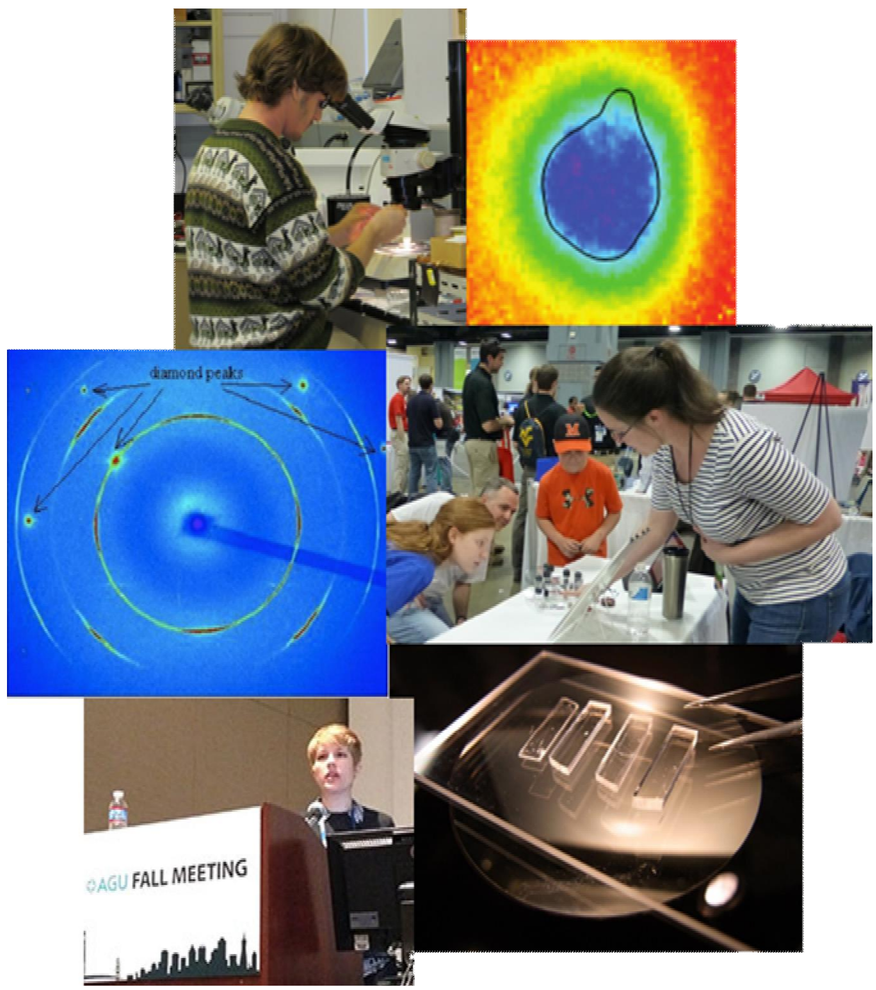
CDAC

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

Russell J. Hemley,
Director
Stephen A. Gramsch,
Coordinator
Morgan Phillips Hoople,
Administrator

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.

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.

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

Figure 3. *2013-2014 CDAC Partners.*

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.

1.2 Highlights from 2013-2014

Training, Outreach, and Personnel

- 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**,

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.*

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.

<u>Scientific Program</u>

- 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]

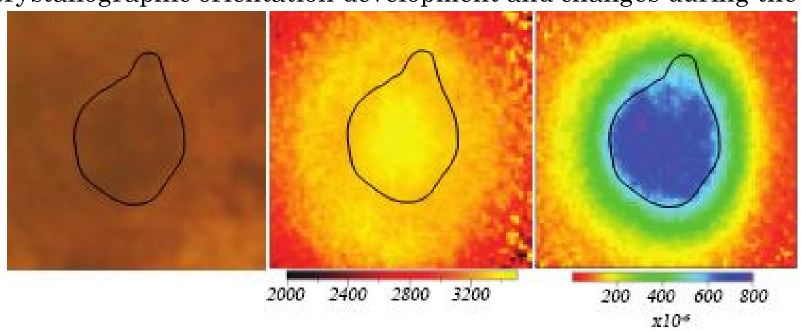


Figure 6. *Comparison of optical, temperature and emissivity maps across a melted sample of SiC at 12 GPa. The image is approximately 40 microns across.*[4]

- 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

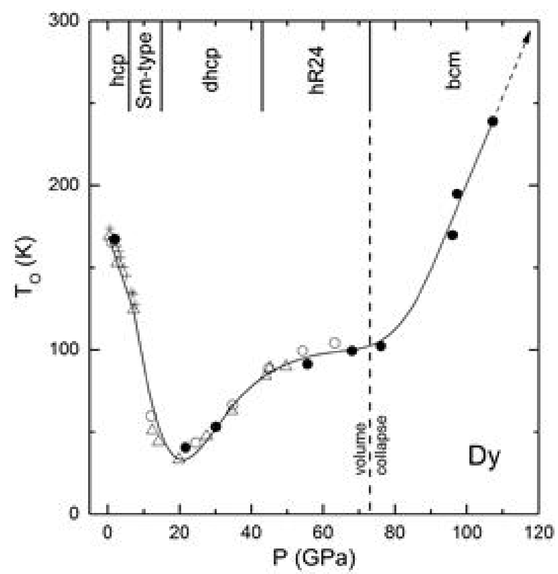


Figure 7. *Magnetic ordering temperature of Dy versus pressure.*[8]

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]

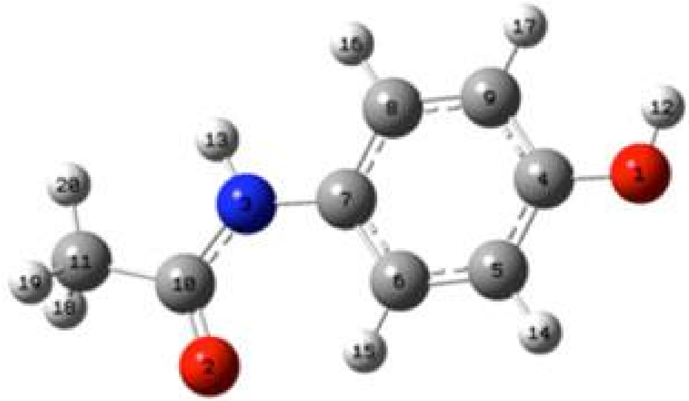


Figure 8. *Paracetemol structure. Carbon, grey spheres; oxygen, red; nitrogen, blue; hydrogen, white.*[9]

- 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]

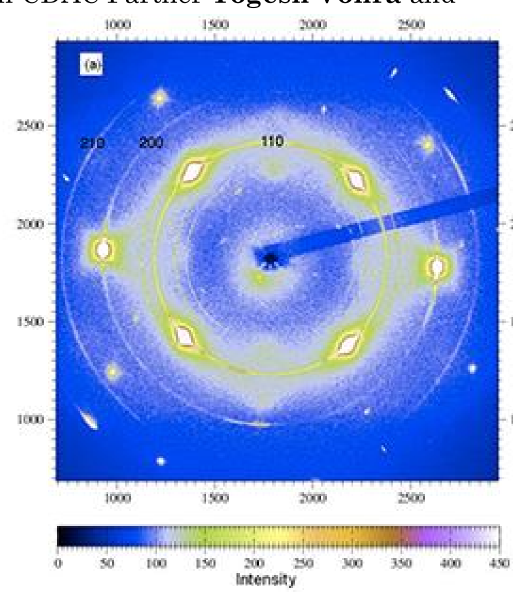


Figure 9. *Diffuse scattering obtained from a [001]-oriented crystal of Fe-Ga alloy at 0.8 GPa.*[10]

- **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 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]

<u>Technique Development</u>

- 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.

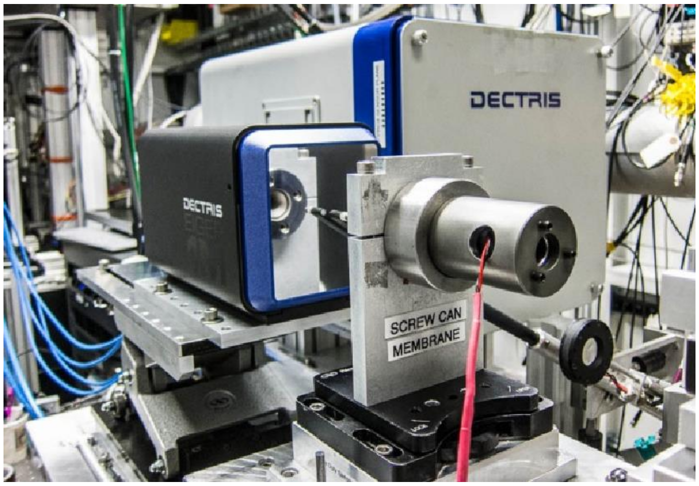


Figure 10. *A diamond anvil cell mounted in a piezoelectric pressure control apparatus for generating ultrahigh compression rates, together with the Pilatus 1M (right) and the Eiger 1M (left, prototype) high frequency area detectors.*

- 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 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]

References

1. Yoder Jr., H. S., *Centenial History of the Carnegie Institution of Washington: The Geophysical Laboratory* (Cambridge University Press, New York, 2004).
2. Rhodes, R., *The Making of the Atomic Bomb* (Simon and Schuster, New York, 1986).
3. Wenk, H. R., P. Kaercher, J. Kanitpanyacharoen, E. Zepeda-Alarcon, and Y. Wang, Orientation relations during the a-w phase transition of zirconium: In situ texture observations at high pressure and temperature, *Phys. Rev. Lett.* **111**, 195701 (2013).
4. Du, Z., L. Miyag, G. Amulele, and K. K. M. Lee, Efficient graphite ring heater suitable for diamond-anvil cells to 1300 K, *Rev. Sci. Instrum.* **84**, 024502 (2013).
5. Smith, R. F., J. H. Eggert, R. Jeanloz, T. S. Duffy, D. G. Braun, J. R. Patterson, R. E. Rudd, J. Biener, A. E. Lazicki, A. V. Hamza, J. Wang, T. Braun, L. X. Benedict, P. M. Celliers, and G. W. Collins, Ramp compression of diamond to five terapascals, *Nature* **511**, 330-333 (2014).
6. Zha, C. S., R. E. Cohen, H. K. Mao, and R. J. Hemley, Raman measurements of phase transitions in dense solid hydrogen and deuterium to 325 GPa, *Proc. Nat. Acad. Sci.* **111**, 4792-4797 (2014).
7. Cadien, A., Q. Y. Hu, Y. Meng, Y. Q. Cheng, M. W. Chen, J. F. Shu, H. K. Mao, and H. W. Sheng, First-order liquid-liquid phase transition in cerium, *Phys. Rev. Lett.* **110**, 125503 (2013).
8. Lim, J., G. Fabbris, D. Haskel, and J. S. Schilling, Magnetic ordering at anomalously high temperatures in Dy at extreme pressures: A new Kondo-lattice state?, *Cond. Mat. Str. El.*, arXiv:1404.4256 (2014).
9. Smith, S. J., M. M. Bishop, J. M. Montgomery, T. P. Hamilton, and Y. K. Vohra, Polymorphism in paracetamol: Evidence of additional forms IV and V at high pressure, *J. Phys. Chem. A* **118**, 6068-6077 (2014).
10. 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).
11. Rainey, E. S. G., J. W. Hernlund, and A. Kavner, Temperature distributions in the laser-heated diamond anvil cell from 3-D numerical modeling, *J. Appl. Phys.* **114**, 204905 (2013).
12. Schmandt, B., S. D. Jacobsen, T. W. Becker, Z. Liu, and K. G. Dueker, Dehydration melting at the top of the lower mantle, *Science* **344**, 1265-1268 (2014).
13. Yang, W., X. Huang, R. Harder, I. K. Robinson, J. Clark, and H. K. Mao, Coherent difraction imaging of nanoscale strain evolution in a single crystal under high pressure *Nature Mat.* **4**, 1680 (2013).