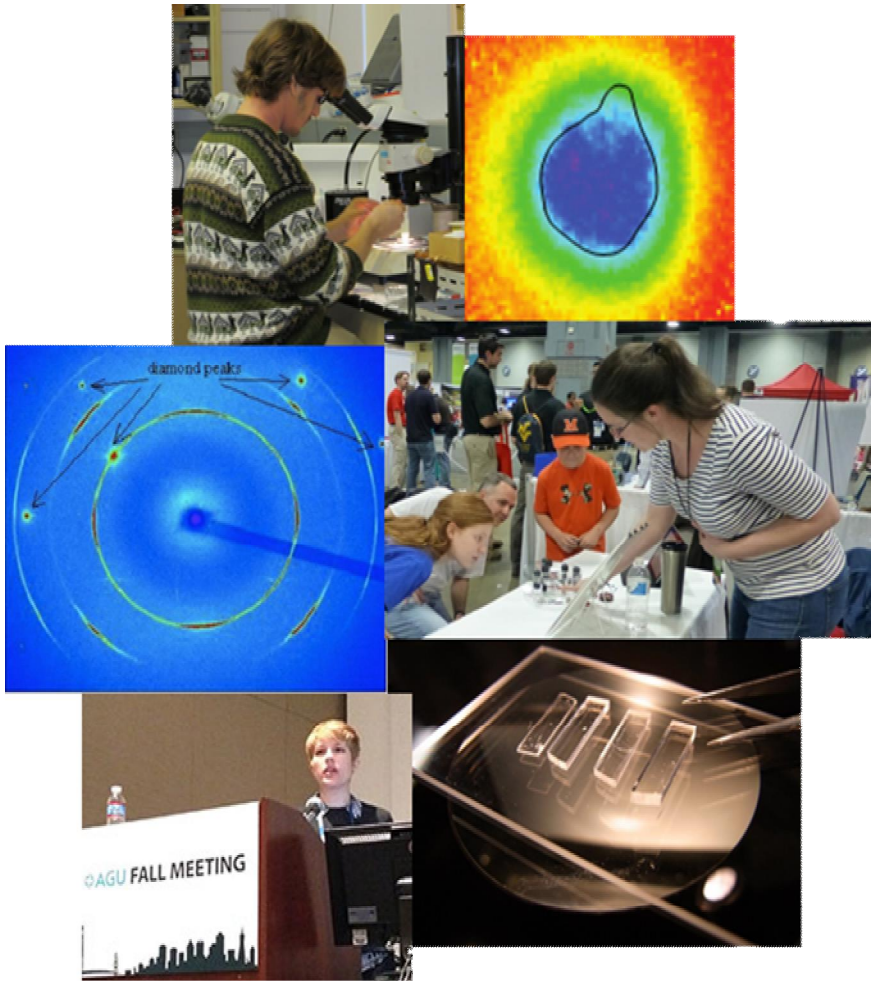
CDAC

CARNEGIE/DOE ALLIANCE CENTER

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

Annual Report
2013-2014



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Director
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CARNEGIE INSTITUTION FOR SCIENCE

NNSA

On the Cover

Clockwise, from top left: 1) Carnegie visiting student Eugene Vinitsky prepares a sample of $BaReH_9$ for investigations of high-pressure phase transitions using Raman and infrared spectroscopy. Vinitsky is spending a year at Carnegie following his undergraduate work at Caltech. 2) Emissivity map across a melted sample of SiC at 12 GPa. Studies of the melting of highly refractory materials is part of the dissertation research of Kierstin Daviau, a graduate student in the group of Academic Partner Kanani Lee at Yale University. 3) Carnegie postdoctoral fellow Caitlin Murphy participates in the 2014 USA Science and Engineering Festival, held in Washington DC. Murphy presented a demonstration on the effects of pressure on materials with defects and impurities. 4) Nearly-pure crystals of acetaminophen are used as models for molecular constituents of plastic-bonded explosives in a collaboration between graduate student John Lazarz and Academic Partner Steve Jacobsen at Northwestern and Dan Hooks, Kyle Ramos and Cindy Bolme at Los Alamos. The collaboration focuses on the use of GHz interferometry to determine high-accuracy elastic constants. 5) Graduate student Emma Rainey, from the group of Academic Partner Abby Kavner at UCLA, presents her work on temperature calibration in the laser-heated diamond anvil cell at the 2013 Fall Meeting of the American Geophysical Union in San Francisco, CA. 6) X-ray diffuse scattering from an Fe-Ga alloy obtained by CDAC Research Scientist Muhtar Ahart at Beamline 16-BM-D at HPCAT confirm the existence of structural inhomogeneity caused by the presence of nanoscale atomic clusters in the solid. Highly optimized diffraction and spectroscopy instrumentation at HPCAT makes possible the investigation of condensed matter at extreme conditions in unprecedented detail.

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

2013-2014 ANNUAL REPORT

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1. OVERVIEW

Since 2003, the Carnegie-DOE Alliance Center (CDAC) has pushed the frontiers of materials science at extreme conditions through advanced research and training. Headquartered at the Carnegie Institution of Washington (Fig. 1), CDAC is the Center of Excellence for materials within the Stockpile Stewardship Academic Programs of the Department of Energy/National Nuclear Security Administration (DOE/NNSA). The Center continues Carnegie's tradition of more than a century of advancing fundamental science "for the improvement of mankind," and in service to the nation, while at the same time promoting unfettered freedom in basic research.[1]

Figure 1. *The Carnegie Institution of Washington's Broad Branch Road campus celebrated its 100th anniversary this year.*

1.1 CDAC in Year 11

CDAC continues to pursue the core mission articulated at its inception, expanding our understanding of materials behavior at extreme pressure-temperature (*P-T*) conditions, developing new facilities and methods to advance high *P-T* materials science, and supporting the education and training of the next generation of scientists in the field. A network of Academic Partners, NNSA Laboratory Partners and Carnegie personnel and facilities comprise the Center. CDAC's program of education, research and technical development support the fundamental science that underlies the mission of the NNSA in stockpile stewardship and its legacy in national security.[2] CDAC personnel study structural, electronic and optical phenomena at extreme conditions in a broad range of materials, including metals, alloys, dense oxides, molecular systems and polymers, and energetic materials - in bulk, on surfaces and at interfaces.

Figure 2. Top to bottom: *Advanced Photon Source (APS), the site of the x-ray sector HPCAT; National Synchrotron Light Source (NSLS), the location of IR beamline U2A; and National Synchrotron Light Source II (NSLS II), the site of FIS, the new IR beamline.*

CDAC is managed at Carnegie by **Russell J. Hemley** (Director), **Stephen Gramsch** (Coordinator) and **Morgan Phillips Hoople** (Administrator). CDAC facilities at Carnegie are supported by Research Scientists **Maddury Somayazulu**, **Muhtar Ahart**, and **Chang-sheng Zha**, who support students, postdocs, and visitors from across the Center, including its offsite facilities (Fig. 2).

At the heart of the CDAC program is the Academic Partner group, 14 faculty representing some of the leading extreme conditions research programs from around the

Box 1. CDAC Academic Partners for 2013-2014

- **David Cahill** (University of Illinois)
- **Przemek Dera** (University of Hawai'i)
- **Dana Dlott** (University of Illinois)
- **Brent Fultz** (California Institute of Technology)
- **Steven Jacobsen** (Northwestern University)
- **Raymond Jeanloz** (University of California – Berkeley)
- **Abby Kavner** (University of California – Los Angeles)
- **Kanani Lee** (Yale University)
- **Lowell Miyagi** (University of Utah)
- **James Schilling** (Washington University in St. Louis)
- **Yogesh Vohra** (University of Alabama – Birmingham)
- **Hans-Rudolf Wenk** (University of California – Berkeley)
- **Choong-shik Yoo** (Washington State University)
- **Eva Zurek** (SUNY – University at Buffalo)

country (Fig. 3 and Box 1). CDAC Academic Partners provide the key education and training function of the Center, and prepare highly qualified graduate students for work in areas of fundamental scientific importance for the NNSA mission. CDAC enhances this preparation by providing access to beam time at CDAC-supported facilities, supporting travel to national user facilities for collaboration with other Center participants, and creating opportunities for interaction with students from other groups and with staff from the NNSA Laboratories.

The CDAC partner group has also evolved significantly. We have expanded our program to include more theory and computation in modern high *P-T* materials science and have added a computational chemist to the Partner group. In addition, at Carnegie, theorist **Ivan Naumov** has been added as a CDAC Research Scientist. Also, the disciplines pursued by CDAC Partners have become more diverse as the nature of extreme conditions science has expanded in recent years to address an ever-broadening array of problems. Both of these developments promise to enhance the interactions between CDAC groups and scientists in the NNSA Laboratories.

We continue to engage with our Laboratory Partner scientists in high *P-T* research groups at all three NNSA Laboratories. Our Laboratory Partners serve on the CDAC Steering Committee, providing valuable input on the direction of the scientific program and serve as points of contact in the NNSA Laboratories for our academic groups. The Laboratory Partners also benefit from the availability of discretionary beam time at CDAC user facilities for both programatic and individual research. They participate in CDAC outreach events and interact directly with graduate students and Academic Partners, providing important insight into the mission and research environment at the NNSA Laboratories.

Figure 3. *2013-2014 CDAC Partners.*

Researchers throughout the Center can access specialized facilities at HPCAT, the dedicated extreme conditions beamline at the Advanced Photon Source (APS), Argonne National Laboratory (ANL) managed by **Guoyin Shen**, and U2A, the synchrotron infrared beamline at the National Synchrotron Light Source (NSLS), Brookhaven National Laboratory (Fig. 2) managed by **Zhenxian Liu**. We are now preparing for the transition to NSLS II and a new IR

Box 2. CDAC Statistics for 2013-2014

- Publications for 2013-2014 – **250**
  - *PNAS* – **11**
  - *Science* – **5**
  - *Nature* – **18**
  - *Physical Review Letters* – **8**
- Presentations for 2013-2014 – **212**
- Student Publications for 2013-2014 – **52**
- Student Presentations for 2013-2014 – **71**
- Collaborators for 2013-2014 – **671** from **173** Institutions
- PhDs Supported – **41**
- CDAC Students 2013-2014 – **19**

facility. Participants in CDAC also have performed experiments at the Lujan Neutron Scattering Center, Los Alamos National Laboratory (LANL). CDAC has supported these DOE/Office of Science (SC) facilities since the inception of the Center in 2003, a fact that highlights one of our important goals—to facilitate partnerships between SC and DOE/NNSA programs. New facilities such as the Dynamic Compression Sector at APS (DCS@APS) and those in the planning stages (MaRIE at LANL), which, along with access to time for fundamental science experiments at Z at Sandia National Laboratories (SNL) and the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory (LLNL), are bringing new capabilities to the field and advancing our understanding of extreme conditions phenomena into new regimes of pressure and temperature.

The overall structure of the Center has proved scientifically productive as well as very effective in achieving our goals in the area of education and outreach (Box 2). On the other hand, the true strength of CDAC has been the results of our efforts at growing the high pressure research community in this country and merging various aspects of it to meet NNSA needs in areas of science crucial to stockpile stewardship.

This report describes the progress of the Carnegie-DOE Alliance Center during the period March 2013-May 2014, including efforts in the Academic Partner groups and among Laboratory Partners. Research of the Laboratory Partners pursued outside CDAC-supported facilities is not addressed.

Figure 4. *CDAC participants at the 2014 SSAP Symposium. Clockwise from top right: Students* ***Walter Uhoya*** *(UAB),* ***Eloisa Zepeda-Alarcon*** *(UC-Berkeley), and* ***Will Shaw*** *(Illinois-Champaign) explain their posters;* ***Zach Geballe*** *(UC-Berkeley) with Carnegie-CDAC Scientists* ***Muhtar Ahart*** *and* ***Maddury Somayazulu;*** ***Andrew Shamp*** *(SUNY-Buffalo) and* ***Spencer Smith*** *(UAB) present their posters.*

1.2 Highlights from 2013-2014

<u>Training, Outreach, and Personnel</u>

- In 2013-2014, CDAC supported the work of 18 graduate students in 14 Academic Partner groups. During this time, 16 CDAC-supported students received the PhD degree, bringing to 41 the total number of degrees earned by CDAC graduate students over the 11 years since the beginning of the Center's program in 2003.
- At the annual SSAP Symposia in Albuquerque, NM (2013) and Bethesda, MD (2014), CDAC graduate students presented a total of 16 and 17 posters, respectively. In 2013, Best Poster citations were awarded to CDAC students **Lisa Mauger** (Caltech), **Pamela Kaercher** (UC-Berkeley), **Zeyu Li** (Michigan) and **Eloisa Zepeda-Alarcon** (UC-Berkeley). In 2014, **Pamela Kaercher**,

Emma Rainey (UCLA) and **Dane Tomasino** (Washington State) received Best Poster Awards (Fig. 4).

- During 2014, CDAC supported the participation of three undergraduate students in Carnegie's Summer Scholars Program, which is supervised by CDAC Coordinator **Stephen Gramsch**.
- CDAC supported the *Paris-Edinburgh Cell Workshop*, which was held in May 2013 at APS and hosted by HPCAT. More than 45 participants attended the two-day workshop. The workshop was composed of four technical training courses, and was attended by 32 graduate students, postdocs, and both early career and senior researchers. The unique opportunity provided by the new instrumental setup established at HPCAT was also introduced to the hands-on participants. The workshop was organized by Carnegie's **Changyong Park**, **Yoshio Kono**, and **Guoyin Shen** (HPCAT), along with **Yanbin Wang** from GSECARS.
- Carnegie Postdoctoral Fellow **Caitlin Murphy** represented the Geophysical Laboratory at the third annual USA Science and Engineering Festival (Fig. 5). The festival, held April 26-27, 2014 in Washington DC, is the largest science, technology, engineering, and math education event of its kind in the US. Caitlin's topic was "How does high pressure affect materials that have defects and impurities?" **Robert Hanrahan**, former Program Manager for CDAC at NNSA, discussed stockpile stewardship and non-proliferation at the State Department's booth in the National Security section of the festival.

Figure 5. *CDAC-Carnegie Postdoctoral Fellow* ***Caitlin Murphy*** *at the third annual USA Science and Engineering Festival in Washington, DC.*

- CDAC Partners **Przemek Dera** (University of Hawai'i) and **Lowell Miyagi** (University of Utah) have been named as the speakers for the 2014-2015 COMPRES Distinguished Lecture series in the field of Mineral Physics. The talks feature topics that emphasize the exciting high-pressure geoscience research being conducted within the COMPRES community and its significance for understanding fundamental Earth and planetary processes. Since its inception in 2008, seven CDAC Academic Partners and/or faculty who were supported as postdoctoral fellows through CDAC have served as Distinguished Lecturers.

- CDAC Academic Partner **Steven Jacobsen** from Northwestern University received a Friedrich Wilhelm Bessel Research Award for 2014. The Bessel Award is granted by the Alexander von Humbolt Foundation, and allows the recipient to spend a year working at a research institution in Germany. He will spend the coming year at the Bayeriches Geoinstitut in Bayreuth, Germany, where he was a Humboldt Postdoctoral Fellow from 2002-2004.
- **Eva Zurek**, a CDAC Academic Partner from the University at Buffalo received the 2014 Young Leaders Professional Development Award of The Minerals, Metals and Materials Society (TMS). She was presented with the award at the 2014 annual meeting of the TMS in San Diego, CA.

Scientific Program

- A group including CDAC Partner **Hans-Rudolf Wenk**, current CDAC students **Pamela Kaercher** and **Eloisa Zepeda-Alarcon**, and former CDAC student **Jane Kanitpanyacharoen** from UC-Berkeley carried out high *P-T* diffraction experiments on polycrystals to explore *in situ* crystallographic orientation development and changes during the α–ω and ω–α phase transitions in Zr. Viscoplastic Self-Consistent modeling of uniaxial compression data shows that upon decompression, the ω-phase reverts back to the α-phase with a texture identical to that of the starting phase, documenting a perfect texture memory after cycling through the ω phase.[3]

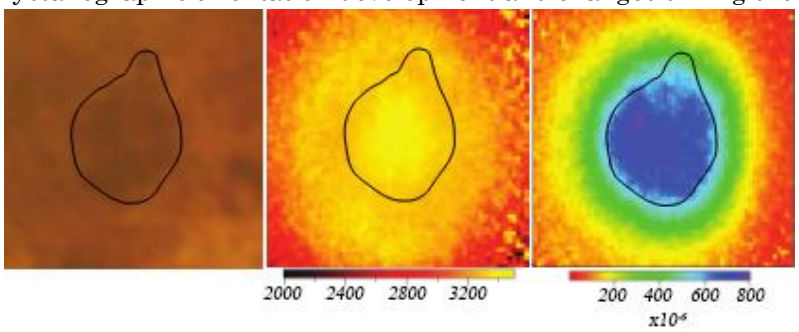


Figure 6. *Comparison of optical, temperature and emissivity maps across a melted sample of SiC at 12 GPa. The image is approximately 40 microns across.*[4]

- CDAC graduate student **Kierstin Daviau** from Yale has carried out a multi-technique, high *P-T* investigation of the highly refractory material SiC using new experimental capabilities, including a 4-color temperature mapping technique[4] in the laboratory of CDAC Academic Partner **Kanani Lee** (Fig 6). Preliminary results show that at low pressures and below 1500 K, SiC forms a new phase, and then decomposes to Si and C at higher temperatures.
- A group from Lawrence Livermore National Laboratory and UC-Berkeley, including current and former CDAC Academic Partners **Raymond Jeanloz** and **Tom Duffy**, former Carnegie-CDAC Postdoc **Amy Lazicki** (LLNL) and CDAC Steering Committee members **Jon Eggert** and **G. W. (Rip) Collins** (both from LLNL), carried out ramp compression experiments on carbon to 5 TPa at the National Ignition Facility. In these experiments, data was obtained on carbon at peak stresses of 2.7, 3.7 and 5 TPa, resulting in a 3.7-fold compression of the material and a density of 12 g/cm^3, greater than the density of lead at ambient pressure.[5]
- In recent work at Carnegie, CDAC Director **Russell Hemley**, and Research Scientist **Chang-sheng Zha**, together with Carnegie's **Ronald Cohen**, report Raman measurements on hydrogen and deuterium to 325

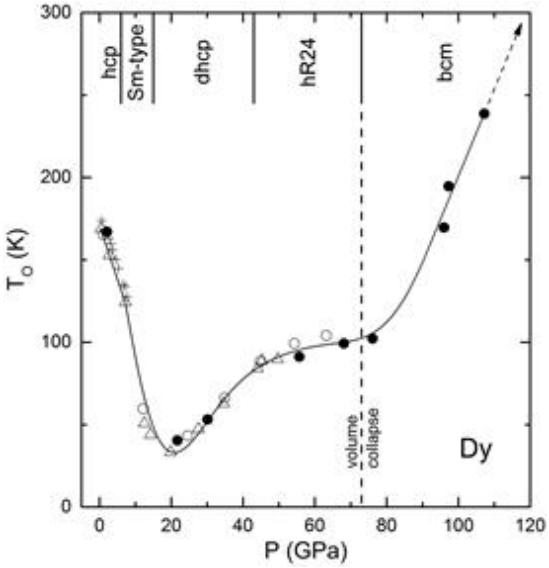


Figure 7. *Magnetic ordering temperature of Dy versus pressure.*[8]

GPa at 300 K, which provide structural information on hydrogen with increasing density along the I-III-IV transition pathway. Changes in intensities and linewidths of the hydrogen vibron with increasing pressure are accompanied by discontinuities in pressure shifts, which indicate changes in structure and bonding, molecular orientation and electronic structure in the compressed solid. The results further point to the formation of new phases, which may be either completely new structures, or variations of the structure of phase IV.[6]

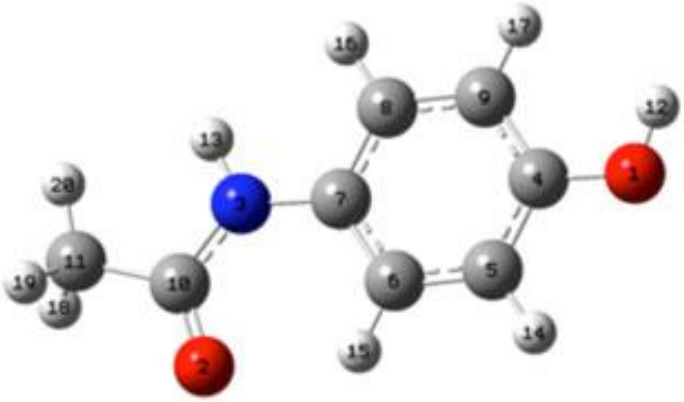


Figure 8. *Paracetemol structure. Carbon, grey spheres; oxygen, red; nitrogen, blue; hydrogen, white.*[9]

- Experiments carried out by **Yue Meng** (HPCAT) and co-workers from Carnegie and colleagues from George Mason University, Oak Ridge National Laboratory, and Tohoku University successfully identified a liquid-liquid phase transition in Ce metal. At 13 GPa, upon increasing temperatures from 1550 to 1900 K, a high-density liquid transforms to a low-density liquid, with a density change of 14%. Theoretical results suggest that the transition is first order and terminates in a critical point. Computational work further points to the delocalization of *f* electrons and a fluctuation in the valence state of the Ce atom as the origin of the transition to a low-density liquid state at high pressure and temperature.[7]
- CDAC graduate student **Jinhyuk Lim** from the **Schilling** group at Washington University in St. Louis carried out four-point electrical resistivity measurements on Dy metal up to 157 GPa and has observed a record-high magnetic ordering temperature between 400-500 K at this pressure. The ordering temperature increases dramatically at $P > 73$ GPa, at which pressure the volume decreases by 6%. The highest previously observed ordering temperature was 292 K at ambient pressure for gadolinium metal (Fig. 7).[8]
- CDAC graduate student **Spencer Smith**, along with CDAC Partner **Yogesh Vohra** and colleagues from the University of Alabama – Birmingham used Raman spectroscopy, synchrotron x-ray diffraction (XRD), and *ab initio* harmonic frequency calculations to explore the solid-state transition behavior of paracetamol (Fig. 8) a commonly used analgesic and anti-pyretic) at hydrostatic pressures up to 21 GPa. The results of this work are being used by the pharmaceutical industry to understand pressure-induced phase transitions that take place at low pressure during the tableting process.[9]
- **Muhtar Ahart** (Carnegie) and CDAC Director **Russell J. Hemley**, along with colleagues from Virginia Tech and the National Institute for Standards and Technology, employed high-pressure XRD techniques to investigate the phase behavior of $Fe_{0.81}Ga_{0.19}$ alloy (Galfenol) (Fig. 9) at 300 K. Diffuse scattering measurements carried out at

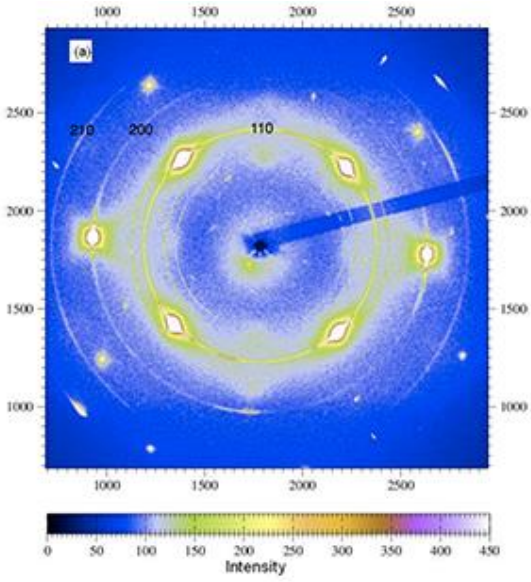


Figure 9. *Diffuse scattering obtained from a [001]-oriented crystal of Fe-Ga alloy at 0.8 GPa.*[10]

beamline 16-BM-D at HPCAT reveal that a coarsening-resistant, nanometer-scale clustering of bulk defects is responsible for enhanced magnetostrictive behavior in the alloy as compared to pure iron. The work explains earlier suggestions of an underlying structural in homogeneity proposed on the basis of earlier neutron diffraction results.[10]

- Long-standing discrepancies in the melting curves of refractory metals have been addressed at Carnegie with the use of an advanced laser flash-heating technique. Predoctoral fellow **Amol Karandikar** and Carnegie's **Reinhard Boehler** concurrently developed an analysis procedure that has reduced the uncertainty in the melting curve of Ta metal to less than 200 K.
- UCLA graduate student **Emma Rainey** has quantitatively explored the temperature gradients in laser-heated dia mond anvil cells using numerical modeling techniques. Rainey's model solves the steady-state heat conduction equation over the sample chamber, gasket, and diamond anvils. The results show that laser heating in a "flat-top" mode does not produce a temperature gradient that is flatter or more uniform than would be produced by a Gaussian beam profile of similar width.[11]
- CDAC Partner **Steve Jacobsen** (Northwestern), CDAC Research Scientist **Zhenxian Liu** (NSLS) and colleagues from the University of New Mexico, University of Southern California, and University of Wyoming used a unique combination of synchrotron IR spectroscopy, TEM, numerical modeling, and seismic P-to-S conversions recorded by a dense seismic array in North America to examine the effects of downwelling from the transition zone into the lower mantle. In experiments, the transition of hydrous ringwoodite to perovskite and (Mg,Fe)O produces intergranular melt. Detections of abrupt decreases in seismic velocity where downwelling mantle is inferred are consistent with partial melt below 660 kilometers. These results suggest hydration of a large region of the transition zone and that dehydration melting may act to trap H_2O in the transition zone.[12]

Technique Development

- The Frontier Synchrotron Infrared Spectroscopy (FIS) Beamline under Extreme Conditions has been approved as one of the eight NxtGen beamlines to be developed and constructed at NSLS-II (Fig. 2). FIS is the successor of the IR facility (U2A) at NSLS, the highly productive, Carnegie-managed user facility supported by COMPRES and CDAC, and the only dedicated high-pressure synchrotron IR facility in the world. Construction of the beamline hutch on bending magnet port 22 will be completed and all existing equipment at U2A moved in by early 2015.
- The laser shock compression facility operated by the **Dlott** group at Illinois has undergone several improvements. The group has added a femtosecond IR laser which can now be used to carry out IR absorption spectroscopy of shocked solids and liquids. Also under development is a 1 ns, 32 channel optical pyrometer that can be used to study the temperature dynamics of shocked materials.
- Graduate student **Lisa Mauger**, from the **Fultz** group at Caltech, has developed a specialized furnace that can be interfaced to beamline 16-ID-D at HPCAT to carry out NRIXS measurements at elevated temperature. The work was carried

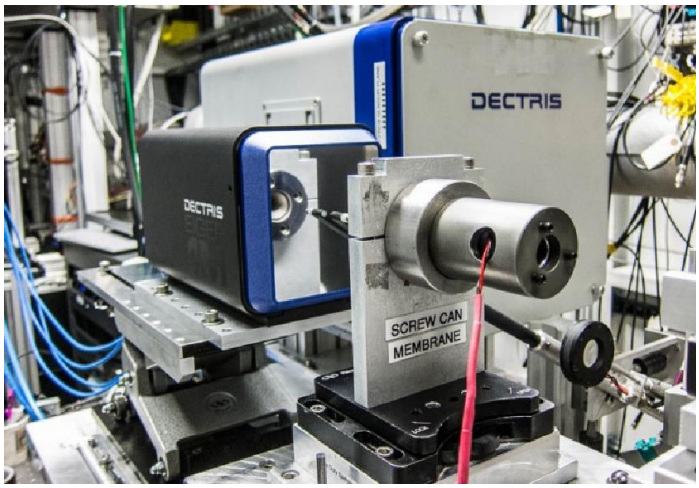


Figure 10. *A diamond anvil cell mounted in a piezoelectric pressure control apparatus for generating ultrahigh compression rates, together with the Pilatus 1M (right) and the Eiger 1M (left, prototype) high frequency area detectors.*

out in collaboration with former CDAC student **Matt Lucas** at the Air Force Research Laboratory.

- A recently installed quad-diode beam position monitor and feedback software on beamline 16-ID-D at HPCAT ensures a stable beam position, and optimizes the intensity of the beam on the sample, both critical in high pressure spectroscopy experiments.
- On beamline 16-BM-B at HPCAT, **Nenad Velisavljevic** (LANL) has led the development of simultaneous XRD, x-ray radiography, electrical resistance, and thermal measurements with the Paris-Edinburg (PE) cell along with student **Jason Baker** and beamline staff at HPCAT. Preliminary experiments have shown that the apparatus performs with high efficiency up to 6 GPa and 1000°C.
- At HPCAT beamline 16-ID-B, progress continues on the development of techniques for time-resolved diffraction. Rapid on-line data analysis has been achieved through optimizing existing software to generate high-quality pressure-temperature-volume relations. An area detector prototype with imaging capability of 800 Hz has been tested and allows the collection of data for compression rates exceeding tens of TPa/s (Fig. 10).
- A group led by **Wenge Yang** (HPSynC) and including researchers from Carnegie, the APS, and University College London has used a new signal averaging technique to eliminate the severe distortions of the high-energy x-rays employed in x-ray imaging to study a 400 nm gold nanocrystal to 6.4 GPa. The averaging algorithm, used on data from APS beamline 34-ID-C, improves spatial resolution over previous methods by more than two orders of magnitude.[13]

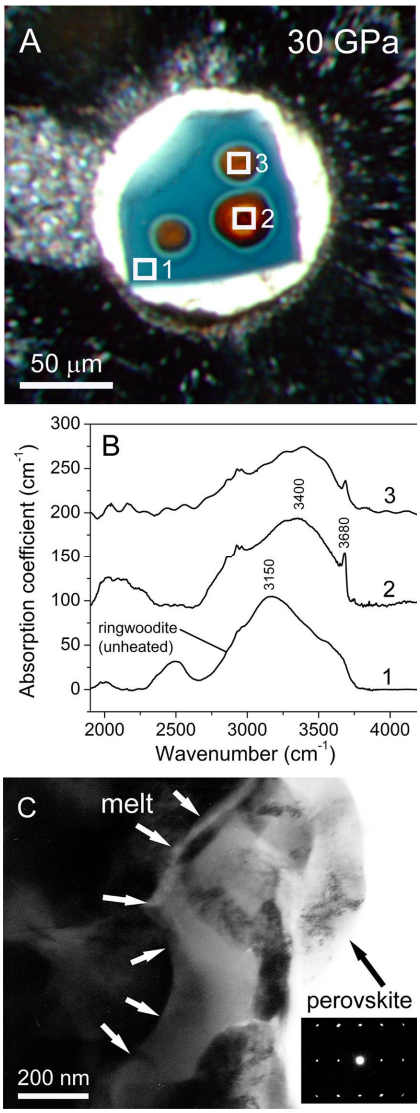


Figure 11. *A) Single-crystal hydrous ringwoodite (blue crystal) containing 1 wt% H_2O inside a DAC at 30 GPa. The sample was laser-heated to 1600°C in several spots (orange circles) to perform direct transformation to perovskite and (Mg,Fe)O. B). Spectrum 1 is an unheated spot, characteristic of hydrous ringwoodite. Spectra 2 and 3 show characteristics of OH in quenched glass). C) On conversion to perovskite plus (Mg,Fe)O, dehydration melting occurred as inter granular melt.*

2. SCIENTIFIC PROGRESS

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

Dehydration Melting in the Deep Earth — The high water storage capacity of minerals in Earth's mantle transition zone (410- to 660-kilometer depth) implies the possibility of a deep H_2O reservoir, which could cause dehydration melting of vertically flowing mantle. Ongoing work in the group of CDAC Partner **Steve Jacobsen** (Northwestern) seeks to model these processes using high *P-T* techniques. Together with Carnegie-CDAC Research Scientist **Zhenxian Liu** (NSLS) and colleagues from the University of New Mexico, University of Southern California, and University of Wyoming, the group has used a unique combination of synchrotron infrared spectroscopy, TEM,

numerical modeling, and seismic P-to-S conversions recorded by a dense seismic array in North America to examine the effects of downwelling from the transition zone into the lower mantle. In experiments, the transition of hydrous ringwoodite to perovskite and (Mg,Fe)O produces intergranular melt (Fig. 11). Detections of abrupt decreases in seismic velocity where downwelling mantle is inferred are consistent with partial melt below 660 kilometers. These results suggest hydration of a large region of the transition zone and that dehydration melting may act to trap H_2O in the transition zone.[12]

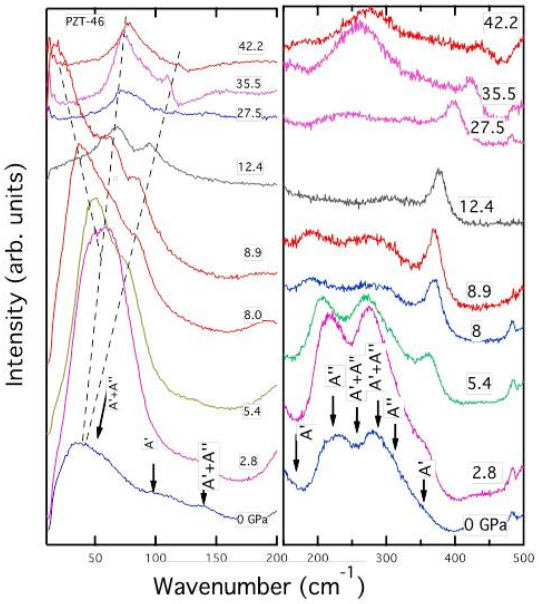


Figure 12. *Detailed display of Raman spectra of $PbZr_{1-x}Ti_xO_3$ at selected pressures. Dashed lines are guides to the eye.*

Phase Transitions in Relaxor Ferroelectrics – Relaxor ferroelectrics such as $Pb(Mg_{1/3}Nb_{2/3})O_3$-x—$PbTiO_3$ (PMN-PT) solid solutions show not only superior piezoelectric properties but also broad frequency dispersive dielectric properties with a low concentration of PT. On the other hand, the $PbZr_{1-x}Ti_xO_3$ system behaves similarly to normal ferroelectrics such as $PbTiO_3$. Many of these materials exhibit structural transitions under pressure.[14] For example, $PbTiO_3$ undergoes second order phase transitions at 12 GPa at 300 K and 16 GPa at 10 K.[15] Carnegie's **Muhtar Ahart** has shown that the structural transitions in the $PbZr_{1-x}Ti_xO_3$ system at 9 GPa are driven by soft mode behavior.[16] Diffraction data were combined with the results of Raman scattering measurements to uncover the transition mechanism.

Diffraction measurements were carried out at HPCAT beamlines 16-ID-B and 16-BM-D. Raman scattering, which was carried out at Carnegie, allowed observation of optical phonons near the Γ point of the Brillouin zone, revealing dynamics that occur in nm sized local structure. Analysis of the spectra was carried out according to the well-established procedure of Lima *et al.*[17] Assignments for the monoclinic phase at ambient pressure are shown in Fig. 12.

These results suggest that the transition from the monoclinic to the rhombohedral phase in $PbZr_{0.54}Ti_{0.46}O_3$ at 3 GPa is related to octahedral tilting, but the second transition that takes place at 9 GPa is driven by a soft optical phonon. The higher pressure transition around 27 GPa, which involves a drastic change in the Raman spectrum and a splitting of diffraction peaks, is associated with a lower symmetry transition. It is proposed that the third transition is from a centro-symmetric rhombohedral to a possible monoclinic or orthorhombic phase induced by pressures above 27 GPa.

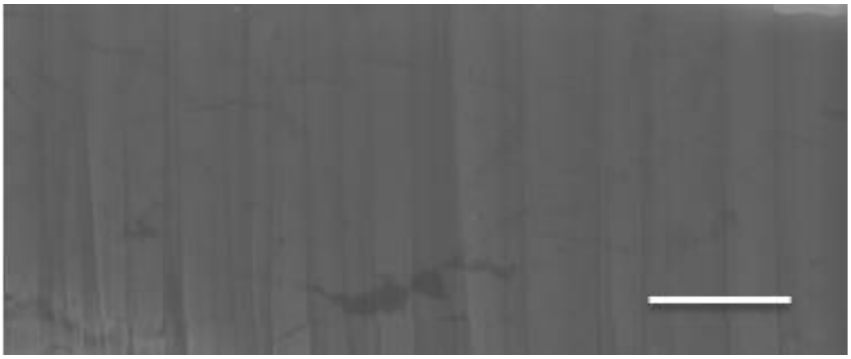


Figure 13. *Cross section of β-SiC quenched from 30 GPa and heated to temperatures of ~2600 K. Note darker crystals, measured by EDS to be C-rich. Scale bar is 2 μm.*

High-Pressure Melting of SiC – CDAC graduate student **Kierstin Daviau** at **Yale** is carrying out a multi-technique study of the high-pressure, high-temperature behavior of silicon carbide (SiC) melting using new techniques developed in the laboratory of Academic Partner **Kanani Lee**.[18] SiC melting at high pressures is not well understood, and existing

studies have inconsistent findings, particularly concerning the Clapeyron slope for the melting curve. Given the discrepant results, it has not been clear whether SiC melts congruently (*i.e.*, SiC *solid* → SiC *liquid*) or incongruently (*e.g.*, SiC *solid* → Si *liquid* + C *solid*). It appears that at low temperatures (less than ~1500 K), SiC sluggishly forms a new solid phase, still undetermined, that has been observed via Raman spectroscopy and XRD. Additionally, it appears that upon further heating, SiC breaks down. Diffraction shows evidence of lonsdaleite, a high pressure polymorph of carbon, and scanning electron microscopy, shows small grains of carbon intermixed within a SiC matrix (Fig. 13). While it appears that it has been possible to melt SiC, investigation of the additional phases and the possible dissociation of SiC at high pressures and temperatures is ongoing.

Experiments with the laser-heated diamond anvil cell (DAC) are challenging, but practical with DAC technology. Due to the small sample chamber size (~10s to 100s of microns) and the high thermal conductivity of diamond, large radial and axial temperature gradients have long plagued DAC experiments. This is due to the thinning of thermal insulation layers that surround the sample against the effects of the highly conductive diamonds at high pressure. In order to overcome these constraints, short-duration laser heating, along with an updated four-color temperature mapping measurement technique (Fig. 6) have been developed, and electron microscopy of quenched samples is used to observe texture and composition. In order to investigate heating along the compression direction, focused ion beam milling techniques allow viewing a cross section of each sample, making features due to melting easier to identify.

New Findings in Dense Hydrogen — Using the U2A facility at NSLS, **Chang-sheng Zha**, **Zhenxian Liu**, **Muhtar Ahart**, **Reinhard Boehler**, and **Russell Hemley** have examined the structure, bonding and electronic properties of highly compressed hydrogen. Experimental results (Fig. 14) show that one type of molecule interacts very weakly with its neighboring molecules, which is unusual for molecules at this very high compression. The other type of molecule bonds with its neighbors, forming surprising planar sheets that comprise the structure. The measurements also show that solid hydrogen at these conditions is on the borderline between a semiconductor and a semimetal. The results disprove earlier claims that hydrogen forms a dense atomic metal at 300 GPa and room temperature.[19]

As a result of recent advances in DAC techniques, measurements on hydrogen to above 300 GPa at room temperature are now possible. Raman measurements of hydrogen and deuterium to 325

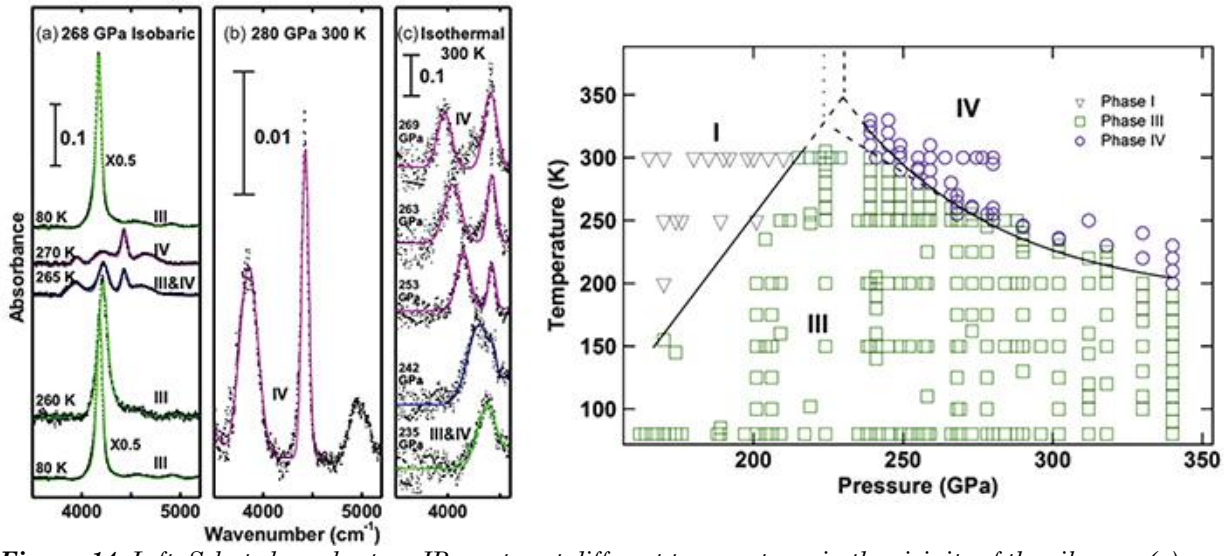


Figure 14. *Left: Selected synchrotron IR spectra at different temperatures in the vicinity of the vibrons. (a) Isobaric measurements of 268 GPa through the III-IV phase transition. (b) Detail in the vibron region at 280 GPa and 295 K. (c) Isothermal compression showing the evolution of the spectrum through phases III and IV at 300 K. The fitted lines show the peaks attributed to each phase. The bar gives the absorbance scale for each panel. Right: Phase diagram of hydrogen to multimegabar pressures.*

GPa at 300 K, representing new regimes of pressure and temperature, have been carried out by **Zha** and **Hemley**, together with Carnegie's **Ronald E. Cohen** and **Ho-kwang Mao**. These measurements provide structural information on hydrogen with increasing density along the I-III-IV transition pathway. A detailed analysis of the spectra indicate that transitions in hydrogen proceed by the formation of a sequence of disordered stackings of molecular and distorted layers. Changes in intensities and linewidths of the hydrogen vibron with increasing pressure (Fig. 15) are accompanied by discontinuities in pressure shifts, which indicate changes in structure and bonding, molecular orientation and electronic structure in the compressed solid. The results further point to the formation of new phases, which may be either completely new structures, or variations of the structure of phase IV. Further work will seek to not only clarify known regions of the phase diagram and explore new pressure-temperature regimes, but also to improve existing theoretical models.[6]

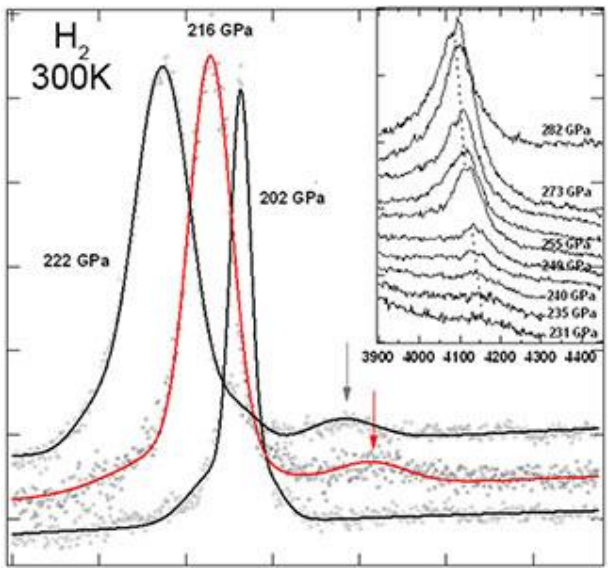


Figure 15. *Hydrogen vibron spectra across the I-III-IV transition.*[19]

Boron Carbide under Pressure – Because of its outstanding hardness, thermodynamic stability, low density, and electronic properties, boron carbide has many uses: *i.e.* as a refractory material, in abrasive powders and ballistics, as a neutron radiation absorbent, and in electronic applications. The space group of boron carbide is generally suggested to be *R3m*, and it is thought to be composed of icosahedra and three atom chains. However, the broad range of compositions possible (from 8-20 at. % carbon) coupled with the fact that it is impossible to distinguish between boron and carbon using diffraction, leaves many open questions about the structure of boron carbide at 1 atm. In addition very little is known about its behavior under hydrostatic pressure. CDAC graduate student **Andrew Shamp** at **Buffalo** has worked towards predicting the most stable structures and important metastable species of boron carbide in a wide pressure range (1 atm – 10 TPa), and studied their electronic structures. The work carried out to date has focused on the idealized carbon-rich B_4C stoichiometry. In the most stable structure found in DFT calculations, the linear chain has a 'CBC' arrangement, and one carbon atom is found in the polar site (Fig. 16). Interestingly, this phase becomes unstable with respect to decomposition into pure carbon and boron around 50

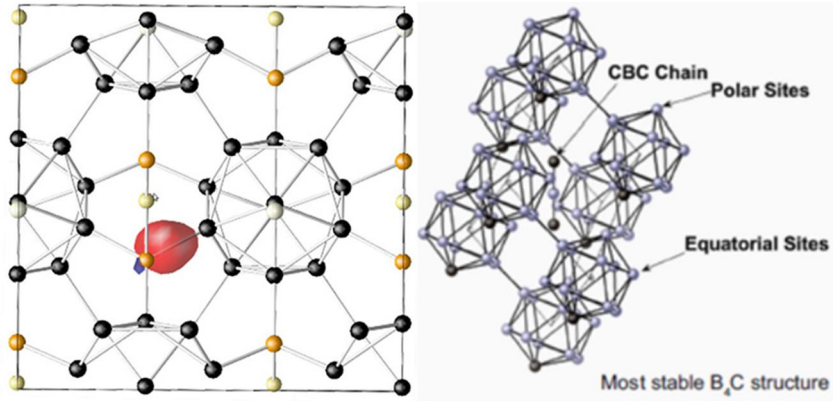


Figure 16. *Top right: the CBC_p configuration shown is the most stable structure below 50 GPa. At higher pressures, segregated boron and carbon are enthalpically preferred. Top left: the same CBC_p configuration with a Wannier function describing one of the carbon sp^3 hybrid orbitals in the chain. This Wannier function shows the bond between the chain carbon and polar boron in the icosahedron.Bottom left: CDAC graduate student* ***Andrew Shamp (Buffalo).***

GPa, but it remains dynamically stable up to at least 100 GPa. Shamp and CDAC Partner **Eva Zurek** are currently analyzing the response of different structures to pressure. In most configurations the three atom chain is predicted to bend, and linearity is only maintained in a structure containing a CCC motif. The configuration which is the most stable at 1 atm remains enthalpically preferred under pressure. This structure also shows the greatest bending of the CBC chain, and it therefore has the smallest volume. Using qualitative analysis techniques (such as generation of 'Fat bands', COHPs and Wannier functions via the LMTO and NMTO methods), it is possible to get a better understanding of the electronic structure of various phases under pressure.

Structure and Physical Properties of Hydrogen-Bearing Post-Perovskite – CDAC graduate student **Joshua Townsend (Northwestern)** is carrying out experiments and theoretical calculations on hydrogen incorporation into the post-perovskite structure of $MgSiO_3$, which may be stable at the core-mantle boundary. By studying the effects of chemical substitutions on post-perovskite material properties at extreme conditions, results are being applied to interpreting the heterogeneous seismic structure of the core-mantle boundary region. Using density functional theory, Townsend has found a stable hydrogen defect structure of post-perovskite containing 1600 ppm H_2O. Vibrational and elastic properties have been calculated for the structure up to 120 GPa, showing an 8% reduction in the bulk modulus for the H-bearing structure compared with ideal $MgSiO_3$ (Fig. 17). At the NSLS beamline U2A, in collaboration with **Zhenxian Liu**, Townsend has co-developed a new CO_2 laser heating sy stem, which he is using to try and synthesize hydrogen-bearing post-perovskite for comparison with his theoretical c_alculations. Through chemical interactions at the core-mantle boundary, primordial hydrogen from the core may enter the post-perovskite structure and influence properties of the core-mantle boundary including viscosity, electrical conductivity, and melting.

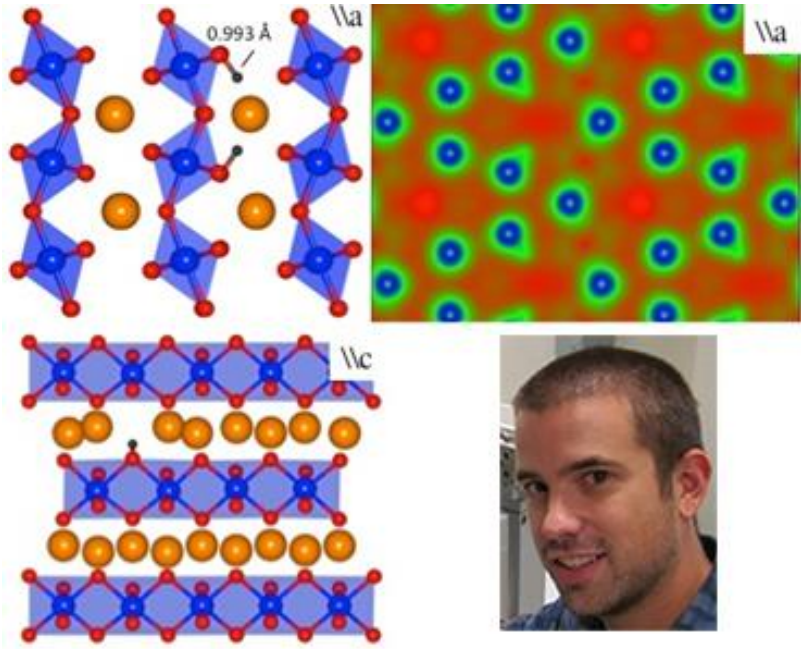


Figure 17. *Predicted stable hydrogen defect structure of post-perovskite at 120 GPa. Left: crystal structure. Top right: electron density map showing defect positions in blue. Bottom right: CDAC graduate student* ***Joshua Townsend (Northwestern)****.*

Liquid-Liquid Critical Point in Ce Metal – Understanding polymorphism in liquids provides key insights into the complex nature of the liquid state, and may now be studied in detail as a result of advances in synchrotron XRD techniques. The observation of a liquid-liquid transition in a material having two distinct liquid phases of differing density is experimentally challenging and requires simultaneous high pressure and high temperature conditions and instantaneous capture of the diffuse scattering from both liquid phases. Recent experiments carried out by **Yue Meng** (HPCAT), and co-workers from Carnegie, along with colleagues from George Mason University, Oak Ridge National Laboratory, and Tohoku University have now successfully identified a liquid-liquid phase transition in cerium metal.

At 13 GPa, upon increasing temperatures from 1550 to 1900 K, a high-density liquid transforms to a low-density liquid (Fig. 18) with a density change of 14%. Theoretical results suggest that the transition is first order and terminates in a critical point (LLCP). Computational work

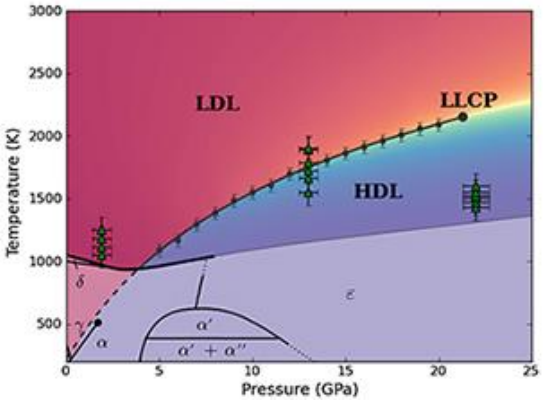


Figure 18*. Ce phase diagram superimposed on the liquid-liquid phase boundary estimated from free-energy calculations. The liquid-liquid phase transition ends at a liquid-liquid critical point (LLCP) near 21.3 GPa and 2100 K. The transition curve is dashed in the supercooled region. Experimental data are shown as green circles.*

further points to the delocalization of *f* electrons and a fluctuation in the valence state of the Ce atom as the origin of the transition to a low-density liquid state at high pressure and temperature.[7]

Giant Magnetostriction in Fe-Ga Alloy – Galfenol is a new class of iron-based, magnetic $Fe_{1-x}Ga_x$ alloy that exhibits giant magnetostriction and has attracted considerable attention because of its potential for use in mechanical devices where resistance to fracture is an important criterion. Maximum values of the magnetostriction coefficient (3/2∂100) of 400 ppm (more than one order of magnitud_e higher than that for pure Ŭ-Fe) have been observed in bulk single crystals with $x = 0.19$. A structurally heterogeneous model has been proposed to explain the enhanced magnetostriction and elastic softening for $Fe_{1-x}GaM_x$ alloys. This model assumes that heat treatment produces a structurally and chemically heterogeneous state consisting of coarsening-resistant, nanometer-scale DO_3 precipitates in FeGa alloy. Recent neutron diffuse scattering measurements on FeGa alloys confirm that the enhanced magnetostriction is directly related to the presence of an underlying structural heterogeneity.

Motivated by a strong interest in understanding the effects of pressure on these materials, CDAC Research Scientist **Muhtar Ahart** and CDAC Director **Russell J. Hemley**, along with colleagues from Virginia Tech and the National Institute for Standards and Technology, employed high-pressure XRD techniques to investigate the phase behavior of the $Fe_{0.81}Ga_{0.19}$ alloy at 300 K. The goal was to study determine how the addition of Ga affects the pressure-induced bcc-to-hcp phase transition in Fe, how pressure affects the diffuse scattering, and to search for new phases in order to uncover the underlying microscopic mechanism responsible for the giant magnetostriction

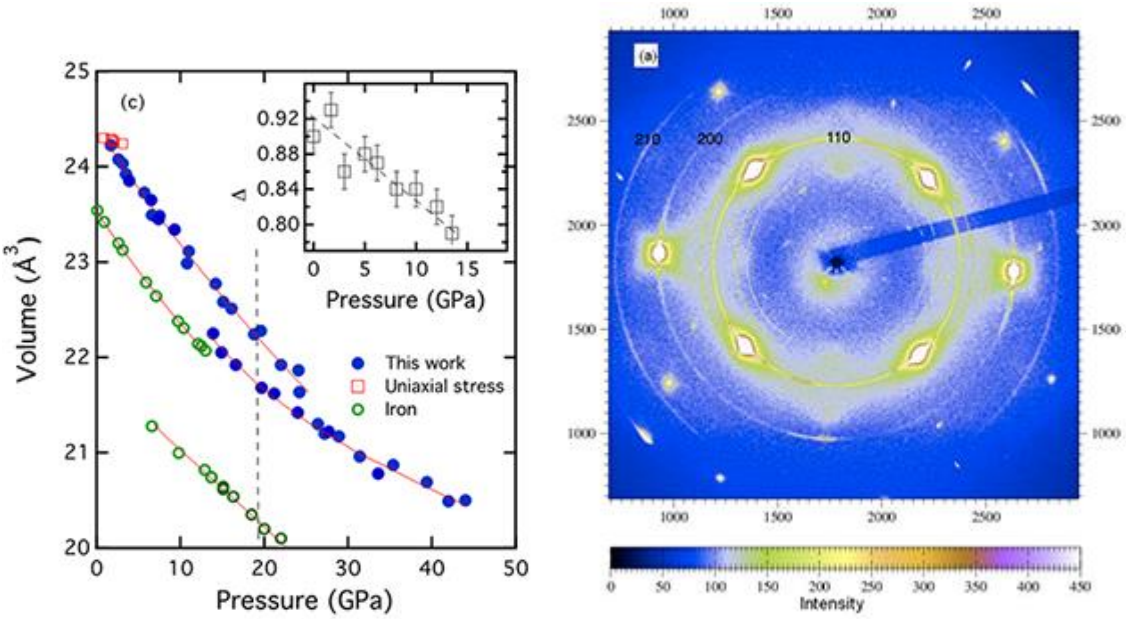


Figure 19. *Left: Pressure dependencies of unit cell volume of bcc and hcp structures in $Fe_{0.21}Ga_{0.19}$ alloy. Right: Diffuse scattering obtained from a [001]-orientated 300 μm sample at 0.8 GPa.*

in the alloy. XRD measurements were carried out at HPCAT beamline 16-BM-D. The x-ray measurements reveal several interesting facts: (1) The bcc-to-hcp phase transition pressure of 18.5 GPa (Fig. 1) for single-crystal $Fe_{0.81}Ga_{0.19}$ is 6.5 GPa higher than that for pure iron (13 GPa). (2) The pressure of the bcc-to-hcp phase transition on compression and decompression differs by roughly 10 GPa, whereas for pure iron this difference is only 5 to 6 GPa; such hysteretic behavior is characteristic of martensitic transformations. (3) The volume difference between the cubic and hexagonal phases of $Fe_{0.81}Ga_{0.19}$ at the transition point is much smaller than that for pure iron (Fig. 19, left); this itself is very interesting and indicates the strong effect of adding Ga. (4) Remarkably clear diffuse scattering (Fig. 19, right) was observed in the 300 ε m thick samples, and this diffuse scattering is associated with the DO_3 precipitates.

By analogy with the phase transition in pure iron, a mechanism for the transition is proposed in which the hcp structure can be derived from the bcc lattice through a compression along the [001] direction, followed by shear along the [1-10] direction. An explanation consistent with experimental observations is that the larger atomic size of Ga is responsible for the higher bcc-to-hcp transition pressure compared to that for pure iron. A modest uniaxial stress of ~3 GPa is sufficient to suppress the presence of DO_3 nanoprecipitates, and eliminate diffuse scattering.[10]

2.2 P-V-T EOS Measurements

Carbon to 50 Megabars – Increased study of the nature of planetary interiors, as well as the current effort to produce inertial confinement fusion, both call for an understanding of matter at ultra-dense states, characterized by pressures in the TPa range. The possible existence of carbon-rich planets has created interest in the behavior of carbon at these conditions. Pursuing this work is a group from Lawrence Livermore National Laboratory and UC-Berkeley, including current and former CDAC Academic Partners **Raymond Jeanloz** and **Tom Duffy**, former Carnegie-CDAC Postdoc **Amy Lazicki** (**LLNL**) and CDAC Steering Committee members **Jon Eggert** and **G. W. (Rip) Collins** (both from **LLNL**). Ramp compression experiments on carbon have been carried out to 5 TPa at the NIF. NIF, which houses the world's largest and most powerful laser, was constructed to realize inertial confinement fusion of hydrogen as an energy source, but discovery science experiments are also provided time on the facility through a proposal review process.

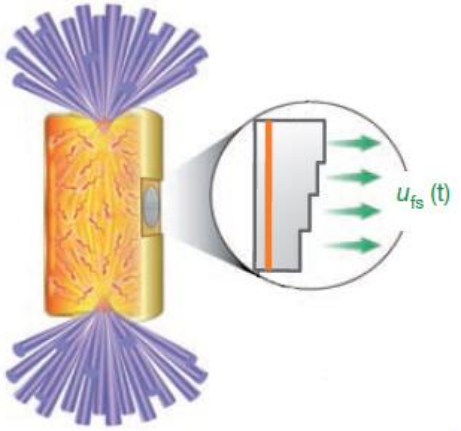


Figure 20*. The 6 mm diameter, 11 mm high, gold-coated hohlraum, containing the synthetic diamond target.*

In the experiments at NIF, 176 laser beams converge simultaneously onto a hohlraum target, which converts the ultraviolet radiation to x-rays; the x-rays ablate the sample and result in dynamic compression of the material. Four thicknesses of the diamond sample effectively allow multiple sample runs within the same experiment (Fig. 20). Velocity interferometry is then used to create a stress-density profile that characterizes the load on the sample. Because ramp compression is more controlled than shock compression, NIF allows observations in pressure ranges where shock compression data are unreliable and static compression data are not available. In these experiments, data was obtained on carbon at peak stresses of 2.7, 3.7 and 5 TPa, resulting in a 3.7-fold compression of the material and a density of 12 g/cm^3, greater than the density of lead at ambient pressure. One of the primary uses of the data obtained at NIF is to provide stringent tests of modern condensed matter theory and models of planetary formation. The LLNL team is also collaborating with the CDAC group at Carnegie on experiments on hydrogen and hydrogen-containing compounds to be carried out at NIF in the future.[5]

Temperature Distribution in the Laser-Heated DAC – One of the key goals of the **Kavner** group at UCLA is pressure and temperature calibration of laser-heating experiments using

the DAC, and to elucidate the principles governing the mechanical behavior of engineering materials at ultrahigh pressures and high temperatures. While previous efforts have focused on mechanical properties of composite materials at high pressures in the diamond cell, during the past two years the CDAC-supported effort in the group has shifted focus toward studying the temperature distribution in the laser heated DAC, and the mechanical properties of samples subject to both high pressures and temperatures.

To design experiments and test hypotheses, CDAC graduate student **Emma Rainey** has created and validated a 3-D numerical model, *TempDAC*, for calculating temperature distributions within the laser-heated DAC (LHDAC) applicable to continuous wave laser heating experiments. *TempDAC* solves the steady-state heat conduction equation over the sample chamber, gasket, and diamond anvils. Sample geometries, laser beam profiles, and laser absorption properties are flexible, allowing *TempDAC* to accurately model a wide range of experimental conditions. Thermal conductivities in *TempDAC* are both material- and temperature-dependent, and can also be anisotropic.

Example calculations illustrate several interesting properties of the extreme temperature gradients that form during DAC laser heating experiments, and underscore the need for considering heat conduction in three dimensions when predicting LHDAC temperature gradients and interpreting XRD data obtained during laser heating. In particular, the results show that a "flat-top" laser beam, while it can produce a shallow temperature gradient near the center of the sample, does not produce a temperature gradient that is flatter or more uniform than would be produced by a Gaussian beam profile of similar width (Fig. 21).

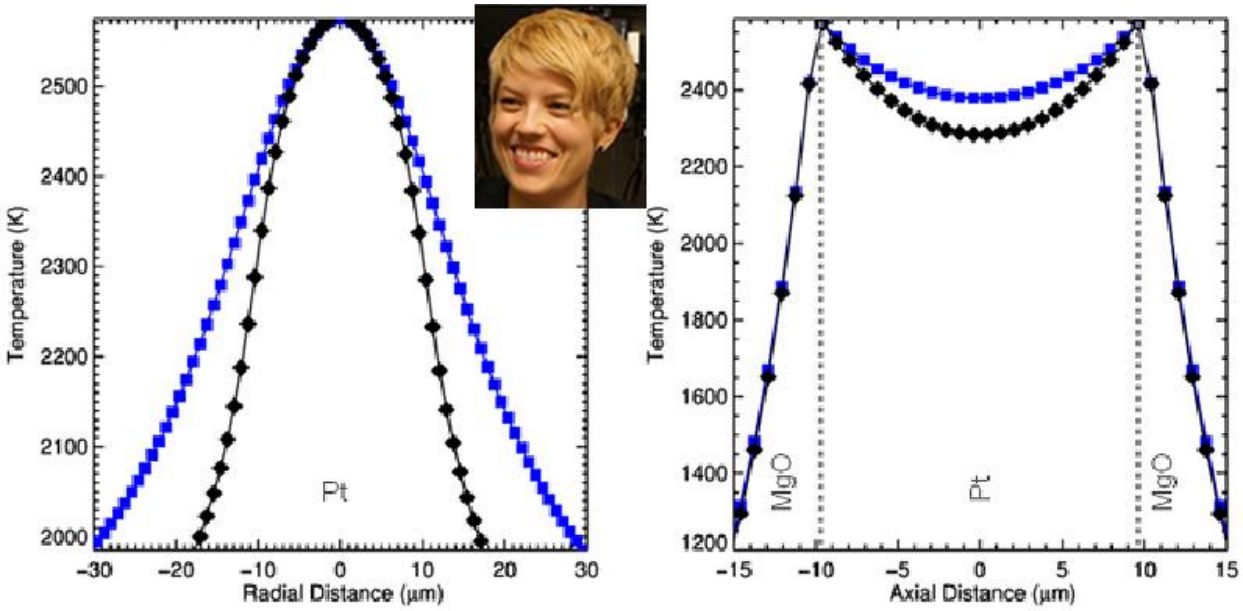


Figure 21. *Left, calculated radial temperature profiles at the surface of a Pt foil for flat-top (black line and symbols) and Gaussian (blue line and symbols) laser beams. Right, corresponding axial temperature profiles through the center of the sample. Inset: CDAC graduate student* ***Emma Rainey (UCLA).***

Paracetamol's Hidden Polymorphs – The study of the behavior of polymorphic organic solids at high pressure is a relatively new and rapidly growing area of interest. The applications span a wide ranging field which includes the pharmaceutical industry, where often times different crystal phases of the same drug can have different physiological effects.

CDAC Graduate Student **Spencer Smith**, along with CDAC Academic Partner **Yogesh Vohra** and colleagues from the University of Alabama - Birmingham, used Raman spectroscopy, synchrotron XRD, and multiple *ab initio* harmonic frequency calculations to explore the solid-state

transition behavior of paracetamol (a commonly used analgesic and anti-pyretic) at hydrostatic pressures up to 21 GPa (Fig. 8).

Spectral measurements provide further evidence for a highly kinetically driven Form I — Form II transition occurring as a mixed phase from 4.8 to 6.5 GPa, as well as new evidence for previously unobserved Form IV and Form V occurring at pressures of 8.1 and 11 GPa, respectively. [9]

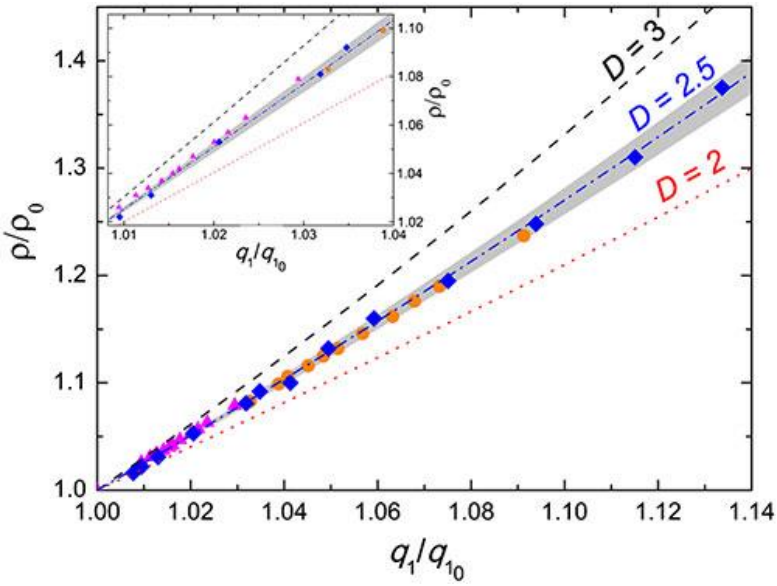


Figure 22. *The density change (ρ=ρ0) as functions of the principal diffraction position for the metallic glass samples, with all three following the 5/2 power law well. The inset shows the details of the low density/low q region.*

Unexpected Densities of Bulk Metallic Glasses – In any material, the increase in density with decreasing volume is directly related to the nature of the interatomic interactions. For typical crystalline materials, the volume varies as the cube of the change in interatomic distance. In amorphous materials, however, an irregular network of interatomic interactions can lead to deviations from this well-established relationship. For bulk metallic glasses (BMGs), a 2.3 (as opposed to the expected 3) power law relationship has been proposed based on studies of materials with different compositions. At high pressure, however, the problem of accurate measurement of density and volume in the DAC has made such studies difficult (Fig. 22).

In recent work at HPCAT 16-BM-D, a group from **Carnegie** and **Stanford** has used a unique combination of XRD, ultrasonic interferometry/x-ray radiography and transmission x-ray microscopy to determine the density and volume of BMGs at high pressure. Studies of several different compositions from 0.7 up to 22 GPa show that a 5/2 power law relationship describes the compression behavior of BMGs quite closely, suggesting a universal type of behavior for these and perhaps other, related materials.[20]

2.3 Phonons, Vibrational Thermodynamics, and Elasticity

Pressure Dependence of the Thermal Conductance of Interfaces between Highly Dissimilar Materials – CDAC student **Greg Hohensee** from the **Cahill** group at **Illinois** is combining the experimental techniques of time-domain thermoreflectance (TDTR) and the high-pressure environment of DACs to advance fundamental understanding of the thermal conductivity of materials and the thermal conductance of interfaces. TDTR is an optical pump-probe technique that can be used to measure the thermal conductivity of almost any type of material with a smooth surface.[21, 22] The high spatial resolution of TDTR enables measurements of samples with volumes as small as 10×10×1 μm^3.

Cahill's group has previously shown that weak interfacial bonding can suppress G by an order of magnitude below the value predicted by conventional models.[23] Anvil cell techniques can easily generate pressures (typically 10 GPa), needed to increase the small force constants characteristic of van der Waals interactions to values more typical of strong chemical or ionic bonds. As the strength of interface bonding increases at high pressures, G of weakly-bonded interfaces approaches the thermal conductance of clean and strongly-bonded interfaces between materials.[23]

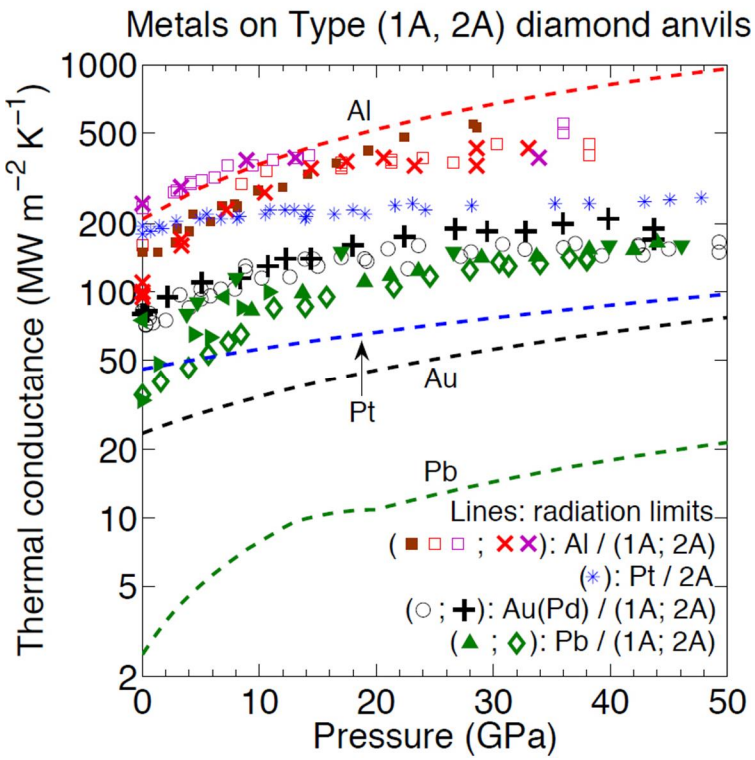


Figure 23. *Measurements of the thermal conductance G of Pb, Au(Pd) alloy, Pt, and Al films deposited on the face of a Type 1A and 2A diamond anvils with comparisons to the predicted phonon radiation limit (PRL, dashed-lines). The x-axis is the hydrostatic pressure within the volume of the diamond anvil cell as measured by ruby fluorescence. G for Al/diamond is described well by the PRL. G of Au(Pd)/diamond and Pb/diamond greatly exceeds the PRL and saturates at a common value of ≈150 MW m^{-2} K^{-1} in the high pressure limit. G of Pt exceeds the PRL by a factor of ≈2 and shows less pressure dependence than the PRL. Left: CDAC graduate student* ***Greg Hohensee (Illinois).***

Currently, the focus is on a long-standing problem in the field of nanoscale thermal transport: when the phonon spectra on the two sides of the interface are highly dissimilar, the observed values for G are much larger than the maximum predicted by elastic (harmonic) phonon-scattering,[24, 25] the so-called "phonon-radiation-limit" (PRL). The phonon-radiation-limit is reached when the transmission coefficient of phonons incident on the interface from the material with high vibrational frequencies is close to unity for all phonon frequencies that are below the upper cut-off frequency Ω of the vibrational spectrum in the material with low vibrational frequencies. The conductance in the phonon-radiation-limit scales with Ω^3. If the thermal conductance greatly exceeds the phonon-radiation-limit, the usual assumption in the field has been that inelastic (anharmonic) interactions between phonons create additional channels for heat transport. In the prototypical example of Pb/diamond, the assumption is that one phonon in diamond interacts with two (or more) phonons in Pb. The radiation limit for this type of three-phonon process is simply 2^3=8 times larger than the conventional elastic phonon radiation limit. Theoretical understanding of the magnitude of the inelastic channel is lacking.

High pressure provides a method of varying the phonon frequencies and anharmonicity of materials and therefore we can gain new insight on this long-standing problem by measuring how G varies with pressure. Data for interfaces between Pb, Au(Pd), Pt, and Al metal films and diamond at pressures up to 50 GPa are compiled in Fig. 23. The upper cut-off frequency Ω increases in the sequence Pb, Au, Pt, to Al. (The Au(Pd) film is a dilute alloy of Pd in Au that is used to increase the optical absorption of Au.) Data for Al closely resemble the phonon-radiation limit. The deviation between the data and phonon radiation limit becomes larger as Ω decreases. For Pb/diamond, the deviation is on the order of a factor of 8 at all pressures.

For some samples, the conductance increases steeply at first, presumably because of stiffening of weak interfacial bonding as we previously observed for Al/graphene/SiC interfaces.[23] In all cases, the conductance at high pressure is flatter than the trend predicted by the phonon radiation limit. Work is ongoing to understand this weak pressure dependence. The working

hypothesis is that there are competing effects: i) pressure increases Ω and therefore enhances the elastic channel for heat transport and ii) pressure decreases the anharmonicity of the metal and therefore reduces the inelastic channel for heat transport.

In the case of Au(Pd), an additional contribution to G may be coming from the relatively low lattice thermal conductivity Λ_l combined with the small value of the electron-phonon coupling parameter g. The series conductance created by electron-phonon non-equilibrium near an interface is given by $G_{NE}=(g\Lambda_l)^{1/2}$. For Au at ambient pressure, $G_{NE}\approx 300$ MW m^{-2} K^{-1}. Λ_l is expected to to increase with pressure and to decrease with pressure. Current work focuses on an evaluation of the variation in G_{NE} with pressure and the importance of G_{NE} in these measurements.

Interestingly, the thermal conductivity of the Type 1A diamonds, ≈500 W m^{-1} K^{-1}, is a factor of 4-5 smaller than the intrinsic value, and ≈2000 W m^{-1} K^{-1} for Type 2A diamonds. Characterization by infrared spectroscopy suggests that the Type 1A anvils contain approximately 1500 ppm of nitrogen impurities. These impurities strongly suppress thermal conductivity and could potentially reduce G because of a greater mismatch between the phonons that carry heat across the interface and the phonons that carry heat in the diamond crystal. That phonon non-equilibrium effect, if present, is not obvious in the data. The conductance of interfaces with diamond appears to be insensitive to the diamond purity.

Nonharmonic Vibrational Properties of a-Fe – The thermodynamics of iron and its phase transitions are of longstanding interest. The entropy of iron originates with the degrees of freedom of phonons, electrons, and spins, and is also affected by interactions between them. Vibrational entropy makes the largest contribution to the high temperature thermodynamics of metallic iron, and the vibrational entropy can be obtained directly from the phonon density-of-states (DOS) obtained by nuclear resonant inelastic x-ray scattering (NRIXS).

During the last year CDAC student **Lisa Mauger** at **Caltech** completed a substantial experimental effort to study the vibrational properties of bcc Fe and their impact on the thermodynamics. This included the development of a new high temperature NRIXS furnace in collaboration with former CDAC student **Matthew Lucas** (**Air Force Research Lab**). The furnace was commissioned at AFRL and used for GUP / CDAC beamtime at HPCAT in April 2013 to collect NRIXS spectra of bcc Fe and cementite (Fe_3C) at elevated temperatures.

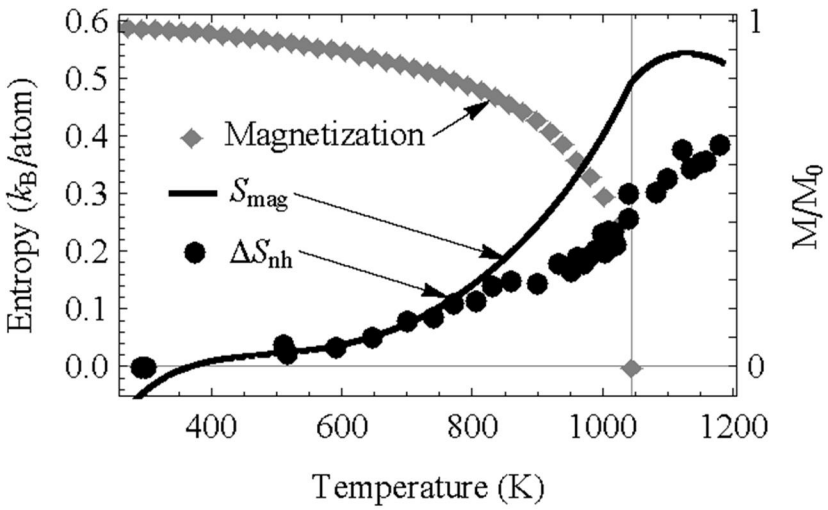


Figure 24. The nonharmonic vibrational entropy, ΔS_{nh} (calculated by subtracting the quasiharmonic vibrational entropy from the total vibrational entropy from phonon DOS measurements), compared with the magnetization of bcc Fe, and the magnetic entropy of bcc Fe.

The detailed study of the phonon DOS of iron at 38 temperatures between 30K and the fcc transition at 1184K showed that bcc iron has a significant nonharmonic contribution to the vibrational entropy. It is poorly modeled by the quasi-harmonic theory typical of conventional *ab-initio* calculations. It does not track the typical trends of phonon-phonon anharmonicity, either, and there is little thermal broadening of the spectrum. By elimination, this leaves a large magnon-phonon interaction in bcc iron as anomalous source of phonon entropy. In fact, the anharmonic contribution to the vibrational entropy of bcc Fe tracks the magnetic entropy as shown in Fig. 24. Evidently a large magnon-phonon coupling in bcc iron makes a significant contribution to the

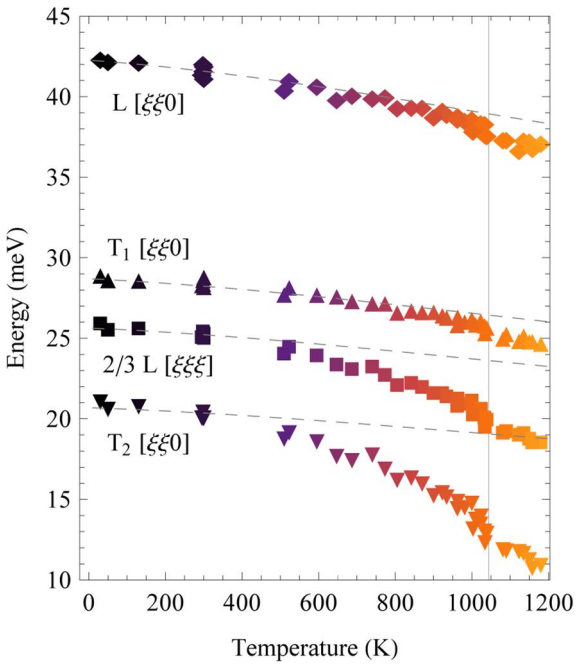
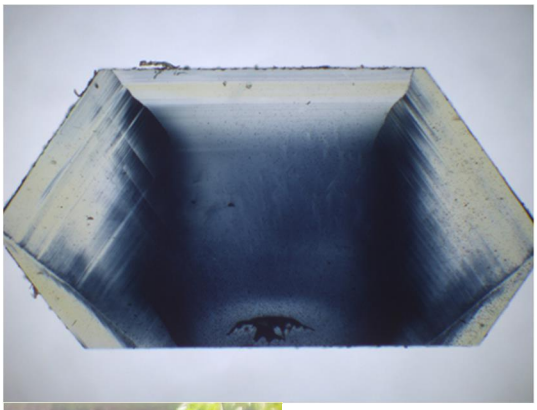


Figure 25. *Energies of specific phonon modes versus temperature. The modes are compared with their quasiharmonic estimates (gray dashed lines).*

thermodynamics of the system at temperatures around the Curie transition, approximately 35 meV/atom in the free energy.

Beyond the thermodynamic analysis, a genetic algorithm optimization to extract interatomic force constants from our phonon DOS measurements has also been implemented. The model optimizes Born-von Karman interatomic force constants through a least-squares comparison with the measured phonon DOS, providing information on interatomic interactions. These force constants were also used to generate phonon dispersions at elevated temperatures that were in excellent agreement with the few triple axis neutron studies of phonons in iron at high temperature.[26] The thermal trends in our phonon dispersions exhibit anomalously large anharmonic behavior at some points in k-space (*e.g.*, T_2[ξξ0] in Fig. 25) while other phonons were as expected from quasiharmonic estimates (L[ξξ0] in Fig. 25). The rapid softening of the second nearest neighbor axial force constants in iron near the magnetic transition corresponds with the observed rapid softening of the low energy transverse Γ-N phonon branch (T_2[ξξ0] in Fig. 25). Apparently the magnon-phonon interaction has considerable variation in k-space.

Elastic and Mechanical Properties of Boron-Doped Diamond – Among various dopants possible in diamond, boron is important because at modest levels boron-doped diamond is a semiconductor. CDAC graduate student **Yun-Yuan Chang**, along with postdoctoral researcher **Xiaobing Liu**, at Northwestern University, are investigating the influence of boron on diamond's elastic and mechanical properties. Using GHz-ultrasonic interferometry, the elastic constants of boron-doped diamond with a gradient of boron concentration is currently under investigation. In regions with



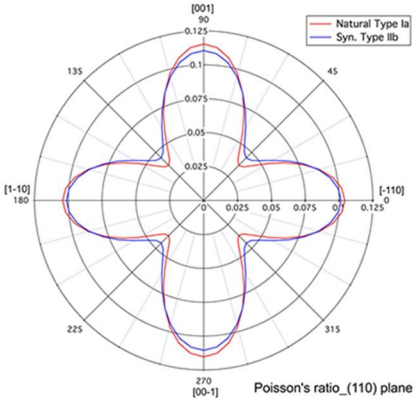


Figure 26. *Top left: boron-doped diamond with a compositional gradient spanning one order of magnitude, from about 100 to 1000 ppm boron. The crystal measures 2 mm across. Spatially resolved acoustic and mechanical properties measurements are being carried out at* ***Northwestern*** *to correlate the influence of defects on elastic properties of semi-conducting, single-crystal boron-doped diamond. Top right: comparison of the anisotropy of Poisson's ratio between natural type Ia diamond (red curve) and heavily boron-doped diamond (>2000 ppm), blue curve. The figure was calculated from the elastic tensor measured by GHz-ultrasonic interferometry. The result illustrates how boron reduces the elastic moduli of diamond as well as its elastic anisotropy. Bottom left: CDAC graduate student* ***Yun-Yuan Chang*** *(****Northwestern****).*

relatively low boron (150-300 ppm) the bulk and shear moduli are 444(3) and 530(2) GPa, respectively. Whereas, in regions of higher boron concentration (Fig. 26, top left) dark blue areas in the figure, 1500-2000 ppm B), the elastic moduli are reduced to about 436(3) GPa (bulk) and 521(2) GPa (shear). Experimental studies of hardness are currently underway, with preliminary results showing that the Vicker's hardness in high-boron doped region is measurably lower than in the low-boron region (Fig. 26, top right). The research will further the understanding of how defects influence elastic properties of superhard materials and further inform relationships between mechanical and elastic properties.

High P-T Elastic Properties of Majorite Garnet – CDAC graduate student **John Lazarz** (**Northwestern**) is using online Brillouin scattering at the APS to measure the sound velocities of majorite garnet at simultaneous high pressure and high temperature conditions of the Earth's mantle. The majorite, nominally $Mg_3(Fe,Al,Si)_2(SiO_4)_3$, also contains hydrogen at the level of ~1000 ppm, so the experiments are testing the influence of H-related defects on the elastic properties of this important mantle phase. In the transition zone (410-660 km depth), observed seismic velocities appear too fast to be explained by the standard mantle rock model, called dry pyrolite. It is possible that H_2O, incorporated into the high-pressure phases of the transition zone could reduce velocities to better match seismic observations. Because majorite is slower than the co-existing ringwoodite (spinel), a higher basaltic (majorite-rich) component in the mantle from descending slabs could also reduce velocities to better match observations. These experiments on the sound wave velocities of majorite at pressures up to 15 GPa and 700 K will thus be useful for placing tighter constraints on the composition of the Earth's mantle. Lazarz has constructed a resistive-heated DAC for the measurements.

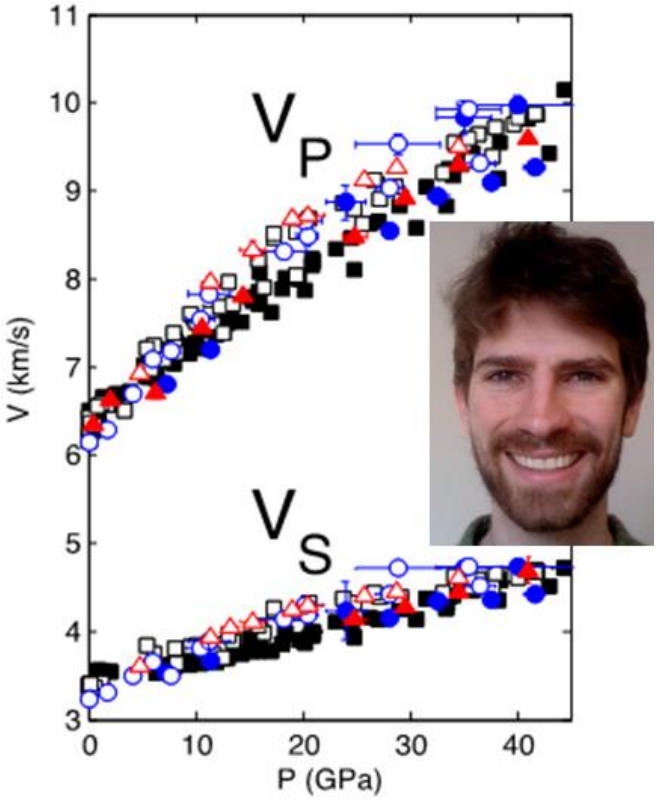


Figure 27*. Longitudinal (V_P) and shear (V_S) wave speeds of amorphous $CaSiO_3$ as a function of pressure during compression (solid symbols) and decompression (open symbols) at room temperature. Colors and shapes indicate starting material: melt-quenched $CaSiO_3$ glass (black squares), non-hydrostatically compressed powder (blue circles), and pressure-amorphized wollastonite in a pressure transmitting medium (red triangles). Inset: CDAC graduate student* ***Zack Geballe (Berkeley)****.*

Brillouin Spectroscopy of **$CaSiO_3$** – A Brillouin study of $CaSiO_3$ glass carried out by CDAC graduate student **Zack Geballe** at **Berkeley** provides evidence that amorphous $CaSiO_3$, though metastable at room temperature, is a thermodynamic phase in the sense that it can be described by a single energy surface, *G(P,T)*, independent of synthesis conditions. The proposed energy surface is consistent with observed transitions between amorphous and crystalline phases at both low and high pressures, and consistent with the acoustic measurements (Fig. 27) that constrain the curvature of energy versus pressure. The acoustic data thus constrain the Gibbs free energy estimates for crystalline and amorphous phases.

Single-Crystal Elastic Constants of Molecular Crystals – Knowledge of elastic constants of molecular crystals is important in the area of energetic materials used in plastic-bonded explosives. In particular, accurate determination of constituent material properties of heterogeneous media will improve mesoscale simulations of growth and formation of hot spots during weak initiation. CDAC Academic Partner **Steve Jacobsen** and graduate students **Yun-Yuan Chang** and

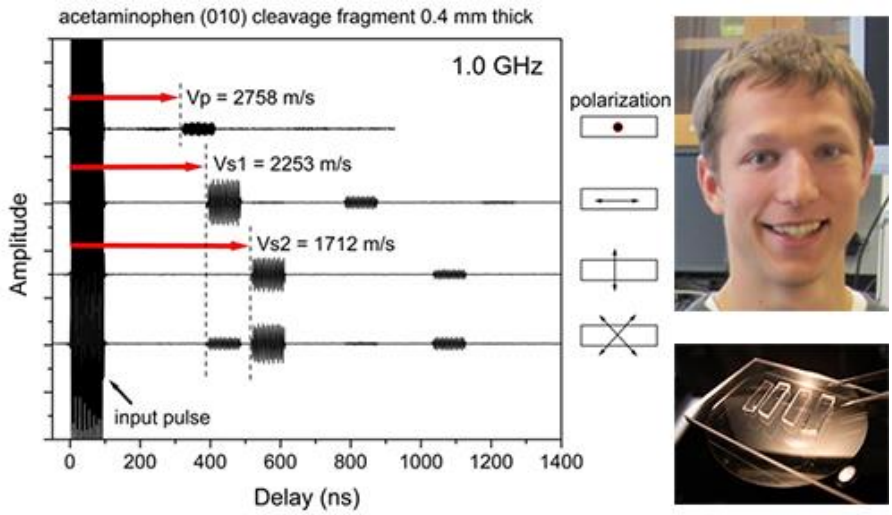


Figure 28. *Single-crystal acetaminophen (bottom right) synthesized by the LANL group for GHz-ultrasonic measurements (0.5-2 GHz) at Northwestern to determine the elastic tensor. Acoustic waveforms from different polarizations taken at 1 GHz are shown. Top right: CDAC graduate student* ***John Lazarz*** *(**Northwestern**).*

John Lazarz at Northwestern are collaborat_ ing with **Kyle Ramos, Cindy Bolme,** and **Dan Hooks** at **LLNL** to combine Brilliouin scattering measurements (at LANL) and GHz-ultrasonic measurements (at Northwestern) to determine the full elastic tensors of molecular crystals beginning with acetaminophen (Fig. 28) as an analog to many energetic materials.

Thermal Conductivity in Earth's Mantle – One key to understanding Earth's evolution is to look at how heat is conducted in the deep lower mantle, 660 to 2,900 kilometers below the surface. CDAC post-doctoral associate **Allen Dalton** (now at Defense Threat Reduction Agency), Carnegie's **Alexander Goncharov**, CDAC Academic Partner **David Cahill** (**Illinois**), and CDAC students **Gregory Hohensee** and **Wen-Pin Hsieh**, have for the first time experimentally measured the conductivity of a key Earth material (MgO) at these conditions. The results suggest that heat transfer in Earth's mantle is lower than other predictions, with total heat flow across the Earth of about 10.4 terawatts, which is about 60 % of the power used today by civilization. Conductivity also has less dependence on pressure conditions than predicted.

This work provides important bounds on the degree to which heat is transferred by convection as opposed to conduction in the lower mantle. Further work will focus on examining the effects of different mineral components on the thermal conductivity and to better understand the atomic scale basis of convective motion of these materials within the broader context of mantle dynamics. The results suggest that this technique could advance other high pressure and temperature studies of the deep Earth and provide a better understanding of the finer details of Earth's evolution.[27]

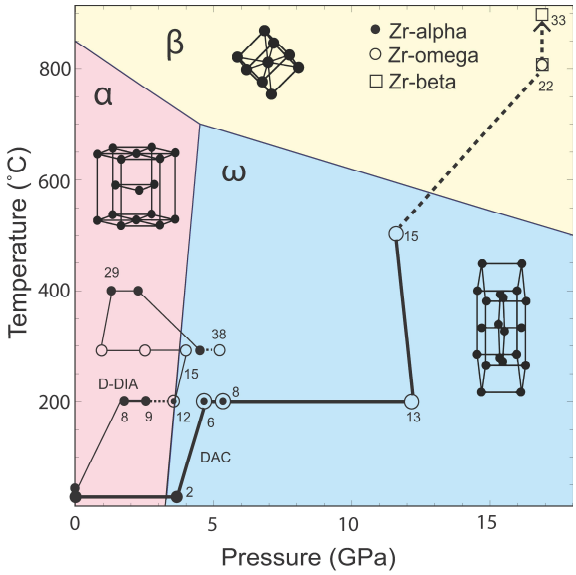


Figure 29*. P-T-phase diagram for Zr incorporating recent D-DIA and DAC experiments with resistive and laser heating.*

2.4 Plasticity, Yield Strength and Deformation

Deformation of Hexagonal Metals at High Pressure – For many years, the **Wenk** group at **Berkeley** has been interested in phase transitions in metals, and particularly orientation relations if materials are under stress and at high pressure. The original DAC deformation experiments on iron,[28] and more recent work[29] were used to understand seismic anisotropy in the Earth's

inner core. Since then investigations have moved on to deformation mechanisms in other hexagonal metals at high pressure.[30] Transition metals Ti, Zr, and Hf have a hexagonal close-packed structure (α) at ambient conditions, but undergo phase transformations with temperature and pressure. Of particular significance is the high- pressure ω phase which is brittle compared to the α phase (Fig. 29). There has been a long debate about transformation mechanisms and orientation relations between the two crystal structures, but new high pressure DAC and D-DIA experiments resolved this with *in situ* synchrotron XRD texture studies on polycrystalline aggregates.[3] Following crystal orientation changes in Zr confirmed that the original suggestion for an α → ω martensitic transition for Ti, with $(0001)_\alpha \| (11\bar{2}0)_\omega$, and a remarkable orientation memory when ω reverts back to α.

Deformation and Transformation Textures in $NaMgF_3$ Perovskite and Post-Perovskite – $MgSiO_3$ post-perovskite (pPv) is believed to be the major phase in the Earth's lowermost mantle. Thus it is critically important to understand the plastic deformation properties of pPv in order to understand the rheology and seismic anisotropy of this region. However, the $MgSiO_3$ system is difficult to study due to the extreme pressures needed to stabilize the pPv phase (~130 GPa). Furthermore, current high temperature deformation DAC technology is limited to *P-T* conditions of ~65 GPa and ~2000 K,[31] thus deformation behavior of $MgSiO_3$ pPv currently cannot be studied at high pressure and temperature. Over the last year CDAC graduate student **Michael Jugle** at **Utah** has been studying high pressure texture development in $NaMgF_3$ perovskite (Pv) and pPv as a potential analog system for $MgSiO_3$ Pv and pPv. Previously. transformation textures in $NaMgF_3$ during the phase transformation from Pv to pPv have been documented. Texture changes during the phase transformation indicate that {100}Pv → {110}pPv. This transformation relation is consistent with previous theoretical and experimental work on the Pv to pPv transformation mechanisms.[32-35] In February 2014, deformation experiments were performed on $NaMgF_3$ pPv up to 66 GPa at HPCAT. Figures 30a and 30b show the results of the deformation experiment. After transformation at 37 GPa, $NaMgF_3$ pPv exhibits a transformation texture with a maximum near 110. Upon compression to 66 GPa this texture disperses and develops a maximum toward 001 with a minimum near 100. To determine the deformation mechanisms associated with this texture change, poly-crystal plasticity modeling using the Visco-Plastic Self Consistent (VPSC) code was performed. The transformation texture shown in Fig. 30a was used as a starting texture for the simulations. Results for dominant (010)<101> slip and (001)<100> slip are shown in Figs. 30c and 30d.

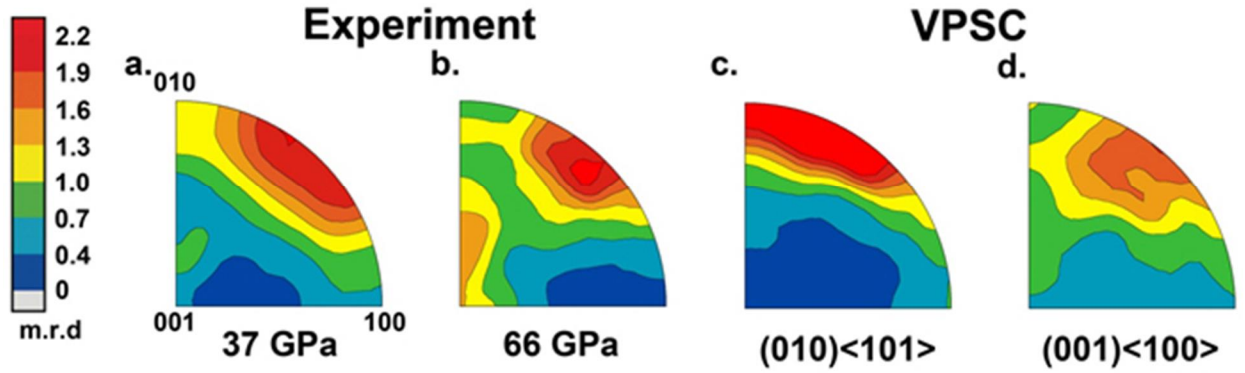


Figure 30. *Top: inverse pole figures of $NaMgF_3$ pPv from experiment (a, b) and from VPSC simulations (c, d). a, transformation texture immediately after conversion from the Pv phase. b, texture after compression to 66 GPa. c and d, simulations for dominant (010)<101> slip and dominant (001)<100> slip respectively. Dominant (001)<100> provides the closest match to (b). Pole densities are given in multiples of random distribution (m.r.d.) where an m.r.d. of 1 is random and a higher number indicates a greater number of orientations (stronger texture). Left: CDAC graduate student* ***Mike Jugle (Utah)****.*

(010)<101> slip has been previously observed in $CaIrO_3$ pPv[36] and (001)<100> slip has been inferred for $MgGeO_3$ and $MgSiO_3$ pPv.[34, 37] (010)<101> slip generates a strong maximum at 010 and a minimum at 001 as in Fig. 30c. Slip on (001)<100> results in a maxima near 110 with a shoulder close to 001 (Fig. 30a), similar to the experimental deformation texture (Fig. 30b). It is thus concluded that $NaMgF_3$ pPv slips predominantly on the (001) plane. This is consistent with $MgSiO_3$ pPv[37] providing strong evidence that $NaMgF_3$ is a good analog for deformation behavior of $MgSiO_3$ pPv, and a good candidate for future high *P-T* deformation experiments.

Deformation of Two Phase Materials – The **Utah** group has recently been joined by summer undergraduate intern **Max Giannetta**, who is working closely with **Michael Jugle** to analyze diffraction data from deformation experiments on mechanical mixtures with a range of volume fractions of NaCl + MgO. The Earth's lower mantle is composed of primarily $MgSiO_3$ Pv (~70-80 vol %) and MgO (~30-20 vol %). $MgSiO_3$ Pv is believed to be the mechanically harder phase while MgO is believed to be the softer phase. These experiments on the simple solids NaCl and MgO seek to elucidate the fundamental deformation behavior of poly-phase materials with a phase contrast, and to determine which phase controls deformation, in particular how texture development is affected by the presence of a harder or softer phase. Texture analysis has been performed on the first of these compression datasets, a mechanical mixture of 75 vol. % NaCl + 25 vol. % MgO (Fig. 31). In this experiment, NaCl rapidly develops a 100 texture maximum with a shoulder toward 110, consistent with slip on {110}<1-10>.[38] Unsurprisingly MgO, which is the harder phase and volumetrically minor remains essentially random. Thus the majority of strain is partitioned into the softer NaCl and MgO is only passively involved in deformation. At pressures greater than ~30 GPa, the B1 to B2 transformation in NaCl is observed. By 34 GPa, the transformation to B2 is complete. The B2 phase of NaCl exhibits a texture maximum at 110 with a shoulder toward 111. This indicates transformation relationships of {001}B1 → {110}B2 and {110}B1 → {111}B2 consistent with previously proposed mechanisms for B1-B2 transformations based on molecular dynamics simulations.[39]

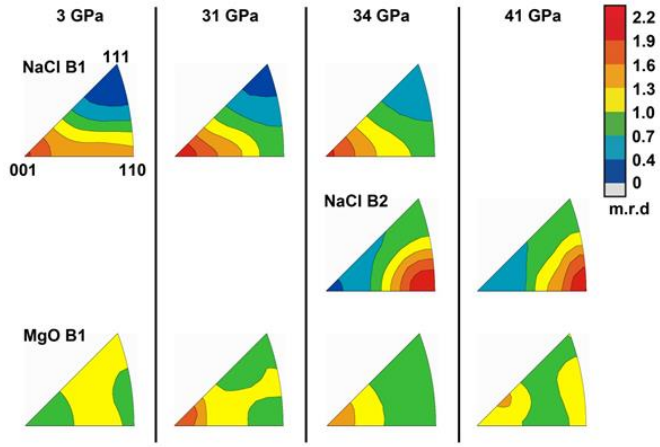


Figure 31. *Inverse pole figures showing texture evolution during axial compression for a mechanical mixture of 75 volume % NaCl and 25 volume % MgO. Top row, texture development in NaCl in the B1 structure. At pressure > 31GPa, NaCl undergoes a B1 to B2 transition. Bottom row, texture evolution in MgO.*

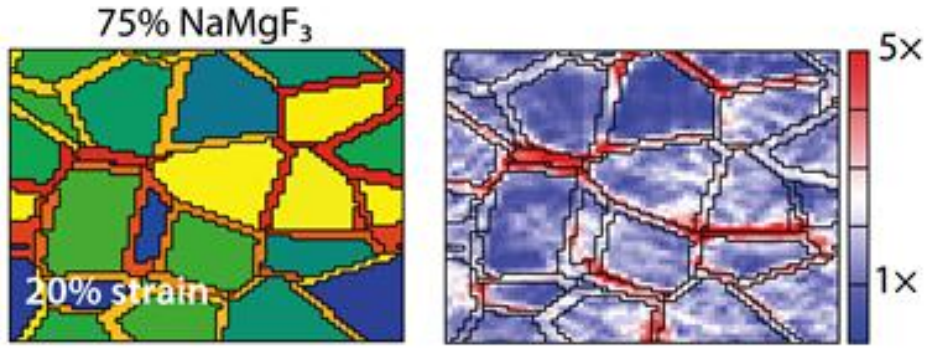


Figure 32. *Modeling deformation of a percolate 2-phase mixture with the FFT polycrystal plasticity model. The deformation concentrates on the soft phase (blue) distributed on grain boundaries.*

Deformation of Polyphase Materials – Despite recent progress, polyphase deformation is still very enigmatic. In the **Wenk** group at **Berkeley**, DAC experiments on periclase + perovskite mixtures and D-DIA experiments on

mantle analogs are ongoing, along with modeling simulations in collaboration with **Ricardo Lebensohn** and **Carlos Tome** at LANL. It turns out that in such mixtures preferred orientation development is highly reduced due to local stress-strain heterogeneities. Figure 32 shows results of a fast Fourier transform model that documents that heterogeneous Von Mises strain concentrates on the soft phase, while the hard phase barely deforms. These are important components of the PhD thesis of **Pamela Kaercher**. **Eloisa Zepeda-Alarcon** is continuing with the project. A comparative microtomography study on the same samples at APS, ALS and SLS documented amazing resolution and reproducibility.[40] The Wenk group has dedicated considerable effort in making their sophisticated diffraction data analysis more widely available. Tutorials on Rietveld texture analysis have recently been published.[41, 42]

2.5 Electronic and Magnetic Structure and Dynamics

Parallel Suppression of Superconductivity and Fe Moment in Sr-substituted $CaFe_2As_2$ – The Fe-pnictide superconductors present systems that challenge the notion of the antithetical nature of superconductivity and magnetism. These systems are composed of corrugated Fe-As layers arranged in a tetragonal unit cell, and at low temperature, they display antiferromagnetic order. With doping or pressure, however, the antiferromagnetism can be suppressed, and superconductivity can develop.

Jason Jeffries from **LLNL** has been carrying out non-resonant Fe K_β x-ray emission spectroscopy (XES) experiments at HPCAT 16 ID-D of the APS, which reveal that Sr substitution into $CaFe_2As_2$ decouples the Fe moment from the volume collapse transition, yielding a collapsed-tetragonal, paramagnetic normal state out of which superconductivity develops (Fig. 33). XRD measurements at Sector 16 BM-D implicate the *c*-axis lattice parameter as the controlling criterion for the Fe moment, promoting a generic description for the appearance of pressure-induced superconductivity in the alkaline-earth-based 122 ferropnictides (AFe_2As_2). This work suggests that both the destruction of antiferromagnetism and the presence of the Fe moment are requisite for the development of high-temperature superconductivity in these systems. That the pressure-dependent suppression of T_c tracks that of the Fe moment supports the picture of an unconventional superconducting state mediated by magnetic fluctuations. This generic picture suggests that driving the CT phase to ambient pressure while maintaining an Fe moment should be a promising route to high-temperature, magnetically mediated superconductivity in the 122 systems.

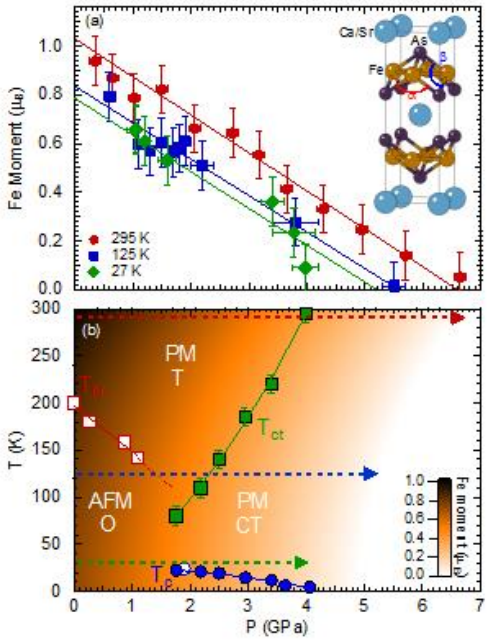


***Figure 33**. a) Variation of the Fe magnetic moment with pressure. b) Temperature of paramagnetic tetragonal to collapsed tetragonal transition (green); superconducting transition temperature (blue) and Neel temperature (red) with pressure for Sr-substituted $CaFe_2As_2$.*

High Pressure Effects on the Superconductivity in Rare Earth Doped $CaFe_2As_2$ – High pressure superconductivity in a rare-earth doped $Ca_{0.86}Pr_{0.14}Fe_2As_2$ single crystal sample has been studied up to 12 GPa and temperatures down to 11 K using designer DAC technology under quasi-hydrostatic pressure conditions. The electrical resistance measurements were complemented by high pressure and low temperature XRD studies at HPCAT 16 BM-B. Electrical resistance measurements show an intriguing observation of superconductivity under pressure, with T_c as high as ~51 K at 1.9 GPa, presenting the highest T_c reported in the intermetallic class of 1-2-2 iron-based superconductors (Fig. 34). The resistive transition observed suggests the possible existence of two superconducting phases at 0.5 GPa: one phase starting at T_{c1} ~ 48 K and

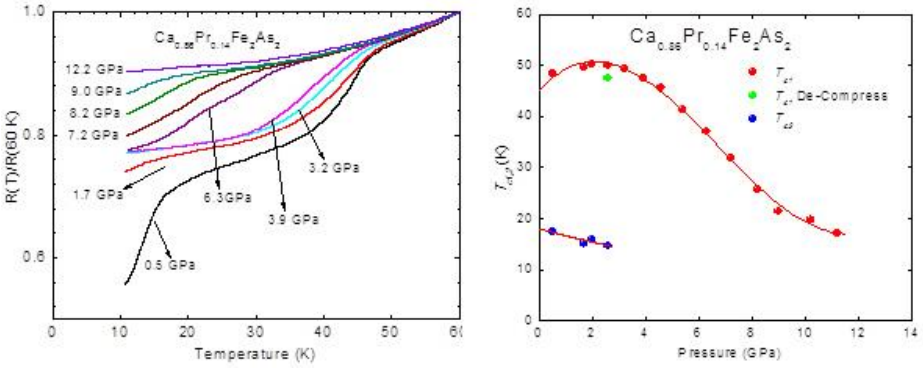


Figure 34. Left: Temperature dependence of the electrical resistance of rare earth doped $Ca_{0.86}Pr_{0.14}Fe_2As_2$ at various applied pressures. Steatite was used as the pressure medium. The two superconducting transitions (T_{c1} and T_{c2}) are clearly observed at low pressures below 2 GPa. Right: Variation of measured superconducting transition temperatures T_{c1} and T_{c2} for $Ca_{0.86}Pr_{0.14}Fe_2As_2$ with pressure.

the other starting at T_{c2} ~ 16 K. The two superconducting transitions show distinct variations with increasing pressure. High pressure-low temperature structural studies indicate that the superconducting phase has a collapsed tetragonal $ThCr_2Si_2$-type (122) crystal structure. Further studies at various Pr-doping levels are currently underway.

Robust Ferromagnetism in the Compressed Permanent Magnet Sm_2Co_{17} – Permanent magnets have found applications since antiquity, but the purview of their technological impact has exploded in recent decades. Most of this newfound application space has been enabled by the development, and subsequent deployment, of high-strength permanent magnets based on intermetallic compounds composed of rare-earth (RE) and transition-metal (TM) elements. The compound Sm_2Co_{17} displays magnetic properties amenable to permanent magnet applications owing to both the 3*d*-electrons of Co and the 4*f*-electrons of Sm. The long-standing description of the magnetic interactions between the Sm and Co ions implies a truly ferromagnetic configuration, but some recent calculations challenge this, suggesting at least a propensity for ferrimagnetic behavior. **Jason Jeffries** from **LLNL** has used high-pressure synchrotron x-ray techniques to characterize the magnetic and structural properties of Sm_2Co_{17}. The results reveal a robust ferromagnetic state. L_Y XES at Sector 16 ID-D has been used to probe the Sm *f*-state under pressure. The local Sm moment is at most weakly affected by compression. These results, combined with data from x-ray magnetic circular dichroism (XMCD) and XRD experiments, indicate that the ordered moments show a surprising resilience to volumetric compressions of nearly 20%.

Magnetic Properties of Rare Earth Materials at High Pressures – During the past year, CDAC graduate student **Jinhyuk Lim**, from the **Schilling** group at **Washington University in St. Louis**, has made progress in the understanding of magnetism in rare earth materials through several different projects.

Record High Magnetic Ordering Temperature in Dy at 157 GPa: In some of the most precise four-point measurements of the electrical resistivity ever obtained at extreme pressure (see Fig. 7), **Lim** has succeeded in subjecting the lanthanide metal Dy to pressures as high as 157 GPa.[8] After initially decreasing under pressure and passing through a minimum near 20 GPa, Dy's magnetic ordering temperature T_o begins to increase dramatically for P > 73 GPa, the pressure at which Dy's volume suddenly collapses by 6%. As the pressure increases further, T_o increases through ambient temperature near 110 GPa, reaching at 157 GPa an estimated maximum value of 400 - 500 K, by far the highest ordering temperature of any lanthanide, the highest previous value being T_o = 292 K for Gd at ambient pressure.

The reason for this dramatic increase appears to be that Dy under extreme pressure enters a Kondo lattice or dense Kondo state. The negative mixing exchange interaction associated with this state becomes anomalously large as Dy is pushed by pressure toward a magnetic instability, leading to the record high value of the magnetic ordering temperature.

In contrast, the lanthanide metal Gd shows no such anomalous pressure dependence of T_o for pressures just above 59 GPa where its volume collapses. The extreme magnetic stability of Gd does not allow the Kondo lattice to develop so that the magnetic ordering temperature follows a conventional pressure dependence where, under extreme pressure, T_o never comes close to reaching its ambient pressure value of 292 K. These experiments were carried out in collaboration with **Gilberto Fabbris** and **Daniel Haskel** at the APS.

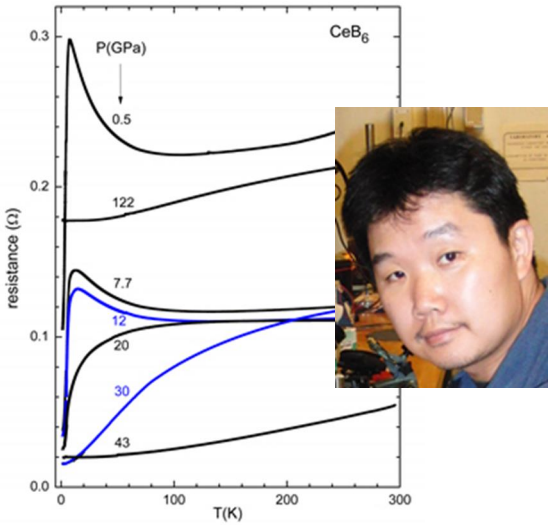


Figure 35. *Electrical resistance of CeB_6 versus temperature at pressures measured at 295 K. Inset: CDAC graduate student* ***Jinhyuk Lim (Washington University in St. Louis)***

Pressure-Induced Volume Collapse in Gd and Tb: Most elemental lanthanide metals suffer a volume collapse at a critical pressure, for Gd at 59 GPa and for Tb at 53 GPa. There is much controversy regarding the mechanism(s) responsible for this volume collapse. Candidates are: (a) valence change, (b) 4*f* local-itinerant transition, (c) Kondo resonance, (d) *s-d* electron transfer. X-ray absorption near-edge structure (XANES) and XES measurements at the APS by G. Fabbris *et al.*[8] Tb and by Maddox *et al.*[43] on Gd speak against (a) and (b). The true state of the lanthanide ion under pressure can be inferred from the degree of suppression of the superconductivity in a very dilute magnetic alloy for pressures just exceeding the critical pressure for the volume collapse. Experiments by **Gilberto Fabbris** and **Jinhyuk Lim** on the dilute magnetic alloys Y(0.5 at.% Tb) and Y(0.5 at.% Gd) reveal that there is very strong suppression of superconductivity *only* in the former alloy. One can infer that the volume collapse in Tb can be best described by the Kondo volume collapse model of Allen and Martin,[44] whereas in Gd the volume collapse arises from simple *s-d* charge transfer [5] under pressure. Very recent parallel experiments on Dy and the dilute magnetic alloy Y(1 at.% Dy) lead to the same conclusions as for Tb.[45]

Pressure-Quenched Dense Kondo State in CeB_6: CeB_6 is a well-known dense Kondo system, as evidenced by its temperature-dependent electrical resistivity that initially decreases on cooling from ambient temperature and passes through a "Kondo" minimum near 100 K before rising steeply to a sharp maximum near 6 K and then dropping precipitously (see Fig. 35 at 0.5 GPa). However, the application of 43 GPa pressure changes this behavior (Fig 35). The highly anomalous temperature dependence of the resistivity is completely suppressed, leaving only conventional Fermi-liquid-like behavior to the highest pressure studied (122 GPa).[46]

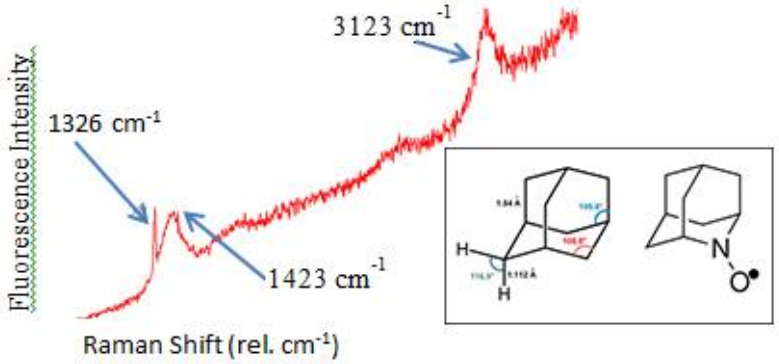


Figure 36. *Raman spectrum of nanodiamonds synthesized from adamantine and its mitroxylradical. Inset: molecular structures of adamantane and the nitroxyl radical.*

The primary reason for studying this compound under extreme pressure was to search for a transition to possible topological insulating behavior as has been observed for SmB_6 at ambient pressure. Although this transition was not observed in the present experiment, the destruction of the dense Kondo state is also of considerable interest since its evolution can be continuously tuned using pressure as a parameter. These measurements

were carried out by postdoctoral associate **Neda Foroozani** with assistance from **Jinhyuk Lim** in collaboration with **Z. Fisk** at **UC-Irvine.**

Synthesis of Nanophase Diamond with NV- Centers – Nanodiamond (ND) synthesis has a variety of applications such as biological markers, drug delivery facilitation, and nanotesla metrology.[47] Metrology and biological markers use the coherent properties and optical polarization of the negatively charged Nitrogen Vacancy center defect (NV^-). At **Carnegie**, visiting graduate student **Todd Zapata** from **Texas A & M** has been working on the synthesis of nanodiamond with NV^- centers using adamantane, $C_{10}H_{16}$, and its nitroxyl radical (2-azaadamantane-N-oxyl), which are shown in the inset of Fig. 36. Ultimately, the material may be used as an *in-situ* sensor for measuring very weak magnetic signals from DAC samples. The synthesis is carried out using the DAC and either laser or resistive heating. The ultimate goal of this work is to work out the growth conditions that will produce the smallest possible ND which may at the same time hold NV^- centers (~ 5 nm), with as little agglomeration as possible, and coherence which rivals the NV^- center in bulk diamond. Raman spectroscopy is used to follow the evolution of the adamantine-nanodiamond transition. T_1 and T_2 coherence times of the NV^- centers are measured using Hahn Echo experiments. Anti-bunching experiments are performed to determine the number of NV^- centers per ND, and AFM/SEM images are taken to determine the size and agglomeration of the ND. The analysis of the NV^- is carried out at the **University of Ulm** with the help of **Fedor Jelezko**.

Although this project is still in its early stages, there have been several important results thus far. With regards to synthesis, it is necessary to include hydrogen within the DAC sample chamber to terminate the ND and hinder the transformation of ND to onion-like carbon. Raman analysis (532 nm excitation) confirms the existence of nanometer-sized diamonds from the shift in the diamond peak to about 1326 cm^{-1}. There is typically also a large shoulder following the diamond peak centered around 3120 cm^{-1} (Fig. 36) due to fluorescence from the NV^-. Some of the ND also exhibits a strong Raman peak in the 1420 cm^{-1} range, which is associated with the neutral NV (NV^0).

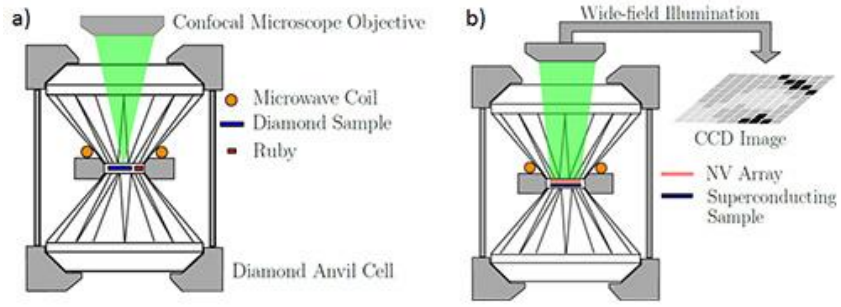


Figure 37. *A) Schematic of the DAC arrangement used in the experiments. ODMR was performed via microwave excitation provided by a wire or coil embedded in an insulating gasket or wound around a culet. B) Schematic of the proposed design of a diamond chip containing an NV—array, which is used to switch between pressure monitoring and wide field imaging of the magnetic field at the surface of a high pressure superconductor.*

NV- Centers as Quantum Sensors –**Viktor Struzhkin** and **Russell J. Hemley**, along with colleagues from the Austrialian National University, the University of Melbourne, and the University of Ulm have investigated the behavior of NV- centers in diamond under high-pressure and normal temperatures, with the goal of developing a method for the measurement of electronic and magnetic properties of materials at high pressures, particularly superconductivity. Experiments utilizing laser excitation of a CVD diamond sample at pressures up to 60 GPa and then scans of the microwave frequencies emitted by the sample (Fig. 37) show that electrons at the NV^- centers, which are very sensitive to magnetic fields, electrical fields and stress, interact not only with the atoms immediately surrounding the vacancy, but also with atoms more removed from the vacancy. In addition, results show that the distance over which the electrons from the NV- centers interact with the surrounding atoms decreases with increasing pressure. A related benefit is that the NV- center can be used as a quantum sensor of high pressure phenomena.[48]

2.6 High *P-T* Chemistry

Hydrides with Novel Stoichiometries – It is widely believed that metallic hydrogen will be superconducting at high temperatures. One way to metallize hydrogen may be to access the appropriate region of the temperature/pressure phase diagram. However, a *chemical* route towards this 'holy grail' is also being sought out. One may wonder if compressed hydrogen can be metallized via doping by a particular element, if the resulting phases also have the propensity to be superconducting at high temperatures, and if they could be stabilized at 1 atm. In order to advance research in this field **Andrew Shamp** at **Buffalo** has computationally studied mixtures of hydrogen and iodine under pressure. At 150 GPa, the H_2I and H_4I stoichiometries become thermodynamically stable. In the H_2I phase the iodine atoms form buckled triangular nets. Bonding between the nets results in a host structure, and 1-D chains of H_2 molecules with slightly stretched bonds (0.80 Å) behave as the guests. H_4I consists of layers of H_2 molecules (which measure 0.81 Å) arranged in a hexagonal lattice, with the I atoms forming layers below and above the hexagons. It resembles the AlB_2 structure, where iodine assumes the position of the aluminum atoms, and the center of the H_2 bond is found in the same spot as boron. Calculations reveal that at 150 GPa H_4I has a high DOS at E_F hinting that it may be superconducting. Calculations of the T_c of H_4I are currently underway

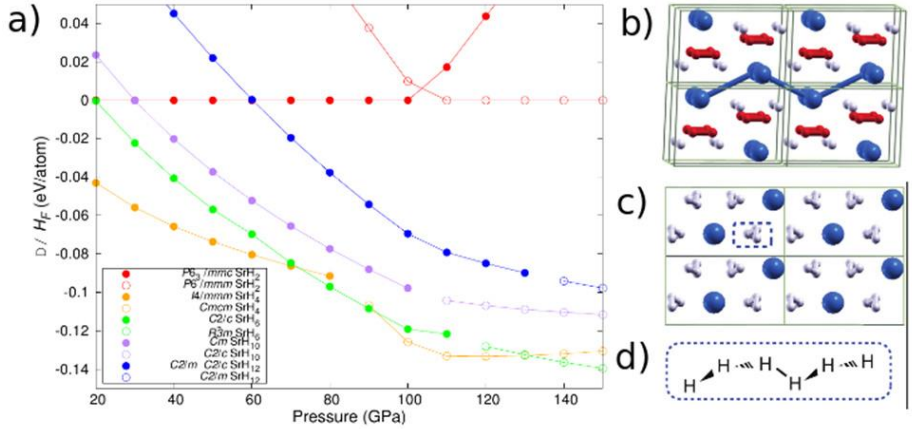


Figure 38. *a) ΔH_F for the reaction $SrH_2 + ½ (H_2)_{n-2} \rightarrow SrH_n$ at pressures up to 150 GPa. b) SrH_4 lies on the convex hull at 150GPa (Sr/H atoms are shown as blue/white and H_2 molecules are shown in red). c) R3m-SrH_6, stable at 250 GPa, contains. d) 1D hydrogen chains that give rise to a high density of states at the Fermi level. This phase may be superconducting at high temperatures.*

Furthermore, Andrew has worked with other members of the **Zurek** group to predict the structures of the strontium polyhydrides, SrH_n with n>2, under pressure. A number of phases with even n were found to be thermodynamically stable below 150 GPa. Particularly interesting is the SrH_4 stoichiometry (Fig. 38), which comprises the convex hull at 50, 100, 150 GPa. Its hydrogenic sublattice contains H_2 and H^- units, and throughout the pressure range considered it adopted one of the two configurations which were previously predicted by for CaH_4 under pressure. At 150 GPa, the SrH_6 stoichiometry has the lowest enthalpy of formation. The most stable configuration assumes *P3* symmetry, and its lattice consists of one-dimensional $H_2 \cdots H^-$ hydrogenic chains. Symmetrization of these chains results in the formation of $[H^-]$ helices, which are reminiscent of the trigonal phase of sulfur. The *R3m*-SrH_6 phase, which is comprised of these helices, becomes dynamically stable by 250 GPa, and has a high density of states at the Fermi level. We explored the geometric relationships between *R3m*-SrH_6 and the *Im3m*-CaH_6 and *Imm2*-BaH_6 structures found in prior investigations.[49]

High Pressure Kinetic Studies using the Dynamic DAC – Current research supported by CDAC in the group of Academic Partner **Choong-shik Yoo** at **Washington State** focuses on the study of solid-state transformations and dense solid-solid interfaces of multi-phases and/or mixtures, across the melting/solidification, phase transitions, amorphization, and chemical reactions, utilizing the dynamic-DAC *(d*-DAC) coupled with time-resolved spectroscopy and time-resolved synchrotron XRD. The *d*-DAC is capable of precise controls of pressure and compression rates in time-scales that are ideal for diffusion-controlled solid-state transformations, complementing conventional DAC and shock wave studies. To probe the structural evolution of solids undergoing phase and chemical

changes, the *d*-DAC is coupled with time-resolved Raman spectroscopy, time-resolved synchrotron XRD, and time-resolved high-speed microphotography. Combining with a pulse (or ramp) laser-heating method, it is possible to produce tailored dynamic thermo-mechanical conditions for specific transformations of interest such as dynamic shear-induced deformation, interfacial mixing and bonding, and structural and chemical transformations. This work has been the focus of the dissertation research of CDAC graduate student **Dane Tomasino**.

Melting and Phase Transitions in Ramp-Heated Nitrogen at High Pressures – Raman studies of nitrogen were performed to investigate the melting curve and solid-solid phase transitions in the pressure-temperature range of 25 to 103 GPa and 300 to 2000 K. The solid-liquid phase boundary has been probed with time-resolved Raman spectroscopy on ramp-heated nitrogen in the DAC, showing a melting maximum at 73 GPa and 1690 K. The solid-solid phase boundaries have been measured with spatially resolved micro-confocal Raman spectroscopy in the resistively heated DAC, in order to investigate the δ-ε phase line to 47 GPa and 914 K. At higher pressures the θ-phase was produced upon a repeated thermal heating of the ζ-phase, yet no evidence was found for the ι-phase.

Time-Resolved XRD across Phase Transitions in H_2O – The *d*-DAC with time-resolved XRD (Fig. 39) to determine time evolutions of structural and chemical changes in H_2O under rapidly modulating pressures across a series of phase transitions (*HDW—metastable ice VII—HDA—ice VI—ice VII,* HDW = high density water, HAD = high density amorphous ice) over a wide range of compression rates (10^{-2} to 10^4 GPa/s). We have obtained a large number of time-resolved x-ray data on H_2O, and the major findings include: The structural evolution of ice VI to ice-VII, however, occurs rather coarsely. The diffraction data shows an anisotropic compression behavior of ice VI; the c-axis is more compressible than the a-axis at the same compression rate. Nevertheless, the present equations of state of both ice VI and ice VII obtained under dynamic loadings agree well with those previously obtained under static conditions.[50]

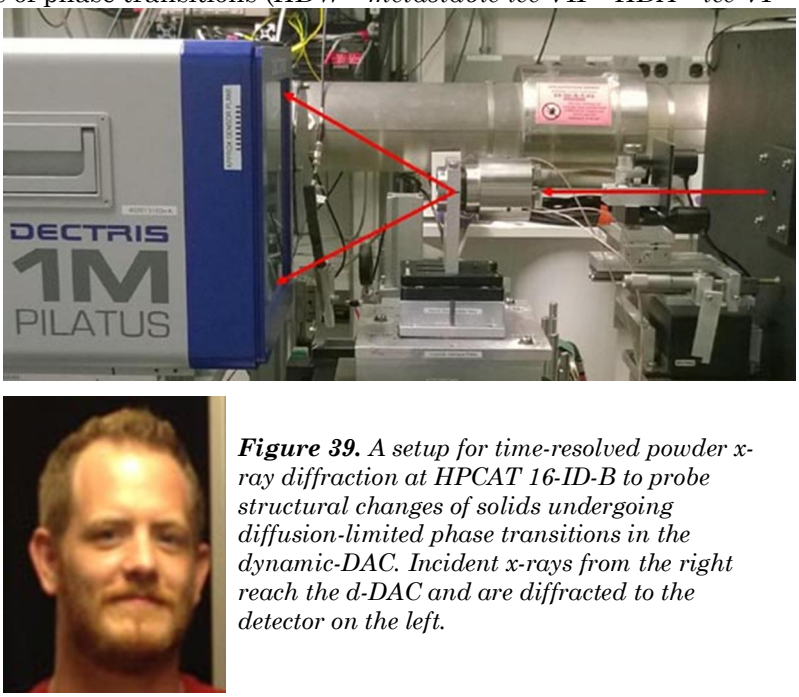


Figure 39. *A setup for time-resolved powder x-ray diffraction at HPCAT 16-ID-B to probe structural changes of solids undergoing diffusion-limited phase transitions in the dynamic-DAC. Incident x-rays from the right reach the d-DAC and are diffracted to the detector on the left.*

Characterization of a Mineral-Fluid Interface by X-ray Reflectivity – Termination and hydration of the forsteritic ($Fo_{90}Fa_{10}$) olivine (010) surface have been investigated by **Changyong Park** at HPCAT with high-resolution specular x-ray reflectivity and atomic force microscopy under room temperature and pressure conditions. The surface was prepared by polishing a naturally grown {010} face, which was found in an acidic (pH 3.5) alumina suspension to exhibit regular steps while the basic (pH 9.5) silica polished surface is irregularly roughened. This indicates that there are two distinguishable mechanochemical processes for the surface dissolution. The quantitative interpretation of the regular steps from the alumina-polished surface suggests that the observed step heights correspond to multiples of the crystallographic unit cell. The terrace surface was investigated with high-resolution specular x-ray reflectivity to determine the termination and hydration conditions (Fig. 40). The model-dependent fit of the reflectivity data suggests that the alumina-polished olivine (010) surface in equilibrium with water is terminated at a partially depleted (~24% with respect to stoichiometric) M1 metal atom plane. Vacancies created by this depletion and the removal of surface SiO_4^{4-} oxygen atoms are filled by adsorbed water species. The terminating plane

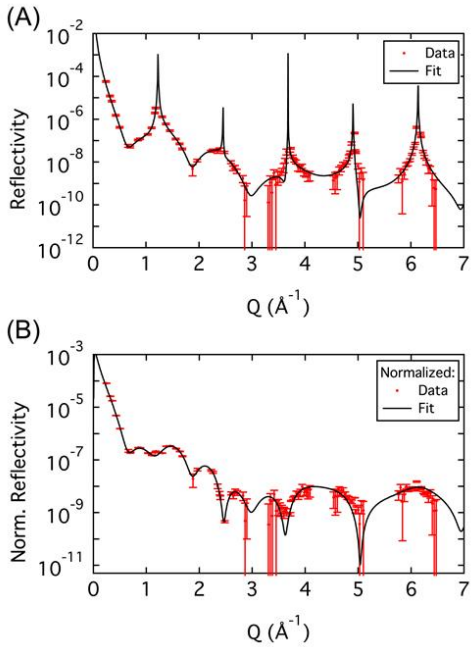


Figure 40. *A) Model of interface structure. B) Electron density profile from fit.*

generates two distinct atomic layers in the laterally averaged electron density profile, on which two highly ordered adsorbed water layers are formed. The first layer formation is likely through interaction with the M1 plane and the second layer is due to the hydrogen bonding interaction with the oxygen apex of the surface silicate tetrahedron. With this multilayered adsorbed water structure, the surface metal ion is partially hydrated by the vacancy filling and the adsorbed water molecules. The bulk water links to these distinct adsorbed water layers, with weak density oscillations that almost completely damp out after the first bulk water layer. The total thickness of the layered water structure including the two distinct adsorbed layers and the first layer of bulk water is slightly less than 1 nm, which corresponds to roughly three molecular layers of water. These results describe the steric constraints of the surface metal ion hydration and the iron redox environment during water-olivine interactions in this particular crystallographic orientation.

Shock Initiation of Reactive Nanomaterials – During the past year, the **Dlott** group at **Illinois** has been using their laser-launched flyer plate apparatus (see section 4) to to study shock initiation of reactive nanomaterials (*e.g.* Al + Fe_2O_3) by detecting and time-resolving the burst of light that accompanies initiation.[51] Also under investigation are the complex material dynamics of a high molecular weight polymer using noninvasive emissive spectroscopic probes embedded in the polymer.[52] As shown in Fig. 41, the dye emission spectrum is monitored, while an algorithm assists in the computation of the emission peak redshift versus time. The figure shows how the peak shift varies with time in PMMA for different shock pressures and different flyer speeds. This work is part of the dissertation research of CDAC graduate students **Will Shaw** and **Will Bassett** (Fig. 42).

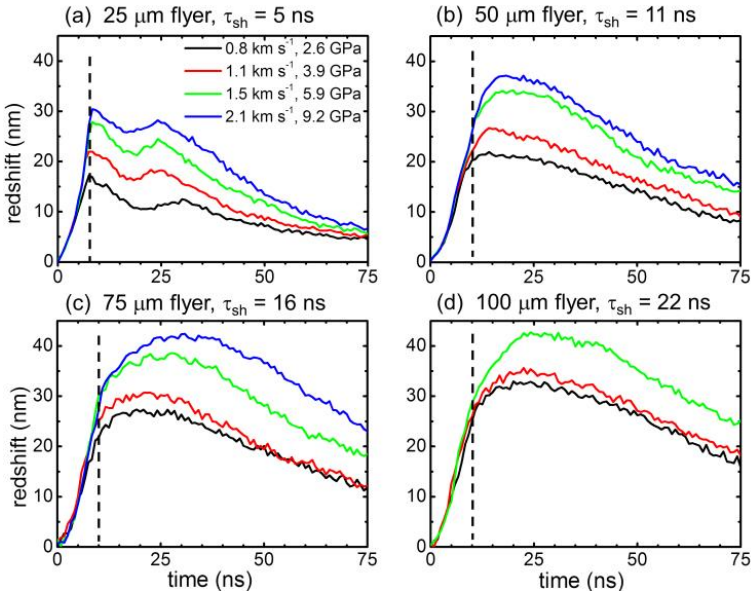


Figure 39. *Dye emission redshift transients at different pressures (impact velocities) with (a) 25 μm thick flyers, (b) 50 μm thick flyers (c) 75 μm thick flyers and (d) 100 μm thick flyers. The dashed line at 7 ns in (a) is a guide to the rising edge. The dashed lines at 10 ns in (b)-(d) indicate the change in slope associated with the transition from elastic to viscous compression.*

High-Pressure Polymorphism in Paracetamol – The structural phase stability of *N*-(4-hydroxyphenyl) acetamide (paracetamol, Fig. 8) has been studied by CDAC graduate student **Spencer Smith** (**UAB**) at ambient temperature up to 12 GPa using Raman spectroscopy. Spectral changes have provided further evidence for a highly kinetically driven Form I → II transition that occurs as a mixed phase from 4.8 – 6.5 GPa, and might be completed as low as 7 GPa. Upon further compression to 8.1 GPa, a drastic shift in spectral signature was observed providing the first evidence for a previously undiscovered Form IV of paracetamol. Additional shifts in

mode intensities were observed near 11 GPa indicating a potential restructuring of the hydrogen bonding network and/or structural modification to a potentially new Form V. Multiple *ab initio* harmonic frequency calculations at different levels of theory were performed with a B3LYP/6-31G** basis set used to provide a more robust mode assignment to experimentally obtained Raman modes. High pressure XRD was performed up to 21 GPa which provided further evidence for a highly kinetically driven Form I → II transition in agreement with Raman measurements. In addition, the XRD provided further evidence for the existence of Form IV near 8 GPa and Form V near 11 GPa with Form V persisting up to 21 GPa.

3. EDUCATION, TRAINING, AND OUTREACH

CDAC works to support the education and training of the next generation of scientists for work in areas of fundamental science that are important for Stockpile Stewardship. In addition to direct support of graduate students in the Academic Partner groups, we also seek opportunities to support outreach to the broader high pressure community in the US.

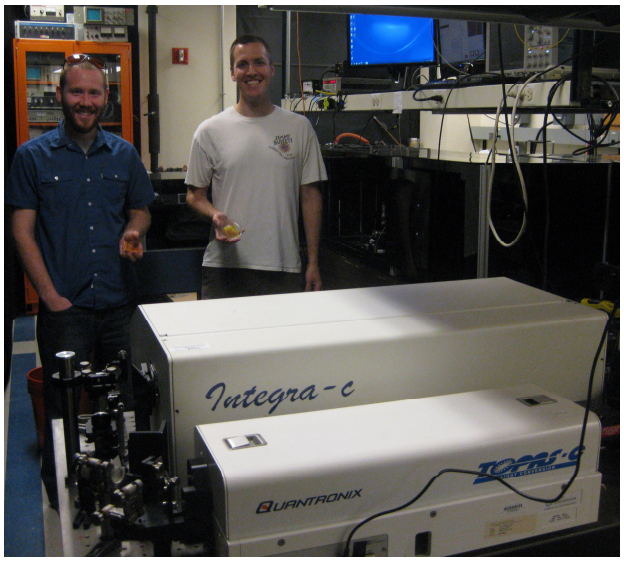


Figure 42. *CDAC graduate students from the* ***Dlott*** *group at* ***Illinois****,* ***Will Shaw*** *and* ***Will Bassett****.*

3.1 CDAC Graduate Students and Postdoctoral Fellows

The primary focus of CDAC is the support of graduate student preparation in the groups of the Academic Partners. As outlined in our technical section, CDAC graduate students pursue many different types of problems in areas of high *P-T* research relevant to stockpile stewardship, and their work represents the fields of materials science, physics and chemistry as well as high-pressure mineral physics and geophysics. One-third of the CDAC award goes to the support of graduate students in our Academic Partner groups. To date, 41 students have received the PhD degree with either full or partial support from CDAC.

During 2013-2014, the following graduate students were supported either fully or in part through CDAC for their work toward the PhD degree in the groups of in the research groups of CDAC Academic Partners.

Caltech (Fultz)	Lisa Mauger Max Murialdo
UC-Berkeley (Wenk)	Eloisa Zepeda-Alarcon Pamela Kaercher
Alabama–Birmingham (Vohra)	Spencer Smith Samuel Moore
Illinois (Dlott)	Will Shaw Will Bassett
Yale (Lee)	Kierstin Daviau
UCLA (Kavner)	Emma Rainey
Northwestern (Jacobsen)	Yun-yuan Chang John Lazarz

	Josh Townsend
Washington Univ. (Schilling)	Jinhyuk Lim
Illinois (Cahill)	Greg Hohensee
Washington State (Yoo)	Gustav Borstad Dane Tomasino
Hawai'i (Dera)	Yi Hu Hannah Shelton (undergraduate)
Utah (Miyagi)	Mike Jugle
University at Buffalo (Zurek)	Andrew Shamp
UC-Berkeley (Jeanloz)	Zack Geballe

As of May, 2014, 41 graduate students have received the PhD degree,supported fully or in part by CDAC funds to the Academic Partner groups. They are:

James Patterson (Illinois, 2004)
Raja Chellappa (Nevada-Reno, 2004)
Wendy Mao (Chicago, 2005)
Jenny Pehl (Berkeley, 2005)
Tabitha Swan-Wood (Caltech, 2005)
Sergio Speziale (Princeton, 2006)
Alexander Papandrew (Caltech, 2006)
Nenad Velisavljevic (Alabama–Birmingham, 2006)
Emre Selvi (Texas Tech, 2007)
Joanna Dodd (Caltech, 2007)
Matthew Lucas (Caltech, 2008)
Resul Aksoy (Texas Tech, 2008)
Lowell Miyagi (Berkeley, 2009)
Chris Seagle (Chicago, 2009)
Bin Chen (Illinois, 2009)
Zhu Mao (Princeton, 2009)
Lyci George (Florida International, 2010)
Michael Winterrose (Caltech, 2010)
Erin Oelker (Arizona State, 2010)
Arianna Gleason (Berkeley, 2010)
Yahya Al-Khatatbeh (New Mexico State, 2010)
Susannah Dorfman (Princeton, 2011)
Xinyang Chen (Michigan, 2011)
Daniel Reaman (Ohio State, 2011)
Wenli Bi (Washington University, 2011)
Jeffrey Carter (Illinois, 2011)
Kathryn Brown (Illinois, 2012)
Wen-Pin Hsieh (Illinois, 2012)
Samrat Amin (Arizona State, 2012)
Yu Lin (Stanford, 2012)
Rostislav Hrubiak (Florida International, 2012)
Matt Armentrout (UCLA, 2012)
Walter Uhoya (Alabama-Birmingham, 2013)
Jane Kanitpanyacharoen (UC-Berkeley, 2013)
Jeffrey Finklestein (Princeton, 2013)
Andrew Stemshorn (Alabama-Birmingham, 2014)
Jorge Muñoz (Caltech, 2014)

Figure 43. *CDAC graduate student* ***Emma Rainey (UCLA)*** *presenting a talk at the 2013 American Geophysical Union Meeting.*

Chris Berg (Illinois, 2014)
Yun-Yuan Chang (Northwestern, 2014)
Pamela Kaercher (UC-Berkeley, 2014)
Zach Geballe (UC-Berkeley, 2014)

A number of CDAC graduate students have gone on to postions within the NNSA Laboratories or within Department of Energy facilities in general.

CDAC Students to Postdoctoral Positions at NNSA Labs
Raja Chellappa
Wendy Mao
Nenad Velisavljevic
Jeffrey Carter
Kathryn Brown

CDAC Students to Postdoctoral Positions at Other Federal Government or Government-Supported Labs or Facilities
James Patterson (WSU Shock Physics)
Matt Lucas (ORNL)
Bin Chen (LBL)
Michael Winterrose (Lincoln Laboratory)
Wenli Bi (APS, ANL)
Chris Berg (DOE/BES Office, Washington DC)

CDAC Students Obtaining Staff Positions at NNSA Labs
Raja Chellappa (LANL)
Nenad Velisavljevic (LANL)
Chris Seagle (SNL)

Carnegie Postdoctoral Fellows Obtaining Staff Positions at NNSA Labs
Michael Furlanetto (LANL)
Amy Lazicki (LLNL)
Chris Seagle (SNL)
Luke Shulenberger (SNL)

Figure 44. *Former CDAC-supported graduate students* ***Nenad Velisavljevic*** *and* ***Raja Chellappa****, along with* ***Ramon Saavedra****, were presented with a DOE-NNSA Defense Program Award of Excellence by* ***Donald L. Cook****, Deputy Administrator for Defense Programs. Both* ***Velisavljevic*** *and* ***Chellappa*** *are now on the scientific staff at* ***LANL****.*

Carnegie Postdoctoral Fellows at Other Federal Government Labs or Facilities
Caitlin Murphy (AIP Congressional Fellow)
Douglas Allan Dalton (Defense Threat Reduction Agency)

Publications and presentations involving CDAC-supported students and postdoctoral fellows during 2013-2014 are as follows:

Student Publications

Armentrout, M. M., E. S. G. Rainey, and A. Kavner, High-pressure and high-temperature equation of state of cobalt oxide: Implications for redox relations in Earth's mantle, *Am. Mineral.* **98**, 993-999 (2013).

Banishev, A. A., W. L. Shaw, and D. D. Dlott, Dynamics of polymer response to nanosecond shock compression, *Appl. Phys. Lett.* **104**, 101914 (2014).

Berg, C. M., A. Lagutchev, and D. D. Dlott, Probing of molecular adsorbates on Au surfaces with large-amplitude temperature jumps, *J. Appl. Phys.* **113**, 183509 (2013).

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Berg, C. M., Y. Sun, and D. D. Dlott, Temperature-dependent dynamic response to flash heating of molecular monolayers on metal surfaces: Vibrational energy exchang, *J. Phys. Chem. B* **500**, 142011 (2014).

Berg, C. M., Y. Sun, and D. D. Dlott, Picosecond dynamics of shock-compressed and flash-heated nanometer thick films of HMX, *J. Phys.: Conf. Series* **500**, 142004 (2014).

Berg, C., Shock compression and flash-heating of molcular adsorbates on the picosecond time scale, *Ph.D. Thesis, University of Illinois at Urbana-Champaign* (2014).
Chang, Y. Y., S. D. Jacobsen, M. Kimura, T. Irifune, and I. Ohno, Elastic properties of transparent nano-polycrystalline diamond measured by GHz-ultrasonic interferometry and resonant sphere methods, *Phys. Earth Planet. Inter.* **228**, 47-55 (2014).
Chang, Y. Y., S. D. Jacobsen, J. F. Lin, C. R. Bina, S. M. Thomas, J. Wu, G. Shen, Y. Xiao, P. Chow, D. J. Frost, C. A. McCammon, and P. Dera, Spin transition of Fe_3^+ in Al=bearing phase D: An alternative explanation for small-scale seismic scatterers in the mid-lower mantle, *Earth Planet. Sci. Lett.* **382**, 1-9 (2013).
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Curtis, A. D., W. L. Shaw, A. A. Banishev, and D. D. Dlott, Dynamics of shocks in laser-launched flyer plates probed by photon Doppler velocimetry, *J. Phys.: Conf. Series*, in press.
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Delaire, O., I. I. Al-Qasir, J. Ma, A. M. dos Santos, B. C. Sales, L. Mauger, M. B. Stone, D. L. Abernathy, Y. Xiao, and M. Somayaulu, Effects of temperature and pressure on phonons in $FeSi_{1-x}Al_x$, *Phys. Rev. B* **87**, 184304 (2013).
Dera, P., G. J. Finkelstein, T. S. Duffy, R. T. Downs, Y. Meng, V. Prakapenka, and S. N. Tkachev, Metastable high-pressure transformations of orthoferrosilite Fs_{82}, *Phys. Earth Planet. Inter.* **221**, 15-21 (2013).

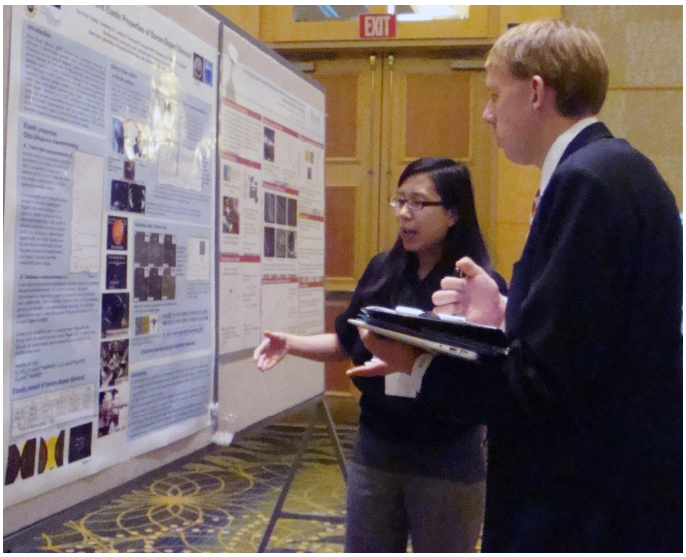

Figure 45. *CDAC graduate student* ***Yun-yuan Chang (Northwestern)*** *presenting her poster at the 2014 SSAP Symposium in Bethesda, MD.*

Dera, P., M. Manghnani, A. Hushur, Y. Hu, and S. N. Tkachev, New insights into the enigma of boron carbide inverse, *J. Solid State Chem.* **215**, 85-93 (2014).
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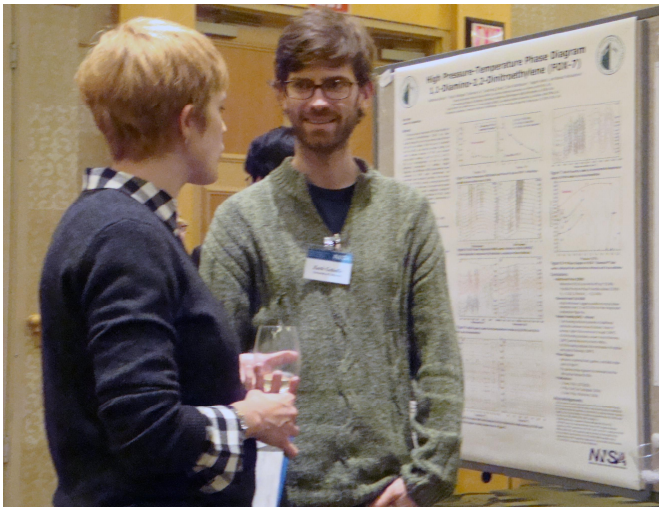

Figure 47. *CDAC graduate students* ***Emma Rainey (UCLA)*** *and* ***Zack Geballe (Berkeley)*** *discuss their research at the 2014 SSAP Symposium in Bethesda, MD.*

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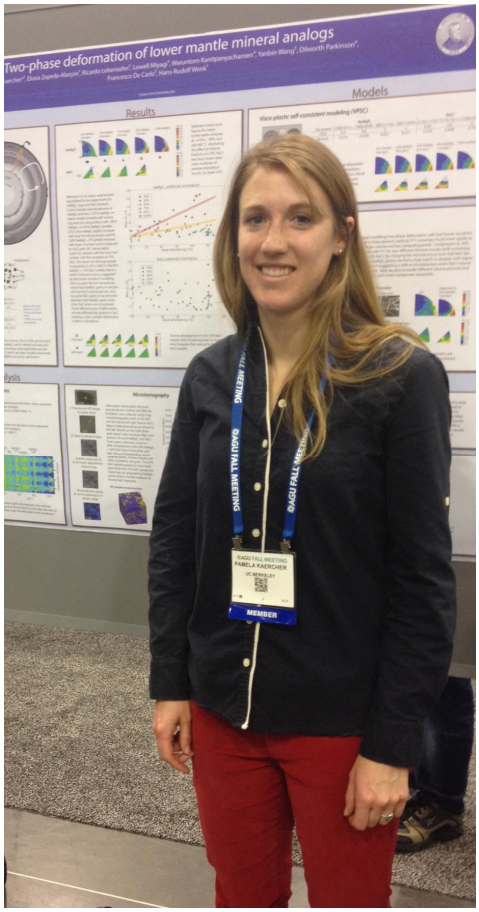

Figure 48. *Former CDAC graduate student* ***Pamela Kaercher (Berkeley)*** *at the 2013 American Geophysical Union Meeting.*

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Figure 49. *CDAC graduate student* ***Max Murialdo (Caltech).***

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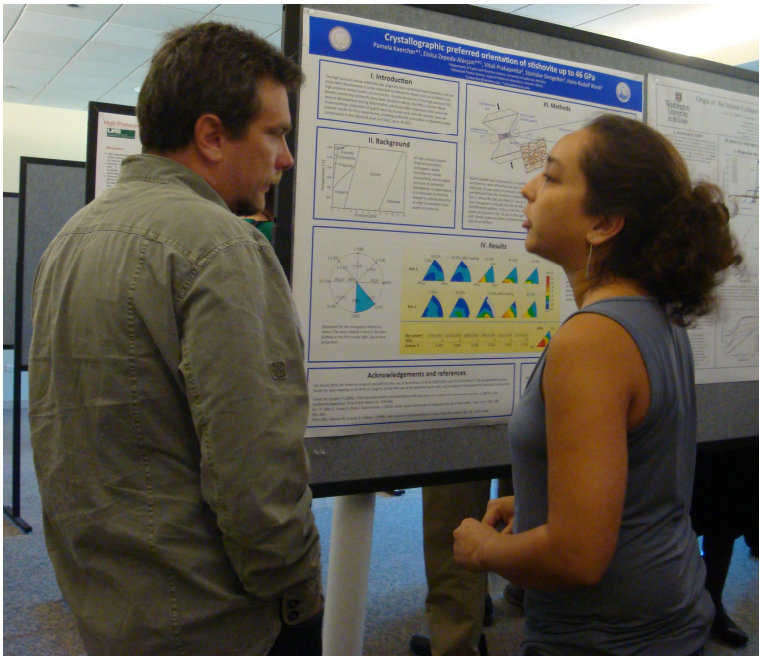

Figure 50. *CDAC graduate student* ***Eloisa Zepeda-Alarcon (Berkeley)*** *discusses her poster with CDAC partner* ***Przemek Dera (Hawai'i)*** *at the CDAC Year 11 Review.*

Shelton, H., P. Dera, M. C. Barkley, and R. T. Downs, Phase transition and hydrogen bonding behavior in Be(OH), $Zn(OH)_2$, and SiO_2 cristobalite at high temperatures and pressures, *COMPRES Annual Meeting* (Skamania Lodge, WA, June 16-19, 2014).
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Uhoya, W. O., G. M. Tsoi, Y. K. Vohra, J. E. Mitchell, A. Safa-Sefat, and S. Weir, High pressure low temperature studies on 1-2-2- iron-based superconductors using diamond anvil cells, *Materials Research Socieity Proceedings*, 1582 (2013).
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Wu, X., J. F. Lin, Z. Mao, J. Liu, P. M. Kaercher, H. R. Wenk, V. Prakapenka, and K. K. Zhuravlev, Deformation and seismic anisotropy of silicate post-perovskite in the Earth's lowermost mantle, *Eos Trans. AGU Fall Meet., Suppl.* **94** (2013).
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Zepeda-Alarcon, E., H. Nakotte, S. C. Vogel, and H. R. Wenk, Magnetic structure of goethit □-FeOOH: A neutron diffraction study, *Eos Trans. AGU Fall Meet., Suppl.* **94** (2013).

3.2 Undergraduate Student Summer Scholars

Some of the university students participating in the Carnegie Summer Scholars Program each year carry out their projects in the high pressure group at Carnegie with CDAC personnel. The Summer Scholars Program, which is run by CDAC Coordinator **Stephen Gramsch**, seeks to identify promising students who may not have had the opportunity to engage in research at their home institutions. At **Carnegie**, such students experience a rigorous introduction to scientific research, and through attendance at CDAC group meetings, are learning about the research process as well as the important problems in the field.

Figure 51. *Top, Kevin Hernandez, Olivia Reyes-Becerra, and Joseph Romero. Bottom: Brooke Sherman and Brandon Wilfong.*

During the summer of 2014, the following students worked with the Carnegie group (Fig. 51). Students funded by CDAC are designated with an asterisk in the list below (*).

Kevin Hernandez*, California State University-Sacramento *Reactivity of Hematite and Silica at High Pressure and Temperature*

Olivia Reyes-Becerra*, Stanford University
Synthesis of Single-Crystal Na_4Si_{24} Clathrate

Joseph Romero, Augustana College
The Effect of Clay on Glycerol/Carboxylic Acid Polymerization

Brooke Sherman, George Mason University
Microbes in the Deep Sea: Analyzing Bacteria from an Inactive Chimney Structure Located Along the East Pacific Rise

Brandon Wilfong*, Washington College
In-situ Raman Spectroscopic Investigation of Relaxor Multiferroic $Pb(Fe_{0.5}Nb_{0.5})O_3$ under High Pressure and Temperature Conditions

3.3 CDAC Collaborators

The CDAC collaborators from 2013-2014 include the following faculty and students from institutions around the world:

Aarhus Universitet, Denmark
A. Svane
Academy of Science of Moldova
I. M. Tiginyanu
V. V. Ursaki
Air Force Research Laboratory
J. Horwath
S. O. Leontser
M. Lucas
S. L. Semiatin
Ames Laboratory
K. A. Gschneider, Jr.
Y. Mudryk
D. Paudyal
V. K. Pecharsky
Amherst College
D. Ang
J. Gordon
L. Hunter
S. Peck
Aarhus Universitet, Denmark
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A. Alatas
E. E. Alp
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C. C. Chen
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Y. Ding
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G. Fabbris
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B. J. Ingram
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X. Zhang
Bhabha Atomic Resarch Center, India
G. K. Dey
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J. Gyanchandani
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Z. Fang
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C. Lin
C. Q. Lin
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L. Liu
Q. Q. Liu
Z. X. Qin
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W. Xiao
K. Yang
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Z. Zeng
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A. Cadien
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T. Pandy
A. K. Singh
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Institut Jožef Stefan, Slovenia
Z. Mazej
Institut Laue Langevin, France
A. Bytchkov
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M. Diaz-Michelena
Iowa State University
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Japan Synchrotron Radiation Research Institute, Japan
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Y. Ohishi
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Y. L. Li
Jilin University, China
X. Bai
X. Chen
H. Cui
Q. Cui
T. Cui
D. Duan
F. Huang
X. Huang
X. Jin
F. Li
L. Li
Q. Li
S. Li
Z. Li
B. Liu
C. Ma
F. Ma
Y. Ma
Z. Men
H. Song
C. Sun
F. Tian
J. Wang
K. Wang
W. Wang
X. Wang
X. Wu
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M. Zhou
Q. Zhou
H. Zhu
B. Zou
G. Zou
Kean University
J. Ha

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H. S. Kim
KTH Royal Institute of Technology, Sweden
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Kurchatov Institute, Russia
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J. Knight
A. MacDowell
D. Y. Parkinson
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Y. A. Freiman
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S. M. Tretyak
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M. He
National Chiao Tung University, Taiwan
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F. S. Elkin
A. G. Gavriliuk
A. G. Ivanova
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S. M. Stishov
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Z. Zeng
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C. Chen
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K. Lipinska
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Y. Wang
Y. Zhang
Y. Zhao
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G. Subrahmanyam
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D. Akinwande
J. G. Cheng
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C. Jin
P. P. Kong
K. E. Kweon
S. Larregola
J. F. Lin
J. Liu
Y. Liu
C. Lu
Z. Mao
A. Manthiram
A. P. Nayak
J. Wu
J. Yang
J. S. Zhou
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G. T. Seidler
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M. van Zant
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Yale University
G. Amulele
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Zheijiang University, China
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J. Z. Jiang
H. Luo
Q. Tao
X. D. Wang
Z. A. Xu
D. X. Zhang
Z. Zhang

3.4 Visitors to CDAC

Carnegie also receives many visiting scientists each year, who utilize laboratory facilities to prepare and perform experiments that would be impossible to do at their home institutions. Scientists from around the country and the world have visited **Carnegie** to take advantage of this program. Such visitors often make formal presentations, which enrich the scientific work of the group as a whole.

A. Palke	Stanford University	Ferric-iron perovskite synthesis with Yingwei Fei	January 7-28, 2013
E. J. Kim	Seoul National University	High pressure samples of silicates with CO_2 with Yingwei Fei	January 21-25, 2013
J. Wu	University of Texas at Austin	Experiments for superconductors with Viktor Struzhkin	January 21-25, 2013
K. Post	University of California – San Diego	High pressure measurements of intermetallic compounds	January 30-February 8, 2013
D. Wai	Shanghai Jiaotong University	Computational physics of materials and high-pressure Fe-S with Yingwei Fei	February 19-March 1, 2013
T. Zapata	Texas A&M	Materials under high pressure using a DAC with Viktor Struzhkin	February 18-22, 2013
R. Chellappa	LANL	Work with Maddury Somayazulu	February 26-March 2, 2013
S. Starchikov	Institute of Crystallography, RAS	DAC experiments with Viktor Struzhkin	March 18-31, 2013
C. Ji	ANL	Sample loading with Ho-kwang Mao	March 18-22, 2013
L. Gasparov N. Timmins	University of North Florida	High pressure study of magnetie with Viktor Struzhkin	April 29-May 10, 2013
F. Huang	Johns Hopkins University	High *P-T* experiments with Yingwei Fei	May 21-August 20, 2013
R. Caracas	Ecole Normale Superieure de Lyon	Work on carbonatite melts with Ronald E. Cohen	June 3-7, 2013
R. Boles	University of Nevada – Reno	Properties of amorphous metal ribbons at high pressures with Maddury Somayazulu	June 10-28, 2013
J. Holaday	Walt Whitman High School	High pressure synthesis experiments with Timothy Strobel	June 24-August 25, 2013
W. Grochala	University of Warsaw	High pressure conductivity studies of AgF_2 and AgF; Transport optical measurements with Viktor Struzhkin	June 24-July 5, 2013
C. Tulk	Oak Ridge National Laboratory	Work with Maddury Somayazulu	August 12-14, 2013
Y. Davyolova	Moscow Engineering Physics Institute	High pressure optical experiments with Viktor Struzhkin	September 17-October 17, 2013
A. Kyono	University of Tsukuba	Single crystal XRD experiments with Timothy Strobel and Stephen Gramsch	September 18-24, 2013

N. Holtgrew	Howard University	Laser optics in Raman pump-probe experiments with Alexander Goncharov	October 1, 2013-September 30, 2014
K. Chang	New York Times	Interview with Russell J. Hemley	October 10, 2013
S. Cervera	University of Paris	Measurements of elasticity of Fe by an ultrafast laser pump-probe technique with Alexander Goncharov	November 18-29, 2013
S. M. Thomas	University of Nevada – Las Vegas	Measurements of radiative thermal conductivity of the Earth's minerals with Alexander Goncharov	January 31-February 28, 2014
Z. Konopkova	DESY	Resolved laser heating of samples under pressure with Alexander Goncharov	February 18-June 30, 2014
D. Keefer	Pennsylvania State University	High pressure work with Timothy Strobel	February 18-21, 2014
E. Monroe	Woodrow Wilson Senior High School	Studies of NV centers in diamond under compression with Viktor Struzhkin	July 15-August 15, 2014

3.5 2013 and 2014 SSAA Symposia

The 2013 SSAA Program Symposium took place in Albuquerque, NM on June 27-28 (Fig. 52), and in 2014, the Symposium was held in North Bethesda, MD on February 19-20 (Fig. 4). At both meetings, individual grant recipients and center directors from the three divisions of the program (High Energy Density Physics, Low Energy Nuclear Science, and Materials Properties under Extreme Conditions) gave updates on center or group activities and progress.

In 2013, the symposium was opened with a welcome address from **Ralph Schneider**, the Director of the Office of Defense Science at the NNSA. **Paul Hommert**, Director of Sandia National Laboratories, gave the keynote talk before the poster session. CDAC students and partners were joined by two CDAC and HPCAT scientists and presented 18 posters during the poster session on the first night of the symposium. CDAC Director **Russell Hemley** gave two invited talks, one an overview of CDAC and one with **Yogendra Gupta** (Washington State University) on unique opportunities at the APS, featuring HPCAT and DCS. CDAC Students **Pamela Kaercher** (Berkeley), **Zeyu Li** (Michigan), **Lisa Mauger** (Caltech), and **Eloisa Zepeda-Alarcon** (Berkeley) all received Best Poster awards during the poster session. This was the second year in a row that Pamela earned this honor.

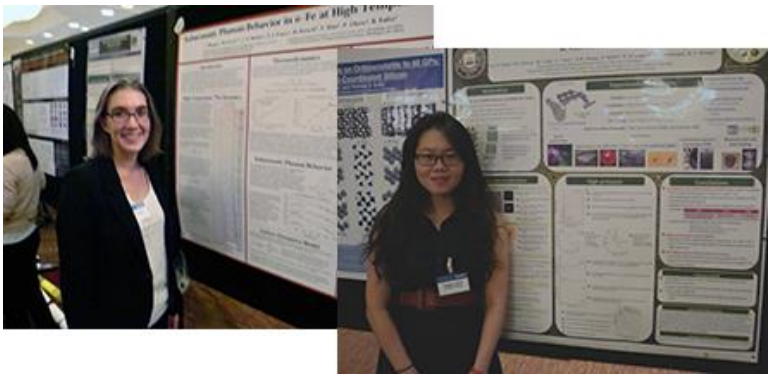

Figure 52. *CDAC graduate students* ***Sulgiye Park (Michigan)*** *and* ***Lisa Mauger (Caltech)*** *with their posters at the 2013 SSAP Symposium in Albequerque, NM.*

In 2014, the Symposium was held in North Bethesda, MD from February 19-20, 2014. The symposium was opened with a welcome address from **Keith LeChien**, the Program Manager in the Defense Science Division at the NNSA. **Bruce Held**, Acting Administrator (NNSA) and Acting Undersecretary for Nuclear Security (DOE), gave the keynote talk before the poster session. CDAC students and scientists presented 18 posters during the poster session. In addition, CDAC

Director **Russell Hemley** gave an invited talk, presenting an overview of CDAC. CDAC Students **Pamela Kaercher** (Berkeley), **Emma Rainey** (UCLA), and **Dane Tomasino** (WSU) all received Best Poster awards during the poster session. Pamela received a Best Poster award for the third consecutive year.

CDAC Posters Presented at the 2013 SSAA Program Symposium

Berg, C., Shock-loading of energetic materials with picosecond temporal resolution, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Bishop, M., 1,1-diamino-2,2-dinitroethylene (FOX-7) under high pressure-temperature, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Du, Z., Mapping temperatures and temperature gradients during flash heating in a diamond-anvil cell, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Finklestein, G., Single-crystal x-ray diffraction experiments on orthoenstatite to 48 GPa: New high-pressure phases and 4-, 5-, and 6-coordinated silicon, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Hemley, R. J., Carnegie/DOE Alliance Center - A center of excellence for high pressure science and technology (invited), *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Hemley, R. J. and Y. Gupta, Unique opportunities at APS - HPCAT and DCS (invited), *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Hohensee, G., High pressure thermal transport properties of interfaces and mixed crystals by time-domain thermoreflectance, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Hrubiak, R., Thermodynamics of the C-H-O fluids: High pressure experimetns on dissociation of carbonates and hydrides, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Kaercher, P. and E. Zepeda-Alarcon, Crystallographic preferred orientation in stishovite: In situ observations at high pressure, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Li, Z., Carbide-dominant inner core inferred from anomalously low shear-wave velocity of dense Fe_7C_3, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Lim, J., Origin of the volume collapse under pressure in elemental Pr, Gd, Tb, and Dy, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Liu, J., Elasticity of bcc Fe and Fe-Si alloy at high *P-T* by mean of inelastic x-ray scattering, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Mauger, L., High temperature phonon behavior in iron and cementite, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Park, S., Structural response of layered perovskite $La_2Ti_2O_7$, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Shaw, W., Time-resolved spectroscopy of shock compreessed materials, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Shen, G., HPCAT - an integrated synchrotron facility for high pressure research, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Somayazulu, M., Novel xenon compounds syntesized at high pressures and high temperatures, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Stan, C., High-pressure phase transition in PbF_2 at room and high temperatures, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Townsend, J., Properties of ultra-high pressure hydrous silicates: Experiment and theory, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

Yang, J., Single-crystal elasticity of the deep-mantle magnesite at high pressure and temperature, *Stewardship Science Academic Programs Annual Review Symposium* (Albuquerque, NM, June 27-28, 2013).

CDAC Posters Presented at the 2014 SSAA Program Symposium

Bishop, M., High pressure-temperature phase diagram of 1,1-diamino-2,2-dinitroethylene (FOX-7), *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Borstad, G., Mixtures of D_2-H_2O, D_2-NH_3 and D_2-CH_4 under high pressure, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Chang, Y. Y., Hardness and elastic properties of boron-doped diamond, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Daviau, K., Preliminary work on the melting of SiC at high pressure, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Geballe, Z., Brillouin studies of a highly-stable glass, $CaSiO_3$, from 0 to 44 GPa, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Hohensee, G., Metal-diamond interface thermal conductance with nitrogen defects at high pressures by time-domain thermoreflectance, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Jugle, M., Deformation and transformation textures in the $NaMgF_3$ perovskite to post-perovskite system, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Kaercher, P., Understanding lower mantle rheology from two-phase deformation experiments, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Lim, J., Origin of pressure-induced volume collapse in Dy, Tb, Gd, and destruction of dense kondo state in CeBa, to 120 GPa, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Murialdo, M., A thermodynamic study of high pressure physisorption on nanostructured carbon, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Rainey, E., High-pressure thermal conductivity of $(Mg,Fe)SiO_3$ perovskite measured in the laser-heated diamond anvil cell, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Shamp, A., Boron carbide: The evolution of structure under pressure, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Shaw, W., Laser-driven flyer-plates for shock induced chemistry, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Shen, G., HPCAT facility at the Advanced Photon Source: Exploring matter under extreme conditions, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Smith, S., Polymorphism in paracetamol: Evidence of additional forms IV and V at high pressure, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Tomasino, D., Dynamic thermo-mechanical loading of simple molecular systems, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Uhoya, W., High pressure effects on the superconductivity in rare earth doped $CaFe_2As_2$, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

Zepeda-Alarcon, E., High pressure deformation of two-phase mineral assemblages: Lower mantle implications, *Stewardship Science Academic Programs Symposium* (North Bethesda, MD, February 19-20, 2014).

3.6 Paris-Edinburgh Cell Workshop

The CDAC-supported *Paris-Edinburgh Cell Workshop 2013* was held on May 23-24 at the APS and HPCAT 16BM-B, (Fig. 53). More than 45 participants attended the two-day workshop. The workshop was composed of four technical training courses, as well as a discussion forum related to current Paris-Edinburgh cell applications in high-pressure research. 32 graduate students, post-docs, and young and senior researchers, among the participants who had little to no experience with Paris-Edinburgh (PE) cell applications, took hands-on courses. This training included instruction in a standard sample cell assembly (established for HPCAT PE cell application), high *P-T* control, ultrasonic measurement, and EDXD data analysis. A falling sphere viscometry technique was also demonstrated. The unique opportunity provided by the new instrumental setup established at HPCAT was also introduced to the hands-on participants through these courses. The workshop, which was organized by HPCAT's **Changyong**

***Figure 53. Paul Chow** discusses x-ray spectroscopy as part of a tour of HPCAT at the Paris-Edinburg Cell Workshop.*

Park, **Yoshio Kono**, and **Guoyin Shen** (HPCAT), along with **Yanbin Wang** from GSECARS, was a successful outreach to the potential user community.

3.7 CDAC Year 11 Review

On September 16-17, 2013, CDAC hosted its Year 11 Review at the Advanced Photon Source at ANL (Fig. 54). In addition to a program overview by Director Russell Hemley, and a presentation on education and outreach activities by Coordinator Stephen Gramsch, HPCAT Director Guoyin Shen also provided an update on HPCAT capabilities and an overview of the APS and HPCAT upgrade plans. Ten of the Academic Partners also made presentations to the review committee. The presentations from the partners included six continuing partners and four new partners that joined the program in 2013. Nenad Velisavljevic (LANL) and Chris Seagle (SNL), two former CDAC students who now hold staff positions in the NNSA Labs, also made presentations on the work that they have carried out with CDAC beam time. The poster session included presentations by 16 current and former CDAC students.

Monday, September 16, 2013:

8:00-8:30	Review Committee Executive Session
8:30-9:15	Russell Hemley – Overview
9:15-9:45	Steve Gramsch – Education and Outreach
9:45-10:15	Guyoin Shen – Update on HPCAT Capabilities
10:30-11:00	Dana Dlott -- University of Illinois
11:00-11:30	Yogesh Vohra -- University of Alabama-Birmingham
11:30-12:00	Jim Schilling -- Washington University in St. Louis
12:00-12:30	Abby Kavner -- University of California-Los Angeles
12:30-2:30	Lunch and Student Poster Session
2:30-3:00	Steve Jacobsen – Northwestern University
3:00-3:30	David Cahill – University of Illinois
3:30-4:00	Nenad Velisavljevic – Los Alamos National Laboratory
4:00-4:30	Chris Seagle – Sandia National Laboratories
4:30-5:00	Review Committee Executive Session

Tuesday, September 17, 2013:

8:30-9:00	Eva Zurek – University at Buffalo
9:00-9:30	Lowell Miyagi – University of Utah
9:30-10:00	Choong-shik Yoo – Washington State University
10:00-10:30	Przemek Dera – University of Hawai'i
10:30-10:45	Russell Hemley – Summary
11:00-11:30	Tour of HPCAT
11:30-12:00	Review Committee Meeting
12:00-12:30	Review Committee Executive Session

Posters Presented at the CDAC Review

Berg, C., Picosecond dynamics of shock compressed and flash-heated nanometer thick films of HMX, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Bi, W., Applications of nuclear resonant scattering in high pressure research at Sector 3 of the Advanced Photon Source, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Brown, K., Transient absorption and hugoniot equations of state of shocked reactive liquids, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Chang, Y., Elastic properties of transparent nano-polycrystalline diamond measured by GHz-ultrasonic interferometry and resonant sphere methods, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Hohensee, G., High pressure thermal transport properties of interfaces and mixed crystals by time-domain thermoreflectance, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Kaercher, P. and E. Zepeda-Alarcon, Crystallographic preferred orientation in stishovite up to 46 GPa, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Lazarz, J., Compression mechanism and equation of state of thaumasite up to 10 GPa, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Lim, J., Origin of the volume collapse under pressure in elemental Dy, Tb, Pr, and Gd, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Liu, X., Synthesis and characterization of cubic B-C-N crystals, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).
Mauger, L., High temperature phonon behavior in iron and cementite, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).
Park, S., Compex oxides under extreme conditions of high pressure and irradiation, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).
Rainey, E. S., Measuring temperature, emissivity, and thermal conductivity at high pressure and temperature in the laser-heated diamond anvil cell, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).
Shaw, W., Using laser-driven flyer plates to study the shock initiation of nanoenergetic materials, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).
Smith, S., High pressure Raman spectroscopy and x-ray diffraction studies on paracetamol, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Figure 54. *Scenes from the CDAC Year 11 Review.*

Stemshorn, A., High pressure high temperature iron-based metallic glass studies, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).
Townsend, J., Hydrogen in Earth's lowermost mantle, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).
Uhoya, W., High pressure-low temperature studies on rare earth doped 1-2-2 iron-based superconductors, *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

3.8 USA Science and Engineering Festival

Carnegie Postdoctoral Fellow **Caitlin Murphy** was among a number of Carnegie scientists participating in the third annual USA Science and Engineering Festival, held at the Washington Convention Center in Washington, DC, from April 26-27, 2014 (Fig. 5). This is the largest science, technology, engineering, and math education event of its kind in the US. Caitlin presented a demonstration on her topic, "How does high pressure affect materials that have defects and impurities?" **Robert Hanrahan**, former Program Manager for CDAC at NNSA, discussed stockpile stewardship and non-proliferation at the State Department's booth in the National Security Section of the event.

3.9 2014 Neutron and X-ray Scattering School

HPCAT Beamline Scientists **Changyong Park** and **Dmitry Popov** hosted a group of eight graduate students during the 2014 Neutron and X-ray School. The NX School was held on June 19-20 at the APS. During the two-day class, HPCAT 16-BM-D hosted groups of students who learned about XRD with hands-on training for high-pressure experiments using the DAC and received a practical introduction to data analysis.

3.10 Honors and Awards

CDAC Academic Partner **Steven Jacobsen** from **Northwestern** received a Friedrich Wilhelm Bessel Research Award for 2014. The Bessel Award is granted by the Alexander von

Humbolt Foundation, and allows the recipient to spend a year working at a research institution in Germany. He will spend the coming year at the **Bayeriches Geoinstitut** in Bayreuth, where he was a Humboldt Postdoctoral Fellow from 2002-2004. **Eva Zurek**, a CDAC Academic Partner from the **University at Buffalo**, received the 2014 Young Leaders Professional Development Award of The Minerals, Metals and Materials Society (TMS). She was presented with the award at the 2014 annual meeting of the TMS in San Diego, CA.

CDAC Partners **Przemek Dera** (**University of Hawai'i**) and **Lowell Miyagi** (**University of Utah)** have been named as the speakers for the 2014-2015 COMPRES Distinguished Lecture series in the field of Mineral Physics. The talks feature topics that emphasize the exciting high-pressure geoscience research being conducted within the COMPRES community and its significance for understanding fundamental Earth and planetary processes. Since its inception in 2008, seven CDAC Academic Partners and/or faculty who were supported as postdoctoral fellows through CDAC have served as Distinguished Lecturers.

Figure 55. *Clockwise from top left:* ***Steven Jacobsen, Eva Zurek, Przemek Dera****, and* ***Lowell Miyagi****.*

4. TECHNOLOGY DEVELOPMENT

Technical development remains an important focus area in CDAC. At HPCAT, NSLS and in the Academic Partner groups, an ongoing significant effort in this area has resulted in many breakthroughs in measurement capabilities, which enable the cutting edge science pursued across the Center. In this section, we outline some of the technology development efforts that have taken place in the Center during 2013-2014.

4.1 Technical Improvements at HPCAT

The objective of **HPCAT** is to provide a state-of-the-art user facility for advancing fundamental knowledge of materials behavior in a broad range of environments, such as pressure, temperature, radiation, and deviatoric stress, including both static and dynamic phenomena. **HPCAT** has continued to stay at the leading position in the world, and is the most productive sector at the APS in terms of the number publications in "high-impact" journals as well as the total number of publications. Over the past year, each of the beamlines at HPCAT has undergone significant improvements in capabilities and performance.

16-1D-D: High Pressure X-ray Spectroscopy – HPCAT beamline 16-ID-D specializes in hard x-ray spectroscopy experiments with samples under high pressure in DACs. In the current configuration, three types of measurements can now be carried out: nuclear forward/nuclear resonant inelastic scattering, x-ray resonant/non-resonant emission and energy loss spectroscopy with 1.4 eV energy resolution. 16-ID-D is one branch of a canted line, with a 3.0 mm period APS undulator and a liquid nitrogen-cooled Si(111) high heat load monochromator delivering x-ray energies of 4.5-37 keV. Several combinations of focusing mirrors are used for various needs in user operation. Typically for flux hungry measurements, the beamline features 1-meter long vertical and horizontal mirrors to achieve 35μVx55μH focus size at the sample position. For a smaller beam at the expense of incoming flux, the setup consists of a pair of 200 mm mirrors for a 3μV x 5μH focus. A combination of one short and one long mirror may be used for special geometries.

In the past year, a number of development projects and improvements have been made to enhance the performance of the beamline and extend its capabilities.

- Working with the APS, design and testing of a pre-figured mirror, to focus the beam suitable for megabar pressures, has begun.
- A multiple-analyzer emission spectrometer is in the final construction stage, and will increase the efficiency of data collection by a factor of 7.
- A low-momentum transfer, 100 meV resolution energy-loss x-ray spectrometer is under commissioning for the study of collective and single particle electronic excitations.
- Automated beamline control software has been progressively upgraded to PyEpics standards. This will allow users the flexibility and ease of writing scripts for various purposes, including data collections and evaluations. The recently installed quad-diode beam position monitor and feedback software ensures a stable beam position, and optimizes the intensity of the beam on the sample (Fig. 57).

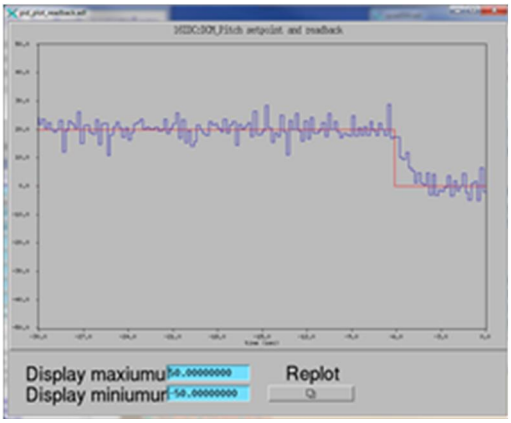

Figure 56. *Response of the position of the beam (blue) using feedback to a change in the target position (red). Stablility in both position and intensity is critical in high pressure spectroscopy experiments.*

16-ID-B: General Purpose Microdiffraction – 16-ID-B is an undulator beamline dedicated to x-ray microdiffraction over a vast range of pressure and temperature conditions. The General Purpose (GP) Table is one of two measurement stations in the experimental hutch and is optimized to handle various types of diffraction experiments (single-crystal and powder) over broad pressure and temperature ranges (ambient pressure to several hundred GPa and ~4 to 1,000 K) with DACs in axial or radial geometry. Continual development at the GP Table makes it a highly productive, high-throughput beamline.

The 200 mm Pt-coated focusing mirrors have been upgraded to 320 mm Pt/Rh-coated mirrors. This combination of increased length and coating yields an increase in flux by about a factor of five. Also, the robust mechanical design offers a more stable beam position and focal spot size. Mirrors, sample, and detector have been mounted on a common table which, in turn, has been stabilized by decoupling it from its translation mechanisms when not in use. This has resulted in an extremely stable experimental configuration that can remain internally stable to within the repeatability of the mechanical stages (micron level) even after displacement of a large mass (~50 kg) across the optical table.

Specialized developments at the GP table are also focused on the emerging field of time-resolved diffraction. Now, timing electronics and pressure control (pneumatic membrane or piezoelectric stack) can be remotely and conveniently controlled using a GUI from the control station. High-frequency (125 Hz) diffraction imaging can be synchronized with ramp compression or stroboscopic pressure cycling using an arbitrary-wave function generator and an 8-channel delay generator. Rapid on-line data analysis has been achieved through optimizing existing software (*e.g.*, batch processing of thousands of images and diffraction patterns) to generate high-quality pressure-temperature-volume relations. One highlight was the recent test of an area detector prototype with imaging capability of 800 Hz, allowing the demonstration of compression rates exceeding tens TPa/s (Fig. 10).

16-ID-B: Microdiffraction with Double-Sided Laser Heating – The laser heating table at HPCAT is heavily used during each run cycle, and the apparatus undergoes continuous improvement in response to the needs of many users (Fig. 58). Recent developments on the laser heating table include:

- *In-situ* variation of the laser heating spot size allows changing the heating spot size anytime as needed, even during heating. This is an effective way to eliminate or minimize the effect of temperature gradients on samples, especially those with complex chemistry. The alignment of

laser and x-ray beams to one spot on sample and maint aining the alignment during an experiment are critical for obtaining meaningful and reliable data. As sample size getting smaller to micron level, maintaining the alignment becomes more challenging.

- Laser power can now be modulated into short pulses or various ramp (up or down) paths and synchronized with diffraction and temperature measurements. This capability is a useful tool for studies of high-pressure melting phenomena and also enables time-resolved studies.
- The capability to synchronize the XRD measurement at 500 ns exposure with the APS hybrid singlet mode (8 groups of 7 consecutive bunches in 500 ns) has been established. This capability can be used for time-resolved and pump-probe studies.
- Synchronized laser pulse with thermal imaging allows for monitoring the temperature distribution on samples during pulsed laser heating experiments. The setup allows the recording of thermal images from the heated samples with exposure times down to 1 µs, which is crucial for controlling the sample heating, temperature homogeneity and position alignment in time-resolved experiments.

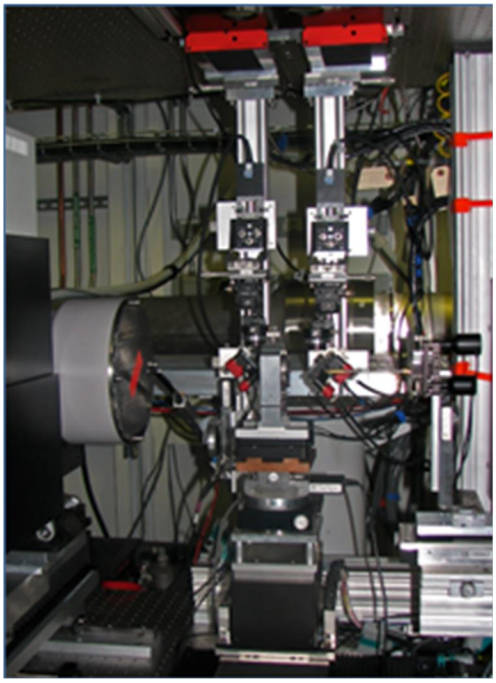

Figure 58. *View of heating mirrors in double-sided laser heating setup at 16-ID-B. The heating lasers and other associated optics are conveniently located on an elevated table, above the table holding the sample stage and detector.*

16-BM-D: X-ray Absorption and Microdiffraction – With the commissioning of x-ray absorption techniques at 16-BM-D, this station has become heavily subscribed for a variety of challenging measurements at high pressure. Important new developments at 16-ID-B include the following.

A Perkin-Elmer amorphous Si pixel array detector (2048 × 2048 pixels with 200 µm fixed size) at the 16-BM-D station now readily achieves high-resolution XRD at the level of $\Delta q/q \sim 2.5\times10^{-3}$ angular resolution as a result of locating the detector at a large sample-to-detector distance (up to ~900 mm). The new instrumental setup substantially reduces the data acquisition and reduction time.

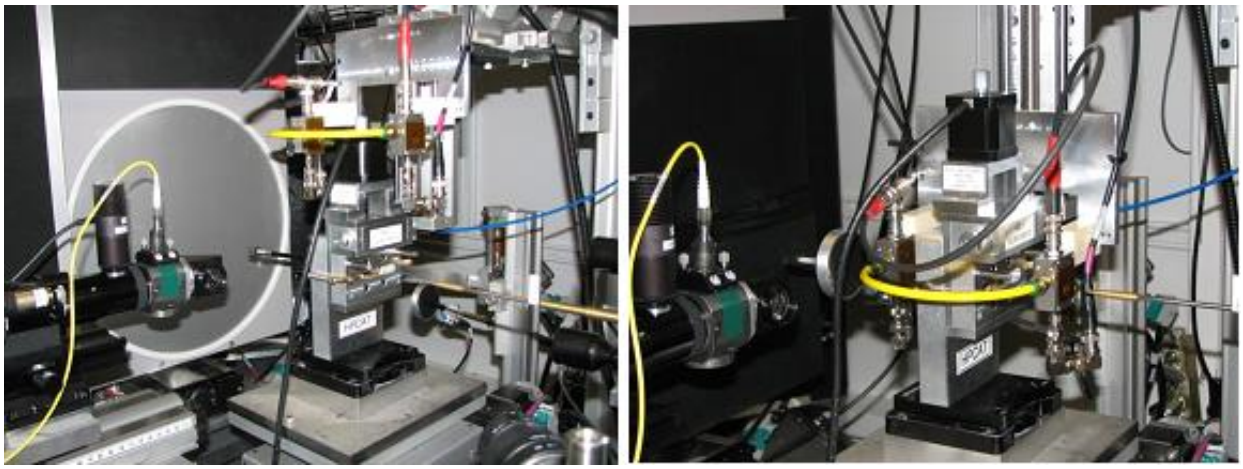

Figure 59. *Interchangeable micro-XRD (left) and XANES (right) setup at 16-BM-D provides a simultaneous probe of atomic and electronic structure at the same sample conditions.*

The XANES measurement has been newly introduced for the 16-BM-D station. The focused (4-5 μm horizontal and 12-15 μm vertical) monochromatic x-ray beam, for which the energy is determined by a Si (111) double crystal monochromator in pseudo-channel cut mode, is delivered to the sample stage with minimal offset of beam height (~2 μm per 1 keV scan range). The capability of performing an energy scan while keeping the finest focus of beam at the sample enables conducting the XANES measurement with DAC samples. The capability of high-energy XANES measurements for K-edge absorption spectroscopy of heavy elements (*e.g.*, Ce K absorption edge at 40.443 keV) is unique to16-BM-D compared to other stations. The ion-chamber detectors for the XANES measurement are mounted on an in-and-out type pneumatic stage, which is fully compatible with the standard XRD setup at 16-BM-D, so that the XANES measurement can be easily combined with high-resolution XRD measurements without disturbing the sample (Fig. 59).

16-BM-B: White-Beam Laue Diffraction – Currently, the white beam diffraction setup is under commissioning at 16-BM-B. This is intended for time resolved studies of crystal lattice defects and deformation *in situ* under external stress. Potential areas of application may include studies of mechanisms defining kinetics of pressure-induced phase transitions or phase transformations under high pressure such as melting or crystal growth, mechanisms of deformation, and shock compression.

Over the past year some measurements on single crystals during pressure induced phase transitions have been performed. For example, spatially resolved white beam Laue data from Si during the α-β phase transition have been obtained. A series of consecutive 2D translational scans have been collected on a Si single crystal until the phase transition was completed. The alteration due to the phase transition was indicated by the appearance of additional diffuse reflections, and at the same time the original single crystal of α-Si exhibited splitting into distorted blocks (Fig. 60). The altered areas have been located right between the blocks of the α-phase.

Improvements in the data reduction process have focused on the development of an approach to quantify crystal lattice rotations. Precision better than 0.05° was obtained from one diffraction pattern typically collected in 0.5 seconds of exposure. Important to note is the fact that such a measurement with a monochromatic beam would require fine angular slicing and it would take at least tens of seconds to get enough data. Total data collection time would be 1-2 orders of magnitude longer than with the Laue technique, and even then most of the observed changes during the studied phase transitions would not be identified.

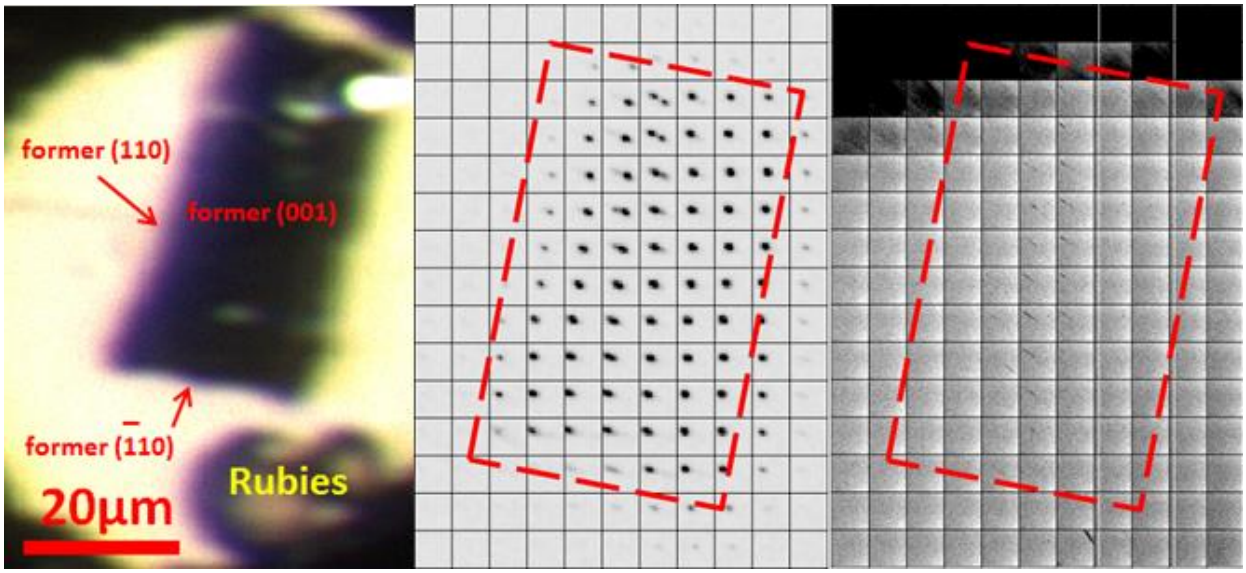

Figure 60. *Left: Si single crystal at pressure right above the α-β phase transition. Center: composite frame of the (862) reflection of α-Si. Right: composite frame of diffuse reflection from the altered area. Red frames on the center and right images reproduce the shape of the original sample.*

16-BM-D: Paris-Edinburgh Cell Program – Techniques for measuring liquid structure, elastic wave velocity, and viscosity under high pressure have been optimized for the Paris-Edinburgh cell at 16-BM-B. The Paris-Edinburgh press allows for compressing large volume samples (up to 2 mm in both diameter and thickness) up to ~7 GPa and 2000 °C.

Ongoing development for anvil and cell design recently enabled measurements at up to ~12 GPa and 1800 °C. Multi-angle energy dispersive XRD provides structure factors of liquids to a large Q of ~20 $Å^{-1}$. Ultrasonic techniques have been developed to investigate elastic wave velocities of amorphous solids and liquids combined with the x-ray imaging. Falling sphere viscometry, using high-speed x-ray imaging (>1000 frames/second), enables investigations over a wide range of viscosity, from those of high viscosity silicate or oxide melts to low viscosity (<1 mPa s) liquids and fluids such as liquid metals or salts. The integration of these multiple techniques has promoted comprehensive studies of structure and physical properties of liquids as well as amorphous materials at high pressures and high temperatures, making it possible to investigate correlations between structure and physical properties of liquids and amorphous solids.

This phase contrast imaging setup has allowed observations of the behavior of low density contrast liquids such as water and oil, which will eventually enable studies of phase separation and liquid-liquid immiscibility at high pressures and high temperatures.

Preliminary experiments with the dynamic DAC were conducted for water by optical imaging (Fig. 61). The sample was rapidly decompressed, and high-speed optical imaging (5000 frames/second) successfully monitored the melting behavior of water, and subsequent falling of a ruby ball in water, which provides important information for determining viscosity. High-speed x-ray imaging allows observations of not only optically transparent materials but also opaque materials such as liquid metals. The combination of high-speed x-ray imaging and the dynamic DAC opens up new techniques for studying the nature of melting/crystallization and the behavior of liquids at high pressures.

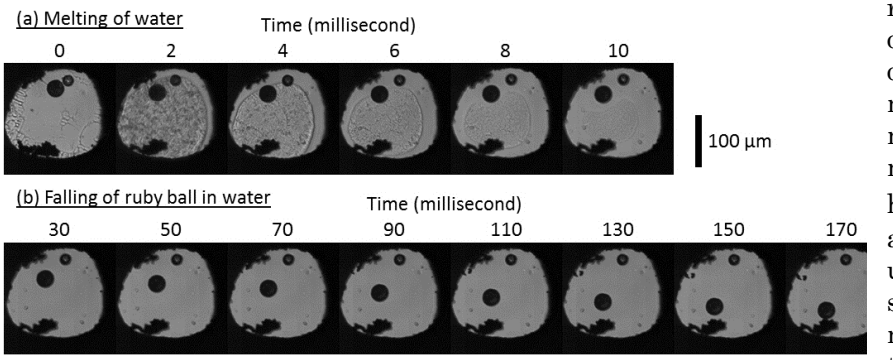

Figure 61. *a) High-speed imaging of the melting of water. b) Subsequent falling of a ruby sphere in water.*

Supporting Facilities at HPCAT – Ancillary capabilities at HPCAT are crucial to the success of the overall experimental program, and all personnel dedicate significant effort to improve these facilities on an ongoing basis to expand the available *P-T* range of the experimental conditions, increase efficiency and productivity of the beamlines, improve the quality of experimental data, and integrate additional methods of sample characterization with synchrotron investigations.

In order to fully utilize remote pressure control capabilities, a number of portable online optical systems for ruby fluorescence pressure measurements and *in-situ* Raman sample characterization have been designed. Now, online optical systems are available for every experimental station at HPCAT. Combined with remote pressure control systems, they significantly increase the productivity of beamlines during high-pressure experiments.

Techniques and instrumentation have been developed for collecting high-quality, time-resolved x-ray scattering data and bridging the gap between static and dynamic high-pressure measurements by enabling rapid controlled uni- and bi-directional or cyclic sample compression/ decompression up to extreme compression rates in excess of a TPa per second. These time-resolved

techniques are currently used for synthesis/observation of metastable high pressure phases, and studying phase transition kinetics and fast rheology.

Because sample quality is a major factor in success of any experiment, HPCAT has established state- of-the-art sample preparation and characterization facilities, which include numerous modern microscopes, a glovebox, sample polishing facilities, a laser drilling and micromachining unit, and offline laser heating and Raman systems.

4.2 HPCAT-CDAC Collaborations

High Pressure Mineral-Fluid Interface Cell – The electron density profile of a mineral-water interface and the element-specific sub-profile can be measured with synchrotron-based high- resolution x-ray reflectivity (HRXR) and resonant anomalous x-ray reflectivity (RAXR) techniques, and it has been known that the interfacial structure and processes are highly specific to the system due to inherent complexity of solid surface. T he convoluted effects of a surface termination, morphology, chemistry, and charge distribution typically result in a unique interfacial profile and process for each individual system. However, the experimental approaches with HRXR and RAXR have been limited to the sample conditions only with ambient pressure and temperatures lower than 100 °C due to limited sample cell capabilities, which in turn limits the utilization of the experimental techniques only to non-hydrothermal systems. To overcome this limitation, **Changyong Park** at Carnegie has developed a high *P-T* aqueous interface cell that can maintain static pressure and temperature conditions up to 40 MPa and 500 °C (Fig. 62). Pilot tests of the new cell and the preliminary applications to the olivine (010)-water interface have been made at HPCAT ID-D and APS Sector 5-ID-C.

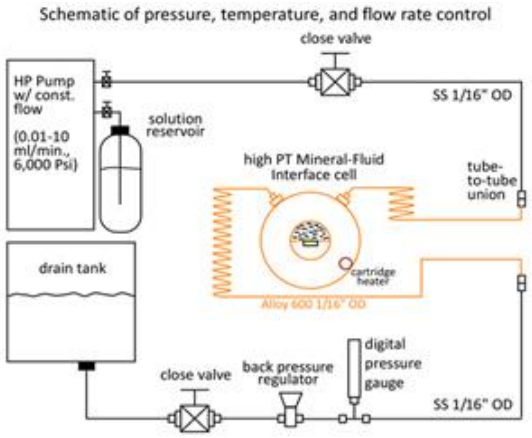

Figure 62. *Schematic diagram of the pressure, temperature and flow control of the high pressure mineral-fluid interface cell.*

High P-T Thermal Measurements in the Paris-Edinburgh Cell – Discretionary CDAC beam time was utilized the development of simultaneous XRD, x-ray radiography, electrical resistance, and thermal measurements with the Paris-Edinburg (PE) cell. Laboratory Partner **Nenad Velsavljevic** (LANL) and student **Jason Baker** collaborated with **Ravi Kumar** (UNLV), **Changyong Park** to improve the experimental setup and establish the feasibility of performing the

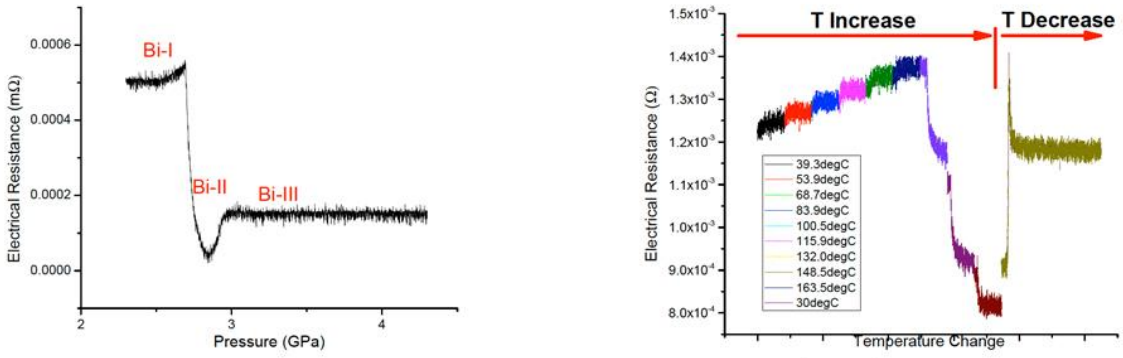

Fig. 63*. Left, Variation in electrical resistance in Bi during isothermal (298 K) compression as the sample undergoes the I→II→II structural transitions. Right, isobaric (2.2 GPa) heating results in a gradual change in electrical resistance as the sample undergoes the I→II transition.*

combined measurements with PE cell. Preliminary measurements were performed on Bi metal and feasibility was demonstrated up t to ~6 GPa and ~1000°C (Fig. 63).

A New Furnace for High-Temperature NRIXS Measurements – Graduate student **Lisa Mauger**, from the **Fultz** group at Caltech, has developed a specialized furnace that can be interfaced to beamline 16-ID-D at HPCAT to carry out NRIXS measurements at elevated temperatures (Fig. 46). The work was carried out in collaboration with former CDAC student **Matt Lucas** at the Air Force Research Laboratory.

4.3 Frontier Synchrotron Infrared Spectroscopy under Extreme Conditions

The Frontier Synchrotron Infrared Spectroscopy (**FIS**) Beamline for Extreme Conditions has been approved as one of the eight NxtGen beamlines to be developed and constructed at NSLS-II. **FIS** is the successor of the IR-DAC facility (U2A) at NSLS, the highly productive, Carnegie-managed user facility supported by COMPRES and CDAC, and the only dedicated high-pressure synchrotron IR facility in the world.

As announced in May 2012 at the NSLS/CFN Joint Users' Meeting by Dr. Steve Dierker, Associate Laboratory Director for Photon Sciences, NxtGen is a set of eight beamlines at NSLS-II that will be based on components from beamlines at NSLS. Carnegie's **Zhenxian Liu** and **Russell Hemley** and the FIS team have been working closely with the BNL Photon Sciences staff to move forward with the development of FIS. A Beamline Execution Plan detailing the **FIS** project is in the advanced draft stage.FIS will adapt one of the novel design features of NSLS II – the large-gap IR dipole. Construction of the beamline hutch on Bending Magnet Port 22 will be completed and all existing equipment at U2A moved in by early 2015. At that time, the integrated optical facility for far-IR to UV absorption and reflectance spectroscopy with conventional sources, together with laser Raman and photoluminescence spectroscopy will open to users for experiments – *i.e.*, during the NSLS/NSLS-II "dark period." Full synchrotron IR capability will be available no later than 2017, with early completion anticipated pending efforts to obtain supplemental funding.

The FIS beamline will enable *in-situ* optical studies of a wide variety of mateirals by spectroscopic techniques at extreme *P-T* conditions, from ambient to several megabars, and from 4-6000 K. Measurements from the far-infrared to visible range will be possible with diffraction-limited resolution. The combination of the high brightness and low noise of NSLS-II with dedicated high pressure facilities will be unique in the world.

4.4 Technique Development at Carnegie

Melting of Refractory Transition Metals – The mechanical strength of materials is known to decrease drastically at temperatures as low as half of their melting points, and the melting behavior of various metals has shown a large variation in their dependence on stress. The direct and accurate measurement of melting temperatures of these metals under extreme stress is therefore not only imperative in understanding the fundamentals of melting but also important

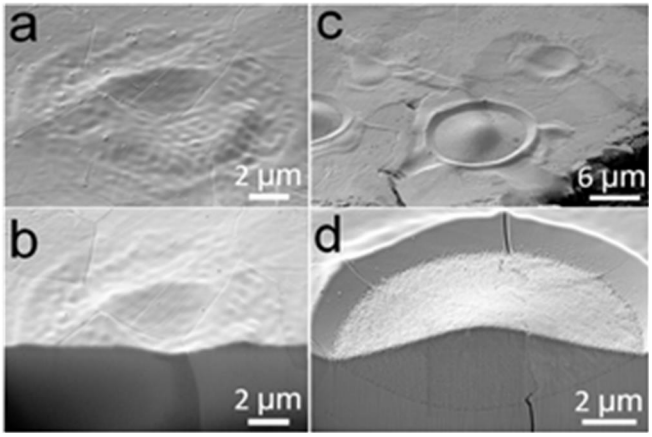

Figure 64. *SEM photos of laser-heated spots at 3538 K (a, b) and 4326 K (c, d) on the Re sample recovered from 22 GPa. Surfaces are shown in (a, c), and cross sections through the laser heated spots are shown in (b, d). Recrystalliazation to sub-μm depth with no change in textural appearance is evident in (b), compared with the unheated portion. Complete restructuring of the metal with a sharp boundary to a depth of several μm between the quenched liquid and the unmolten sample is shown in (d).*

for synthesizing new strong materials. Measuring melting under high pressure is challenging, however. Typical notorious problems associated with prolonged measurements (a few seconds) in a LHDAC are chemical reactions, sample instability and thermal runaway, while using too short a laser heating time (~μs) increases temperature uncertainty. To address these problems, Carnegie's **Reinhard Boehler** and graduate student **Amol Karandikar** have developed a new "flash heating" method for melting studies at high pressure in the LHDAC.[53]

Polished metallic samples (50-60μm diameter, 8-10μm thick) are loaded in the DAC in an inert argon pressure medium that also provides thermal insulation from the diamond on the side to be heated. A heating laser (1070 nm) is aligned with an optical setup for measuring temperatures. The sample is heated with a 20 ms rectangular laser pulse, and the thermal response is monitored with a fast photomultiplier while measuring the steady state temperature with a CCD spectrometer. The 20 ms pulse is long enough to measure the temperature reliably and short enough to avoid any chemical reaction and thermal instabilities in the sample. For each new unheated area on the sample, the laser power is increased to produce a temperature rise of ~100 K. Typically, one sample disc is sufficient for 8-10 heated spots while recording both temperatures and locations.

Samples are then recovered to ambient conditions and are analyzed using Scanning Electron Microscopy (SEM) for imaging the surface topography of the heated areas. Energy dispersive x-ray spectroscopy (EDS) is performed to check for evidence of any chemical reaction. Focused Ion Beam (FIB) techniques are used to examine cross-sections of heated spots, both laterally and vertically. The first appearance of beadlike features several μm in depth is attributed to melting due to the textural similarities observed with the samples heated at one atmosphere. The melting temperature is determined by averaging the highest temperature without appearance of any bead (solid) and the lowest temperature with appearance of a bead (liquid).

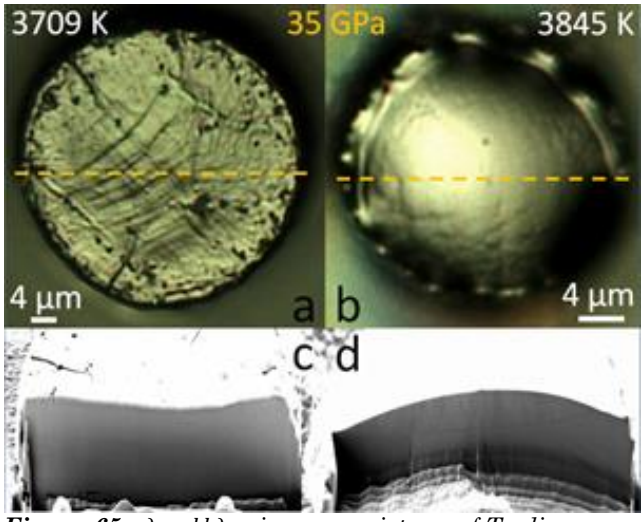

Figure 65. *a) and b): microscope pictures of Ta discs recovered from 35 GPa and heated at 3709 K (below melting) and 3845 K (above melting), respectively. c) and d): corresponding FIB cross-sections viewed across the dotted yellow lines.*

Using the flash heating method, the melting of rhenium (Re) was measured to 47.4 GPa and 4600 K, a 5-fold extension of previous data (Fig. 64). Flash heating was successfully used in reproducing the previous melting curve of Mo measured by different techniques in the LHDAC, up to 45 GPa.

The difficulty in measuring melting temperatures of refractory metals in the LHDAC is perhaps best demonstrated by the discrepancy in the reported measurements on Ta. Using various methods to detect melting and measure temperatures, large differences in the melting slopes have been observed above 50 GPa, the chemical reactivity of Ta being the main difficulty. Flash heating measurements have now been successfully performed on Ta up to 85 GPa and 4318 K. Instead of heating the same sample at different locations at different temperatures, a given Ta sample was heated only at a single spot a single time at a predetermined temperature and pressure and then recovered to ambient conditions for further SEM, EDS and FIB processing and analysis (Fig. 65).

Heating at sub-liquidus temperatures only alters the surface to sub-micrometer levels, whereas melting produces significant structural changes several μm below the surface and a complete restructuring of the surface. EDS performed on T_a samples showed no sign of chemical reaction. The melting curve thus constructed explicably disagrees with previous experimental reports.

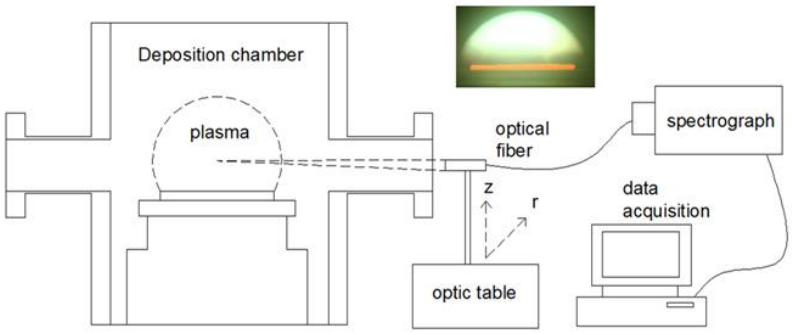

Figure 66. *Optical emission spectroscopy setup for plasma diagnostics during single crystal diamond growth. The inset photograph shows plasma and substrate inside the MPCVD deposition chamber.*

The flash heating method can be employed with minimal modification of a standard LHDAC setup. It allows chemically clean, reliable and reproducible measurements of melting curves of metals with error less than 200°.

Optical Emission Diagnostics of CVD Diamond Growth – A key aspect of single crystal diamond growth via microwave plasma assisted chemical vapor deposition (MPCVD) is in-process control of the local plasma-substrate environment, that is, plasma gas phase concentrations of activated species at the plasma boundary layer near the substrate surface. The underlying mechanisms controlling the size, position, and properties of the plasma discharge, particularly at the boundary layer near the substrate that affect diamond growth rate, are still not well understood. To investigate these processes, a non-intrusive diagnostic, such as optical emission spectroscopy (OES) has been developed at Carnegie. OES is a simple, *in situ* method that does not perturb the highly reactive plasma and probes electronically excited atoms and molecules, species concentrations, atomic relative densities, gas temperature, and the electron temperature of plasma discharge.

The emission intensity signal was collected using a fiber optic cable across a line of sight passing through the window of the observation port and pointed to the discharge inside the deposition chamber 15 cm away and 90º to the axis of the reactor (Fig. 66). A computer connected to the spectrometer was used for data acquisition with typical collection time of 100 ms.

Argon was added into the plasma in order to investigate the emission behavior of the plasma and its influence on the CVD diamond growth rate. Ar was selected due to its inertness, which does not perturb the plasma. Ar is excited to its radiative excited states mainly by a direct electron impact process. The radiative states of Ar have excitation thresholds close to that of the H atom in the $n = 3$ level.[54]

Visual observation showed that the luminous intensity of the plasma discharge increases as Ar is injected into the process chamber. The measured intensities of the three Ar lines also increase by adding argon into the deposition process chamber. However, the Hα, Hβ, and Hγ emissions stay constant. This suggests that Ar has little influence on the H chemistry and the contribution of argon to the excitation of H ($n = 3$) is negligible. Hence, Ar can be used as an actinometer, allowing the estimation of the relative concentration of species in their ground states within the plasma discharge.[54, 55]

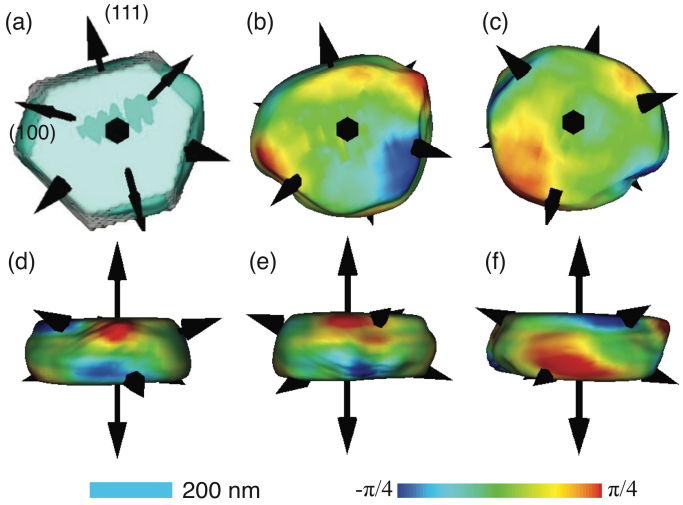

Figure 67. *Strain distribution in a 400 nm gold single crystal at 1.7 GPa, as detected by the recently developed coherent diffraction imaging technique. (a) Crystal shape and surface truncated (100) and (111) plances. (b) and (c), top and bottom views. (d) – (f), side views, rotated 120º along the surface normal direction. Color represents the lattice strain (phase shift) from –π/4 to π /4.*

X-Ray Nanoimaging – At HPSynC, **Wenge Yang** and co-workers from Carnegie, the APS, and University College London have made a major breakthrough in measuring the structure of nanomaterials under pressure. For the first time, a way to get around the severe distortions produced by high-energy x-rays that are used to image structures has been developed. The technique will eventually lead to new nanomaterials created under pressure and a greater understanding of material deformation. By averaging the diffraction patterns of the same single crystal using different sample alignments and using an algorithm developed by a group at the London Centre for Nanotechnology, it is possible to compensate for distortion and improve spatial resolution by two orders of magnitude. The technique was used to study a 400 nm gold nanocrystal from about 800 MPa to 6.4 GPa (Fig. 67).

These measurements were carried out on Beamline 34-ID-C at the APS. At first, as expected, the edges of the crystal become sharp and strained, but disappear under further compression. The crystal develops a more rounded shape at the highest pressure, implying an unusual plastic-like flow. In fact, nanoscale gold particles are very useful materials as they are about 60% stiffer compared with other micron–sized particles and could prove pivotal for constructing improved molecular electrodes, nanoscale coatings, and other advanced engineering materials.

4.5 Technical Development at Academic Nodes

Shock Wave Spectroscopy – Over the past few years, the **Dlott** group at Illinois has developed a shock wave spectroscopy apparatus that uses a one-box laser to launch flyer plates.[56, 57] An 8 GHz photon Doppler velocimeter (PDV) is used to monitor the launch, flight and impact of 0.7 mm diameter Al flyer plates with various sample materials. The current arrangement of the system standard is shown in Fig. 68. The apparatus can be interfaced with a variety of spectroscopic tools. Under conditions used in the apparatus, the flyers are launched by a shock from the glass substrate right under the metal foil, so the flyers see very little laser intensity. They do not melt or vaporize. By stretching the laser pulses using an external pulse stretcher, the group has shown that it is possible to find conditions that eliminate the effects of reverberating shocks. The tilt is minimal, <1 μm, so that it introduces a time dispersion of 1 ns or less.

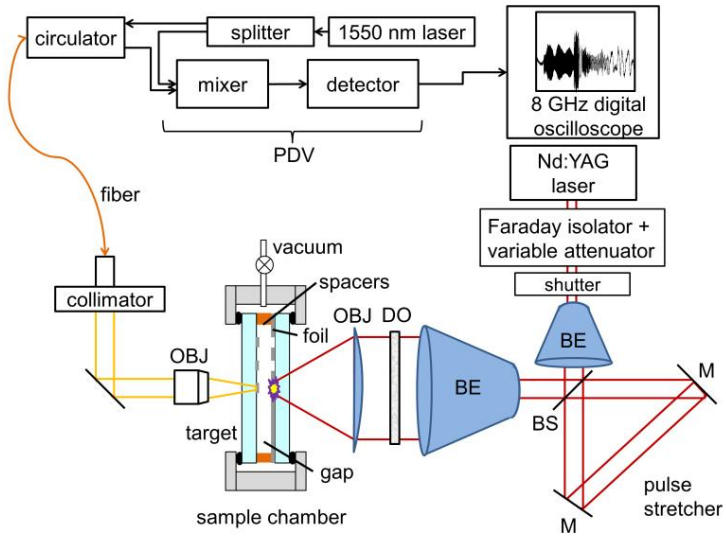

Figure 68. *Schematic of laser flyer launch system with photonic Doppler velocimeter (PDV). M = mirror, BS = beam splitter, BE = beam expander, DO = diffractive optic, OBJ = objective lens.*

New diagnostic capabilities are under development. High-speed thermal imaging is used to measure temperature profiles in shocked inhomogeneous materials. Also, a Raman system is under construction and a few preliminary measurements have been made. Currently CDAC graduate students **Will Shaw** and **Will Bassett** are interfacing a femtosecond IR laser that will be used for IR absorption spectroscopy of shocked materials and liquids. Also, a 1 ns, 32 channel optical pyrometer to study the temperature dynamics of shocked reactive materials is also under development. All these improvements will expand the range of materials and conditions under which shock compression may be explored.

Finally, new sample fabrication techniques suitable for the study of powders and liquids are under development. These involve producing large-area samples having arrays of wells of known

thickness that can be filled with sample materials. For instance, a sample might consist of a 50 x 50 mm^2 glass square having 100 wells, each slightly larger than the flyer plate and 50 µm thick. This becomes tricky when the sample is a volatile liquid, and for this application microfluidic arrays have been developed. This technology will be used to study particulate media that mimic soils and sand or solid propellants, and liquid media such as aqueous solutions and liquid explosives.

Diamond Anvil Cell Calorimeter **– Zack Geballe,** a student in the **Jeanloz** group at UC-Berkeley, has been developing a calorimeter for DACs, building on past modeling of heat transport.[58] In collaboration with LLNL (**Rip Collins**) and the EECS department at UC Berkeley, he is making high-frequency, high-dynamic-range electrical diagnostics in order to measure heat capacity at high pressures. Together with **Andrew Townley** (EECS), he is using a combination of waveform generators, op-amps, electrical filters and digitizers to send up to 1 A of current through thin metal samples pressed against the table of a diamond anvil (which acts as a heat sink), and measuring the first and third harmonics of voltage across a 4-point probe. The goal is to adapt the method to high pressures in order to study pre-melting, melting and partial melting phenomena using up to 100 MHz modulated Joule heating. Currently, the EECS group is designing a suitably buffered voltage source with high harmonic purity at high frequency. In particular, they are modeling all details of the experiment, combining heat flow models, analytical calculations and LTSpice, a powerful electrical engineering code that represents a new tool for high-pressure research. More broadly, once developed, high-frequency electronics adapted to the diamond cell geometry could be useful for a range of dynamic heating, electrical and/or magnetic experiments inside DACs.

5. MANAGEMENT AND OVERSIGHT

5.1 CDAC Organization and Staff

CDAC is managed at **Carnegie** by a small staff comprised of the Director, Coordinator, Administrative Assistant and two Research Scientist/Laboratory Managers and two Research Scientist (Fig. 69). Daily operations of the Center are carried out by the Director, Coordinator and Assistant, while CDAC laboratory facilities at Carnegie are supervised by the Laboratory Managers. Research Scientists spearhead specific projects of interest to the CDAC research program. In addition to oversight of CDAC facilities at Carnegie, the Laboratory Managers assist CDAC visitors with experiments and sample preparation, in addition to training summer undergraduate students as part of the Carnegie Summer Scholars Program.

Russell Hemley, CDAC Director, is also a Staff Scientist at the Geophysical Laboratory at Carnegie. Other members of the Scientific Staff at Carnegie that are involved directly with CDAC are:

- **Ronald Cohen** Computational Theory
- **Yingwei Fei** Geochemistry, Petrology and Materials Science
- **Timothy Strobel** Energy Materials
- **Viktor Struzhkin** Electronic, Magnetic, and Structural Properties
- **Takamitsu Yamanaka** Senior Visiting Fellow

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

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

Postdoctoral fellows, predoctoral students and visitors at Carnegie supported by the Institution, other grants, or outside fellowships often work with the CDAC group as part of their

research program. Their contributions also include training CDAC students, undergraduate summer scholars, and visitors in high-pressure experimental techniques:

- **Kadek Hemawan** (CVD Diamond)
- **Caitlin Murphy** (Geophysics)
- **Todd Zapata** (Magnetic/Electronic Properties of Materials)

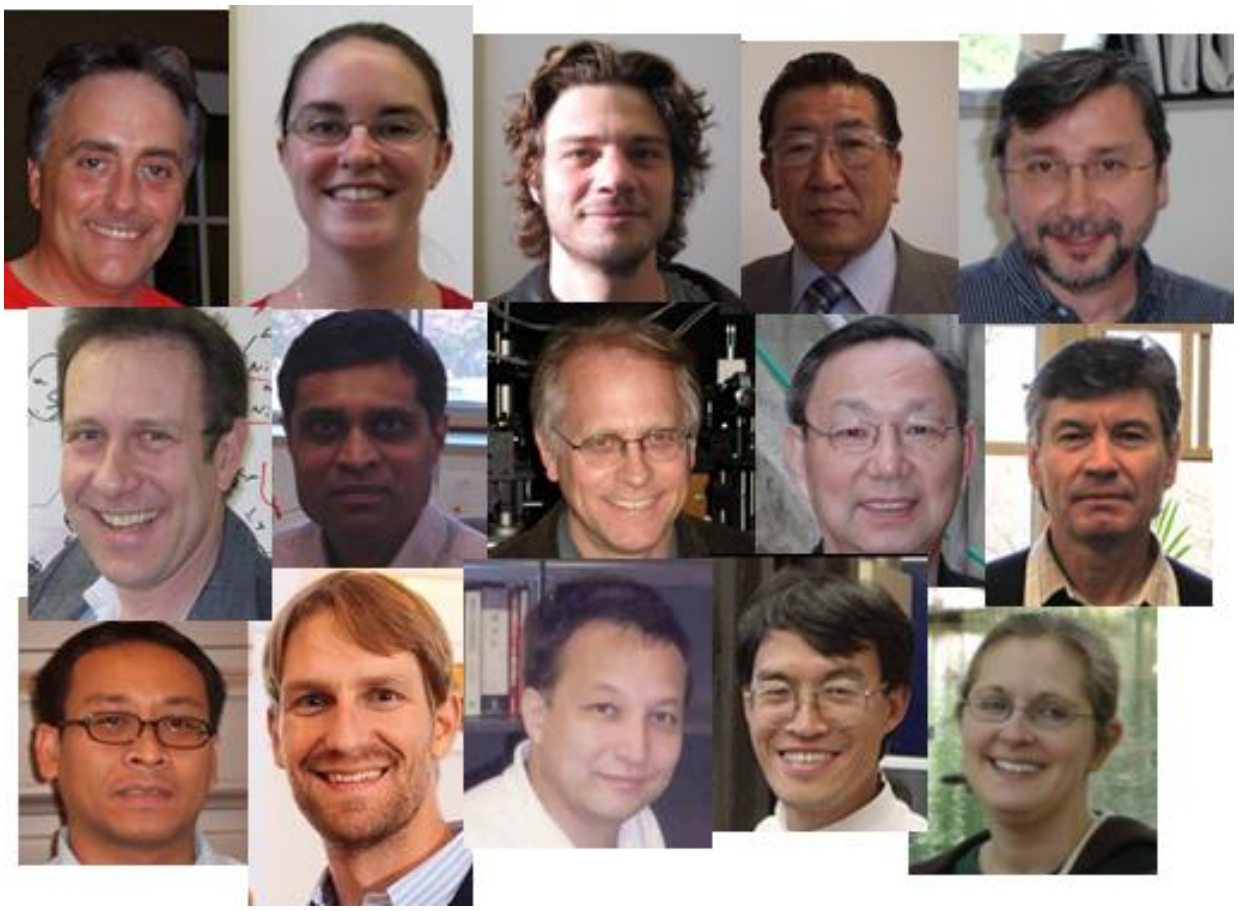

Figure 69. *CDAC affiliated personnel at* ***Carnegie*** *for 2013-2014.*

5.2 CDAC Oversight

CDAC Steering and Advisory Committees have been instrumental in providing input on the direction of the CDAC research program (Fig. 70). Steering Committee members informally advise CDAC management on near-term operational issues and act as points of contact with their respective Directorates and Divisions. Steering Committee members also evaluate yearly proposals for graduate student support from the Academic Partners. The CDAC Steering Committee consists of:

- **Neal Chesnut** (University of West Georgia)
- **Gilbert W. (Rip) Collins** (LLNL)
- **Dana Dattelbaum** (LANL)
- **Daniel Dolan** (SNL)
- **Jon H. Eggert** (LLNL)
- **Marcus Knudson** (SNL)
- **Nenad Velisavljevic** (LANL)

The Advisory Committee assists with long-term strategic planning and provides points of contact between CDAC and the NNSA Labs, other SSAA Centers, and the broader academic community. Current members of the CDAC Advisory Committee are

- **Neil W. Ashcroft** (Cornell)
- **Robert Cauble** (LLNL)
- **Dawn Flicker** (Sandia)
- **David Funk** (LANL)
- **Alan J. Hurd** (LANL)
- **Chi-chang Kao** (SLAC)
- **Christian Mailhiot** (LLNL)
- **Tom Mehlhorn** (SNL)

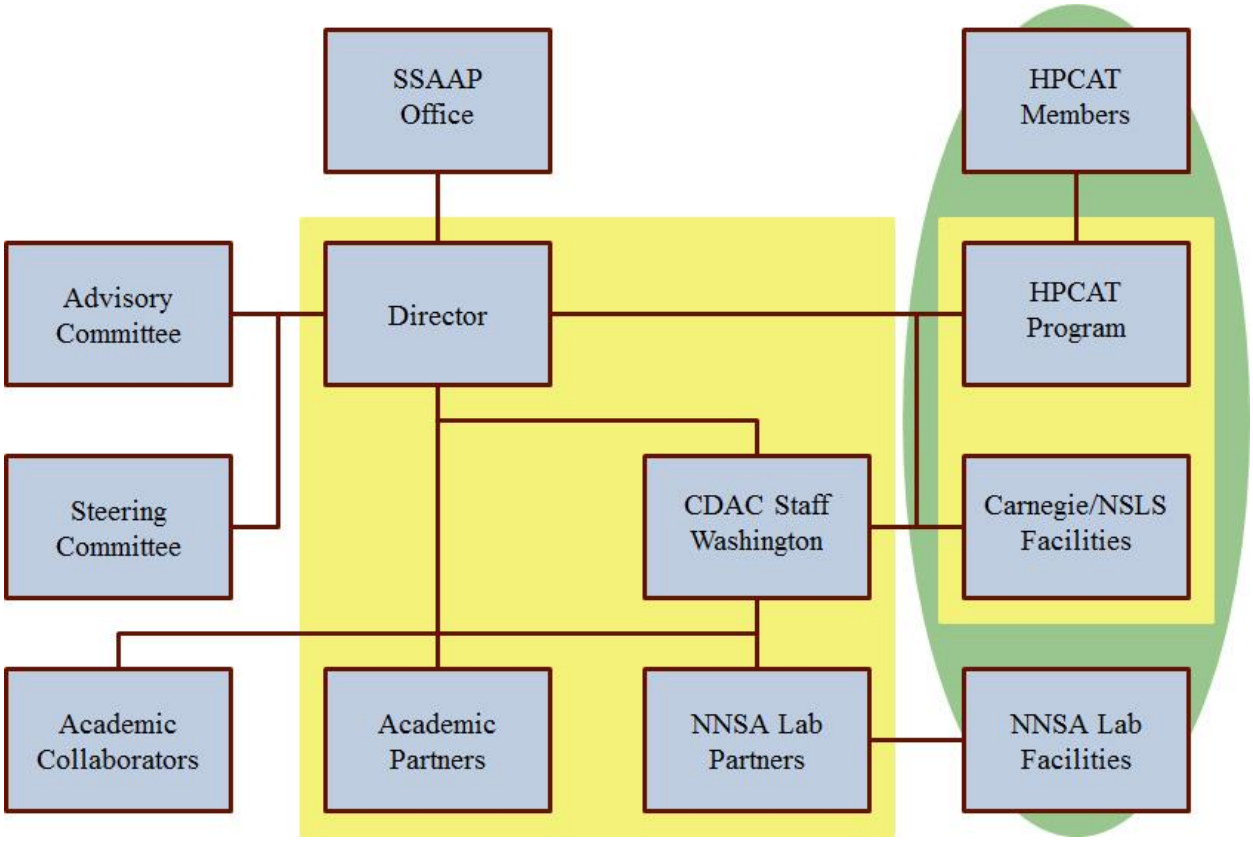

Figure 70. CDAC organizational chart. The yellow areas designate the principal components of CDAC. The oval area encompasses the three different groups of experimental facilities associated with CDAC.

We encourage members of both CDAC oversight committees to attend regular **HPCAT** meetings and invite them to attend all CDAC functions. Members of both committees are updated regularly on progress in the scientific program, innovations in technique development, and plans for outreach.

APPENDIX I: CDAC Publications and Presentations for 2013-2014

We list publications and presentations for 2013-2014, including all work supported fully or in part by CDAC. This list therefore includes work carried out at HPCAT by all of its members and users during this period.

A. CDAC Publications

Ahart, M., C. DeVreugd, J. Li, D. D. Viehland, P. M. Gehring, and R. J. Hemley, X-ray diffraction study of the pressure-induced bcc-to-hcp phase transition in highly magnetostrictive $Fe_{0.81}Ga_{0.19}$ alloy, *Phys. Rev. B* **88**, 184102 (2013).

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Armentrout, M. M., E. S. G. Rainey, and A. Kavner, High-pressure and high-temperature equation of state of cobalt oxide: Implications for redox relations in Earth's mantle, *Am. Mineral.* **98**, 993-999 (2013).

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Baker, J., R. S. Kumar, N. Velisavljevic, C. Park, C. Kenney-Benson, Y. Kono, A. Cornelius, and Y. Zhao, In situ x-ray diffraction, electrical resistivity and thermal measurements using a Paris-Edinburgh cell at HPCAT 16BM-B beamline, *J. Phys.: Conf. Series* **500**, 142003 (2014).

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Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides and subhydrides (invited), *Joint APS-SCCM & AIRAPT-24 Conference* (Seattle, WA, July 7-12, 2013).

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Zurek, E., Structure prediction from first principles calculations (invited_, *MRSEC/CNFM Conference for Undergraduate Women in Physical Sciences - WoPhys* (Lincoln, NE, October, 2013).

Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides and subhydrides (invited), *Department of Chemistry Seminar, SUNY Geneseo* (Geneseo, NY, October, 2013).

Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides and subhydrides (invited), *Inorganic/Physical Seminar, University of Rochester* (Rochester, NY, September, 2013).

Zurek, E., Building a chemical intuition under pressure: Prediction of alkali metal polyhydrides and subhydrides (invited), *High Pressure Seminar, Max Planck Instutit fur Chemie* (Mainz, Germany, June 2013).

Zurek, E., Structure prediction from first principles (invited), *The Minerals, Metals and Materials Society Annual Meeting* (San Diego, CA, February, 2014).

Zurek, E., Boron nitride under extreme conditions (invited), *2013 CDAC Annual Review* (Argonne, IL, September 16, 2013).

Zurek, E., Structure prediction from first principles (invited), *Texas Women's University* (Dallas, TX, March, 2014).

APPENDIX II: CDAC Synchrotron Users/Experiments (APS and NSLS) for 2013-2014

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 in HPCAT obtained by CDAC, the support generated by SSAP funding made possible significant scientific productivity of the state-of-the-art high-pressure facility.

User Name	Affiliations	Project	Dates
Z. Chen B. Chen	HPSTAR	Metallization of Nanocrystals	May 30-31, 2013
Z. Zhao	Stanford University	High pressure study of Sb_2O_3 and $MoSe_2$	May 30-June 1, 2013
Z. Jenei	LLNL	Ultrasound study of Pr	May 31-June 4, 2013
J. Zhu	LANL	Nano-size effects of ferrelectric $BiScO_3$-$PbTiO_3$ composites	June 1-3, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	June 1-3, 2013
Y. Peng	HPsynC	IXS investigating TiM edge	June 1-5, 2013
Y. Ding	ANL	High-pressure IXS study of Fe M23 edge	June 1-6, 2013
C. Tracy M. Lang A. Romanenko	University of Michigan GSI Darmstadt	The response of actinide oxides to irradiation fields of fission track energies	June 1-8, 2013
Y. Kono	HPCAT	Development of ultrasonic measurement of liquid	June 5-6, 2013
S. MacLeod	Atomic Weapons Establishment, UK	Melting of uranium	June 5-8, 2013
H. Cynn	LLNL	5*f* metal compression	June 6-9, 2013
W. Yang	HPSynC	High *P-T* study of SiSn liquid phase	June 6-9, 2013
M. Pravica L. Bai	University of Nevada – Las Vegas	Studies of oxygen- and nitrogen-containing compounds subjected to extreme conditions using x-ray Raman spectroscopy	June 6-9, 2013
Q. Smith	University of Nevada – Las Vegas	X-ray induced decomposition	June 6-9, 2013
G. Guardala	University of Nevada – Las Vegas	High pressure studies of nitrogen-, oxygen-, and fluorine-containing compounds	June 7-9, 2013
Q. Hu	George Mason University	High pressure behaviors of coesite	June 8-10, 2013
X. Chen	Carnegie	TaS_2 diffraction under pressure	June 8-10, 2013
Y. Ye S. H. Shim Q. Zhang C. Nisr	Arizona State University	High pressure properties of mineral physics in subduction oceanic crust	June 8-11, 2013
Y. Peng	HPsynC	TiH_2 diffraction under high pressure and high temperature	June 9-10, 2013
S. Yu E. J. Kim	Seoul National University, Korea	Inelastic x-ray scattering study of Fe bearing multi-component silicate glasses at 1 ATM and high pressure	June 9-13, 2013
J. Y. Chen	LLNL	Time-resolved XRD measurements	June 10-14, 2013
L. Wang	HPSynC	Synthesis of polymerized C60 at high pressure and temperature conditions	June 10-30, 2013

C. Stan	Princeton University	(Mg,Fe)GeO_2 perovskite-postperovskite compression	June 12-14, 2013
T. Duffy G. Finkelstein	Princeton University	High pressure phase transition in YIG	June 12-14, 2013
Y. Kono	KPCAT	Development in PE cell techniques	June 12-16, 2013
R. Chellappa N. Velisavljevic	LANL	XRS measurements of FOX-7	June 12-17, 2013
L. Bai	University of Nevada – Las Vegas	High pressure XRD and XANES studies of MoS_2	June 14-15, 2013
B. Chen	University of Illinois – Urbana-Champaign	High-pressure single-crystal x-ray microdiffraction investigation of s-triazine derivatives	June 14-15, 2013
P. Dera	University of Chicago	High-pressure single-crystal x-ray microdiffraction investigation of s-triazine derivatives	June 14-16, 2013
B. Li	HPSTAR	High pressure study of Se	June 16-17, 2013
J. Liu Z. Li	University of Michigan	Thermal equation of state of $Fe7C_3$ up to 100 GPa and 1000 K	June 16-18, 2013
A. Connolly	University of Nevada – Las Vegas	High *P-T* thermal and electrical measurements with a Paris-Edinburgh cell	June 16-18, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	June 16-18, 2013
J. Baker	University of Nevada – Las Vegas	High *P-T* thermo-electric measurements of Cu, Bi, and organics	June 16-24, 2013
C. Park	HPCAT	Structure and reactivity of high *P-T* water at mafic and ultramafic mineral surfaces	June 17-20, 2013
H. yan	HPCAT	Mineral-water interface at high *P-T*	June 17-22, 2013
C. Ji	HPSynC	Crystal structure of hydrogen under high pressure	June 18, 2013
M. Somayazulu	Carnegie	Synthesis of Xe-Cl and Xe-I compounds	June 19-21, 2013
G. Fabbris J. Lim	Washington University in St. Louis	Search for high-pressure ferromagnetic ground state in potassium	June 19-21, 2013
M. Somayazulu	Carnegie	Studies on CO-D_2O, Co-Zr-Nb metallic glass interaction with H_2	June 20-21, 2013
S. Wang J. Liu	Stanford University University of Michigan	High pressure and low temperature XRD study of the diagram of CeRuPO	June 21-22, 2013
C. McDonald F. Nasreen D. Antonio	University of Nevada – Las Vegas	High pressure and low temperature resonant inelastic x-ray spectroscopy in uranium intermetallic compounds	June 21-24, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	June 22-24, 2013
C. Ji	HPSynC	Crystal structure of zirconium under ultrahigh pressure	June 22-24, 2013
B. Li	HPSTAR	High pressure study of H_2O	June 22-24, 2013
J. Jeffries	LLNL	Pu microdiffraction	June 23-27, 2013
H. Cynn	LANL	5f metal at high pressure	June 26-29, 2013
R. Kumar N. Bandaru	University of Nevada – Las Vegas	Structural studies on $MoSe_2$, WS_2, $Ce_2Ni_3Ge_5$, and $EuFe_2As_2$ compounds at high pressure and high temperatures	June 27-28, 2013

B. Cochain H. Spice	University of Edinburgh, UK	Effect of high pressure and temperature on the viscosity of molten fayalite and ferrosilite	June 27-July 1, 2013
L. Wang T. C. Weng	HPSynC Stanford University	IXS study of hydrogen under high pressure	June 27-July 4, 2013
J. H. Klepeis	LLNL	Compression studies of U compounds under pressure and temperature	June 28-July 1, 2013
C. Ji	HPSynC	Crystal structure of solid hydrogen under high pressure	June 29-30, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	June 29-July 1, 2013
B. Li	HPSTAR	High pressure study of H_2O	June 30-July 1, 2013
L. Bai	University of Nevada – Las Vegas	Studies of x-ray induced decomposition	July 1-3, 2013
G. Guardala	University of Nevada – Las Vegas	Irradiation of perfluorocarbons	July 1-3, 2013
Q. Smith	University of Nevada – Las Vegas	C_8F_{18}, C_6F_{14} decomposition	July 1-3, 2013
M. Somayazulu	Carnegie	Melting of Ta, W, and Pt under high pressure	July 1-4, 2013
Q. Hu J. Zhang H. Zheng	George Mason University HPSynC	High pressure XRD using angle-dispersive diffraction	July 1-4, 2013
A. Karandikar	Carnegie	Synchronizing synchrotron XRD with flash melting technique	July 2-4, 2013
Y. Gao	Carnegie	$MnWO_4$ and cBN under high pressure	July 3-4, 2013
L. Liu	HPSynC	Liquid structure of sulfur at high *P-T*	July 3-4, 2013
I. Efthymiopoulos Y. Wang T. Lochbiler	Oakland University	Compression of multiferroic $HgCr_2S_4$ and $HgCr_2Se_4$ spinels at ambient temperature	July 5-7, 2013
Y. Shibazaki	Carnegie	Structure measurements of molten FeHx alloys at high *P-T*	July 5-9, 2013
P. Cho	HPCAT	Development of polycap optics for IXS and study of beam stability	July 5-12, 2013
F. Yang	Stanford University	Study of pressure induced structural evolution of [121] tetramantane by high pressure single crystal XRD	July 7-9, 2013
S. Feng J. Zhu	Chinese Academy of Sciences	The crystal structural properties of diluted magnetic semiconductors under high pressure	July 8-10, 2013
Y. Kono	HPCAT	Development using Paris-Edinburgh cell	July 10-12, 2013
Z. Zhao	Carnegie	Structure evolution of glass carbon under high pressure	July 10-13, 2013
T. Fitzgibbons	Pennsylvania State University	Cold compression of single walled carbon nanotubes	July 11-13, 2013
Z. Li J. Liu B. Chen	University of Michigan University of Illinois – Urbana-Champaign	Magnetic transitions of Fe_7C_3 up to 1 Mbar by XES	July 12-16, 2013
L. Deng	Chinese Academy of Sciences	XRD for meteorite	July 13-14, 2013
D. Mast	University of Nevada – Las Vegas	Single crystal and powder compressibilities of Fe_4O_5, $ReCl_3$, $ReBr_3$, and ReI_3	July 13-15, 2013
B. Lavina	University of Nevada – Las Vegas	Synthesis of enriched Fe_4O_5 for NFS studies	July 13-15, 2013

D. Hummer A. Kavner	University of California – Los Angeles	Structure of carbonate-silicate melts at high *P-T* conditions using x-ray diffuse scattering	July 13-16, 2013
J. Lazarz	Northwestern University	High pressure ZrCl crystal structure	July 14-16, 2013
C. Park	HPCAT	Bi XANES at high pressures	July 17-19, 2013
Y. Y. Chang X. Liu	Northwestern University	Comparable compressibility of diamond and diamond-like superhard materials to 600 GPa	July 17-19, 2013
D. Mortensen	University of Washington	Studying *f*-electron delocalization under pressure with x-ray emission	July 17-22, 2013
J. Y. Chen	LLNL	Ultrasound measurements of Ce	July 17-22, 2013
M. Lipp	LLNL	XES of 4*f* metals	July 17-22, 2013
H. Cynn W. Evans	LLNL	Compression behavior of *f*-metal at high *P-T* using a DAC	July 19-22, 2013
M. Baldini	HPSynC	Investigating the *P-T* phase diagram of La_2CuO_4	July 20-21, 2013
C. Ji	HPSynC	High pressure study of sirconium	July 20-22, 2013
Y. Gao	Texas Tech University	High pressure effect of $MnWO_4$	July 21-22, 2013
S. Wang	University of Nevada – Las Vegas	Study of structural and elastic properties of PbTe under high *P-T* conditions	July 24-25, 2013
D. Antonio F. Nazreen	University of Nevada – Las Vegas	High pressure XRD in ytterbium and uranium intermetallic compounds	July 24-26, 2013
N. Velisavljevic	LANL	XRD on transition metals and alloys	July 24-28, 2013
X. Wu	Peking University	Spin and valence states of iron in single-crystal silicate perovskite at high pressures and temperatures by SMS	July 25-29, 2013
I. Kun Q. Huang D. Yu J. He M. Hu	Yanshan University	Ordering transformation of bulky glassy carbon under high *P-T*	July 26-30, 2013
L. Zhang	Carnegie	Physical Properties of silicates at high pressure	July 27-29, 2013
X. Wu	Peking University	Spin transition of ferric iron in Al-bearing phase D at high pressure by SMS	July 28-30, 2013
D. Ikuta	HPCAT	Single crystal XRD at high pressure	July 28-30, 2013
Z. Mao	University of Science and Technology of China	Synchrotron Mossbauer study of silicate perovskite	July 28-30, 2013
D. Dattelbaum R. Chellappa	LANL	High pressure behavior of explosives	July 29-August , 20131
J. L. Zhu J. Zhu	Chinese Academy of Sciences	NFS on Fe-based superconductor	July 31-August 3, 2013
V. Iota	University of Nevada – Las Vegas	Single crystal diffraction	July 31-August 3, 2013

C. Rotundu	University of California – Los Angeles	Single crystal diffraction on correlated compounds at high pressure	July 31-August 3, 2013
O. Tschauner	University of Nevada – Las Vegas	Laue diffraction in a DAC	August 1-3, 2013
O. Tschauner	University of Nevada – Las Vegas	Micro diffraction mapping	August 2-3, 2013
V. Iota	University of Nevada – Las Vegas	Phase transitions in 4*f* doped cuprates	August 2-4, 2013
Q. Smith G. Guardala	University of Nevada – Las Vegas	X-ray induced decomposition	August 3-5, 2013
M. Pravica	University of Nevada – Las Vegas	Studies of x-ray induced decomposition of inorganic materials using Raman spectroscopy	August 3-5, 2013
A. Shahar M. Reagan A. Gleason	Carnegie Stanford University	The effect of spin transition on iron isotope fractionation	August 3-9, 2013
W. Yang Y. Peng	HPSynC	Powder diffraction of MoS_2 under high pressure	August 4-5, 2013
K. Lipinska	University of Nevada – Las Vegas	High pressure XRD of mullite-type ceramics	August 5-6, 2013
X. Liu Y. Y. Chang	Northwestern University	Compression behaviors of unfilled and filled skuterudite $CoSb_3$ up to 80 GPa	August 5-8, 2013
M. Guthrie B. Haberl J. Bardby	Carnegie Australian National University	The temperature-dependent phase transition behavior and possible polyamorphism of fully coordinated amorphous silicon	August 7-9, 2013
A. Furukawa	Japan Atomic Energy Agency	The effect of spin transition on iron isotope fractionation	August 7-11, 2013
P. Lipinska-Kalita	University of Nevada – Las Vegas	High pressure XRD of mullite-type ceramics	August 8-9, 2013
L. Wang S. Wang	University of Nevada – Las Vegas	Phase transitions in $PbCrO_3$ at low temperature and high pressure	August 8-11, 2013
J. Shu J. Wang C. Ji	Carnegie HPSynC	Crystal structure of solid hydrogen under pressures	August 9-11, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	August 9-11, 2013
S. Smith	University of Alabama – Birmingham	High-pressure resistance and structure measurements in bismuth and gallium	August 10-12, 2013
J. Zhang	HPSynC	High pressure diffraction on superconductors	August 11-12, 2013
N. Velisavljevic	LANL	High pressure XRD and electrical-r of metals	August 11-13, 2013
K. Kothapalli B. Lavina F. Nasreen	University of Nevada – Las Vegas	Nuclear forward scattering studies of Fe_4O_5 up to 15 GPa	August 11-13, 2013
J. Montgomery	University of Alabama – Birmingham	High-pressure resistance and structure measurements in bismuth and gallium	August 11-14, 2013
M. Baldini	HPSynC	High pressure diffraction of superconductors	August 12-13, 2013
M. Lipp	LLNL	RXES of 5*f* metal	August 14-17, 2013
T. Strobel S. Stefanoski	Carnegie	XRD of carbon and silicon compounds	August 15-18, 2013

H. Cynn S. Weir W. Evans	LLNL	5*f* metal compression behavior at high *P-T*	August 16-19, 2013
J. Zhu	Chinese Academy of Sciences	Structure properties of FeSe under high pressure and low temperature	August 17-20, 2013
J. Jeffries	LLNL	SmB6 RXES under pressure	August 17-21, 2013
C. Park	HPCAT	Small angle x-ray scattering development	August 19-21, 2013
D. Ikuta	HPCAT	Recrystallization of the sample by high temperature	September 14-20, 2013
Y. Kono	HPCAT	Development of Paris-Edinburgh cell experiments	October 1-8, 2013
L. Liu	Carnegie	Liquid structure study of P and Se at high *P-T*	October 2-8, 2013
J. Montgomery	University of Alabama – Birmingham	High *P-T* experiments on bismuth, gallium, gadolinium, and VO_2	October 3-5, 2013
N. Velisavljevic R. Saavedra J. Montgomery N. Brady	LANL University of Alabama – Birmingham	High pressure electrical XRD measurements on metals	October 3-5, 2013
J. Chen R. Li S. Feng	Harbin Institute of Technology Chinese Academy of Sciences	SMS of a NaFeAs under high pressure and low temperature	October 3-7, 2013
S. Li Y. Wang	University of Nevada – Las Vegas	High-pressure study of VN and $PbCrO_3$ at low temperature	October 4-7, 2013
H. Cynn	LLNL	Compression behavior of *f*-metal at high *P-T* using a DAC	October 5-7, 2013
J. Zhang	HPSynC	Single diffraction for bi2201 under high pressure	October 7-8, 2013
Z. Mao	University of Science and Technology of China	Spin and valence state of perovskite using synchrotron Mossbauer spectroscopy	October 7-11, 2013
X. Wu	Peking University	Spin states of iron in single-crystal silicate perovskite at *P-T* conditions relevant to the Earth's lower mantle	October 7-11, 2013
Z. Jenei	LLNL	DAC radiography	October 9-11, 2013
X. Liu Y. Y. Chang	Northwestern University	Comparable compressibility of diamond and diamond-like materials	October 9-11, 2013
G. Tsoi G. Samudrala	University of Alabama – Birmingham	High-pressure studies of lanthanum and lutenium	October 9-12, 2013
O. Tschauner	University of Nevada – Las Vegas	Structure of CO_2	October 11-12, 2013
V. Iota	University of Nevada – Las Vegas	Single crystal laser heated molecular crystals at high pressure	October 11-12, 2013
J. Shu	Carnegie	H_2	October 11-13, 2013
D. Tomassino Y. J. Ryu	Washington State University	Nuclear forward scattering	October 11-15, 2013
K. Li H. Zheng	Carnegie	Structural study of CaC_2 under high pressure	October 12-13, 2013

C. Ji	HPSynC	Crystal structure of solid hydrogen at high pressures	October 12-14, 2013
L. Zhang	Carnegie	Physical properties of silicates at high *P-T*	October 12-14, 2013
Z. Zhao	Carnegie	Structure study of glass carbon under high *P-T*	October 12-15, 2013
Q. Hu J. Shu	Carnegie	High pressure XRD using angle-dispersive diffraction	October 14-15, 2013
W. Yang	HPSynC	X-ray powder diffraction of metallic alloys	October 16-17, 2013
C. Ji	HPSynC	Study of tantalum under zirconium under differential stress at high pressure	October 16-17, 2013
T. Yu	University of Chicago	Hedenbergite melt structure under high pressure	October 16-18, 2013
A. Shahar	Carnegie	Iron isotope fractionation of FeO at high pressure	October 16-20, 2013
A. Furukawa	Carnegie	NRIXS of FeO	October 16-20, 2013
L. Tang	Florida International University	Exploring the structural phase transition of Te doping 11-type iron selenide superconductors driven by pressure	October 17-18, 2013
Y. J. Ru D. Tomasino	Washington State University	X-ray characterization of nitrogen and molecular soids	October 17-19, 2013
M. Reagan	Stanford University	Isotope fractionation of FeO	October 17-20, 2013
F. Yang	Stanford University	High pressure study of diamondoids	October 18-20, 2013
L. Liu	Carnegie	Liquid structure study of S, P, and Se at high *P-T*	October 18-21, 2013
C. Ji J. Shu	HPSynC Carnegie	Crystal structure of solid hydrogen under high pressures	October 19-21, 2013
L. Zhang	Carnegie	Physical properties of silicates at high *P-T*	October 19-21, 2013
E. Tanis J. Knipping	University of Michigan	Partitioning of Zr between rutile and fluid at high *P-T*	October 20-28, 2013
Z. Li J. Liu	University of Michigan	Thermal equation of state of Fe_7C_3 up to 100 GPa and 1000 K	October 21-22, 2013
L. Deng	Chinese Academy of Sciences	Temperature dependence of sound velocity of $Fe_{91}Si_9$	October 21-25, 2013
X. Liu J. Zadronzny M. Fataftah S. Coste	Northwestern University	Compression behaviors of $Co_3Co_4O_9$ and Bi_2Te_3 nanoparticles	October 21-25, 2013
D. Antonio R. Kumar	University of Nevada – Las Vegas	High pressure and low temperature structural studies on $LaBiOS_2$	October 23-25, 2013
C. Ji	HPSynC	Crystal structure of solid hydrogen at high pressures	October 25-27, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	October 25-27, 2013
G. Fabbris	Washington University in St. Louis	Ferromagnetic ground state structure of potassium	October 25-28, 2013
L. Veiga	University of Campinas	Search for high-pressure ferromagnetic ground state structure in potassium	October 25-28, 2013
Z. Jennei	LLNL	Ultrasonic measurements on transition metals in a Paris-Edinburgh cell	October 25-28, 2013
Z. Li	University of Michigan	Stability of germanium analogues of dense hydrous magnesium silicates	October 30-31, 2013

K. Lee K. Daviau T. Gu	Yale University	High-pressure investigation of lower mantle compositions, SiC, and $Fe_{43}(S,P)$	October 30-November 1, 2013
M. Lipp	LLNL	L gamma XES of 4*f* metals	October 30-November 3, 2013
D. Mortensen	University of Washington	Studying *f*-electron delocalization under pressure with x-ray emission	October 30-November 3, 2013
J. Baker A. Connolly	University of Nevada – Las Vegas	Thermal and electrical measurements using modified Paris-Edinburgh assembly	October 30-November 3, 2013
Z. Yu L. Wang	HPSTAR HPSynC	Structural transitions of carbon nanotubes under high pressure	October 31-November 2, 2013
D. Antonio R. Kumar	University of Nevada – Las Vegas	Structural studies of $LxBiOS_2$ at high pressure and low temperature	November 1-3, 2013
Y. Wang	University of Nevada – Las Vegas	ADXRD studies of potassium perchlorate and C_6F_6 at high pressure	November 2-3, 2013
M. Pravica	University of Nevada – Las Vegas	Studies of x-ray induced decomposition of inorganic materials using Raman spectroscopy	November 2-3, 2013
L. Tang	Florida International University	The crystallographic structure of iron arsenides under pressure	November 3-4, 2013
Y. Ren C. Yu	ANL Northern Illinois University	High pressure study of the strain coupling in nanocomposite Nb-NiTi	November 3-4, 2013
N. R. Bandaru D. Antonio R. Kumar	University of Nevada – Las Vegas	Structural studies of $MoSe_2$ and WSe_2	November 3-5, 2013
J. Baker	University of Nevada – Las Vegas	Thermal and electrical measurements using modified Paris-Edinburgh assembly	November 3-5, 2013
B. Aoun	ANL	Voltage fade	November 4-5, 2013
C. Ji	HPSynC	Crystal structure of tantalum under shear stress	November 4-6, 2013
J. Jeffries	LLNL	Sm L-gamma XES to probe the local moment of the topological insulator SmB_6	November 4-9, 2013
B. Baer J. H. Klepeis	LLNL	Equation of states of actinide compounds	November 6-8, 2013
K. Li	Carnegie	Structure characterization of CD_3CN under high pressure	November 7-8, 2013
Y. Shibazaki	Carnegie	Viscosity and structure measurements of Fe_3C liquid at high *P-T*	November 7-11, 2013
Z. Li	University of Michigan	Melting temperature of Ca-carbonate at 10-30 GPa	November 8-9, 2013
X. Yan	HPSTAR	Structural studies of Er_2O_3 at high pressures	November 8-11, 2013
H. Cynn	LLNL	Time-resolved XRD of 5*f* metals	November 9-11, 2013
K. Li	Carnegie	Structure analysis of CaC_2 and $Li2C_2$ under high pressure	November 13-14, 2013
K. Li	Carnegie	Structure characterization of CD_3CN under high pressure	November 13-14, 2013
Y. Shi	Stanford University	Earth core formation mechanism	November 13-15, 2013

D. Hummer	University of California – Los Angeles	Structure of carbonate-silicate liquids at high *P-T* conditions using *in situ* diffuse x-ray scattering	November 13-16, 2013
R. Li	Chinese Academy of Sciences	Ge single crystal XRD study	November 14-15, 2013
Y. Lin	Stanford University	XRS of water at ultrahigh pressures	November 14-16, 2013
J. Hall M. Lang R. Palomares	University of Tennessee – Knoxville	Actinide oxide chemistry	November 15-19, 2013
B. Lu	HPSTAR	High pressure study of hydrogen and Os	November 16-17, 2013
L. Liu	HPCAT	Structural study of Ta at high *P-T*	November 16-17, 2013
D. Hummer	University of California – Los Angeles	*In situ* investigation of germinate melt structure at high *P-T* using diffuse x-ray scattering	November 16-18, 2013
Y. Wang M. Pravica	University of Nevada – Las Vegas	Studies of hydroflurocarbons at extreme conditions using x-ray Raman spectroscopy	November 16-18, 2013
C. Ji	HPSynC	Crystal structure of solid hydrogen under high pressures	November 16-18, 2013
S. Palaich A. Watenphul	University of California – Los Angeles	Germanium melt coordination at high *P-T*	November 16-19, 2013
Z. Yu M. Feng L. Wang	HPSTAR HPSynC	Inelastic x-ray scattering of solvated C_{60} and C_{70} at high pressure	November 18-22, 2013
J. Fonseca, Jr. L. Veiga	LNLS University of Campinas	Coupled/decoupled hysteric pressure behaviors of magneto-electronic and crystallographic properties in a hybrid ferromagnet	November 20-21, 2013
Z. Jenei	LLNL	Us of transition metals	November 20-22, 2013
W. Yang	HPSynC	IXS study of laser shocked diamond	November 22-23, 2013
M. Somayazulu	Carnegie	Equation of state of $BaReH_9$; high pressure behavior of CO-H_2O clathrate and high *P-T* synthesis of xenon carbonyl	November 21, 2013
J. Jeffries	LLNL	Equation of state of complex materials	November 22, 2013
Q. Zeng Z. Zeng	Stanford University	Volume of metallic glass under high pressure	November 22-25, 2013
Y. Ding	ANL	High pressure IXS of H_2	November 22-30, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	November 23-25, 2013
C. Ji	HPSynC	Inelastic scattering study of solid hydrogen under high pressures	November 23-30, 2013
B. Li	HPSTAR	High pressure IXS study of hydrogen	November 24-30, 2013
S. Hirai	Stanford University	Low temperature lattice evolution of Sr-based iron arsenide	November 25-26, 2013
B. Lavina D. Mast E. Siska	University of Nevada – Las Vegas	Technetium compressibility and Fe_4O_5 synthesis	November 25-28, 2013
Z. Yu M. Feng	HPSTAR	Pair distribution functions of C_{60} at high *P-T* conditions	November 25-December 1, 2013

L. Wang Z. Wu	HPSynC HPSTAR	Phase stability of iron-based superconductor FeSw, WS_2, and Cr_2S_3 at high pressures	November 26-28, 2013
Z. Zhao	Stanford University	High pressure study on $MoSe_2$ and WSe_2	November 29-December 1, 2013
L. Zhang	Carnegie	Physical properties of silicates at high pressure	November 29-December 1, 2013
C. Ji	HPSynC	Study of zirconium under ultra-high pressures	November 29-December 1, 2013
Q. Zhang C. Nisr Y. Ye	Arizona State University	Oceanic subcondition materials	December 1-3, 2013
C. Fancher	North Carolina State University	The origin of ferroelectrics in Si doped HfO_2	December 1-3, 2013
S. H. Shim	Arizona State University	Basaltic perovskite	December 1-3, 2013
P. Chow	HPCAT	Low-q inelastic scattering from metals	December 1-5, 2013
Y. Xiao	HPCAT	Low moment transfer IXS development	December 1-5, 2013
Y. Kono	HPCAT	Development using Paris-Edinburgh cell	December 1-6, 2013
C. Park	HPCAT	Paris-Edinburgh cell liquid density development	December 4-6, 2013
Y. Kono	HPCAT	Development of liquid density measurement in a Paris-Edinburgh cell at BMD	December 4-6, 2013
B. Chen	University of Illinois – Urbana-Champaign	Crystal structure of $CaSiO_3$ perovskite	December 4-6, 2013
P. Dera	University of Hawai'i at Manoa	Compression behavior of s-triazine derivatives	December 5-7, 2013
X. Lu	University of Nevada – Las Vegas	XES study of $YbFeO_3$	December 5-8, 2013
W. Yang	HPSynC	X-ray while Laue diffraction on single crystal under high pressure	December 5-8, 2013
Z. Jenei	LLNL	Radial XRD of transition metals	December 6-9, 2013
X. Lu	University of Nevada – Las Vegas	XRD of Ta_2O_5 with various structures under high *P-T*	December 8-10, 2013
Y. Wang	University of Nevada – Las Vegas	Pressure-induced amorphization of Ta_2O_5 and the pressure-induced amorphization mechanism investigation	December 8-10, 2013
M. Reagan	Stanford University	High-pressure behavior of FeOOH	December 11-, 201312
T. Strobel H. Guo	Carnegie	XRD study of carbon-rich materials	December 11-13, 2013
R. Chellappa N. Velisavljevic	LANL	High-pressure XANES study on CeO_2	December 11-14, 2013
C. Park	HPCAT	High energy XANES development	December 13-14, 2013
Q. Smith M. Pravica D. Sneed	University of Nevada – Las Vegas	Studies of the mobility of x-ray induced oxygen	December 13-16, 2013
M. Lipp	LLNL	*f*-metal RXES	December 13-16, 2013

Y. Wang M. Pravica	University of Nevada – Las Vegas	Studies of x-ray irradiated potassium halates under extreme conditions using *in situ* Raman spectroscopy	December 13-17, 2013
H. Cynn M. Lipp	LLNL	Laser heating study of 5*f* metal using a triply sealed DAC	December 14-16, 2013
J. Liu F. Zhang Z. Li	University of Michigan	Stability and thermal equation of state of Fe_7C_3 approaching *P-T* conditions of Earth's core	January 30-February 1, 2014
E. Tanis Y. Yang A. Wong	University of Michigan	Partitioning of Zr between rutile and aqueous fluid at high *P-T*	January 30-February 6, 2014
D. Ikuta	HPCAT	The structure of liquid Sn	January 31-February 2, 2014
W. Yang	HPSynC	Powder diffraction on oxides	February 1-4, 2014
Z. Li	University of Texas at Austin	High pressure XRD using angle-dispersive diffraction	February 1-4, 2014
H. Cynn	LLNL	5*f* metal laser heating	February 1-4, 2014
S. Gramsch	Carnegie	$FeAlO_3$ at high pressure	February 5-7, 2014
C. Park	HPCAT	High-energy XANES development	February 5-7, 2014
W. Bi G. Fabbris Q. Jia	University of Illinois – Urbana-Champaign APS Chinese Academy of Sciences	XES of europium under pressure	February 6-10, 2014
B. Li	HPSynC	High pressure study of water and vanadium	February 7-9, 2014
C. Ji	HPSynC	Crystal structure of solid hydrogen at high pressures	February 7-9, 2014
J. H. Klepeis	LLNL	Equation of state studies of complex metal compounds	February 7-9, 2014
Z. Zhao	Carnegie	Ultrasound and structure measurements of glass carbon at high *P-T*	February 7-10, 2014
T. Strobel H. Guo	Carnegie	Molecular polymerization mechanisms	February 9-11, 2014
S. Wang L. Wang	University of Nevada – Las Vegas	Phase relations in some perovskites and nitrides	February 9-11, 2014
Y. Kono	HPCAT	Paris-Edinburgh cell development	February 10-11, 2014
C. Park	HPCAT	High-resolution x-ray reflectivity from olivine-water interface at elevated temperature and pressure	February 10-15, 2014
H. Yan	Carnegie	Water-mineral interfaces under high *P-T* conditions using high-resolution x-ray reflectivity	February 10-16, 2014
S. Weir	LLNL	Magnetism in *f*-electron systems	February 11-15, 2014
Z. Jenei	LLNL	Ultrasonic studies of Pr in a Paris-Edinburgh cell	February 12-14, 2014
P. Dera H. Shelton	University of Hawai'I at Manoa	High-pressure single-crystal x-ray microdiffraction investigation of s-triazine derivatives	February 12-14, 2014
J. Jeffries	LLNL	High-pressure equation of state of strong spin-orbit compounds	February 12-15, 2014

J. Baker V. Mkrtchyan	University of Nevada – Las Vegas	Electrical and thermal measurements using a Paris-Edinburgh cell	February 14-18, 2014
R. Hrubiak	HPCAT	High pressure melting study	February 14-March 9, 2014
L. Miyagi M. Jugle	University of Utah	Deformation of two phase materials: Texture in post-perovskite and ferropericlase	February 15-17, 2014
M. Lang A. Cusik	University of Tennessee University of Michigan	Structural response of $A_2B_2O_7$ (A= La, Gd, Sm, Er) induced by combined swift heavy ion irradiation and high pressure	February 15-17, 2014
D. Ikuta	HPCAT	Single crystal XRD	February 17-18, 2014
Y. Meng	HPCAT	IXS of oxygen under high pressure	February 18-19, 2014
L. Bai	HPCAT	Pressure-induced phase transition of VO_2	February 19-20, 2014
J. Pigott A. Campbell R. Fisher B. Chidester	Ohio State University University of Chicago	Equations of state of Ni and SiO_2 at 80 GPa and 3000 K using controlled geometry samples	February 19-21, 2014
Y. Wang M. Pravica	University of Nevada – Las Vegas	X-ray Raman studies of fluorocarbons at extreme conditions	February 19-22, 2014
Y. Kono	HPCAT	Development of high q amorphous structure measurement	February 19-24, 2014
X. Liu	Northwestern University	Compression behaviors of polycrystalline and nanocrystalline $Ca_3Co_4O_9$ up to 50 GPa	February 20-21, 2014
G. Fabbris L. Veiga	ANL Labrotorio Nacional de Luz Sincotron	Tuning spin-orbit, crystal field, exchange interactions and lattice distortions in iron-osmium based double perovskites	February 20-22, 2014
D. Ikuta	HPCAT	The structure of liquid Sn	February 21-24, 2014
J. Y. Chen	LLNL	Time-resolved XRD	February 22-24, 2014
Y. Lin	Stanford University	High pressure XRD on H2O	February 22-26, 2014
M. Somayazulu	Carnegie	High-pressure diffraction studies of CO-H2O, Ti, Nd-Ti-Zr alloys	February 26-28, 2014
C. Ji	HPSynC	Phase transition of azide materials under pressure	February 26-March 3, 2014
W. Yang	HPsynC	High *P-T* study on CsN_3	February 26-March 3, 2014
L. Wang	HPSynC	Inelastic x-ray scattering of N_2 at high pressure	February 26-March 6, 2014
J. Liu F. Zhang M. Lang	University of Michigan University of Tennessee	Defects, uranium covalency and phase transformations of non-stoichiometric UO_{2+x} under high *P-T*	February 28-March 2, 2014
H. Cynn	LLNL	Time-resolved diffraction of 5*f* metals	February 28-March 2, 2014
F. Yang	Stanford University	Study of pressure-induced structural evolution of self-assembled metal diamondoid chalcogenides by single crystal x-ray	March 2-4, 2014
B. Li	HPSynC	High-pressure study of Te	March 3-4, 2014
J. Liu Z. Li	University of Michigan	Thermal expansion of Fe_3C and implications for the Earth's inner core	March 5-7, 2014

T. Strobel H.Guo D. Keefer	Carnegie Pennsylvania State University	Molecular polymerization mechanisms II	March 5-7, 2014
M. Wilding	Aberystwyth University	Ultrasonic and XRD measurements of amorphous B_2O_3	March 5-8, 2014
L. Kong G. Liu	HPSTAR	The compression of TiO	March 7-9, 2014
L. Zhang	HPSTAR	Physical properties of silicates at high *P-T*	March 7-9, 2014
P. Chow	HPCAT	Cyrostat polycap inelastic scattering development	March 7-13, 2014
L. Wang Z. Yu	HPSynC HPSTAR	PDF measurements for C_{60} at high *P-T*	March 8-11, 2014
H. K. Mao	Carnegie	XRD of hydrogen and deep mantle mineralogy	March 9-11, 2014
C. Ji	HPSynC	Crystal structure of solid hydrogen at high pressures	March 9-11, 2014
R. Li	Chinese Academy of Sciences	Study of the ß-tin phase of germanium	March 9-13, 2014
C. Tracy	University of Michigan	Structural and chemical response of actinide materials to highly ionizing radiation	March 10-11, 2014
Z. Jenei	LLNL	DAC radiography	March 12-14, 2014
Y. Wang	University of Nevada – Las Vegas	Experiments in hard x-ray induced chemistry	March 13-15, 2014
M. Pravica	University of Nevada – Las Vegas	X-ray induced decomposition of $KClO_4$	March 13-15, 2014
D. Tomasino	Washington State University	DAC phase transitions	March 13-15, 2014
B. Lavina E. Siska	University of Nevada – Las Vegas	Orthorhombic iron oxides, defect structures and compressibility	March 14-16, 2014
D. Hummer	University of California – Los Angeles	Structure and viscosity of carbonate-silicate melts at high *P-T* conditions using x-ray diffuse scattering	March 14-17, 2014
N. Velisavljevic	LANL	Zr recrystallization and phase transformation under high *P-T*	March 15-16, 2014
N. Bandaru	University of Nevada – Las Vegas	Structural studies on WSe_2 and related compounds under high pressure	March 16-20, 2014
M. Guthrie	Carnegie	Recoverable phases of silicon	March 17-18, 2014
Y. Kono	HPCAT	Development of liquid structure measurement	March 17-18, 2014
D. Antonio R. Kumar	University of Nevada – Las Vegas	Structural studies on $MoSe_2$ and WSe_2 compounds at high *P-T*	March 17-20, 2014
Y. Wu	Peking University	Spin state of iron	March 17-20, 2014
J. Bradby B. Haberal S. Wong	Australian National University	Novel metastable phases: Temperature and rate dependent phase transitions in silicon	March 17-21, 2014
D. Mast B. Lavina E. Siska P. Ellison P. Forester	University of Nevada – Las Vegas	T_c compression	March 19-22, 2014
T. Sakamaki	Tohoku University	Viscosity and structure measurements of Fe-Si liquid	March 19-24, 2014

J. Jeffries	LLNL	Studying *f*-electron moment under pressure with x-ray emission	March 21-24, 2014
H. K. Mao	Carnegie	Single crystal diffraction of hydrogen	March 22-23, 2014
H. Cynn	LLNL	Single crystal XRD of Group 4 compounds at high pressure	March 22-23, 2014
L. Zhang	HPSTAR	Physical properties of silicates at high *P-T*	March 22-23, 2014
C. Ji	HPSynC	Crystal structure of solid hydrogen under high pressures	March 22-24, 2014
W. Yang	HPSynC	Ice nanowire confined in mesoporous silica tube	March 23-24, 2014
B. Li	HPSynC	High pressure study of Ir	March 23-24, 2014
M. Somayazulu	Carnegie	Radial diffraction of Ti, Ta, B4C	March 26-28, 2014
Y. Kono	HPCAT	Paris-Edinburgh cell development projects	March 26-29, 2014
Y. Wu	Peking University	NSF of perovskite	March 27-30, 2014
G. Lu	HPSTAR	High pressure XRD using angle-dispersive mode	March 28-30, 2014
Z. Jenei H. Cynn	LLNL	Fast compression of simple metals	March 28-31, 2014
T. Yu	University of Chicago	A study of hedenbergite melt structure under high pressure	March 29-April 1, 2014
L. Tang	Florida International University	Investigating the structural transition of $Ba_{0.3}K_{0.7}Fe_2As_2$ under pressure	March 30-April 1, 2014
K. Li H. Zheng	Carnegie	Mossbauer study of $K_3Fe(CN)_6$ under high pressure	March 30-April 1, 2014
W. Yang	HPSynC	High pressure powder diffraction	March 31-April 1, 2014
K. Li	HPSTAR	High pressure study of CaC_2	April 2-4, 2014
Y. Kono	HPCAT	Development of DAC imaging	April 2-4, 2014
D. Ikuta	HPCAT	The structure of liquid bismuth	April 2-4, 2014
K. Kothapalli	Carnegie	Nuclear forward scattering low temperature studies of Fe_4O_5	April 2-5, 2014
X. Lu Y. Wang	University of Nevada – Las Vegas	XRD of black TiO_2 with different crystal sizes	April 3-4, 2014
X. Li	Chinese Academy of Sciences	Structure and electron delocation research of single-crystal Cr_2O_3 under pressure	April 4-5, 2014
H. Li J. Liu	Beijing University of Technology Chinese Academy of Sciences	High pressure single crystal diffraction	April 4-5, 2014
O. Tschauner	University of Nevada – Las Vegas	Micro XRD mapping of shocked meteorite	April 4-5, 2014
B. Lavina	University of Nevada – Las Vegas	Single crystal diffraction at high pressure of a few oxides and phosphates	April 5-6, 2014
E.Siska	University of Nevada – Las Vegas	Compression of single crystals	April 5-6, 2014
H. K. Mao C. Ji	Carnegie HPSynC	Crystal structure of solid hydrogen at high pressures	April 6-8, 2014
K. Li	HPSTAR	Crystal structure of CaC_2 under high pressure	April 6-8, 2014

M. Ahart	Carnegie	Pressure-induced transitions in $Pb(Zr_{0.6}Ti_{0.4})O_3$ crystals	April 6-10, 2014
A. Shahar M. Reagan	Carnegie Stanford University	The effect of spin transition on iron fractionation	April 9-14, 2014
C. Park	HPCAT	High-pressure XANES-XRD development	April 10-13, 2014
S. Wang	Stanford University	Diffuse scattering of oxygen chain order in $HgBa_2CuO_4$ at high pressure	April 11-13, 2014
M. White D. Sneed	University of Nevada – Las Vegas	Studies in useful hard x-ray chemistry	April 11-15, 2014
M. Somayazulu	Carnegie	XRD of $BaReH_9$, $CO\text{-}H_2O$	April 13-15, 2014
C. Ji	HPSynC	Crystal structure of solid hydrogen at high pressures	April 16-17, 2014
L. Yang	Carnegie	Radial diffraction on iron with laser heating	April 16-18, 2014
M. Lipp	LLNL	Iron K beta and lanthanide L gamma	April 16-21, 2014
B. Li	HPSynC	High pressure study of Ta	April 17-18, 2014
D. Antonio	University of Nevada – Las Vegas	Structural studies of Ce and Yb based heavy fermion compounds at high pressure	April 17-19, 2014
J. Zhang Y. Wang	University of Nevada – Las Vegas	High pressure study of PbTe, VO_2 and some antiperovskites	April 18-19, 2014
H. Cynn	LLNL	Phase diagram of Ti, Hf, and Zr at high temperatures and high pressures	April 19-21, 2014
D. Dattelbaum	LANL	High *P-T* studies of polymer and explosives	April 19-24, 2014

B. U2A Infrared Beamline

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 provides partial salary support for Beamline Scientist **Zhenxian Liu**, as well as beamline upgrades and supplies.

User Name	Affiliations	Project	Dates
M. Ahart	Carnegie	Infrared reflectivity measurements of D_2O under high pressure	March 3-4, 2013
T. Yu T. Wu T. Tyson	New Jersey Institute of Technology	High pressure IR and XRD studies of multiferroic orthorhombic $REMnO_3$	March 4-7, 2013
C. Ma	Jilin University	The behavior of hydrogen bond under extreme conditions in typical linear or cyclic organic compounds under extreme conditions	March 7-10, 2013
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	March 11-14,
F. Zhang	University of Michigan	Response of minerals to extreme conditions of ion irradiation and high pressure: A novel approach in geosciences	March 22-25, 2013
R. Chellappa M. Bishop N. Velisavljevic D. Dattelbaum	LANL	High *P-T* phase stability and decomposition boundary investigation of FOX 7	Mar. 28-31, 2013
A. Plonka	State University of New York at Stony Brook	Pressure induced polymerization of dyines in assembled cocrystals	April 2-5, 2013
Y. Yu	State University of New York at Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application	April 9, 2013
B.Grocholski E. Stevenson	National Museum of Natural History	Water storage capacity of lower mantle perovskite and stishovite	April 10-12
M. Ahart	Carnegie	Infrared reflectivity measurements of D_2O under high pressure	April 19-21, 2013
Z. Liu V. Struzhkin M. Ahart C. Zha	Carnegie	Infrared study for dense hydrogen under wide simultaneous *P-T* conditions	April 21-23, 2013
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	April 24-25, 2013
Z. Liu	Carnegie	Infrared study for dense hydrogen under wide simultaneous *P-T* conditions	May 1-5, 2013
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	May 13-14, 2013
H. Feng	Montclair State University	Chemical study of mental chelation on functionalized graphene surface for development of metal catalysis and sensors	May 20-21, 2013
W. Yang Z. Liu	HPSynC Carnegie	The pressure dependence of hydrogen vibron at room temperature	May 23-25, 2012

J. Townsend Z. Liu	Northwestern University Carnegie	Water in post-perovskite: A hydrogen trap at the core-mantle boundary?	May 28-June 1, 2013
J. Musfeldt K. O'Neal	University of Tennessee	Pressure-induced in the magnetoelastic coupling of $Co(dca)_2$ by synchrotron infrared spectroscopy	June 3-7, 2013
M. Bishop N. Velisavljevic	LANL	High *P-T* phase stability and decomposition boundary continuation investigation of FOX 7	June 8-12, 2013
J. Tse Z. Liu	University of Saskatchewan Carnegie	Pressure induced magnetic and insulator to nano-organometallic radical complexes	June 13-16, 2013
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	June 17-22,
S. Wang Z. Zhao	Stanford University	Monitoring the bandgap of mixed valent $CsAuI_3$ and $CsAuBr_3$ at high pressure	June 26-28, 2013
Z. Zhao S. Wang	Stanford University	High pressure infrared spectroscopic study on metallization of 3D topological insulators Ag2Te and Ag2Se	June 29-30, 2013
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	July 7-16, 2013
R. Liu Q. Li	Jilin University	Pressure induced metal-insulator transition in VO_2 bulks and nanomaterials	July 17-25, 2013
P. Bowden N. Mack	LANL	High pressure chemistry of simple molecules: Hydrazine and its methylated derivatives	July 25-30, 2013
T. Yu T. Wu T. Tyson	New Jersey Institute of Technology	High pressure IR and XRD studies of multiferroic orthorhombic $REMnO_3$	July 31-August 2, 2013
W. Du	State University of New York at Stony Brook	Investigation of water content of high pressure experiment recovered sample	August 2, 2013
Z. Liu	Carnegie	Infrared study for dense hydrogen under wide simultaneous *P-T* conditions	August 7-10, 2013
R. Chellappa D. Dattelbaum P. Bowden F. Rein	LANL	Role of mode anharmonicity in initiation of high explosives	August 11-18, 2013
M. Bishop N. Velisavljevic Z. Dreger	LANL Washington State University	High *P-T* phase stability and decomposition boundary investigation of FOX 7	August 21-25, 2013
H. Feng	Montclair State University	Chemical study of mental chelation on functionalized graphene surface for development of metal catalysis and sensors	September 12-13, 2013
Z. Liu	Carnegie	Infrared study for dense hydrogen under wide simultaneous *P-T* conditions	September 13-15, 2013
W. Du	State University of New York at Stony Brook	Investigation of water content of high pressure experiment recovered sample	September 16, 2013
Z. Liu	Carnegie	Infrared study for dense hydrogen under wide simultaneous *P-T* conditions	September 17-19 2013

X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	September 23-27, 2013
W. Du	State University of New York at Stony Brook	Investigation of water content of high pressure experiment recovered sample	September 30, 2013
J. Townsend Z. Liu	Northwestern University Carnegie	Water in post-perovskite: A hydrogen trap at the core-mantle boundary?	October 8-11, 2013
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	October 12-15, 2013
J. Musfeldt K. O'Neal	University of Tennessee	Pressure-induced in the magnetoelastic coupling of $Co(dca)_2$ by synchrotron infrared spectroscopy	October 19-25, 2013
B. Chen L. Kong G. Liu	HPSTAR	High pressure IR and XRD study of mix-stacking Nano-ZnS	October 26-28, 2013
J. Townsend Z. Liu	Northwestern University Carnegie	Water in post-perovskite: A hydrogen trap at the core-mantle boundary?	October 29-31, 2013
B. Chen L. Kong G. Liu	HPSTAR	High pressure IR and XRD study of mix-stacking Nano-ZnS	November 2-3, 2013
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	January 24-February 9, 2014
H. Feng	Montclair State University	Chemical study of mental chelation on functionalized graphene surface for development of metal catalysis and sensors	February 10-11, 2014
D. Reaman	Army Research Laboratory	High pressure IR analysis of compressed gas mixtures with application to high-energy and super-hard materials	February 12-14, 2014
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	February 15-18, 2014
H. Zheng K. Li	HPSTAR	The reaction mechanism and dynamics of acetonitrile under high pressure	February 18-21, 2014
J. Zhu S. Zhang	LANL Chinese Academy of Sciences	Anomalous antiferromagnetic metallic evolution of $CaCrO_3$ single crystal under high pressure: an IR spectroscopy study	February 22-March 1, 2014
J. Thomas A. Kronenberg	Rensselaer Polytechnic Institute Texas A&M University	High-Resolution FTIR Study of Water Contents of Caledonide and Himalayan Mylonites	Mar. 2-5, 2014
J. Tse J. Zhao	University of Saskatchewan	Pressure induced magnetic and insulator to nano-organometallic radical complexes	Mar. 6-8, 2014 Mar. 9, 2014
D. Reaman	Army Research Laboratory	High pressure IR analysis of compressed gas mixtures with application to high-energy and super-hard materials	Mar. 10-13, 2014
J. Townsend Z. Liu	Northwestern University Carnegie	Water in post-perovskite: A hydrogen trap at the core-mantle boundary?	Mar. 14-16, 2014
A. Plonka	State University of New York at Stony Brook	Pressure induced polymerization of dyines in assembled cocrystals	Mar. 19-21, 2014
Z. Liu X. Xi	Carnegie BNL	Infrared spectroscopy of H_2O up to 100 GPa	Mar. 22-25, 2014

M. Sangwan	Carneige	Kinetic Study of methanol synthesis from carbon dioxide and hydrogen at elevated temperature and pressures	Mar. 26-27, 2014
L. Kong G. Liu	HPSTAR	High pressure IR and XRD study of mix-stacking nano-ZnS	Mar. 28-30, Mar. 31-Apr.1, 2014
Z. Liu Y. Ma Y. Lee	Carneige Yonsei University	Pressure-induced trapping of large cations and molecules in small-pore zeolites	Apr. 1-2, 2014
C. Ma B. Yang J. Chen H. Zhu Q. Cui	HPSTAR Jilin University	High pressure infrared spectroscopy studies of cyclopentane	Apr. 3-5, 2014 Apr. 6, 2014
A. Campbell B. Chidester E. Tompson R. Fisher	University of Chicago	High pressure optical absorption across an electronic spin transition in (Mg,Mn)O	Apr. 7-9, 2014
A. Campbell B. Chidester E. Tompson R. Fisher	University of Chicago	Spectroscopic properties of pyrite (FeS_2) at high pressure	Apr. 10-11, 2014
X. Xi	BNL	Evolution of superconductivity with pressure in iron-based superconductors studied by infrared spectroscopy	Apr. 12-15, 2014
R. Liu Q. Li	Jilin University	Pressure induced metal-insulator transition in VO_2 bulks and nanomaterials	Apr. 16-18, 2013
Z. Liu X. Xi	Carnegie BNL	Infrared spectroscopy of H_2O up to 100 GPa	Apr. 19-22, 2014
M. Sangwan	Carnegie	Kinetic study of methanol synthesis from carbon dioxide and hydrogen at elevated temperature and pressures	Apr. 24-25, 2014
R. Chellappa M. Bishop N. Velisavljevic	LANL	High *P-T* phase stability and decomposition boundary investigation of FOX 7	Apr. 28-29, Apr. 30, 2014

References

1. Yoder Jr., H. S., *Centenial History of the Carnegie Institution of Washington: The Geophysical Laboratory* (Cambridge University Press, New York, 2004).
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