and titanium oxide at high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Banighan, E. J., R. Caracaz, P. Beck, and R. J. Hemley, Theoretical and experimental Raman study of spinel, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Bass, J. D., S. V. Sinogeikin, D. L. Lakshtanov, V. Prakapenka, G. Shen, C. Sanchez-Valle, J. Perrillat, J. Wang, and B. Chen, Brillouin scattering with simultaneous x-ray diffraction at GSECARS, Advanced Photon Source: Toward determination of absolute pressure scales, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Beck, P., A. F. Goncharov, and R. J. Hemley, High-pressure high-temperature Raman spectroscopy of San Carlos olivine, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Beck, P., A. F. Goncharov, V. V. Struzhkin, B. Militzer, and R. J. Hemley, Measurements of thermal diffusivity under planetary interior P-T conditions, *37th Annual Lunar Planetary Science Conference* (League City, TX, March 12-16, 2007, 2007).
- Benmore, C. J., Q. Mei, J. L. Yarger, S. Sen, and J. Parise, The first and second sharp diffraction peaks in network and molecular glasses, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Bommannavar, A., M. Somayazulu, V. Naik, and R. Naik, High pressure studies on nanoparticles of gamma Fe_2O_3 , *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Brown, J. M., J. Crowhurst, A. Goncharov, and S. D. Jacobsen, Reduced seismic anomalies in the lower mantle: Role of the high-spin to low-spin electronic transition, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Brown, J. M., J. C. Crowhurst, A. F. Goncharov, J. Zaugg, and S. D. Jacobsen, Sound velocities for ferrous periclase through the high spin-low spin transition, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Campbell, A. J., R. B. Thomas, and Y. Fei, Effect of the fcc to hcp phase transition on trace element partitioning between metal and sulfide melt, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Caracas, R. and R. E. Cohen, Searching for ferroelectrics with exotic chemistry, *Fundamental Physics of Ferroelectrics 2006* (Williamsburg, VA, February 12-15, 2006).
- Caracas, R. and R. E. Cohen, Computational study of the pressure behavior of post-perovskite phases, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).

- Caracas, R. and R. E. Cohen, Theoretical determination of the Raman spectra of MgSiO_3 under pressure, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Caracas, R., A. Goncharov, and J. Castillo, Multidisciplinary approaches to the study of planetary ices I, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Caracas, R., A. Goncharov, and J. Castillo, Multidisciplinary approaches to the study of planetary ices II Posters, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Caracas, R. and R. J. Hemley, Theoretical precursors to polymeric nitrogen, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Caracas, R. and B. Mysen, Spectroscopy in mineralogy: theory and experiment I, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Caracaz, R., Dynamic mean-field theory study of FeO, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Carpenter, M. A., T. W. Darling, J. D. Bass, D. L. Lakshtanov, S. V. Sinogeikin, and S. D. Jacobsen, Superattenuation of acoustic resonances and non-linear elasticity associated with the cubic-rhombohedral phase transition in LaAlO_3 perovskite, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Chellappa, R., Pressure-induced transformations and order-disorder phenomena in Li-based complex hydrides: Implications to hydrogen storage, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chellappa, R., D. Chandra, S. Gramsch, M. Somayazulu, and R. J. Hemley, High pressure research on complex hydrides and energy storage materials, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chellappa, R., D. Chandra, S. A. Gramsch, M. S. Somayazulu, and R. J. Hemley, Pressure-induced phase transformations in Li-based complex hydrides, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Chen, X. J., Optical evidence for the metallization of solid silane under pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chen, X. J., Superconductivity and lattice effects in mercury-based superconductors, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chen, X. J., On the oxygen isotope effect in high-Tc superconductors, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Chen, X. J., V. V. Struzhkin, A. Goncharov, Y. Song, Z. Liu, H. K. Mao, and R. J. Hemley, Spectroscopic evidence for pressure-induced metallization in solid silane, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Chen, X. J., V. V. Struzhkin, Z. Wu, R. J. Hemley, H. K. Mao, B. Liang, C. Ulrich, and H. Q. Lin, Oxygen isotope effect in layered cuprate superconductors, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Cody, G., S. Lee, B. Mysen, and Y. Fei, Pressure-induced changes in crystal-melt partitioning coefficient between silicate melts and crystals: A view from solid-state NMR, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Cohen, R. E., Origin of large response in high electromechanical coupling transducer materials, *Fundamental Physics of Ferroelectrics 2006* (Williamsburg, VA, February 12-15, 2006).
- Cohen, R. E., Computation of thermal, elastic, and magnetic properties at high pressure, *Frontiers in High Pressure Research* (Kibbutz Ein-Gued, Dead Sea, Israel, March 2-7, 2006).
- Cohen, R. E., Theory of iron at high pressure and temperature (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Cohen, R. E., Multiscale modeling of magnetism in iron at high pressures, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Cohen, R. E., Enhanced piezoelectricity from polarization rotation in perovskites (invited), *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Cohen, R. E., Theory of minerals at high pressure beyond band theory, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cohen, R. E., Theory and experiments on ferroelectrics and other active materials, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cohen, R. E., Twisted materials by design: Exploring properties of piezoelectrics from first-principles, *Workshop on Fundamental Physics of Ferroelectrics* (Williamsburg, VA, February 11-14, 2007).

- Cohen, R. E., B. Militzer, R. Hennig, C. Umrigar, K. Driver, R. Needs, and M. Towler, Quantum Monte Carlo simulations of phase transitions in silica, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Cohen, R. E., B. Militzer, Z. Wu, K. Driver, P. L. Rios, M. Towler, and R. Needs, Quantum Monte Carlo computations for equations of state, phase transitions, and elasticity of silica, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Cohen, R. E. and X. Sha, Multiscale simulations of iron at high pressures and temperatures, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Cohen, R. E., G. Shen, and R. Caracas, Ironworkers reunion: The behavior of iron and iron-bearing phases in the deep Earth II posters, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Cohen, R. E., M. Towler, P. Lopez Rios, N. Drummond, and R. Needs, Quantum Monte Carlo simulations of the quartz to stishovite transition in SiO₂, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Cohen, R. E. and R. M. Wentzcovitch, Spectroscopy in mineralogy: theory and experiment II, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Cohen, R. E. and Z. Wu, Ferroelectricity in PbTiO₂ and BaTiO₃, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Cohen, R. E. and Z. Wu, Prediction of pressure induced morphotropic phase boundary in PbTiO₃ and the origin of giant electromechanical coupling via polarization rotation, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Cottrell, E. and Y. Fei, Challenges to determining metal-silicate element partition coefficients under extreme P-T conditions, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Cuk, T., V. Struzhkin, T. Devereaux, A. Goncharov, C. Kendziora, H. Eisaki, H. K. Mao, and Z. X. Shen, A pressure induced insulator-to-metal critical point in the copper-oxides, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Cunningham, N., High pressure structural phase transformations in heavy rare earth metal terbium to 154 GPa: Evidence for f-shell delocalization, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Cunningham, N. C., W. Qiu, K. M. Hope, and Y. K. Vohra, Structural trends in heavy rare earth metals at high pressure - possible f-delocalization mechanisms, *Gordon Conference on Research at High Pressure* (Biddeford, ME, June 25-30, 2006).
- Cynn, H. and H. P. Liermann, Mechanical properties under extreme conditions, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Delaire, O., M. Kresch, M. Lucas, R. Stevens, J. Munoz, and B. Fultz, Anharmonic phonons in vanadium alloys and compounds, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Delaire, O., T. Swan-Wood, M. Kresch, and B. Fultz, Thermodynamics of impurities in vanadium, *TMS Annual Meeting* (San Antonio, TX, March 12-16, 2006).
- Deng, L., Z. Gong, and Y. Fei, Direct shock loading of pre-synthesized MgSiO₃-perovskite sample to the Earth's lower mantle conditions and its geophysical implications, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Dera, P., Oscillation Laue analysis (OLA) - a new crystal structure determination method for mineral physics, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Ding, Y., R. Ahuja, J. Shu, P. Chow, W. Luo, and H. K. Mao, The equation of state and structure stability of elemental metal vanadium under high pressure -from experiments to theories, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Ding, Y., H. Liu, J. Xu, R. J. Hemley, H. K. Mao, and C. T. Prewitt, Neutron and x-ray scattering studies for Fe_{1-x}O, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Dlott, D. D., Interfaces at high pressure (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Dlott, D. D., Vibrational energy at interfaces: Material transformation dynamics (invited), *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Dlott, D. D., Vibrational spectroscopy with high time and space resolution (invited), *Carnegie Institute of Washington, Geophysical Laboratory Department Seminar* (Washington, DC, May 8, 2006).
- Dlott, D. D., Ultrafast IR-Raman measurements of water vibrations, *Stockholm Discussion Meeting, Local Structure and Molecular Scale Properties of Liquid Water* (Stockholm, Sweden, June, 2006).

- Dlott, D. D., Vibrational dynamics with high time and space resolution (invited), *Gordon Conference on Liquids, University of New England* (Biddeford, ME, July, 2006).
- Dlott, D. D., Vibrational energy relaxation in condensed phases, *Telluride Workshop on Vibrational Dynamics* (Telluride, Co, July 2006).
- Dlott, D. D., Vibrational energy in liquids, *Telluride Workshop on Vibrational Dynamics* (Telluride, CO, July, 2006).
- Dlott, D. D., Vibrational energy in water, *Telluride Workshop on Vibrational Dynamics* (Telluride, Co, July, 2006).
- Dlott, D. D., Vibrational energy in molecules and molecular nanostructures, *Auburn University* (Auburn, IL, April, 2006).
- Dlott, D. D., Vibrational dynamics with high time and space resolution (invited), *International Workshop on Time-Resolved Spectroscopy, RIKEN* (Wako-shi, Japan, August, 2006).
- Dlott, D. D., Vibrational dynamics with high time and space resolution (invited), *International Conference on Raman Spectroscopy* (Yokohama, Japan, August, 2006).
- Dlott, D. D., Energetic materials: landscapes, surfaces and interfaces (invited), *Joint Army-Navy-NASA-Air Force Interagency Propulsion Committee Workshop on R&D Required to Implement New Energetic Ingredients in Munitions* (Aberdeen, MD, August, 2006).
- Dlott, D. D., Ultrafast dynamics of molecules at interfaces under extreme conditions (invited), *American Chemical Society National Meeting* (San Francisco, CA, September, 2006).
- Dlott, D. D., Vibrational dynamics with high time and space resolution (invited), *Bowling Green State University* (Bowling Green, OH, October, 2006).
- Dlott, D. D., Vibrational dynamics with high time and space resolution (invited), *University of Southern California, Viterbi College of Engineering* (Los Angeles, CA, October, 2006).
- Dlott, D. D., Fundamental dynamic mechanisms of nanoenergetic material initiation and ignition (invited), *Army Research Office review of "Nanotechnology Engineered Energetic Materials"* (Army Research Laboratory, Aberdeen, MD, 2006).
- Dlott, D. D., Vibrational energy in molecules with high time and space resolution (invited), *MIT Seminar on Modern Optics and Spectroscopy, George R. Harrison Spectroscopy Laboratory* (Cambridge, MA, February, 2007).
- Dlott, D. D., Infrared-Raman studies of vibrational energy transfer (invited), *American Chemical Society National Meeting* (Chicago, IL, March, 2007).
- Dlott, D. D., Vibrational sum-frequency generation studies of reactivity and dynamics at interfaces (invited), *Argonne National Laboratory Users' Week, Workshop on In Situ Studies of Interfacial Reactivity* (Argonne, IL, May, 2007).
- Dlott, D. D., Ultrafast shock wave coherent dissociation and spectroscopy of materials, *American Physical Society Topical Meeting on Shock Compression of Condensed Matter* (Hawaii, June, 2007).
- Dlott, D. D., Energy transfer at interfaces, *International Conference on Femtochemistry, "Femto8"* (Oxford, England, July, 2007).
- Dlott, D. D., Vibrational energy in molecules and interfaces *Telluride Vibrational Workshop* (Telluride, CO, August 6-10, 2007).
- Dorfman, S. M., F. Jiang, Z. Mao, A. Kubo, V. Prakapenka, and T. S. Duffy, Phase transitions and equations of state of alkaline earth fluorides CaF_2 and SrF_2 to 95 GPa, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Driver, K., J. W. Wilkins, R. Hennig, C. Umrigar, G. E. Scuseria, R. E. Cohen, and B. Militzer, Simulations of silica phases beyond the generalized-gradient approximation, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Driver, K. P., R. E. Cohen, P. L. Rios, M. Towler, R. Needs, and J. W. Wilkins, Quantum Monte Carlo study of the elastic instability of stishovite under pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Driver, K. P., J. W. Wilkins, R. G. Henning, C. J. Umrigar, G. Scuseria, B. Militzer, and R. E. Cohen, Quantum Monte Carlo benchmarks functionals for silica polymorphs, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Drozd, V., S. K. Saxena, A. Durygin, and S. V. Garimella, Chemical reactions for hydrogen storage and generation, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Duffy, T. and Y. Fei, Mantle phase transitions and seismic discontinuities I, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).

- Duffy, T. S., Elastic properties of hydrous minerals and implications for seismic studies of the upper mantle (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Duffy, T. S., The post-perovskite phase transition and the Earth's core-mantle boundary region (keynote lecture), *European Mineralogy and Petrology Meeting* (Bristol, UK, September 12, 2006).
- Duffy, T. S., The post-perovskite phase transition and Earth's core-mantle boundary region (invited), *Symposiums on Impacts and Deep Earth Geophysics* (Pasadena, CA, May 12, 2006).
- Duffy, T. S., Recent advances in deep Earth studies (invited), *Department of Geophysical Sciences, University of Chicago* (Chicago, IL, February 24, 2006).
- Duffy, T. S., New views of the deep mantle (invited), *Royal Society of London Conference on Origin and Evolution of the Earth* (London, England, September 13, 2007).
- Duffy, T. S., Static strength of materials to Mbar pressures in the diamond cell (invited), *Topical Conference on Shock Compression in Condensed Matter* (Kona, Hawaii, June, 2007).
- Duffy, T. S., Elastic properties of olivine polymorphs: Insights into the structure and composition of the upper mantle (invited), *Department of Geology, University of Maryland* (College Park, MD, March 30, 2007).
- Duffy, T. S., Experimental studies of post-perovskites: Implications for the core-mantle boundary (invited), *Department of Earth, Atmospheric, and Planetary Sciences* (Cambridge, MA, March 15, 2007).
- Duffy, T. S., Static and dynamic equations of state: key challenges and solutions, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Duffy, T. S. and Z. Mao, Elasticity of the olivine (Mg,Fe)₂SiO₄ polymorphs: Current understanding and implications for mantle composition, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Duffy, T. S., Z. Mao, S. D. Jacobsen, F. Jiang, J. R. Smyth, C. M. Holl, and D. J. Frost, Elasticity of hydrous olivine polymorphs: implications for seismic structure of the transition zone, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Esler, K., Computational prediction of material properties under extreme pressure: The equation of state of cubic boron nitride, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Esler, K. P., B. Militzer, and R. E. Cohen, Quantum Monte Carlo determination of the equation of state of cubic boron nitride, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Esler, K. P., B. Militzer, and R. E. Cohen, High-accuracy pressure scale computed with quantum Monte Carlo, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Fei, Y., Challenges in studying the chemistry of deep interior of the Earth (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Fei, Y., NaCl and neon as pressure standards and media, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Fei, Y., Chemistry and physics of the Earth's deep interior, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Fei, Y., A. Ricolleau, E. Cottrell, L. Zhang, A. Corgne, Y. Wang, T. Komabayashi, N. Sata, V. Prakapenka, and Y. Meng, Spin transition and equation of state of ferropericlase at high temperature: implications for density model of the lower mantle, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Feng, Y., R. Jaramillo, T. F. Rosenbaum, O. G. Shpyrko, E. D. Isaacs, G. Srajer, J. Lang, Z. Islam, M. Somayazulu, H. K. Mao, and V. Prakapenka, Evolution of Cr's charge and spin density waves under GPa pressures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Feng, Y., R. Jaramillo, C. T. Seagle, D. M. Silevitch, T. F. Rosenbaum, and D. L. Heinz, High pressure probes of magnetic quantum phase transitions, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Ferroir, T., P. Beck, P. Gillet, A. Simionovici, M. Bohn, L. Dubrovinsky, and A. El Goresy, Polycrystalline and intracrystalline growth of akimotoite in clinoenstatite of the L-6 tenham chondrite, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).

- Fultz, B., Phonon thermodynamics in materials under extreme conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Fultz, B., Mössbauer diffractometry (invited), *Fourth Nassau Mössbauer Symposium* (Garden City, NY, January 14, 2006).
- Fultz, B., Dynamic data-driven data applications systems for the domain of neutron scattering research (invited), *Workshop at the National Science Foundation Headquarters* (Washington, DC, January 19, 2006).
- Fultz, B., Inelastic neutron scattering and entropy (invited), *Indiana University Department of Physics Colloquium* (Bloomington, IN, May 30, 2006).
- Fultz, B., Nanostructured materials for lithium and hydrogen storage (invited - Keynote talk), *MIT Energy Nanotechnology International Conference* (Cambridge, MA, June 27, 2006).
- Gao, C., Y. Ma, Y. Han, M. Li, and G. Zou, In-situ conductivity measurement of matter under extreme conditions by film fabrication of diamond anvil cell, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Gao, C., Y. Ma, J. He, D. Yu, and Y. Tian, In-situ x-ray diffraction of BCN compound under pressure up to 30 GPa, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Gavriliuk, A., V. V. Struzhkin, and I. Lyubutin, Scenario of high pressure phase transitions in multiferroic BiFeO₃, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Goncharov, A., Optical spectroscopy under extreme conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Goncharov, A., Hydrogen-rich molecular systems at high pressure and temperatures, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Goncharov, A., Simple molecular systems under high pressure and temperature, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Goncharov, A., Molecular systems under high compression, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Goncharov, A., Simple molecular systems under simultaneous conditions of high pressure and temperature, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Goncharov, A. and J. Crowhurst, Simple molecular systems at high pressures and temperatures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Goncharov, A. and J. C. Crowhurst, Raman spectroscopy of hot compressed hydrogen and nitrogen - implications for the intramolecular potential, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Goncharov, A. F. and J. Crowhurst, Simple molecular materials under conditions of high pressure and temperature, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Goncharov, A. F. and J. C. Crowhurst, High pressure calibration at high temperatures in the diamond anvil cell using cubic boron nitride, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Gupta, Y. M., Institute for Shock Physics: Research objectives, activities, and capabilities, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Haugen, B., A. F. Goncharov, S. D. Jacobsen, V. V. Struzhkin, and D. P. Dobson, Conduction in the lower mantle: Optical absorption spectra of iron-bearing magnesium silicate perovskite at lower mantle pressures, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- He, C., C. Gao, and Y. Ma, In-situ electrical property study of CdSe under pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- He, C., C. Gao, and Y. Ma, Electrical impedance spectrum study of CdS under high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Heinz, D., Experimental studies of core minerals at core conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Heinz, D. L., C. T. Seagle, A. J. Campbell, N. Miller, V. Prakapenka, and G. Shen, Thermal equations of state in the Fe-FeS, Fe-FeO, and ammonia-water systems, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Hemley, R. J., New findings in materials under pressure (invited), *Massachusetts Institute of Technology* (Cambridge, MA, February 6, 2006).
- Hemley, R. J., Overview of new developments and future prospects in high-pressure research (invited), *Frontiers in High Pressure Research* (Kibbutz Ein-Gued, Dead Sea, Israel, March 2-7, 2006).

- Hemley, R. J., New findings in materials under pressure (invited), *Dalhousie University* (Halifax, Nova Scotia, Canada, March 23, 2006).
- Hemley, R. J., Emerging diamond technology and the science of extreme conditions (invited), *ICOPS* (Traverse City, Michigan, June 4-8, 2006).
- Hemley, R. J., Current problems in high-pressure science (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Hemley, R. J., New findings in molecular systems under pressure (invited), *ACS National Meeting* (San Francisco, CA, September 10-14, 2006).
- Hemley, R. J., New findings in materials under pressure (invited), *University of Virginia, Chemistry Department* (Charlottesville, VA, October 20, 2006).
- Hemley, R. J., New findings in materials under pressure (invited), *53rd Midwest Solid State Conference* (Kansas City, Missouri, October 6-8, 2006).
- Hemley, R. J., New findings in materials under pressure (invited), *Fall 2006 Joint Meeting of the Texas sections of the American Physical Society, American Association of Physics Teachers, Zone-13 of the Society of Physics Students, Forum on Industrial and Applied Physics, National Society of Hispanic Physicists, and National Society of Black Physicists* (Arlington, TX, October 5-7, 2006).
- Hemley, R. J., New studies of low-Z systems under pressure, *Sixth International Conference on Cryocrystals and Quantum Crystals* (Kharkov, Ukraine, September 3-7, 2006).
- Hemley, R. J., New developments at CDAC - The Carnegie/DOE Alliance Center: A center of excellence for high pressure science and technology (invited), *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Hemley, R. J., Ultra high pressure phases: Part I (invited), *Spring College on Water in Physics, Chemistry, and Biology* (Trieste, Italy, April 10-20, 2007).
- Hemley, R. J., Ultra high pressure phases: Part II (invited), *Spring College on Water in Physics, Chemistry, and Biology* (Trieste, Italy, April 10-20, 2007).
- Hemley, R. J. and B. Militzer, Planetary fluids under extreme conditions, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Hemley, R. J., C. S. Yan, and H. K. Mao, The new diamond age - from Earth to CVD (invited), *2006 DeBeers Diamond Conference* (Cambridge, England, July 10-12, 2006).
- Howard, J., S. Sinogeikin, M. Nicol, and O. Tschauner, Structural evolution of schreibersite, Fe₃P, at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Jackson, J., High-pressure investigations of Earth's interior (invited), *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Jackson, J. M., Physical properties of minerals and melts under high-pressure (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Jackson, J. M., The electronic structure of iron in aluminous (Mg, Fe)SiO₃ perovskite at high-pressures and temperatures, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Jackson, J. M., Y. Fei, M. Hu, and H. K. Mao, Sound velocities of upper mantle minerals determined by nuclear resonant inelastic x-ray scattering, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Jackson, J. M., O. Tschauner, Y. Fei, W. Sturhahn, M. Lerche, and J. Zhao, The electronic structure of iron in (Mg,Fe)SiO₃ perovskite and post-perovskite under megabar pressures, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Jackson, J. M. and L. Wagner, Elasticity of orthopyroxene at high-temperature: Novel phase transitions and applications to geophysics, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Jacobsen, S. D., Identifying hydration in the mantle transition zone: Emerging constraints from mineral physics and seismology (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, *Yale University, Department of Geology and Geophysics* (New Haven, CT, January 20, 2006).
- Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, *Northwestern University, Department of Geological Sciences* (Evanston, IL, February 13, 2006).

- Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, *Virginia Polytechnic Institute and State University, Department of Geological Sciences* (Blacksburg, VA, February 23, 2006).
- Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, *University of Minnesota, Department of Geology and Geophysics* (Minneapolis, MN, March 2, 2006).
- Jacobsen, S. D., Seismic structure of a hydrous mantle transition zone: the emerging picture from mineral physics, *University of Illinois Chicago, Department of Earth and Environmental Science* (Chicago, IL, September 7, 2006).
- Jacobsen, S. D., Effect of water on the equation of state of nominally anhydrous minerals, *Mineralogical Society of America Short Course: Water in Nominally Anhydrous Minerals* (Verbania, Italy, October 1-4, 2006).
- Jacobsen, S. D., F. Jiang, J. R. Smyth, T. S. Duffy, Z. Mao, C. M. Holl, and D. J. Frost, Sound velocities of hydrous olivine and the effects of water on the equation of state of nominally anhydrous minerals, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Jacobsen, S. D., J. R. Smyth, and S. van der Lee, Effect of water on the elastic properties of nominally anhydrous minerals (invited), *Eos Trans. AGU Jt. Assem. Suppl., Abstract.*, **87** (2006).
- Japel, S. and B. Keifer, Iron phosphide (Fep) to 60 GPa: Equation of state and phase transition, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Jenkins, T., R. J. Hemley, H. K. Mao, W. Mao, B. Militzer, and V. V. Struzhkin, Clathrate hydrogen storage examined with inelastic neutron scattering and Raman vibrational spectroscopy, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Jenkins, T., R. J. Hemley, H. K. Mao, W. Mao, V. V. Struzhkin, B. Militzer, and J. Leao, Examination of hydrogen clathrates vibrational spectra by inelastic neutron scattering *American Conference on Neutron Scattering* (St. Charles, IL, June 18-22, 2006).
- Jenkins, T., R. J. Hemley, W. Mao, H. K. Mao, B. Militzer, and V. Struzhkin, Clathrate hydrates studied by diffraction and vibrational spectroscopy, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Jenkins, T., W. Mao, H. K. Mao, V. Struzhkin, B. Militzer, and R. J. Hemley, High pressure hydrogen clathrate research using inelastic neutron scattering and x-ray diffraction, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Jiang, F., G. D. Gwanmesia, and T. S. Duffy, Elasticity of stishovite and acoustic mode softening under high pressure by Brillouin scattering, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Jiang, F., G. D. Gwanmesia, and T. S. Duffy, Elasticity of stishovite and acoustic mode softening under high pressure by Brillouin scattering, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Johnson, K., J. Feldman, and R. J. Hemley, Vibron dynamics of hydrogen at high pressures and temperatures, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Jung, H., Y. Fei, P. S. Silver, and H. W. Green, Detecting acoustic emissions at high pressure and high temperature using multianvil press: Application to deep seismicity, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Kalita, P. E., R. Kumar, and A. Cornelius, Ambient and high pressure structural studies on TiH₂, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Kalita, P. E., G. Mariotto, Y. Ohki, and K. E. Lipinska-Kalita, Core/shell nanocrystalline clusters in a glass matrix: a high pressure synchrotron x-ray diffraction study, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Kalita, P. E., S. Sinogeikin, K. E. Lipinska-Kalita, T. Hartmann, and A. Cornelius, On the high-pressure behavior of titanium hydride, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Kalita, P. E., S. Sinogeikin, K. Lipinska-Kalita, T. Hartmann, and A. Cornelius, On the high-pressure behavior of titanium hydride, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Kavner, A. and M. Weinberger, Material yield strength and anisotropy in the nonhydrostatic diamond anvil cell: Implications for mantle and core minerals, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).

- Kharlamova, S. A., A. G. Gavriliuk, S. Sinogeikin, V. V. Struzhkin, I. S. Lyubutin, W. Sturhahn, and S. G. Ovchinnikov, Phase transitions in $\text{GdFe}_3(\text{BO}_3)_4$ under high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Kharlamova, S. A., V. V. Struzhkin, S. Sinogeikin, A. G. Gavriliuk, D. Brown, T. Toellner, J. Zhao, M. Lerche, I. S. Lyubutin, S. G. Ovchinnikov, E. E. Alp, and W. Sturhahn, Pressure-induced phase transitions in gadolinium iron borate, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Kiefer, B. and T. S. Duffy, Finite element situations of the laser-heated diamond cell: Effect of experimental geometry on thermal structure, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- King, S. L. and A. Goncharov, Investigation of the high P-T behavior of binary hydrogen-helium mixtures, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Kollias, A., Ab initio study of the pressure-induced spin transition in $\text{Mg}_{1-x}\text{Fe}_x\text{O}$, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Kollias, A. C. and R. E. Cohen, Dynamical mean-field theory study of the high pressure behavior of FeO , *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Kolorenic, J., L. Mitas, A. C. Kollias, K. P. Esler, and R. E. Cohen, Quantum Monte Carlo study of equilibrium phase stability of crystalline FeO , *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Komabayashi, T. and Y. Fei, Phase relations of iron determined by in-situ x-ray diffraction in an internally-heated diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Krasnicki, S., C. S. Yan, S. S. Ho, J. Lai, H. Y. Shu, T. Yu, H. K. Mao, and R. J. Hemley, Fabrication and properties of large CVD diamond single crystals, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Krasnicki, S., C. S. Yan, J. Lai, H. Y. Shu, T. Yu, S. S. Ho, Y. Meng, H. K. Mao, and R. J. Hemley, fabrication and properties of large CVD diamond single crystals, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Kresch, M., O. Delaire, R. Stevens, J. Lin, and B. Fultz, Phonons in nickel and aluminum at elevated temperatures from neutron scattering, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Kubo, A., T. Duffy, G. Shen, and V. Prakapenka, Stability and Equation of State of post-perovskite phase in the system $\text{MgSiO}_3\text{-Al}_2\text{O}_3$ to 2 Mbar, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Kubo, A., T. S. Duffy, B. Kiefer, S. Shim, G. Shen, V. Prakapenka, and R. J. Cava, Structure refinement of MgGeO_3 post-perovskite to 1 Mbar, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Kubo, A., B. Keifer, S. H. Shim, G. Shen, V. B. Prakapenka, R. J. Cava, and T. S. Duffy, Rietveld structure refinement of MgGeO_3 post perovskite (ppv) phase to 1 Mbar, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Kulkarni, S., Ternary layered carbides - MAX phases, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Kumar, R. and A. Cornelius, High pressure phases of alkali ternary borohydrides, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Kumar, R. S., A. L. Cornelius, M. F. Nicol, M. Y. Hu, P. Chow, E. D. Bauer, and J. L. Sarrao, Valences changes in YbCu_2Si_2 and YbAgCu_4 studied by high pressure x-ray absorption and resonant inelastic x-ray scattering, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Kuznetsova, A. Y., V. Prakapenka, A. J. Campbell, T. S. Duffy, G. Shen, D. L. Heinz, M. L. Rivers, and S. R. Sutton, CO_2 laser heating system at GSECARS, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Lakshtanov, D. L. and P. Dera, Composition and dynamics of Earth's mantle: Current frontiers and grand challenges in elasticity, phase transitions, and rheology studies VI, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Lakshtanov, D. L., S. Sinogeikin, H. Hellwig, T. Katsura, and J. Bass, Elastic properties of SiO_2 stishovite to 50 GPa, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Lakshtanov, D. L., S. V. Sinogeikin, K. D. Litasov, V. Prakapenka, H. Hellwig, J. Wang, C. Sanchez-Valle, J. Perrillat, B. Chen, M. Somayazulu, E. Ohtani, and J. Bass, Anomalously low pressure of rutile- CaCl_2 phase transition in aluminous hydrogen-bearing stishovite, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Lazor, P., H. K. Mao, W. L. Mao, J. Shu, M. Y. Hu, P. Chow, M. Somayazulu, and R. J. Hemley, X-ray induced dissociation of NH_3 at high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).

- Lee, K., Pressure and chemistry-dependent electron capture radioactive decay, *New Mexico Institute of Mining and Technology* (Socorro, NM, March 30, 2006).
- Lee, K., Pressure and chemistry-dependent electron capture radioactive decay, *Ludwig Maximilians University* (Munich, Germany, June 30, 2006).
- Lee, K., Pressure and chemistry-dependent electron capture radioactive decay, *Bayerisches Geoinstitut* (Beyreuth, Germany, July 6, 2006).
- Lee, K., Laser-driven shock studies on planetary ices (invited), *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Lee, K. and G. Steinle-Neumann, Pressure and chemistry-dependent electron-capture radioactive decay: ^7Be , ^{22}Na , and ^{40}K in crystalline materials, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Lee, K. K., R. O. Nelson, R. Rundberg, and G. Steinle-Neuman, First measurements on how pressure affects the half-life of ^{22}Na : Comparison to theory and analog to ^{40}K , *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Lee, K. K. M., Pressure- and chemistry-dependent electron-capture radioactive decay of ^7Be , ^{22}Na and ^{40}K in crystalline materials, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Lee, K. K. M., Is potassium really in the core? Ab-initio predictions of potassium partitioning between $(\text{Mg,Fe})\text{SiO}_3$ perovskite and iron, (2006).
- Lee, S., J. F. Lin, H. K. Mao, P. Eng, and Y. Q. Cai, Structure and properties of amorphous MgSiO_3 in Earth's mantle: A view from synchrotron inelastic x-ray scattering, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Lee, S., B. O. Mysen, Y. Fei, G. D. Cody, H. K. Mao, and P. Eng, Structure of oxide glass and melts at high-pressure: A view from inelastic x-ray scattering and 2d solid-state NMR, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Lei, Y., R. E. Cohen, J. Lee, and Y. Chen, First-principles study and atomistic modeling of $(\text{BiScO}_3)_{1-x}-(\text{PbTiO}_3)_x$ solid solutions, *Workshop on Fundamental Physics of Ferroelectrics* (Williamsburg, VA, February 11-14, 2007).
- Lerche, M., Y. Ding, M. Abliz, L. Wang, G. Shen, R. J. Hemley, and H. K. Mao, The high pressure synergetic center at the Advanced Photon Source, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Lerche, M., W. Sturhahn, G. Shen, V. B. Prakapenka, A. Ryder, and K. S. Suslick, Synchrotron mossbauer spectroscopy of amorphous iron at pressures up to 30 GPa, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Li, J., L. Gao, B. Chen, H. Vescogni, X. Ding, Y. Ding, S. Sinogeikin, W. Yang, and W. Sturhahn, Effect of alloying elements on the magnetic transitions in iron-rich alloys, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Liermann, H., S. Merkel, L. Miyagi, H. R. Wenk, G. Shen, H. Cynn, and W. J. Evans, New experimental method for in situ determination of material textures at simultaneous high-pressure and -temperature by means of radial diffraction in the diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Liermann, H. P., W. Yang, S. Sinogeiken, G. Shen, H. Cynn, S. Merkel, H. R. Wenk, M. Somayazulu, and P. Dera, Measurement of mechanical properties of materials at high-pressure and temperatures in the diamond anvil cell, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Lin, H. Q., X. J. Chen, V. V. Struzhkin, Z. G. Wu, R. J. Hemley, H. K. Mao, B. Liang, C. Ulrich, and C. T. Lin, Theoretical and experimental studies on the oxygen isotope effect in cuprate superconductors, *The 8th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors* (Dresden, Germany, July, 2006).
- Lin, J., S. D. Jacobsen, V. V. Struzhkin, W. Sturhahn, V. Iota, A. G. Gavriliuk, J. M. Jackson, M. Hu, V. Prakapenka, J. Zhao, and C. Yoo, Sound velocities and spin states of magnesiowustite in the Earth's lower mantle, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Lin, J. F., G. Vanko, S. D. Jacobsen, V. Iota, V. V. Struzhkin, V. Prakapenka, A. Y. Kuznetsova, and C. Yoo, Spin transition zone (STZ) in the lower mantle, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Lipinska-Kalita, K., P. E. Kalita, C. Segre, R. J. Hemley, and T. Hartmann, Novel oxide glass-based complex nanocomposite materials: Fabrication and structural characterization, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Lipinska-Kalita, K. E., O. A. Hemmers, P. E. Kalita, G. Mariotto, Y. Ohki, S. A. Gramsch, R. J. Hemley, T. Hartmann, and L. Ma, Amorphous matrix-based composite materials:

- Fabrication, high-pressure structural integrity and structural transformations, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Lipinska-Kalita, K. E., P. E. Kalita, R. J. Hemley, and C. L. Gobin, High pressure-induced phase transition in b-Ga₂O₃: in situ synchrotron x-ray diffraction studies up to 70 GPa, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Liu, H., Synchrotron x-ray scattering studies for minerals under high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Liu, H., X-ray scattering studies for materials under high pressure: From powder to amorphous samples, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Liu, H. and M. Kunz, High-pressure materials science: Synchrotron x-ray scattering studies *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Liu, H., L. Wang, X. Xiao, P. Lee, R. J. Hemley, and H. K. Mao, Compressibility and phase transition studies for amorphous materials under high pressure: Approach combined of synchrotron high energy x-ray diffraction and micro tomography techniques using diamond anvil cell, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Liu, Z., Synchrotron far-infrared spectroscopy and ab initio study of phonon density of states in ice VII at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Lucas, M., O. Delaire, M. Winterrose, I. Halevy, B. Fultz, M. Y. Hu, and J. Hu, Effect of vacancies on the pressure dependence of lattice dynamics in B₂FeAl, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Lyubutin, I., A. Gavriluk, and V. V. Struzhkin, Magnetic collapse and insular-metal transitions in some 3D metal oxides under high pressure, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Ma, Y., High pressure research at Texas Tech University (plenary presentation), *Chinese High Pressure Conference* (Jilin, China, August 1, 2006).
- Ma, Y., Application of synchrotron x-ray in high pressure (invited), *Southwest Jiatong University* (Chengdu, China, July 23, 2006).
- Mao, H. K., Synergy of high-pressure research (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Mao, H. K., The mineral physics exploration of the Earth's deep interior (invited), *Geophysical Laboratory Centennial Celebration* (Carnegie Institution of Washington, Washington DC, May 3, 2006).
- Mao, H. K., High pressure - A new dimension in physics, chemistry, materials science, geoscience, and biology (invited), *Forum on Science Frontier and China's Opportunities in the 21st Century* (Beijing, China, May 24-26, 2006).
- Mao, H. K., High-pressure synergetic consortium - A new approach to high-pressure research at national facilities (invited), *Future Frontiers in High-Pressure Science with ERL X-Ray Beams Workshop* (Cornell University, Ithaca, NY, June 5-6, 2006).
- Mao, H. K., High-pressure - A new dimension in physics, chemistry, materials science, geoscience, and biology (plenary talk), *Academia Sinica's Biannual Meeting* (Taipei, Taiwan, July 1-5, 2006).
- Mao, H. K., New diamond science and technology for the 21st century (invited), *Taipei International Meeting Center* (Taipei, Taiwan, July 7, 2006).
- Mao, H. K., The formation of elasticity, rheology, and dynamics of iron-rich silicate in core-mantle boundary layer (keynote talk), *19th General Meeting of the International Mineralogical Association* (Kobe, Japan, July 23-28, 2006).
- Mao, H. K., Core-mantle interaction - The formation, elasticity, rheology, and dynamics of iron-rich silicate in core-mantle boundary layer (invited), *Fifth International Conference on Synchrotron Radiation in Materials Science (SRMS-5)* (Chicago, IL, July 31, 2006).
- Mao, H. K. and W. L. Mao, Experimental studies at the core-mantle boundary conditions, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Mao, H. K. and W. L. Mao, Hydrogen storage in molecular compounds, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, H. K., G. Shen, and R. J. Hemley, High-Pressure Synergetic Center (HPSynC) - The APS-wide approach to high-pressure synchrotron research, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, W. L., Experimental determination of elasticity of iron at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).

- Mao, W. L., Elasticity of iron-rich silicate in Earth's D" layer, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Mao, W. L., H. K. Mao, Y. Meng, P. Eng, M. Y. Hu, P. Chow, Y. Cai, J. Shu, and R. J. Hemley, X-ray induced dissociation of H₂O and formation of O₂-H₂ compound at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Mao, W. L., H. K. Mao, Y. Meng, P. Eng, M. Y. Hu, P. Chow, Y. Q. Cai, G. Shen, and R. J. Hemley, X-ray induced dissociation of H₂O and formation of an O₂-H₂ compound at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Mao, W. L., H. K. Mao, Y. Meng, P. Eng, M. Y. Hu, P. Chow, Y. Q. Cai, J. Shu, and R. J. Hemley, X-ray induced dissociation of H₂O and formation of an O₂-H₂ compound at high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, W. L., H. K. Mao, J. Shu, Y. Fei, R. J. Hemley, Y. Meng, V. Prakapenka, W. Sturhahn, and J. Zhao, Elasticity of iron-rich silicate in Earth's D" layer, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Mao, W. L., H. K. Mao, W. Sturhahn, J. Zhao, V. B. Prakapenka, Y. Meng, J. Shu, Y. Fei, and R. J. Hemley, Iron-rich silicates at the Earth's core-mantle boundary, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Mao, W. L., V. V. Struzhkin, A. Baron, C. Tommaseo, H. R. Wenk, M. Y. Hu, P. Chow, J. Shu, R. J. Hemley, D. L. Heinz, and H. K. Mao, Experimental determination of elasticity of iron at high pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Mao, W. L., C. Tommaseo, H. R. Wenk, V. V. Struzhkin, A. Baron, P. Chow, M. Hu, W. Sturhahn, J. Shu, R. J. Hemley, and H. K. Mao, Experimental determination of elasticity of iron at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Mao, Z., S. Jacobsen, F. Jiang, C. Holl, J. R. Smyth, and T. S. Duffy, Effect of water on the elastic properties of wadsleyite, B-Mg₂SiO₄, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Mao, Z., S. D. Jacobsen, F. Jiang, J. R. Smyth, C. M. Holl, D. J. Frost, and T. S. Duffy, Single-crystal elasticity of hydrous wadsleyite to 12 GPa, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Mao, Z., F. Jiang, S. D. Jacobsen, J. R. Smyth, C. Holl, T. S. Duffy, and D. J. Frost, Single-crystal elasticity of hydrous wadsleyite by Brillouin scattering, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Meng, Y., M. Y. Hu, P. Chow, E. Rod, A. Bommannavar, and G. Shen, X-ray spectroscopy beamline at HPCAT, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., H. P. Liermann, W. Wang, Y. Ding, E. Rod, A. Bommannavar, and G. Shen, Micro focus x-ray diffraction at high-pressure and low/high temperature at 16BMD (HPCAT): Present and future capabilities, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., S. Sinogeikin, H. Liu, E. Rod, A. Bommannavar, and G. Shen, Micro-focused angle dispersive undulator beamline for x-ray diffraction studies under extreme P-T condition, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., S. V. Sinogeikin, H. P. Liermann, P. Chow, E. Rod, and G. Shen, Online systems at Sector 16 (HPCAT): Efforts to improve beamtime efficiency, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Meng, Y., W. Wang, H. P. Liermann, Y. Ding, E. Rod, A. Bommannavar, and G. Shen, High energy x-ray diffraction at high-pressure and -temperature at 16BMB (HPCAT): Amorphous and melting studies, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Merkel, S., C. Tome, and H. R. Wenk, Evaluation of stress in high pressure radial diffraction: application to hcp Co, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Merkel, S., H. R. Wenk, and C. Tomé, Evaluation of stress in high pressure radial diffraction experiments: Application to Co, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Miltzer, B., Shock hugoniot calculations of dense liquid helium, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Miltzer, B., W. B. Hubbard, and J. Vorberger, Characterization of Materials in Jupiter's Interior with First-Principles Computer Simulations, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).

- Militzer, B. and J. Vorberger, Characterization of Jupiter's interior with first principles computer imulations, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, Co, March 5-9, 2007).
- Militzer, B., J. Vorberger, and W. Hubbard, Modeling Jupiter's interior with a hydrogen-helium equation of state derived from first principles computer simulations, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Miyagi, L., M. Kunz, M. Voltolini, and H. R. Wenk, In-situ laser heating and pressure change with radial diffraction to investigate deformation of deep Earth relevant minerals, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. S. Duffy, and H. R. Wenk, Deformation of the CaIrO_3 post-perovskite phase to 5 GPa and 1300 K in the multi-anvil press, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. S. Duffy, and H. R. Wenk, Texture development in the CaIrO_3 post-perovskite phase deformed in the multi-anvil press up to 5 GPa and 1300 K, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Miyagi, L. and H. R. Wenk, Deformation of Earth materials at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Murakami, M., S. V. Sinogeikin, J. D. Bass, N. Sata, Y. Ohishi, and K. Hirose, Sound velocity of MgSiO_3 post-perovskite phase: Constraints on the D" discontinuity, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Mysen, B. O., S. Lee, G. D. Cody, and Y. Fei, Microscopic origins of configurational thermodynamic properties of silicate melts at ambient and high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Oelker, E., Pressure-induced amorphization of PbGeO_3 crystal, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Oganov, A. R., Y. Ma, J. Chen, Y. Ma, and C. W. Glass, Light elements under pressure: Insights into unusual structures and bonding, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Palasyuk, T., M. Tkacz, L. Dubrovinsky, A. Durygin, and S. K. Saxena, Raman studies of REH_3 under pressure, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Perrillat, J., F. Neestola, S. V. Sinogeikin, and J. D. Bass, Single-crystal elastic properties of $\text{Ca}_{0.07}\text{Mg}_{1.93}\text{Si}_2\text{O}_6$ orthopyroxene, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Prakapenka, V., S. V. Sinogeikin, D. L. Lakshtanov, J. Bass, M. Rivers, and S. Sutton, Self consistent equation of state for dense argon, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Prakapenka, V. B., A. Kunznetsov, S. V. Sinogeikin, M. L. Rivers, and S. R. Sutton, Pressure-assisted synthesis of nano-sized materials in a diamond anvil cell, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Pravica, M., H. Giefers, Z. Quine, E. Romano, B. Yulga, S. Bajar, W. Yang, and H. P. Liermann, Radiation-induced decomposition of energetic materials, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Pravica, M., H. Giefers, E. Romano, B. Yulga, W. Yang, and H. P. Liermann, High pressure and high temperature decomposition studies of PETN and TATB, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Reid, F. R., S. D. Jacobsen, H. C. Watson, Z. Liu, J. Liu, F. Langenhorst, S. Demouchy, J. R. Smyth, Y. Fei, R. J. Hemley, and H. K. Mao, Synthesis and high-pressure synchrotron-infrared studies of OH-bearing silicate perovskite in the laser-heated diamond cell, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Ricolleau, A., Y. Fei, E. Cottrell, A. Corgne, Y. Wang, M. Roskosz, and V. Prakapenka, In-situ x-ray diffraction measurements of ferropericlaase up to 110 GPa and 2000 K, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Ricolleau, A., Y. Fei, E. Cottrell, H. Watson, L. Deng, L. Zhang, G. Fiquet, A. Auzende, M. Roskosz, G. Morard, and V. Prakapenka, New constraints on the pyrolitic model: In situ x-ray diffraction measurements on KLB-1 peridotite under the lower mantle conditions, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Runge, C., A. Kubo, B. Kiefer, V. B. Prakapenka, G. Shen, and T. S. Duffy, Equation of state of MgGeO_3 post perovskite to 65 GPa: Comparason with perovskite phase, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).

- Runge, C. E., A. Kubo, B. Kiefer, T. S. Duffy, V. Prakapenka, G. Shen, and Y. Meng, Equation of state of MgGeO₃ perovskite to 65 GPa: Comparison with the post-perovskite phase, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Said, A., G. Shen, H. Sinn, and A. Alatas, Viscosity of liquid iron derived from the liquid structure data at high pressures, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Sanchez-Valle, C., K. D. Litasov, S. V. Sinogeikin, J. R. Smyth, E. Ohtani, and J. D. Bass, High-pressure sound velocities and single-crystal elastic properties of DHMS phases in subducted slabs, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Schrenk, M. O. and R. J. Hemley, Physiological adaptations of microorganisms to the environmental changes of the deep biosphere, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Scott, H. P., N. Boeteng, M. R. Frank, and Y. Meng, High-pressure stability and equations of state in the Fe-P system: implications for iron meteorites and planetary cores, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Scott, H. P., Z. Liu, R. J. Hemley, and Q. Williams, High pressure infrared spectra of talc and lawsonite, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, N. Miller, and V. Prakapenka, Liquidus temperatures in the iron - sulfur system and melting of Fe₃S at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, and V. Prakapenka, Melting in the Fe-FeO system at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Seagle, C. T., D. L. Heinz, A. J. Campbell, V. B. Prakapenka, and G. Shen, Experimental determination of binary phase diagrams at high pressure, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Seagle, C. T., D. L. Heinz, Z. Liu, and R. J. Hemley, Synchrotron infrared reflectivity of iron at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Sha, X. and R. Cohen, Multiscale modeling of iron at high temperatures and pressures, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Sha, X. and R. E. Cohen, First principles phonon and elasticity computations iron under extreme conditions, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Sha, X. and R. E. Cohen, First-principles study on hcp Fe under Earth's core conditions, *Eos Trans. AGU Jt. Assem. Suppl., Abstract*, **87** (2006).
- Sha, X. and R. E. Cohen, Multiscale modeling of iron at high temperatures and pressures, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Sha, X. and R. E. Cohen, Multi-scale modeling of ferromagnetism in bcc Fe as a function of pressure and temperature, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Shen, G., Experimental studies of phase diagram of iron (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Shen, G., X. Hong, S. V. Sinogeikin, H. P. Liermann, C. Yoo, and H. Cynn, Thermal densification of GeO₂ glass under high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, (2006).
- Shieh, S. R., T. S. Duffy, A. Kubo, and V. Prakapenka, Synthesis of post-perovskite phases from almandine-pyrope garnets at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Shim, S., A. Kubo, T. S. Duffy, and R. J. Cava, Raman spectroscopy of perovskite, post-perovskite, and glass in MgGeO₃ to 1.2 Mbar, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Singh, A. K., H. P. Liermann, Y. Akahama, and S. K. Saxena, The pressure and grain-size dependence of strength of platinum to 330 GPa from the x-ray diffraction data, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Sinogeikin, S., New developments at HPCAT, IDB, and supporting facilities, *Geophysical Laboratory Informal Talk Series* (Washington, DC, October 2, 2007).
- Sinogeikin, S., D. L. Lakshtanov, V. Prakapenka, C. Sanchez-Valle, J. Wang, B. Chen, G. Shen, and J. Bass, Toward a self-consistent pressure scale: elastic moduli and equation of state of MgO by simultaneous x-ray density and Brillouin sound velocity measurements at high-pressure high-temperature conditions, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).

- Soignard, E., J. Yarger, S. Amin, and Q. Mei, Pushing new boundaries in high pressure x-ray diffraction within supercooled liquids and amorphous solids: exploration of phase transformations, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Somayazulu, M., S. Gramsch, H. K. Mao, and R. J. Hemley, High pressure-high temperature studies on Xe-Cl₂, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Somayazulu, M., A. Levedahl, A. Goncharov, H. K. Mao, and R. J. Hemley, High pressure-temperature Raman spectroscopy of H₂-H₂O clathrate, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Somayazulu, M. S., S. A. Gramsch, R. J. Hemley, and H. K. Mao, High pressure-high temperature reactions in xenon-chlorine system, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Speziale, S., F. Jiang, Z. Mao, P. J. Monteiro, H. R. Wenk, T. S. Duffy, and F. Schilling, Single-crystal elasticity of ettringite at ambient conditions, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Speziale, S., H. J. Reichmann, F. Schilling, H. R. Wenk, and P. J. Monteiro, The elastic properties of natural portlandite Ca(OH)₂, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Struzhkin, V. V., X-ray emission spectroscopy, *Frontiers in High Pressure Research* (Kibbutz Ein-Gued, Dead Sea, Israel, March 2-7, 2006).
- Struzhkin, V. V., Magnetism and superconductivity at high pressures (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Struzhkin, V. V., Optimizing hydrogen clathrates for hydrogen storage, *Sixth International Conference on Cryocrystals and Quantum Crystals* (Kharkov, Ukraine, September 3-7, 2006).
- Struzhkin, V. V., Synchrotron x-ray and Mössbauer spectroscopy of iron oxides under high pressure, *MRS Fall Meeting* (Boston, MA, November 27-December 1, 2006).
- Struzhkin, V. V., X. J. Chen, O. Degtyareva, M. Ahart, Y. Song, H. P. Liermann, J. Xu, H. K. Mao, and R. J. Hemley, Optical studies of compressed silane up to 40 GPa, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Struzhkin, V. V., A. G. Gavriiliuk, and I. S. Lyubutin, Pressure-induced spin transition in multiferroics and related compounds, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Surber, E., Surfaces and interfaces of high explosives probed by nonlinear spectroscopy, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Surber, E., Surfaces and interfaces of explosives probed by nonlinear optical spectroscopy, *American Chemical Society* (Chicago, IL, March, 2007).
- Surber, S. E., Surfaces and interfaces of explosives probed by nonlinear optical spectroscopy, *Ohio State University International Symposium on Molecular Spectroscopy* (Columbus OH, June 18-22, 2007).
- Surber, S. E., Sum frequency generation characterization of the surface structure of HMX, *Joint Army Research Office MURI on Insensitive Munitions* (Aberdeen, MD, July 11-13, 2007).
- Tamblyn, I., J. Vorberger, B. Militzer, and S. A. Bonev, Simulations of dense hydrogen and hydrogen-helium mixtures at conditions relevant to gas planet interiors, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Tkachev, S. N. and A. Goncharov, High-pressure Raman spectroscopy of protonic diffusion in ice VII, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Tschauner, O., P. D. Asimow, T. J. Ahrens, N. Kostandova, and S. Sinogeikin, Formation of wadsleyite in a shock experiment - implications for the duration of shock events in meteorite parent bodies, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Tschauner, O., B. Kiefer, H. Liu, M. Somayazulu, and S. N. Luo, Structural polymorphism in Al-bearing magnesiumsilicate post-perovskite, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Vennila, S., A. Durygin, M. Merlini, and S. K. Saxena, High pressure - high temperature study on TiH₂ up to 823 K, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Vennila, S., L. George, V. Drozd, and S. K. Saxena, In situ x-ray diffraction and Raman study on the phase transformation in LiAlH₄ under high pressure - A comparison, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).

- Vohra, Y., Grand challenges in f-electron metals research at high pressures and low temperatures using designer anvil cells (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Vohra, Y., Basic science and applications of vapor grown diamonds of high pressure research (invited), *Gordon Conference on Research at High Pressure* (Biddeford, ME, June 25-30, 2006).
- Vohra, Y. K., Squeezing materials to high pressures using designer diamond anvils, *Materials Science and Engineering Colloquium, University of Alabama* (Birmingham, AL, January 24, 2007).
- Vohra, Y. K. and S. T. Weir, Development of designer diamond technology for high pressure high temperature experiments in support of stockpile stewardship program, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Voltolini, M., H. R. Wenk, N. H. Mondol, K. Bjorlykke, and J. Jahren, Anisotropy in experimentally compressed kaolinite-illite-quartz aggregates: Microstructure, preferred orientation and acoustic velocities, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Vorberger, J., R. E. Cohen, and B. Militzer, Melting of sodium under pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Vorberger, J., I. Tamblyn, S. A. Bonev, and B. Militzer, Hydrogen-helium mixtures under giant gas planet conditions, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Vorberger, J., I. Tamblyn, S. A. Bonev, and B. Militzer, Equation of state calculations for hydrogen and helium under giant planet conditions, *Dalhousie* **87** (2006).
- Vorberger, J., I. Tamblyn, S. A. Bonev, and B. Militzer, Dense fluid hydrogen and helium in the interior of giant planets, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Wan, J. T., T. S. Duffy, S. Scandolo, and R. Car, First-principles study of molten MgSiO₃ in Earth's lower mantle, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Wang, J., S. V. Sinogeikin, T. Inoue, and J. Bass, Elastic properties of hydrous wadsleyite at high pressures, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Wang, L., H. Liu, S. Sinogeikin, J. Shu, and H. K. Mao, Synchrotron x-ray diffraction studies for zincite and ceria under high pressure conditions, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Wang, L., H. Liu, J. S. Tse, and H. K. Mao, Experimental and first-principles calculation studies for several NIST x-ray powder diffraction standards under high pressure conditions, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Wang, Y. and Y. Fei, An experimental investigation of melting relations in the Fe-C system at high pressure and temperatures, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Watson, H. C., Y. Fei, E. Hauri, F. R. Reid, and S. D. Jacobsen, The effect of minor elements on H incorporation in MgSiO₃ perovskite, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Weinberger, M., J. Levine, H. Y. Chung, R. Kaner, A. Kavner, and S. Tolbert, In situ studies of osmium and transition metal diborides under high stress conditions, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Wenk, H. R., Deformation experiments at ultrahigh pressure: Where we are and where we should be going (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Wenk, H. R., I. Lonardelli, M. Mazurek, and L. Van Loon, Preferred orientation and anisotropy in shales, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Wu, Y., Y. Fei, and Z. Jin, Subduction of continental crust into Earth's transition zone: an experimental investigation with implications for the fate of continental subduction, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Wu, Z. and R. E. Cohen, Origin of large response in high electromechanical coupling transducer materials, *Fundamental Physics of Ferroelectrics 2006* (Williamsburg, VA, February 12-15, 2006).
- Wu, Z. and R. E. Cohen, A more accurate generalized gradient approximation for solids, *Bull. Am. Phys. Soc. (APS March Meeting)* (Baltimore, MD, March 13-17, 2006).
- Xu, J., Variability in the vertical structure of the Indonesian throughflow during the last 140 kyr: evidence from the Timor outflow, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Yan, C. S., S. S. Ho, J. Lai, S. Krasnicki, H. K. Mao, and R. J. Hemley, Development of the microwave plasma CVD technique for rapid growth of large single-crystal diamond, *2006 IEEE International Conference on Plasma Science* (Traverse City, MI, June 4-8, 2006).

- Yang, W., W. Liu, B. C. Larson, G. E. Ice, H. P. Liermann, and G. Shen, Deviatoric and dilation strain measurements with x-ray micro-diffraction, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Yarger, J., Structural transformations in liquids and glasses under extreme conditions (invited), *Workshop on Synergy of 21st Century High-Pressure Science and Technology* (Argonne, IL, April 29-May 1, 2006).
- Yarger, J., High-pressure and spin enhanced neutron scattering (invited), *Argonne National Laboratory, Intense Pulsed Neutron Source* (Argonne, IL, April, 2006).
- Yarger, J., High-pressure quenched glasses (invited), *Arizona State University, Chemistry & Biochemistry Symposium* (Tempe, AZ, October, 2006).
- Yarger, J. L., High-pressure phase transformation within supercooled liquid and amorphous solids (invited), *Materials Research Society National Meeting* (Boston, MA, November, 2006).
- Yarger, J. L., Exploring phase transitions in amorphous As_2O_3 (invited), *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Yarger, J. L., Pushing new boundaries in high pressure x-ray diffraction within supercooled liquids and amorphous solids: Exploration of phase transformations (invited), *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
- Yoo, C., J. Lin, H. Fukui, D. Prendergast, T. Okuchi, Y. Cai, A. Hiraoka, P. Eng, M. Hu, and P. Chow, Bonding transition in SiO_2 glass at high pressure: Applications to SiO_2 liquid in Earth's interior, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
- Yoshimura, Y., H. K. Mao, and R. J. Hemley, In situ Raman spectroscopy study on the reversible transition between low-density and high-density amorphous ices at 135 K, *3rd Asian Conference on High Pressure Research* (China, October 16-20, 2006).
- Yulga, B., M. Pravica, Z. Liu, O. Tschauer, and M. Nicol, An infrared study of secondary explosives under high pressure, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
- Zeng, X., R. E. Cohen, Y. Chen, and J. D. Lee, Thermo-electromechanical response of a ferroelectric perovskite from molecular dynamics simulations, *Workshop on Fundamental Physics of Ferroelectrics* (Williamsburg, VA, February 11-14, 2007).
- Zha, C. S., R. J. Hemley, S. A. Gramsch, H. K. Mao, and W. A. Bassett, Optical study of H_2O ice to 120 GPa: Dielectric function, molecular polarizability, and the equation of state, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Zha, C. S., R. J. Hemley, S. A. Gramsch, H. K. Mao, W. A. Bassett, and K. Mebe, New internal resistive heating DAC extends the thermal equation of state of platinum to 80 Pa and 1900 K, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
- Zhang, L. and Y. Fei, Melting behavior of (Mg,Fe)O solid solutions at high pressure, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
- Zhong, Y., Y. S. Chu, A. T. Macrander, and F. Krasnicki, Quantitative strain analysis of single crystals using x-ray topography, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).

APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for Year 4

A. HPCAT (APS)

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

User Name	Affiliations	Project	Dates
B. Yulga E. Romano	University of Nevada – Las Vegas	Single crystal diffraction of epsilon oxygen and nitrogen under high pressure	July 1-2, 2006
J. Pietryga	LANL	DAC, XRD	July 1-3, 2006
K. Zhuravlev	LANL	Quantum dots under pressure	July 1-3, 2006
N. Cunningham W. Qiu N. Velisavljevic	University of Alabama – Birmingham	High pressure x-ray diffraction of metals	July 3-7, 2006
Kimberly Tait	LANL	High <i>P-T</i> phase relationships of first row transition metal monosulfides	July 5-7, 2006
H. Giefers M. Pravica	University of Nevada – Las Vegas	14.4 keV, NRIXS 14.4 keV, NFS	July 5-10, 2006
H. Scott Sabrina Huggins	Indiana University – South Bend	High pressure EOS of Fe ₃ P (ID-B)	July 7-9, 2006
Lysi George Selva Vennila Raju	Florida International University	High pressure and temperature study of MAX phases, hydrides and Perovskite	July 7-10, 2006
Patricia Kalita	University of Nevada – Las Vegas	High-pressure investigations of TiH ₂	July 12-14, 2006
Jennifer Jackson	Carnegie	Raman System	July 10, 2006
M. Jacobsen J. Baker E. Baxter J. Keen	University of Nevada – Las Vegas	High pressure characterization of Bi ₂ Se ₃ , SbTe ₃ , and solid solution 50/50 Bi ₂ Te ₃ /Sb ₂ Te ₃	July 13-14, 2006
H. Giefers	University of Nevada – Las Vegas	High pressure experiments on PbO and Fe-alloys	July 15-17, 2006
J. McClure	University of Nevada – Las Vegas	High pressure investigation of rare earth oxides	July 15-18, 2006
P. Shafe B. Huberti L. Fiorenino	University of Nevada – Las Vegas	Visitors	July 17, 2006
S. K. Lee	Seoul National University	Raman System	July 17, 2006
V. Iota C. Gobin	University of Nevada – Las Vegas	Bonding changes in compressed molecular solids	July 19, 2006
P. Dera	Carnegie	Single Crystal OLA	July 19-22, 2006
W. Evans	LLNL	Ambient and high-temperature crystal structures, phase transitions and EOS of materials at high pressures by EDXD	July 19-23, 2006

W. Xiao	Chinese Academy of Sciences	Investigation of phase transitions of barium chromate under high pressure	July 20, 2006
J. Liu W. Xiao H. Li J. Shu	Chinese Academy of Sciences	High pressure XRD of BaCrO ₄ , BaSO ₄ , CeO ₂ Ho ₂ O ₃ , La ₂ O ₃ , MnO ₂ , Nd ₂ O ₃ , NiO, Sm ₂ O ₃ , SrSO ₄	July 21-27, 2006
Wendy Mao	LANL	High <i>P-T</i> study of Fe-Mg silicate in post-perovskite phase	July 23, 2006
C. S. Yoo	LLNL	F-metal behavior at high pressures and high temperatures using diamond anvil cell	July 25-31, 2006
P. Dera	Carnegie	OLA diffraction study of Cr ₂ O ₃	July 25-28, 2006
Lauren Borkowski	University of Nevada – Las Vegas	Single Crystal OLA	July 26-29, 2006
M. Lipp B. Baer	LLNL	F-metal behavior at high pressures and high temperatures using diamond anvil cell	July 26-31, 2006
J. McClure	University of Nevada – Las Vegas	OLA diffraction study of Cr ₂ O ₃	July 26-31, 2006
J. Shu	Carnegie	EDXD Single Crystal Testing	July 26-31, 2006
X. Li	Chinese Academy of Sciences	High pressure behavior of some rare earth sesquioxides	July 29-31, 2006
A. Gordon J. Larson	University of Nevada – Las Vegas	Angle-dispersive x-ray studies of organic materials	August 1-5, 2006
M. Pravica H. Giefers	University of Nevada – Las Vegas	EDXD of energetics and there decomposition in white radiation	August 2-4, 2006
Amy Lazicki	LLNL	XRS O K-edge, CO ₂ , 24 GPa (IV); a-MgSiO ₃ , 13.5 GPa	August 2-4, 2006
B. Yulga E. Romano	University of Nevada – Las Vegas	Angular dispersive x-ray studies of organic materials	August 3-4, 2006
Patricia Kalita	University of Nevada – Las Vegas	High-pressure investigations of TiH ₂	August 3-4, 2006
D. Eradonea D. Santamaria	University of Valencia	Structural studies of silicides and hydrides under pressure	August 3-8, 2006
R. Kumar	University of Nevada – Las Vegas	Structural studies of silicides and hydrides under pressure	August 4, 2006
L. Friedman S. Mini	IIT NIU	Fluorescence measurements of artifacts	August 4, 2006
Lauren Borkowski P. Dera	University of Nevada – Las Vegas Carnegie	Tests of oscillation Laue analysis approach to structure solution from white beam diffraction	August 4-8, 2006
B. Downs	University of Arizona	Single Xtal	August 4-8, 2006
H. Cynn W. Evans	LLNL	EDXD of W/Re alloy at high-pressure and -temperture, "Dynamic DAC" of metaile Fe	August 7-12, 2006
J. Shu Y. Ding	Carnegie	X-ray diffraction for V under high pressure, NH ₃ -radial diffraction	October 4-7, 2006
P. Lazor H. K. Mao	Uppsala University Carnegie	XRS N K-edge	October 5-9, 2006
X. Li	Chinese Academy of Sciences	GL/Single crystal	October 6-7, 2006
M. Somayazulu S. Gramsch	Carnegie	High pressure EOS of chlorine	October 7-8, 2006
S. Gramsch M. Zomayazulu	Carnegie	Flourecens	October 7-8, 2006

N. Velisavljevic K. Zhuravlev L. Stevens	LANL	High pressure x-ray diffraction on metals, high explosives and polymers	October 8-10, 2006
P. Dera Lauren Borkowski	Carnegie Washington State University	PUP/Single crystal Laue	October 8-13, 2006
Kimberly Tait Q. Guo T. Laetsch	LANL University of Arizona	High pressure x-ray diffraction for synthetic covellite CuS, and synthetic ThSiO ₄ and HfSiO ₄	October 11-13, 2006
Lyci George Selva Vennila Raju	Florida International University	High pressure/temperature study of hydrides	October 13-15, 2006
Yue Meng	HPCAT	XRS N K-edge	October 13-16, 2006
J. Liu	Chinese Academy of Sciences	Single crystal EDXD	October 13-16, 2006
R. Kumar J. Baker	University of Nevada – Las Vegas	EDXD of Au and superconductor in DAC and cryo at high-pressure low-temperature.	October 13-17, 2006
V. Swamy	Monash University, Australia	High pressure XRD nanoscale rutile TiO ₂	October 15-17, 2006
Wendy Mao Q. Guo	LANL	XRS N K-edge	October 18-19, 2006
M. Jacobsen	University of Nevada – Las Vegas	High pressure powder diffraction of thermoelectric materials	October 18-19, 2006
O. Tschauner O. Grubor-Urosevic	University of Nevada – Las Vegas	Single crystal diffraction studies at high pressure	October 19-20, 2006
O. Tschauner	University of Nevada – Las Vegas	XRS C K-edge	October 20, 2006
A. Goncharov	Carnegie	Single crystal Laue on D ₂ and H ₂	October 20-23, 2006
B. Yulga M. Pravica E. D. Romano	University of Nevada – Las Vegas	X-ray powder diffraction of organic materials	October 21, 2006
M. Pravica O. Grubor-Urosevic	University of Nevada – Las Vegas	XRS C K-edge	October 21-22, 2006
J. McClure	University of Nevada – Las Vegas	High pressure investigation of Rare Earth oxides	October 21-22, 2006
Svetlana Kharlamova	APS/ANL	Structural behavior of GdFe ₃ (BO ₃) ₄ at high pressures	October 22-27, 2006
J. Liu	Chinese Academy of Sciences	Single crystal EDXD	October 23-26, 2006
R. Kumar	University of Nevada – Las Vegas	XRS B K-edge	October 25-27, 2006
M. Pravica M. Nicol E. Tanis J. Howard B. Yulga E. Romano	University of Nevada – Las Vegas	Decomposition experiment with EDXD and CCD	October 26-31, 2006
B. Yulga E. D. Romano J. Howard	University of Nevada – Las Vegas	X-ray powder diffraction of organic materials	October 27-28, 2006
G. Lee C. S. Yoo	LLNL	EDXD with dynamic DAC	October 27-31, 2006
H. Giefers Elizabeth Tanis	University of Nevada – Las Vegas	High pressure x-ray diffraction on Dy ₆ Fe ₂₃	October 28, 2006

V. Iota	LLNL	XRS with metal gasket	October 28- November 4, 2006
O. Tschauner P. Dera	University of Nevada – Las Vegas Carnegie	Single crystal diffraction studies at high pressure	October 29, 2006
R. Kumar	University of Nevada – Las Vegas	High pressure diffraction studies on $\text{Na}_{0.85}\text{CoO}_2$	October 29, 2006
O. Tschauner J. McClure	University of Nevada – Las Vegas	X-ray micro diffraction experiments	October 29-31, 2006
V. Prakapenka A. Kuznetsov	GSECARS	Self consistent equitation of state of Ar	November 1, 2006
M. Pravica R. Kumar S. Bajar	University of Nevada – Las Vegas	Continue decomposition experiment with EDXD	November 1-6, 2006
Svetlana Kharlamova	APS/ANL	Structural behavior of $\text{GdFe}_3(\text{BO}_3)_4$ at high pressures	November 2, 2006
R. Kumar	University of Nevada – Las Vegas	EDXD of Au and superconductor in DAC and cryo at high-pressure low-tempeture.	November 2-5, 2006
J. F. Lin	LLNL	XRS O K-edge	November 5-9, 2006
Alice Acatrinei M. Hartl	LANL	EDXD of PbTiO_3 in DAC and cryo at high- pressure low-tempeture	November 5-9, 2006
J. Liu	Chinese Academy of Sciences	Single crystal EDXD	November 6-9, 2006
Alice Acatrinei M. Hartl	LANL	EDXD	November 9-11, 2006
P. Dera B. Downs	Carnegie University of Arizona	PUP/Single crystal Laue	November 9-11, 2006
X. Li	Chinese Academy of Sciences	GL/Single crystal	November 11- 13, 2006
J. Shu H. K. Mao	Carnegie	HP XRD for diuterated H_2O Be, D_2O	November 10- 12, 2006
X. J. Chen	Carnegie	High pressure structure of $\text{Na}_{0.48}\text{CoO}_2$	November 12- 13, 2006
N. Velisavljevic G. N. Chesnut	LANL	Depleted uranium alloy, titanium alloy	November 12- 13, 2006
J. Liu H. Li	Chinese Academy of Science	The investigation of phase transitions of barium chromate (BaCrO_4) under high pressure	November 15- 16, 2006
H. K. Mao	Carnegie	XRS He	November 15- 19, 2006
M. Lipp G. Lee	LLNL	Liquid in DAC with external heating	November 15- 26, 2006
H. K. Mao J. Shu	Carnegie	X-ray diffraction of deuterated H_2O at high pressure	November 16- 18, 2006
H. Cynn	LLNL	EDXD side diffraction	November 17- 22, 2006
J. F. Lin Z. Jenei	LLNL	X-ray diffraction study of H_2O at high pressures	November 18- 22, 2006
A. Gavriluk V. Struzhkin	Russian Academy of Sciences Carnegie	XES Fe K β	November 24- 26, 2006
W. Evans C. S. Yoo Amy Lazicki	LLNL	Low-z hydrides and f-metal behavior at high pressure	November 24- 27, 2006

X. Li	Chinese Academy of Sciences	GL/Single crystal	November 24-27, 2006
J. F. Lin	LLNL	XES Fe Kb	November 27-29, 2006
S. H. D. Shim Krystle Catalli J. Hustoft	Massachusetts Institute of Technology	Effect of ferric iron for the EOS and crystal structure of Mg-Silicate perovskite and post-perovskite at lower mantle	November 29-December 1, 2006
P. Dera O. Tschauner	Carnegie University of Nevada – Las Vegas	UNLV/Single crystal Laue	November 29-December 2, 2006
M. Pravica O. Grubor-Urošević B. Yulga Z. Quine	University of Nevada – Las Vegas	Single crystal EDXD	November 30-December 3, 2006
R. Kumar A. Cornelius	University of Nevada – Las Vegas	RXES Yb LIII/La1	December 1-4, 2006
M. Pravica	University of Nevada – Las Vegas	EDXD of energetics and their decomposition in white radiation	December 2-5, 2006
J. Liu	Chinese Academy of Sciences	Single crystal EDXD	December 3-5, 2006
J. Shu H. K. Mao	Carnegie	High pressure XRD for deuterated H ₂ O	December 3-5, 2006
Jennifer Ciezak	Carnegie	Single crystal EDXD	December 6-8, 2006
Jennifer Ciezak	Carnegie	EDXD of energetics	December 6-8, 2006
C. S. Yoo	LLNL	Classified experiment	December 6-11, 2006
Amy Lazicki	LLNL	RXES Eu LIII/La1	December 7-10, 2006
J. Liu	Chinese Academy of Sciences	Single crystal EDXD	December 8-10, 2006
X. Li	Chinese Academy of Sciences	GL/Single crystal	December 9-11, 2006
K. Zhuravlev N. Velisavljevic L. Sanchez	LANL	EDXD of powder diffraction	December 10-12, 2006
K. Zhuravlev N. Velisavljevic L. Sanchez	LANL	High pressure XRD of europium	December 11-12, 2006
P. Dera	Carnegie	PUP/Single crystal Laue	December 13-15, 2006
R. Kumar J. Baker	University of Nevada – Las Vegas	Low temperature x-ray diffraction studies on CeCu ₂ Si ₂ and CeCu ₂ (SiGe) ₂ compounds	December 13-16, 2006
R. Chellappa	University of Nevada – Las Vegas	Crystal structure/Li-based complex hydrides	December 15-17, 2006
T. Jenkins	Carnegie	High pressure/low temperature powder diffraction on hydrogen clathrate	December 16-19, 2006
H. K. Mao	Carnegie	Chemical composition mapping with microbeam	December 18-19, 2006
H. P. Liermann	HPCAT	Radiation survey, realignment of entire system after switching of experimental table	January 30-February 2, 2007
W. Yand Y. Ding H. K. Mao	APS Carnegie	High Resolution Diffraction	January 31-February 4, 2007

H. K. Mao Q. Zhou Q. Cui	Carnegie Chinese Academy of Sciences	TaN, Ta ₂ N, AlN, and nanowire AlN	February 1-5, 2007
Y. Ma C. Gao	Texas Tech University	Elasticity of Fe in the rotatable DAC.	February 2-5. 2007
Y. Ma C. Gao	Texas Tech University	Fe	February 3-4, 2007
W. Yang	HPCAT	Amorphous study	February 3-6, 2007
Lauren Borkowski Barbara Lavina P. Dera	George Washington University University of Nevada – Las Vegas Carnegie	Single crystal diffraction of Hercynite-Spinel crystals.	February 5-9, 2007
Y. Ding W. Yang	Carnegie HPCAT	Investigation of spin-transition induced structure anomaly in magnetite under high pressure	February 7-8, 2007
Lauren Borkowski Barbara Lavina P. Dera	George Washington University University of Nevada – Las Vegas Carnegie	EDXD studies of marokite	February 7-14, 2007
Dana Dattlebaum	LANL	ATB, THV500 fluoropolymer	February 9-10, 2007
M. Somayazulu	Carnegie	Xenon chloride, Ice in W gasket	February 10- 11, 2007
R. Chellappa	University of Nevada – Reno	LiBH ₄ , NaBH ₄ , Neopentylglycol, XRD+Raman	February 11- 13, 2007
O. Tschauner Laruen Borkowski Barbara Lavina P. Dera	University of Nevada – Las Vegas Carnegie	OLA on single crystals of perovskite and ice.	February 11- 16, 2007
R. Kumar	University of Nevada – Reno	NRIXS Fe ₅₇ - YbFe ₂ Ge ₂ , 1.3.5,13.8 Gpa	February 12- 15, 2007
C. S. Yoo Z. Jenei Amy Lazicki J. H. Klepeis	LLNL	CO ₂ , LiB, N ₂ , B, heating	February 14- 17, 2007
H. P. Liermann P. Dera. Lauren Borkowski Barbara Lavina	HPCAT Carnegie University of Nevada – Las Vegas	Single Crystal diffraction of Marokite at high-pressure.	February 16- 19, 2007
W. Yang	HPCAT	Amorphous study	February 16- 19, 2007
B. Sahoo Elizabeth Tanis J. Croy L. Ono Beatriz Roldan- Cuenya	University of Nevada – Las Vegas	NRIXS Fe ₅₇ - a-Fe ₄₀ Y ₆₀ , ambient, 0.1, 1.7, 2.5, 5.1, 10.3, 20.7, 0.5 GPa	February 16- 20, 2007
Beatriz Roldan- Cuenya J. Croy B. Sahoo Elizabeth Tanis	University of Nevada – Las Vegas	NRIXS Fe ₅₇ - nano-Fe ₈₀ Pt ₂₀ , isolated particles	February 17-18
W. Yang	HPCAT	Fluorescence mapping of suspicious metal particles in a DAC loaded with hydrogen.	February 21- 23, 2007

B. Yulga E. Romano M. Pravica	University of Nevada – Las Vegas	X-ray induced decomposition	February 21- 24, 2007
S. Turneure	Washington State University	Hexamethylenetetramin ((CH ₂) ₆ N ₄)+Cu in N ₂ and Si-oil, Radial diffraction	February 22- 23, 2007
H. Liu	HPCAT	Gearbox, standards CeO ₂ +Au	February 23, 2007
M. Jacobsen	University of Nevada – Las Vegas	High Pressure diffraction of Sb ₂ Te ₃	February 23, 2007
H. P. Liermann	HPCAT	Graphite heater in the membrane DAC, T calibration.	February 23- 27, 2007
B. Yulga E. Romano	University of Nevada – Las Vegas	X-ray powder diffraction of organic materials	February 24, 2007
Elizabeth Tanis Emily Hartnett M. Pravica	University of Nevada – Las Vegas	NFS Fe57- Fe0.953Si0.047, 6.98, 11.3, 15.3, 18.3, 21.4, 24.0, 1.2 GPa	February 24- 26, 2007
W. Yang	HPCAT	Amorphous study in air	February 24- 27, 2007
Andrea Prodi Y. Feng	Massachusetts Institute of Technology	Pressure tuning of spin-Peierls transition on TiOCl single-crystal as imaged by zone-axis x-ray diffraction	February 24- 27, 2007
Wendy Mao H. K. Mao	LANL Carnegie	(Mg, Fe)SiO ₃ perovskite and post perovskite phases at high PT/laser heating and XRD	February 28- March 2, 2007
H. Cynn H. P. Liermann	LLNL HPCAT	EDXD studies of stishovite and osmium	February 28- March 4, 2007
E. D. Romano B. Yulga M. Pravica	University of Nevada – Las Vegas	Radiation-induced Decomposition of energetic materials.	February 28- March 5, 2007
R. Kumar	University of Nevada – Las Vegas	Low temperature x-ray diffraction studies on CeCu ₂ Si ₂ and CeCu ₂ (SiGe) ₂ compounds	March 2-5, 2007
N. Velisavljevic G. N. Chesnut	LANL	EDX study of EOS of Ti alloy	March 5-6, 2007
G. N. Chesnut N. Velisavljevic Dana Dattlebaum	LANL	Compression of TATB, Cu, Ti, Ti alloys, and zirconium in DAC.	March 5-8, 2007
P. Dera H. P. Liermann	Carnegie HPCAT	NIST ruby sphere in air	March 5-8, 2007
Svetlana Kharlamova	APS/ANL	Structural behavior of GdFe ₃ (BO ₃) ₄ at high pressures at low temperatures.	March 7-9, 2007
W. Yang	HPCAT	EDXD study of poly-crystals	March 7-11, 2007
V. Struzhkin A. Gavriluk	Carnegie Russian Academy of Sciences	NFS Fe57- Fe ₂ O ₃ , 15 - 67 GPa, 12 – 300 K; GdFe ₃ (BO ₃) ₄ , 16.9 GPa, 12 – 298 K	March 7-11, 2007
O. Tschauner	University of Nevada – Las Vegas	X-ray diffraction studies at high pressure	March 9-12, 2007
J. McClure	University of Nevada – Las Vegas	High pressure investigation of various rare- earth sesquioxide systems.	March 9-12, 2007
B. Yulga E. Romano Z. Quine	University of Nevada – Las Vegas	Angular-dispersive X-Ray powder diffraction of PbO and several nucleotides	March 14-16, 2007
J. F. Lin	LLNL	NFS Fe57- mw25, 1.1, 19.6, 39.1 GPa, 298 - 800 K; pv10, 0 GPa, 300 K	March 14-16, 2007
O. Tschauner Jennifer Jackson	University of Nevada – Las Vegas California Institute of Technology	High pressure micro-diffraction experiments	March 16-17, 2007

W. Qiu N. Cunningham	University of Alabama – Birmingham	Ho to 135GPa, Fe ₂ P to 70GPa	March 17-18, 2007
N. Velisavljevic L. Stevens G. N. Chesnut	LANL	Compression of TATB, Cu, Ti, Ti alloys, and Zirconium in DAC.	March 17-19, 2007
O. Tschauner A. Simon M. Frank	University of Nevada – Las Vegas Northern Illinois University	X-ray fluorescence mapping	March 19-26, 2007
V. Iota H. Rhee	LLNL	XES Fe, K _{β1,3} , K _{β2,5} - FeO, 0 – 48 GPa	March 21-24, 2007
P. Dera H. P. Liermann	Carnegie HPCAT	NIST ruby sphere in air	March 22-April 2, 2007
Wendy Mao H. K. Mao J. Shu	LANL Carnegie	(Mg, Fe)SiO ₃ perovskite and post perovskite phases at high PT/laser heating and XRD	March 23-25, 2007
R. Kumar	University of Nevada – Las Vegas	RXES Yb LIII/La1- YbFe ₂ Ge ₂ , 0 – 20 GPa; YbRe ₂ Al ₁₀ , 0.8 – 18 GPa	March 25-29, 2007
Lyci George Selva Vennila Raju	Florida International University	Gd ₃ Ga ₅ O ₁₂ , LiAlH ₄ , NH ₃ BH ₃ (High T), SrPbO ₃ /Resistive heating & XRD	March 26-29, 2007
W. Yang	HPCAT	SA-EDXD and beamline operation	March 28-April 7, 2007
Kanani Lee Y. Al-khatbeh	New Mexico State University	TiO ₂ /Laser heating & XRD	March 29-31, 2007
H. Scott	Indiana University – South Bend	Fe ₂ P/XRD	March 29-31, 2007
H. K. Mao Y. Ding	Carnegie	RXES/PFY Fe K/Kα- Fe ₂ O ₃ , ambient; FeS, 0, 2 GPa	March 30-April 18, 2007
M. Ahart	Carnegie	Pressure induced phase transitions in lead titanate at room temperature	April 1-2, 2007
P. Dera Lauren Borkowski Barbara Lavina H. P. Liermann	Carnegie University of Nevada – Las Vegas HPCAT	Single crystal of ruby in DAC	April 4-6, 2007
V. Iota H. Rhee	LLNL	RXES/PFY Fe K/Kα- Fe ₂ O ₃ , ambient; FeS, 0, 2 GPa	April 4-7, 2007
H. Cynn W. Evans B. Baer M. Lipp	LLNL	Special project/laser heating & XRD	April 4-9, 2007
M. Lipp B. Baer W. Evans	LLNL	Pu ₂₃₉ , CaLi ₂ , HP and laser heating	April 4-9, 2007
P. Dera Lauren Borkowski Barbara Lavina H. P. Liermann	Carnegie University of Nevada – Las Vegas HPCAT	Single crystal of ruby in DAC	April 7-10, 2007
Amy Lazicki	LLNL	Eu and Ce under high pressure EDXD	April 7-13, 2007
V. Struzhkin A. Gavriluk P. Lazor	Carnegie Russian Academy of Sciences Upsala University	XES Mn Kβ- MnFe ₂ O ₄ , 13 – 80 GPa; LaMnO ₃ , 7 – 59 GPa; beta-Mn, 0 – 33 GPa;	April 8-12, 2007
L. Miyagi	University of California – Berkeley	Deformation of (Mg, Fe, Al)SiO ₃ provskite/laser heating and XRD	April 9-12, 2007
L. Miyagi	University of California – Berkeley	Natural enstatite, gearbox+radial diffraction, Laser heating. Start gearbox.	April 9-12, 2007

H. P. Liermann S. Merkel	HPCAT University of Lille	Resistive heating side	April 11-14, 2007
C. S. Zha M. Somayazulu H. K. Mao	Carnegie	Water to Megabar pressures/ XRD	April 12-14, 2007
B. Liu L. Wang	Jilin University	EDXD studies of olivine	April 13-16, 2007
B. Liu L. Wang	Jilin University	Be, H ₂ O, Pt, Au, (Mg, Fe)SiO ₃	April 14, 2007
S. Turneaure K. Zimmerman K. Perkins	Washington State University	Shockwave diffraction test	April 13-16, 2007
B. Liu L. Wang	Jilin University	Y ₂ O ₃ , TiO ₂ nanoparticles and nanotubes/XRD	April 14-16, 2007
A. Campbell N. Miller C. Seagle	University of Maryland University of Chicago	Fe ₃ O ₄ , Fe-Si alloy/laser heating & XRD	April 16-17, 2007
J. Howard	University of Nevada – Las Vegas	EDXD of Fe ₃ P	April 16-17, 2007
O. Tschauner	University of Nevada – Las Vegas	X-ray diffraction on samples in diamond cells	May 30-31, 2007
Y. Ding G. Shen H. K. Mao	HPSynC HPCAT Carnegie	FeK alpha, K beta resonant emission	June 1-8, 2007
P. Dera	GSECARS	Ruby test of single crystal program	June 2-7, 2007
H. K. Mao	Carnegie	X-ray diffraction of CH ₄ -H at high pressure	June 2-7, 2007
H. Liu L. Wang S. Sinogeikin	HPCAT	Low temperature, ZnO	June 7-9, 2007
P. Dera	GSECARS	Single crystal of marokite in DAC	June 7-10, 2007
P. Chow	HPCAT	17 element backscattering characterization and beamline alignment	June 8-21, 2007
G. Amulele M. Manghnani J. Balogh A. Wushuer	University of Hawaii	Radial diffraction B4C+Au, 53 Gpa	June 9-11, 2007
Lauren Borkowski	University of Nevada – Las Vegas	Single crystal of hercynite in DAC	June 10-14, 2007
Selva Vennila Raju V. Drozd	Florida International University	Heating Mg(AlH ₄) ₂ , Ca(AlH ₄) ₂ , NaAlH ₄ +Si	June 11-12, 2007
P. Dera	GSECARS	Single crystal of marokite	June 14-17, 2007
R. Kumar	University of Nevada – Las Vegas	Low-temperature x-ray diffraction studies on CeCu ₂ Si ₂	June 14-18, 2007
M. Somayazulu C. S. Zha	Carnegie	H ₂ O+Pt W gasket	June 20-21, 2007
H. Liu	HPCAT	Advances in data reduction from 2-d detectors for high pressure x-ray powder diffraction study: Cases for selected oxides	June 20-21, 2007
Barbara Lavina	University of Nevada – Las Vegas	Single crystal of hercynite in DAC	June 20-22, 2007
N. Velisavljevic	LANL	Ti/Cu	June 21-22
H. K. Mao	Carnegie	4- inch A ₂₃ Si ₅₅₅ analyzer 1 meter, hydrogen helium x-ray Raman	June 21-24, 2007
R. Kumar	University of Nevada – Las Vegas	4- inch A ₂₃ Si ₅₅₅ analyzer 1 meter, Boron X- ray Raman	June 24-29, 2007
H. P. Liermann	HPCAT	Membrane control	June 27-29, 2007

H. P. Liermann	HPCAT	Membrane control	June 27-29, 2007
A. Goncharov	Carnegie	X-ray diffraction and in situ Raman study of polyatomic and nonmolecular phases of nitrogen at high pressure	June 27-29, 2007
D. Brown	LANL	Pseudo-elasticity of Fe-Al	June 29-30, 2007
V. Iota	LLNL	4- inch A ₂₃ Si ₅₅₅ analyzer 1 meter, oxygen x-ray Raman, CO ₂	June 29-July 4, 2007
L. Wang	HPSynC	C60 EDXD in DAC	June 30-July 4, 2007
Patricia Kalita	University of Nevada – Las Vegas	High-pressure x-ray diffraction of zirconium hydride	July 1-3, 2007
J. McClure	University of Nevada – Las Vegas	Structure determination of laser heated lanthanide sesquioxides	July 1-3, 2007
O. Tschauner	University of Nevada – Las Vegas	Diffraction experiments	July 3-4, 2007
S. Gramsch	Carnegie	4- inch A ₂₃ Si ₅₅₅ analyzer 1 meter, oxygen x-ray Raman, B ₆₀	July 5-7, 2007
H. Cynn Chantel Aracne W. Evans M. Lipp B. Baer	LLNL	Pu239	July 5-9, 2007
O. Tschauner A. Simon M. Frank	University of Nevada – Las Vegas Northern Illinois University	X-ray fluorescence measurements on rare earth elements	July 5-10, 2007
Dana Dattlebaum E. Emmons L. Stevens N. Velisavljevic C. Whitney	LLNL	4- inch A ₂₃ Si ₅₅₅ analyzer 1 meter, carbon x-ray Raman, CO ₂	July 7-10, 2007
N. Velisavljevic Dana Dattlebaum Cheryl Whitney E. Emmons L. Stevens	LANL	Cu, polyethylene, triaminotrinitrolue	July 11-13
M. Previsa G. U. Ognjen B. Yulga	University of Nevada – Las Vegas	4- inch A ₂₃ Si ₅₅₅ analyzer 1 meter, carbon x-ray Raman, CO ₂	July 11-14, 2007
H. Cynn	LLNL	Side diffraction	July 12-16, 2007
L. Wang	HPSynC	C60 ADX in DAC	July 12-19, 2007
M. Lucas I. Halevy M. Winterrose	California Institute of Technology	NFS Fe-Os alloys, Fe-Pt, Fe-V, external heating	July 18-23, 2007
O. Tschauner	University of Nevada – Las Vegas	Lanthanide oxide and phosphate in ADX in DAC	July 19-23, 2007
W. Yang	HPCAT	Amorphous diffraction	July 20-24, 2007
Y. Fei T. Komabayashi Elizabeth Cotrell Angele Ricolleau	Carnegie	P-V-T EOS of (Mg, Fe)O up to core-mantle boundary pressures	July 22-24, 2007

J. H. Klepief J. F. Linn	LLNL	NFS ^{57}Fe enriched spinel (FeCr_2O_4) and silicate perovskite ($(\text{Mg,Fe})\text{SiO}_3$) at room temperature	July 23-28, 2007
H. K. Mao J. Shu Y. Ding Yue Meng L. Wang Wendy Mao	Carnegie HPCAT LANL	Radial x-ray diffraction of Fe and Co at high pressures	July 24-27, 2007
M. Pravica	University of Nevada – Las Vegas	Single crystal Laue diffraction with energetic materials	July 25-30, 2007
M. Ahart	Carnegie	$\text{Pb}(\text{Sc}_{0.5}\text{Nb}_{0.5})\text{O}_3$ ADX in DAC	July 27-29, 2007
L. Miyagi H. R. Wenk	University of California – Berkeley	Texture development in perovskite, relevant to deformation conditions in the Earth's lower mantle	July 27-29, 2007
Svetlana Kharlamova A. Goncharov	APS Carnegie	NFS Structural behavior of $\text{GdFe}_3(\text{BO}_3)_4$ at high pressures at low temperature	July 28-August 2, 2007
H. Liu	HPCAT	Perovskite NbTiO_3 , SmTiO_3 ADX in DAC	July 29-31, 2007
M. Somayazulu C. S. Zha	Carnegie	Water to megabar pressures/XRD	July 31, 2007
J. F. Lin V. Iota-Herbei	LLNL	Phase stability and thermal EOS of ferropericlase-(Mg, Fe)O in the Earth's lower mantle	August 1-3, 2007
L. Wang B. Zou Q. Cui L. Tang J. Liu	HPSynC Jilin University Chinese Academy of Sciences	C60, Ag, Mo, Pt, W powder diffraction with EDXD in DACs	August 1-7, 2007
J. Howard	HPCAT	Fe_3P NFS	August 2-3, 2007
W. Qiu	University of Alabama – Birmingham	Rare earth elements Er, Th, Y ADX in DACs	August 3-6, 2007
E. Tanis J. Olitzky	University of Nevada – Las Vegas	NRIXS and NFS on a-Fe Alloys	August 3-7, 2007
J. Liu L. Tang	Chinese Academy of Sciences	In-situ high pressure/temperature investigation of La_2O_3	August 4-6, 2007
W. Xiao J. Liu L. Tang	Chinese Academy of Sciences	BaCrO_3 , SrCrO_3 , PbCrO_3 , laser heating	August 6-7 2007
N. Chesnut	LANL	Elements Ce, Cu, Au, Pt, Ta, W ADX in DACs	August 6-10, 2007
J. Li	University of Illinois – Urbana Champagne	EOS of Fe_3C in DAC	August 8-10, 2007
N. Arganbright K. Perkins C. Bakeman S. Turneure C. S. Yoo K. Zimmerman	Washington State University	Shock wave single bunch x-ray diffraction measurements on shock compressed single Crystals	August 8-14, 2007

W. Yang	HPCAT	Amorphous diffraction in DAC	August 10-12, 2007
M. Lipp	LLNL	EOS of CE with ADX in DACs with high temperature	August 10-18, 2007
W. Xiao J. Liu L. Tang	Chinese Academy of Sciences	BaCrO ₃ , SrCrO ₃ , PbCrO ₃ , laser heating	August 11-12 2007
C. Gao	Texas Tech University	ZnS EDXD in DAC with electric field	August 12-14, 2007
H. Cynn Chantel Aracne W. Evans M. Lipp B. Baer	LLNL	Pu239	August 12-17
V. Struzhkin	Carnegie	Fe Kbeta/valence	August 16-19, 2007
H. Cynn	LLNL	Radial diffraction with EDXD in DAC	August 15-19, 2007
Anna-Gay Nelson Andrea Alsobrook R. Rich P. Dutta Elizabeth Heider J. Kizewski Karah Knope Y. Al Katatbeh J. Haag K. Terrani	Auburn University Texas Christian University South Dakota State University University of Utah North Carolina State University George Washington University New Mexico State University Northwestern University University of California – Berkeley	Phase transition of ZnO at high pressures using x-ray diffraction	August 17-19, 2007
Y. Ding	HpsynC	Zone-axis diffraction of single crystal Fe ₃ O ₄	August 18-20, 2007
E. Soignard	Arizona State University	High-pressure phase transition in BeF ₂ and As ₂ O ₃	August 19-20, 2007
H. K. Mao Y. Ding	Carnegie HPSynC	Resonant Fe K alpha	August 19-21, 2007
H. P. Liermann	HPCAT	Side diffraction	August 19-23, 2007
G. Chesnut N. Velisavljevic	LANL	High-pressure x-ray diffraction of metals	August 20-21, 2007
H. P. Liermann	HPCAT	Side diffraction of Fe in DAC	August 20-23, 2007
H. Scott M. Frank	Indiana University – South Bend Northern Illinois University	High-pressure stability of Fe ₃ P and EOS of Fe ₂ P	August 21-22, 2007

B. U2A Infrared Beamline (NSLS)

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

User Name	Affiliations	Project	Dates
O. Tschauer	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high pressure	July 12-15, 2006
S. Jacobsen Heather Watson Franceseid	Carnegie Carleton College	Synchrotron-IR measurement of OH in Al-bearing silicate perovskite	July 17-20, 2006
X. Chen Z. Liu	Carnegie	High-pressure optical spectroscopy of hydrogen-based electron materials	July 27-29, 2006
B. Chen H. Zhang M. Kruger V. S. M. Dharmaraj	University of California – Berkeley University of Missouri	High Pressure XRD and IR Study of Polytypically Disordered Nano-ZnS	August 1-6, 2005
D. Dolan M. Madlener R. Hacking	Sandia	Characterizing the emissivity of materials under dynamic compression	August 9-13, 2006
D. D. Klug J. Tse	National Research Council of Canada University of Saskatchewan	High-pressure low-temperature studies of novel clathrate hydrates	August 14-20, 2006
P. Allen T. Sun T. Yu	State University of New York – Stony Brook	Light absorption by Fe impurities in MgO at high pressure	August 25-31, 2006
O. Sramek P. Skemer M. Mookherjee	Yale University	Grain boundary water in olivine at high pressure	September 7-8, 2006
D. Dolan M. Madlener M. Roderick R. Hickman J. Gluth R. Hacking	Sandia	Characterizing the emissivity of materials under dynamic compression	September 9-18, 2006
H. Long	State University of New York – Stony Brook	Investigation on cell assemblies for mantle rheology	September 21, 2006
Tao Zhou Z. Qin	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	September 25-29, 2006
T. Tyson P. Gao	New Jersey Institute of Technology	Exploring strain effects in manganite films with Infrared Spectroscopy	October 4-7, 2006
Jennifer Ciezak	Carnegie	High pressure vibrational characterization of energetic materials	October 11-12, 2006
T. Jenkins	Carnegie	Examination of a novel clathrate hydrate phase	October 13-14, 2006
M. Somayazulu	Carnegie	FTIR spectroscopy of XeCl at high pressure	October 16, 2006
J. Smedley	Brookhaven	Characterization of impurities in diamond	October 19-20, 2006
W. Han	Brookhaven	FTIR spectroscopy of nano materials	October 20, 2006

L. Dobrzhinetskaya	University of California – Riverside	Role of water for diamond crystallization: implication for subduction zone processes	October 20, 2006
W. Han	Brookhaven	FTIR spectroscopy of nano materials	October 27, 2006
Tao Zhou Z. Qin	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	November 2-8, 2006
O. Tschauner B. Yulga	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high pressure	November 9-11, 2006
Q. Cui	Jilin University	High-pressure infrared studies on Se, Te, AlN and C ₃ N ₄	November 16-20, 2006
C. Zha	Carnegie	FTIR spectroscopy of hydrogen at high pressure and high temperature	November 21-22, 2006
W. Han	Brookhaven	FTIR spectroscopy of nano materials	January 12-15, 2007
Q. Cui	Jilin University	High-pressure infrared studies on Se, Te, AlN and C ₃ N ₄	January 18-21, 2007
O. Sramek M. Mookherjee	Yale University	Grain boundary water in olivine at high pressure	January 24-55, 2007
T. Tyson P. Gao	New Jersey Institute of Technology	Exploring strain effects in manganite films with infrared spectroscopy	January 29-February 2, 2007
Yufei Meng	Carnegie	Characterization of CVD diamonds	February 3, 2007 February 8, 2007
J. Smedley	Brookhaven	Characterization of impurities in diamond	February 5, 2007
H. Long	State University of New York – Stony Brook	Investigation on cell assemblies for mantle rheology	February 9, 2007
Gianluca Iezzi	CHIETI-PESCARA	The high-pressure behavior of amphiboles	February 12-16, 2007
C. Zha	Carnegie	High temperature infrared study for dense hydrogen	February 26-March 2, 2007
Y. Song Z. Dong D. Shakhvorostov	University of Western Ontario	Structural investigation of zeolites under high pressures by infrared microspectroscopy	March 2-3, 2007
Tao Zhou Z. Qin	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	March 11-18, 2007
Heather Watson	LLNL	Synchrotron-IR measurement of OH in Al-bearing silicate perovskite	March 29-30, 2007
B. Liu	Jilin University	Infrared studies of carbon nano-tubes under high pressure	April 2-4, 2007
Tao Zhou Z. Qin	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	April 5-12, 2007
D. Dolan M. Madlener M. Roderick R. Hickman J. Gluth R. Hacking	Sandia	Characterizing the emissivity of materials under dynamic compression	April 18-27, 2007
J. Chen T. Yu	State University of New York – Stony Brook	IR spectroscopy of new high pressure phase of boron	May 31, 2007

H. Long	State University of New York – Stony Brook	Effect of water fugacity on deformation of olivine at low temperature	June 1, 2007
M. Mookherjee	Yale University	Synchrotron infrared spectroscopy of nominally anhydrous pyrope at high pressure	June 4-10, 2007
C. Yulga M. Pravica	University of Nevada – Las Vegas	Infrared spectroscopy on energetic materials at high pressure and temperature	June 13-15, 2007
M. Mookherjee	Yale University	Grain boundary water in olivine at high pressure	June 22-23, 2007
Tao Zhou Z. Qin	New Jersey Institute of Technology	Infrared and Raman spectroscopic studies of FeS under high pressure	June 26-28, 2007

References

1. Jeanloz, R., *Phys. Today*, **53**, 44 (2000).
2. Lee, K. K., R. O. Nelson, R. Rundberg, and G. Steinle-Neuman, *Eos Trans. AGU Fall Meet., Suppl.*, **88** (2007).
3. Winterrose, M. and B. Fultz, to be published.
4. Kubo, A., Y. Wang, C. E. Runge, T. Uchida, B. Kiefer, N. Nishiyama, and T. S. Duffy, *J. Phys. Chem. Solids*, submitted.
5. Wu, Z. and R. E. Cohen, *Phys. Rev. Lett.*, **95**, 037601 (2005).
6. Ahart, M., R. E. Cohen, and R. J. Hemley, to be published.
7. Dattlebaum, D. M., L. M. Sanchez, G. N. Chesnut, E. N. Brown, and A. M. Schwendt, to be published.
8. Stevens, L. L., E. B. Orler, D. M. Dattlebaum, M. Ahart, and R. J. Hemley, in press.
9. Dattlebaum, D. M., J. D. Jensen, A. M. Schwendt, M. Lewis, E. M. Kober, and R. Menikoff, *J. Chem. Phys.*, **122**, 144903 (2005).
10. Surber, E. and D. D. Dlott, to be published.
11. Chellappa, R., D. Chandra, M. Somayazulu, S. A. Gramsch, and R. J. Hemley, *J. Phys. Chem. B*, **111**, 10785-10789 (2007).
12. Chellappa, R. S., D. Chandra, S. A. Gramsch, R. J. Hemley, J. F. Lin, and Y. Song, *J. Phys. Chem. B*, **110**, 11088-11097 (2006).
13. Zha, C. S., R. J. Hemley, S. A. Gramsch, H. K. Mao, and W. A. Bassett, *J. Chem. Phys.*, **126**, 074506 (2007).
14. Sinogeikin, S., New developments at HPCAT, IDB, and supporting facilities, *Geophysical Laboratory Informal Talk Series* (Washington, DC, October 2, 2007).
15. Lin, J. F., M. Santoro, V. V. Struzhkin, H. K. Mao, and R. J. Hemley, *Rev. Sci. Instrum.*, **75**, 3302-3306 (2004).
16. Santoro, M., J.-F. Lin, H. K. Mao, and R. J. Hemley, *J. Chem. Phys.*, **121**, 2780-2787 (2004).
17. Honnell, K. G., N. Velisavljevic, C. D. Adams, P. A. Rigg, G. N. Chesnut, and R. M. Aikin, Equation of state for Ti-beta-21S, in *Shock Compression of Condensed Matter - 2007* (eds. M. D. Furnish, Elert, M. L., Russell, T. P. and White, C. T.), (AIP, New York, 2007).
18. Velisavljevic, N. and G. N. Chesnut, *Appl. Phys. Lett.*, **91**, 101906 (2007).
19. Chesnut, G. N., N. Velisavljevic, and L. Sanchez, Static high pressure x-ray diffraction of Ti-6Al-4V, in *Shock Compression of Condensed Matter - 2007* (eds. M. D. Furnish, Elert, M. L., Russell, T. P. and White, C. T.), (AIP, New York, 2007).
20. Velisavljevic, N. and G. N. Chesnut, in progress.
21. Velisavljevic, N., G. N. Chesnut, W. Qiu, Y. Vohra, H. P. Liermann, and H. Liu, *J. Appl. Phys.*, submitted.
22. Ahart, M., M. Somayazulu, P. Dera, H. K. Mao, R. E. Cohen, R. J. Hemley, R. Yang, H. P. Liermann, and Z. Wu, *Nature*, in press.
23. Knittle, E. and R. Jeanloz, *J. Geophys. Res.*, **96**, 16169-16180 (1991).
24. Anderson, O. L. and D. G. Isaak, *Am. Mineral.*, **85**, 376-385 (2000).
25. Seagle, C. T., A. J. Campbell, D. L. Heinz, G. Shen, and V. B. Prakapenka, *J. Geophys. Res.*, **111**, B06209 (2006).
26. Campbell, A. J., C. T. Seagle, D. L. Heinz, G. Y. Shen, and V. Prakapenka, *Phys. Earth Planet. Inter.*, **162**, 119-128 (2007).
27. Seagle, C. T., D. L. Heinz, A. J. Campbell, V. B. Prakapenka, and S. T. Wanless, *Earth Planet Sci. Lett.*, submitted.
28. Shen, G., P. Lazor, and S. K. Saxena, *Phys. Chem. Minerals*, **20**, 91-96 (1993).
29. Shen, G., V. B. Prakapenka, M. L. Rivers, and S. R. Sutton, *Phys. Rev. Lett.*, **92**, 185701 (2004).
30. Darken, L. S. and R. W. Gurry, *J. Am. Chem. Soc.*, **68**, 798-816 (1946).
31. Ringwood, A. E. and W. Hibberson, *Phys. Chem. Minerals*, **17**, 313-319 (1990).
32. Tsuno, K., E. Ohtani, and H. Terasaki, *Phys. Earth Planet. Inter.*, **160**, 75-85 (2007).
33. Boehler, R., *Nature*, **363**, 534-536 (1993).
34. Zhang, J. Z. and Y. S. Zhao, *Phys. Chem. Minerals*, **32**, 241-247 (2005).
35. Fei, Y. and H. K. Mao, *Science*, **266**, 1678-1680 (1994).
36. Murakami, M., K. Hirose, S. Ono, J. Tsuchiya, M. Isshiki, and T. Watanuki, *Phys. Earth Planet. Inter.*, **146**, 273-282 (2004).
37. Kondo, T., E. Ohtani, N. Hirao, T. Yagi, and T. Kikegawa, *Phys. Earth Planet. Inter.*, **143-144**, 201-213 (2004).
38. Lee, S. K., P. J. Eng, H. K. Mao, Y. Meng, and J. Shu, *Phys. Rev. Lett.*, **98**, 105502 (2007).
39. Lipp, M. J., W. J. Evans, B. Baer, and C. S. Yoo, *Nature Materials*, **4**, 211 (2005).
40. Iota, V., C. S. Yoo, J. H. P. Klepeis, Z. Jenei, W. Evans, and H. Cynn, *Nature Materials*, **6**, 34-38 (2007).
41. Meng, Y., H. K. Mao, P. J. Eng, T. P. Trainor, M. Newville, M. Y. Hu, C. Kao, J. Shu, D. Häusermann, and R. J. Hemley, *Nature Materials*, **3**, 111-114 (2004).

42. Xu, J., H. K. Mao, and R. J. Hemley, to be published.
43. Ma, Y., M. Somayazulu, G. Shen, H. K. Mao, J. Shu, and R. J. Hemley, *Phys. Earth Planet. Inter.*, **143-144**, 455-467 (2004).
44. Ahart, M., J. L. Yarger, K. M. Lantzky, S. Nakano, H. K. Mao, and R. J. Hemley, *J. Chem. Phys.*, **124**, 14502 (2006).
45. Weinberger, M., S. Tolbert, M. Ahart, J. Yarger, N. Satoshi, and R. J. Hemley, Spectroscopic studies of new forms of SiO₂ and BeH₂, *First Annual SSAAP Symposium* (Albuquerque, NM, March 29-31, 2004).
46. Militzer, B., Quantum monte carlo simulation of high pressure materials, *Contributed talk, meeting of the American Geophysical Union* (San Francisco, CA, December, 2004).
47. Kubo, A., B. Kiefer, G. Shen, V. Prakapenka, R. J. Cava, and T. S. Duffy, *Geophys. Res. Lett.*, **33**, L12S12 (2006).
48. Runge, C. E., A. Kubo, B. Kiefer, Y. Meng, V. Prakapenka, G. Shen, R. J. Cava, and T. S. Duffy, *Phys. Chem. Minerals*, **33**, 699-709 (2006).
49. Stevens, L. L., E. B. Orler, D. M. Dattelbaum, M. Ahart, and R. J. Hemley, *J. Chem. Phys.*, **127**, 104906 (2007).
50. Emmons, E. D., N. Velisavljevic, J. R. Schoonover, and D. M. Dattlebaum, *Appl. Spectroscopy*, submitted.
51. Stevens, L. L., N. Velisavljevic, D. E. Hooks, and D. M. Dattlebaum, in preparation.
52. Ahart, M., *J. Chem. Phys.*, to be published.
53. Scott, H. P., S. Huggins, M. R. Frank, S. J. Maglio, C. D. Martin, Y. Meng, J. Santillan, and Q. Williams, *Geophys. Res. Lett.*, **34**, L06302 (2007).
54. Dubrovinsky, L. S., N. A. Dubrovinskaia, I. A. Abrikosov, M. Vennstrom, F. Westman, S. Carlson, M. vanSchilfgaarde, and B. Johansson, *Phys. Rev. Lett.*, **86**, 4851-4854 (2001).
55. Lucas, M. S., A. B. Papandrew, B. Fultz, and M. Y. Hu, *Phys. Rev. B*, **75**, 054307 (2007).
56. Ruckert, T., W. Keune, W. Sturhahn, M. Hu, J. P. Sutter, T. S. Toellner, and E. E. Alp, *Hyperfine Interact.*, **126**, 363-366 (2000).
57. Shieh, S. R., A. Kubo, T. S. Duffy, V. B. Prakapenka, and G. Shen, *Phys. Rev. B*, **73**, 014105 (2006).
58. Mao, Z., S. D. Jacobsen, F. Jiang, J. R. Smyth, C. Holl, D. J. Frost, and T. Duffy, *Earth Planet. Sci. Lett.*, in press.
59. Jacobsen, S. D., J. R. Smyth, and S. van der Lee, *Eos Trans. AGU Fall Meet., Suppl., Jt. Assem. Suppl.*, **87** (2006).
60. Mao, Z., F. Jiang, and T. Duffy, *Am. Mineral.*, **92**, 570-576 (2007).
61. Ahart, M., A. Asthagiri, Z. G. Ye, P. Dera, H. K. Mao, R. E. Cohen, and R. J. Hemley, *Phys. Rev. B*, **75**, 144410 (2007).
62. Ahart, M., *Phys. Rev. B*, to be submitted.
63. Duffy, T. S., Strength of materials under static loading in the diamond anvil cell, in *Shock Compression of Condensed Matter - 2007* (eds. M. D. Furnish, Elert, M. L., Russell, T. P. and White, C. T.), submitted (AIP, New York).
64. Miyagi, L., N. Nishiyama, Y. Wang, A. Kubo, D. V. West, R. J. Cava, T. Duffy, and H. R. Wenk, *Earth Planet. Sci. Lett.*, submitted.
65. Merkel, S., A. K. McNamera, A. Kubo, S. Speziale, L. Miyagi, Y. Meng, T. S. Duffy, and H. R. Wenk, *Science*, **316**, 1729-1732 (2007).
66. Merkel, S., A. Kubo, L. Miyagi, S. Speziale, T. S. Duffy, H. K. Mao, and H. R. Wenk, *Science*, **311**, 644-646 (2006).
67. Stackhouse, S., J. P. Brodholt, J. Wookey, J. M. Kendall, and G. D. Price, *Earth Planet. Sci. Lett.*, **230**, 1-10 (2005).
68. Wentzcovitch, R. M., T. Tsuchiya, and J. Tsuchiya, *Proc. Nat. Aca. Sci.*, **103**, 543-546 (2006).
69. Cumalioglu, I., A. Ertas, Y. Ma, and T. T. Maxwell, *Transaction of the ASME: Journal of Fuel Cell Science and Technology*, in press.
70. Cumalioglu, I., Y. Ma, A. Ertas, and T. T. Maxwell, *ASMA Journal of Pressure Vessel Technology*, **129**, 216 (2007).
71. Ma, Y. and R. Aksoy, *Solid State Comm.*, **142**, 376-379 (2007).
72. Ma, Y., Q. Cui, and H. Shen, *J. Appl. Phys.*, **102**, 013525 (2007).
73. Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *2007 Stewardship Science Academic Alliances Program Symposium* (Washington, DC, February 5-7, 2007).
74. Aksoy, R., E. Selvi, and Y. Ma, *J. Phys. Chem. Solid*, submitted.
75. Aksoy, R., E. Selvi, R. Knudson, and Y. Ma, *J. Phys. Chem. Solids*, submitted.
76. Gao, C., Y. Ma, Y. Han, M. Li, and G. Zou, *J. Phys. Chem. Solids*, submitted.
77. Gao, C., Y. Ma, D. Yu, J. He, and Y. Tian, *J. Phys. Chem. Solids*, submitted.

78. Selvi, E., R. Aksoy, R. Knudson, and Y. Ma, High pressure x-ray diffraction study of tungsten diselenide, *Study of Matter at Extreme Conditions* (Miami Beach, FL, April 15-20, 2007).
79. Feng, Y., R. Jaramillo, G. Srajer, J. C. Lang, Z. Islam, M. S. Somayazulu, O. G. Shpyrko, J. J. Pluth, H. K. Mao, E. D. Isaacs, G. Aeppli, and T. F. Rosenbaum, *Phys. Rev. Lett.*, **99**, 137201 (2007).
80. Lin, J. F., G. Vankó, S. D. Jacobsen, V. Iota, V. V. Struzhkin, V. Prakapenka, A. Kuznetsov, and C. S. Yoo, *Science*, **317**, 1740 (2007).
81. Goncharov, A. F., V. V. Struzhkin, and S. D. Jacobsen, *Science*, **312**, 1205-1208 (2006).
82. Struzhkin, V. V., H. K. Mao, J. F. Lin, R. J. Hemley, J. S. Tse, Y. Ma, M. Hu, P. Chow, and C. C. Kao, *Phys. Rev. Lett.*, **96**, 137402 (2006).
83. Chen, X. J., V. V. Struzhkin, Z. G. Wu, H. Q. Lin, R. J. Hemley, and H. K. Mao, *Proc. Nat. Acad. Sci.*, **104**, 3732-3735 (2007).
84. Chellappa, R. S., D. Chandra, S. A. Gramsch, M. Somayazulu, and R. J. Hemley, Pressure-induced phase transformations in Li-based complex hydrides, in *Materials Research at High Pressure* (eds. M. R. Manaa, Goncharov, A. F., Hemley, R. J. and Bini, R.), **987**, 133-138 (Materials Research Society, Warrendale, Pennsylvania, 2007).
85. Maurice, D. R. and T. H. Courtney, *Metall. Trans. A*, **21**, 289 (1990).
86. Bhat, M. H., V. Molinero, E. Soignard, V. C. Solomon, J. L. Yarger, and C. A. Angell, *Nature*, **448**, 787-791 (2007).
87. Sheng, H. W., H. Z. Liu, Y. Q. Cheng, J. Wen, P. L. Lee, W. K. Luo, S. D. Shastri, and E. Ma, *Nature Materials*, **6**, 192-197 (2007).
88. McMahan, A. K. and R. LeSar, *Phys. Rev. Lett.*, **54**, 1929-1932 (1985).
89. Mailhot, C., L. H. Yang, and A. K. McMahan, *Phys. Rev. B*, **46**, 14419-14435 (1992).
90. Gregoryanz, E., A. F. Goncharov, C. Sanloup, M. Somayazulu, H. K. Mao, and R. J. Hemley, *J. Chem. Phys.*, **126**, 184505 (2007).
91. Eremets, M. I., A. G. Gavriliuk, and I. A. Trojan, *Appl. Phys. Lett.*, **901**, 171904 (2007).
92. Caracas, R. and R. J. Hemley, *Chem. Phys. Lett.*, **442**, 65-70 (2007).
93. Kingma, K. J., R. E. Cohen, R. J. Hemley, and H. K. Mao, *Nature*, **374**, 243-245 (1995).
94. Mazin, I. I. and R. E. Cohen, *Phys. Rev. B*, **52**, R8597-R8600 (1995).
95. Steinle-Neumann, G., L. Stixrude, and R. E. Cohen, *Phys. Rev. B*, **63**, 054103 (2001).
96. Young, A. F., C. Sanloup, E. Gregoryanz, S. Scandolo, R. J. Hemley, and H. K. Mao, *Phys. Rev. Lett.*, **96**, 155501 (2006).
97. Young, A. F., J. A. Montoya, C. Sanloup, M. Lazzeri, E. Gregoryanz, and S. Scandolo, *Phys. Rev. B*, **73**, 153102 (2006).
98. Yan, C. S., H. K. Mao, W. Li, J. Qian, Y. Zhao, and R. J. Hemley, *Phys. Stat. Sol. (a)*, **201**, R25-R27 (2004).
99. Mao, W. L., H. K. Mao, C. S. Yan, J. Shu, J. Hu, and R. J. Hemley, *Appl. Phys. Lett.*, **83**, 5190-5192 (2003).
100. Charles, S. J., J. E. Butler, B. N. Feygelson, M. Newton, D. L. Carroll, J. W. Steeds, H. Darwsh, C. S. Yan, H. K. Mao, and R. J. Hemley, *Phys. Stat. Sol.*, **242**, 2473-2485 (2004).
101. Yan, C. S., Y. C. Chen, S. S. Ho, H. K. Mao, and R. J. Hemley, Large single crystal CVD diamonds at rapid growth rates, *The 10th International Conference on New Diamond Science and Technology* (AIST, Tsukuba, Japan, May 11-14, 2005).
102. Yan, C. S., Y. C. Chen, S. S. Ho, H. K. Mao, and R. J. Hemley, Large single crystal CVD diamonds at rapid growth rates, *8th Applied Diamond Conference, NanoCarbon 2005* (Argonne National Laboratory, Argonne, Illinois, May 15-19, 2005).
103. Ho, S. S., C. S. Yan, Z. Liu, H. K. Mao, and R. J. Hemley, *Industrial Diamond Review*, **66**, 28-32 (2006).
104. Goncharov, A. F., J. M. Zaug, J. C. Crowhurst, and E. Gregoryanz, *J. Appl. Phys.*, **97**, 094917 (2005).
105. Jacobsen, S. D., H. J. Reichmann, A. Kantor, and H. A. Spetzler, A gigahertz ultrasonic interferometer for the diamond anvil cell and high-pressure elasticity of some iron-oxide minerals, in *Advances in High-Pressure Techniques for Geophysical Applications* (eds. J. Chen, Wang, Y., Duffy, T., Shen, G. and Dobrzhinetskaya, L.), 25-48 (Elsevier, Amsterdam, 2005).
106. Qiu, W., P. A. Baker, N. Velisavljevic, Y. K. Vohra, and S. T. Weir, *J. Appl. Phys.*, **99**, 064906 (2006).
107. Ma, Y., V. I. Levitas, and J. Hashemi, *J. Phys. Chem. Solids*, **67**, 2083-2090 (2006).
108. Beck, P., A. Goncharov, and R. J. Hemley, *Eos Trans. AGU Fall Meet., Suppl.*, **87** (2006).
109. Cuk, T., V. Struzhkin, T. Devereaux, A. Goncharov, C. Kendziora, H. Eisaki, H. K. Mao, and Z. X. Shen, A pressure induced insulator-to-metal critical point in the copper-oxides, *Bull. Am. Phys. Soc. (APS March Meeting)* (Denver, CO, March 5-9, 2007).
110. Patterson, J. E., A. Lagutchev, W. Huang, and D. D. Dlott, *Phys. Rev. Lett.*, **94**, 015501 (2005).
111. Dera, P., C. T. Prewitt, and S. D. Jacobsen, *J. Synch. Radiation*, **12**, 547-548 (2005).
112. Ding, Y., J. Xu, C. T. Prewitt, R. J. Hemley, H. K. Mao, J. A. Cowan, J. Zhang, J. Qian, S. C. Vogel, K. A. Lokshin, and Y. Zhao, *Appl. Phys. Lett.*, **86**, 052505 (2005).

113. Goncharov, A. F. and J. C. Crowhurst, *Rev. Sci. Instrum.*, **76**, 063905 (2005).
114. Xu, J., J. Liu, W. Xiao, J. Shu, Y. Li, X. Li, H. Xie, Y. Bi, T. Hu, Y. Yan, R. J. Hemley, and H. K. Mao, to be published.
115. Wenk, H. R., I. Lonardelli, and D. Williams, *Acta Mater.*, **52**, 1899-1907 (2004).
116. Wenk, H. R., L. Kestens, and I. Huensche, *Trans AIME*, to be published.
117. Matthies, S., J. Pehl, H. R. Wenk, I. Lonardelli, L. Lutterotti, and S. Vogel, *J. Appl. Cryst.*, **38**, 462-475 (2005).
118. Dolan, D., et al., to be published.
119. Turneure, S., Y. M. Gupta, K. Zimmerman, K. Perkins, C. S. Yoo, and G. Shen, to be published.
120. Bassett, W. A., *Eur. J. Mineral.*, **15**, 773-780 (2003).
121. Cunningham, N., N. Velisavljevic, and Y. K. Vohra, *Phys Rev B*, **71**, 012108 (2005).
122. Manley, M. E., B. Fultz, R. J. McQueeney, C. M. Brown, W. L. Hulst, J. L. Smith, D. J. Thoma, R. Osborn, and J. L. Robertson, *Phys. Rev. Lett.*, **86**, 3076-3079 (2001).
123. Wong, J., M. Krisch, D. L. Farber, F. Occelli, A. J. Schwartz, T.-C. Chiang, M. Wal, C. Boro, and R. Xu, *Science*, **301**, 1078-1080 (2003).
124. Wong, J., M. Krisch, D. L. Farber, F. Occelli, R. Xu, T. C. Chiang, D. Clatterbuck, A. J. Schwartz, M. Wall, and C. Boro, *Phys. Rev. B*, **7206**, 4115 (2005).
125. Manley, M. E., G. H. Lander, H. Sinn, A. Alatas, W. L. Hulst, R. J. McQueeney, J. L. Smith, and J. Willit, *Phys. Rev. B*, **67**, 052302 (2003).
126. Manley, M. E., M. Yethiraj, H. Sinn, H. M. Volz, A. Alatas, J. C. Lashley, W. L. Hulst, G. H. Lande, and J. L. Smith, *Phys. Rev. Lett.*, **96**, 125501 (2006).
127. Farber, D. L., M. Krisch, D. Antonangeli, A. Beraud, J. Badro, F. Occelli, and D. Orlikowski, *Phys. Rev. Lett.*, **96**, 115502 (2006).
128. Holt, M., Z. Wu, H. Hong, P. Zschack, P. Jemian, J. Tischler, H. Chen, and T.-C. Chiang, *Phys. Rev. Lett.*, **83**, 3317-3319 (1999).
129. Holt, M., P. Zschack, H. Hong, M. Y. Chou, and T.-C. Chiang, *Phys. Rev. Lett.*, **86**, 3799-3802 (2001).
130. Holt, M., P. Czochke, H. Hong, P. Zschack, H. K. Birnbaum, and T.-C. Chiang, *Phys. Rev. B*, **66**, 064303-064301-064305 (2002).
131. Pfeifer, M. A., G. J. Williams, I. A. Vartanyants, R. Harder, and I. K. Robinson, *Nature*, **442**, 63-66 (2006).
132. Isaacs, E. D., *Nature*, **442**, 35 (2006).
133. Mao, H. K. and P. M. Bell, *Science*, **191**, 851-852 (1976).
134. Mao, H. K. and P. M. Bell, *Science*, **200**, 1145-1147 (1978).
135. Mao, H. K., P. M. Bell, J. W. Shaner, and D. J. Steinberg, *J. Appl. Phys.*, **49**, 3276-3283 (1978).
136. Hemley, R. J., H. K. Mao, G. Shen, J. Badro, P. Gillet, M. Hanfland, and D. Häusermann, *Science*, **276**, 1242-1245 (1997).
137. Papandrew, A. B., M. S. Lucas, R. Stevens, B. Fultz, M. Y. Hu, I. Halevy, R. E. Cohen, and M. Somayazulu, *Phys. Rev. Lett.*, **97**, 087202 (2006).
138. Lin, J. F., W. Sturhahn, J. Zhao, G. Shen, H. K. Mao, and R. J. Hemley, *Science*, **308**, 1892-1894 (2005).
139. Lin, J. F., V. Struzhkin, S. D. Jacobsen, M. Y. Hu, P. Chow, J. Kung, H. Liu, H. K. Mao, and R. J. Hemley, *Nature*, **436**, 377-380 (2005).
140. Mao, W. L., H. K. Mao, W. Sturhahn, J. Zhao, V. B. Prakapenka, Y. Meng, Y. Fei, and R. J. Hemley, *Science*, **312**, 564-565 (2006).
141. Yoo, C. S., B. Maddox, J. H. P. Klepeis, V. Iota, W. Evans, A. McMahan, M. Hu, P. Chow, M. Somayazulu, D. Häusermann, R. T. Scalettar, and W. E. Pickett, *Phys. Rev. Lett.*, **94**, 115502 (2005).
142. Maddox, B. R., A. Lazicki, C. S. Yoo, V. Iota, M. Chen, A. K. McMahan, M. Hu, P. Chow, R. T. Scalettar, and W. E. Pickett, *Phys. Rev. Lett.*, **96**, 215701 (2006).
143. Krishnamurthy, V. V., J. C. Lang, D. Haskel, D. J. Keavney, G. Srajer, J. L. Robertson, B. C. Sales, D. G. Mandrus, D. J. Singh, and D. I. Bilc, *Phys. Rev. Lett.*, **98**, 126403 (2007).
144. Pascarelli, S., O. Mathon, M. Munoz, T. Mairisa, and J. Susin, **13**, 351-358 (2006).
145. Wenk, H. R., I. Lonardelli, J. Pehl, J. Devine, V. Prakapenka, G. Shen, and H. K. Mao, *Earth Planet Sci. Lett.*, **226**, 507-519 (2004).
146. Lonardelli, I., H. R. Wenk, M. Goodwin, and L. Lutterotti, *J. Synch. Radiation*, **12**, 354-360 (2005).
147. Ischia, G., H. R. Wenk, L. Lutterotti, and F. Berberich, *J. Appl. Cryst.*, **38**, 377-380 (2005).
148. Schoenberg, K. F., ed. *LANSCE into the Future*, Los Alamos Science, 30 (Los Alamos, NM, 2006).
149. Hemley, R. J., A. F. Goncharov, R. Lu, M. Li, V. V. Struzhkin, and H. K. Mao, *II Nuovo Cimento D*, **20**, 539 (1998).
150. Lee, K. K. M., L. R. Benedetti, R. Jeanloz, P. M. Celliers, J. H. Eggert, D. G. Hicks, S. J. Moon, A. Mackinnon, L. B. Da Silva, D. K. Bradley, W. Unites, G. W. Collins, E. Henry, M. Koenig, A. Benuzzi-Mounaix, J. Pasley, and D. Neely, *J. Chem. Phys.*, **125**, 014701 (2006).

151. Knudson, M. D., J. R. Asay, and C. Deeney, *J. Appl. Phys.*, **97**, 073514 (2005).
152. Brown, J. M. and R. G. McQueen, *J. Geophys. Res.*, **91**, 7485-7494 (1986).
153. Nguyen, J. H. and N. C. Holmes, *Nature*, **427**, 339-342 (2004).
154. Ahuja, R., *Phys. Rev. B*, **63**, 212101 (2001).
155. Dubrovinsky, L., N. Dubrovinskaia, W. A. Chrichton, A. S. Mikhaylushkin, S. I. Simak, A. A. Abrikosov, J. S. de Almeida, R. Ahuja, W. Luo, and B. Johansson, *Phys. Rev. Lett.*, **98**, 045503 (2007).
156. Hixson, R. S., D. A. Boness, and J. W. Shaner, *Phys. Rev. Lett.*, **62**, 637-640 (1989).
157. Jona, F. and P. M. Marcus, *J. Phys. Cond. Matt.*, **17**, 1049-1057 (2005).
158. Koller, D. D., R. S. Hixson, G. T. Gray III, P. A. Rigg, L. B. Addessio, E. K. Cerreta, J. D. Maestas, and C. A. Yablinsky, *J. Appl. Phys.*, **98**, 103518 (2005).
159. SinitSYna, L. M., S. A. Novikov, G. T. Gray III, E. Cerreta, B. L. Henrie, M. F. Lopez, and C. A. Yablinsky, *AIP Conference Proceedings*, **845**, 771-774 (2006).
160. Spencer, B. H., S. A. Maloy, and G. T. Gray III, *Acta Materialia*, **53**, 3293-3303 (2005).
161. Huang, H. and J. R. Asay, *J. Appl. Phys.*, **98**, 033524 (2005).
162. Chen, X., J. R. Asay, and S. K. Dwivedi, *J. Appl. Phys.*, **99**, 023528 (2006).
163. Ding, J. L. and J. R. Asay, *J. Appl. Phys.*, **101**, 073517 (2007).
164. Oganov, A. R., M. J. Gillan, and G. D. Price, *Phys. Rev. B*, **71**, 064104 (2005).
165. Umemoto, K. and R. M. Wentzcovitch, *Phys. Rev. B*, **74**, 224105 (2006).
166. da Silva, L. B., P. Celliers, G. W. Collins, K. S. Budil, N. C. Holmes, T. W. Barbee, B. A. Hammel, J. D. Kilkenny, R. J. Wallace, M. Ross, R. Cauble, A. Ng, and G. Chiu, *Phys. Rev. Lett.*, **78**, 483-486 (1997).
167. Cauble, R., L. B. da Silva, T. S. Perry, D. R. Bach, P. Celliers, G. W. Collins, A. Ng, T. W. Barbee, B. A. Hammel, N. C. Holmes, J. D. Kilkenny, R. J. Wallace, A. Chiu, and A. Woolsey, *Phys. Plasmas*, **4**, 1857-1861 (1997).
168. Nellis, W. J., S. T. Weir, and A. C. Mitchell, *Phys. Rev. B*, **59**, 3434-3449 (1999).
169. Asay, J. R., C. A. Hall, C. H. Konrad, W. M. Trott, G. A. Chandler, K. J. Fleming, K. G. Holland, L. C. Chhabildas, T. A. Mehlhorn, R. Vesey, T. G. Trucano, A. Hauer, R. Cauble, and M. Foord, *Int. J. Impact Engin.*, **23**, 27-38 (1999).
170. Baer, B. J. and C. S. Yoo, *Phys. Rev. Lett.*, submitted.
171. Lee, G. W., W. J. Evans, and C. S. Yoo, *Proc. Nat. Acad. Sci.*, in press.
172. Hemley, R. J., *Phys. World*, **19**, 26-30 (2006).
173. Santoro, M., E. Gregoryanz, H. K. Mao, and R. J. Hemley, *Phys. Rev. Lett.*, **93**, 265701 (2004).
174. Lin, J. F., W. Sturhahn, J. Zhao, G. Shen, H. K. Mao, and R. J. Hemley, *Geophys. Res. Lett.*, **31**, 14611 (2004).
175. He, D., Y. Zhao, T. D. Sheng, R. B. Schwartz, J. Qian, K. A. Lokshin, S. Bobev, L. L. Daemen, H. K. Mao, J. Z. Hu, J. Shu, and J. Xu, *Rev. Sci. Instrum.*, **74**, 3012-3016 (2003).
176. Lin, J. F., J. Shu, H. K. Mao, R. J. Hemley, and G. Shen, *Rev. Sci. Instrum.*, **74**, 4732-4736 (2003).
177. Goncharov, A. F. and J. C. Crowhurst, to be published.
178. Akella, J., S. T. Weir, Y. K. Vohra, H. Prokop, S. A. Catledge, and G. N. Chesnut, X-ray diffraction studies using diamond coated rhenium gasket to megabar pressures, in *Science and Technology of High Pressure* (eds. M. Manghnani, Nellis, W. B. and Nicol, M. F.), 1073-1076 (University Press, Hyderabad, India, 2000).
179. Kondrat'yev, A. I. and Y. K. Vohra, *High Press. Res.*, submitted.