Annual Progress Report for Year #4 and Program Plan and Budget Request for Year #5 of the Consortium for Materials Properties Research in Earth Sciences (COMPRES) for

Community Facilities and Infrastructure Development for High-Pressure Mineral Physics and Geosciences: COMPRES II

February 2011

2010 Annual Meeting of COMPRES at

Skamania Lodge in Stevenson, WA

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A COMPRES Year 4: Overview

A.1 Executive Summary

In the first 42 months of COMPRES II [June 2007 to December 2010], substantial progress has been made in achieving the objectives and goals of the Consortium for Materials Properties Research in Earth Sciences [COMPRES]. Major technological advances at the community facilities operated by COMPRES at national laboratories and the infrastructure development projects sponsored by COMPRES have enabled new scientific research opportunities in the field of high-pressure mineral physics and chemistry.

It is appropriate to give at the outset of this Summary two of the most significant tasks that were undertaken and completed in the past year: 1) Transfer of the COMPRES Central office to University of Illinois, and 2) A change in the management of the West Coast Synchrotron Facility (beamline 12.2.2 at the Advanced Light Source) from Raymond Jeanloz and Simon Clarke (UC Berkeley) to Quentin Williams (UC Santa Cruz). With the change in management at the West Coast facility, the productivity of the beamline has continued on its upward trajectory, and has made significant progress toward building a stable, robust laser-heating facility that was a top priority for the Earth Sciences user community.

The management of COMPRES community facilities and infrastructure development projects is monitored by Standing Committees elected by the representatives of the member institutions of COMPRES under policies and procedures established by the committees and endorsed by the Executive Committee, to which the Standing Committees report. There are now 56 U. S. institutions which are voting members of COMPRES [the Electorate] and another 38 non-voting institutions overseas which have affiliate membership.

Following the submission of a proposal in August 2006, to renew funding for COMPRES for another 5-year period from 2007 to 2012, the Division of Earth Sciences paid a Site Visit to the National Synchrotron Light Source at the Brookhaven National Laboratory in November 2006 with its Instrumentation and Facilities Panel. Following an exchange of questions from Program Director David Lambert and responses from the Executive Committee, EAR approved a new Cooperative Agreement [CAGR] for funding of COMPRES as follows:

Annual Year begins on June 1 and ends on May 31 of following yea
Year #1: $2,100,000 [1 June 2007 to 31 May 2008]
Year #2: $2,200,000
Year #3: $2,300,000
Year #4: $2,400,000
Year #5: $2,500,000
Total projected funding for Years #1-5 [1 June 2007 to 31 May 2012]: $11,500,000

Actual appropriated funding history:
Year #1: $2,100,000 [1 June 2007 to 31 May 2008 at the CAGR level]
Year #2: $2,100,000 [or $100,000 less than the CAGR level]
Year #3: $2,100,000—anticipated [or $200,000 less than the CAGR level].
$850,000 Supplementary funding for equipment upgrades at COMPRES-supported beamlines at the NSLS and the ALS.
Year #4: $2,400,000 [up to the CAGR level]
Year #5: $2,400,000—anticipated [1 June 2011 to 31 May 2012; less than the CAGR level]

In this section of the Annual Report for Year #4, we present an overview of the activities of COMPRES. Subsequent sections include detailed reports from each of the Community Facilities operations and Infrastructure Development projects supported by COMPRES. The final section presents the budget plan for Year #5 [June 1, 2011 to May 31, 2012]; detailed budgets and justifications are given in the appendices to this report.

A.2 Research Accomplishments

See also new Science Highlights feature on COMPRES website at:
http://www.compres.stonybrook.edu/ScienceHighlights/index.html

Here we highlight a few of the scientific and technological accomplishments of the past year, indicating which section in this report describes the item in more detail.

- Using U2A at the NSLS, researchers from Northwestern and Carnegie Institution of Washington have found that small quantities of water in the mineral enstatite has a large effect on a phase transition to high-pressure clinoenstatite. The X discontinuity in the upper mantle could serve as an indicator of mantle water content. See Jacobsen et al. in Section B.2.

- Deformation experimeints on $MgSiO_3$ post-perovskite, carried out at beanline 12.2.2 of the Advanced Light Source, shows that strong textures develop in ths materials at large strains. These experiments may explain seismic anisotropy in the D'' region at the base of the mantle. See Miyagi et al. (2010) in Sections B.4.

- A team led by Shun Karato of Yale has measured the creep strength of anhydrous olivine, wadsleyite, and ringwoodite to >20 GPa. These results help understand the stability of deep continental roots, and energy dissipation from deep slab deformation. See Section B.3.

- Using samples of nano-crystalline forsterite and two different high-pressure apparatuses at X17B2 and B3 at the NSLS, Couvy et al. from Florida Internatnioal

University found that crystal size has an effect on the bulk modulus of olivine. See Section B.1 and B.3.

● Using new technologies developed at X17B2 of the NSLS, a team led by David Dobson from University College London has derived a method for measuring thermal diffusivity at high pressure and temperature. See section B.3.

● Wicks and co-workes at CalTech and APS have shown that low seismic velocities in D” may be due to Fe-rich ferropericlas. Their research utilized facilities at Sector 3 of the APS and beamline 12.2.2 of the ALS West Coast Syncrotron Facility. See sections B.4 and C.2.

● A team led by David Walker from Columbia has used beamline 12.2.2 to obtain X-ray absorption contrast images of binary chemical reactions. See Walker et al. in Section B.4.

● A team led by Rod Ewing and co-workers from the University of Michigan have developed a new method to quantitatively measure pressure induced atomic disordering in pyrochlore oxides, and have applied the technique to determine the nature of defects as a function of pressure. The work was carried out at beamlines X17B3 and C at the NSLS. See Zhang et al., in Section B.1.

● A team led by Jung-Fu Lin from U Texas, Austin, has studied the shear wave anisotropy of textured iron to understand the anisotrypy of the inner core, in experiments at beamline XOR-3 of the APS with support from the NRIXS development project at UIUC and ANL. See Lin et al. in Section C.2.

● Teams from Northwestern University and Carnegie Institution of Washington used synchrotron Infra Red radiation experiments on methane to explain dark surface features of Titan in terms of polarl lakes and a rain of methane. See Adams et al. in Section B.2.

A.3 Meetings and Workshops

The following meetings and workshops were sponsored, at least in part, by COMPRES since the start of the current Cooperative Agreement [2007].

Workshop on Current Status and Prospects for Establishing Precise and Accurate
Pressure Scales at High Temperatures
January 26-28, 2007
Geophysical Laboratory of the Carnegie Institution of Washington.
Organizing committee:
Alexander Goncharov, *Geophysical Laboratory*
Kurt Leinenweber, *Arizona State University*
Tom Duffy, *Princeton University*
Russell Hemley, *Geophysical Laboratory*
Yingwei Fei, *Geophysical Laboratory*

Workshop on Calorimetry-on-a-Chip
March 15-16, 2007
University of California at Berkeley
Organizers: Alexandra Navrotsky-UC Davis and Francis Hellman-UC Berkeley

Fourth Biennial Conference of CeSMEC
April 15-20, 2007
Organizers: Surendra Saxena and colleagues-Florida International University
Hotel Deauville, Miami Beach
More than 160 scientists from 20 countries attended, with a heavy emphasis on non-U. S. participants. COMPRES was one of the sponsors and more than 29 members of the COMPRES community attended.

7th High Pressure Mineral Physics Seminar (HPMPS-7)
May 8-12, 2007
Matsushima, Japan (near Sendai)
Organizers: E. Ohtani, D. Andrault, M. Brown, D. Rubie, Y. Wang, and T. Yagi.
This 7th in the series begun in 1976 in Hawaii was co-sponsored by COMPRES and 23 U. S. attendees were supported by special funds from the NSF Division of Earth Sciences and Office of International Programs. See details at:
7th High Pressure Mineral Physics Seminar (HPMPS-7) - Matsushima , Japan (near Sendai) May 8 to 12, 2007.

Gordon Conference on Earth's Interior
June 10-15, 2007
Organizers: Bruce Buffett-University of Chicago
Mt Holyoke College, South Hadley, MA
This biennial included many fine invited talks: those from mineral physics were by Greg Hirth, Lars Stixrude, Hans Keppler, Andrea Tommasi, Donald Weidner, and Marc Hirschmann.

Sixth Annual Meeting of COMPRES
June 17-20, 2007
Lake Morey Resort, Vermont
Program Committee: Michael Brown, Jennifer Jackson, Boris Kiefer, Sara Gaudio, Lara O'Dwyer
There were 102 registered participants and many accompanying persons to enjoy this splendid site. One of the new features was a set of keynote talks focused on the mantle, geochemical evolution and the core, with speakers for each topic from both within and outside the mineral physics community. The social events of the meeting were underwritten by 9 industrial sponsors: Almax, Blake Industries, Bruker AXS, D'Anvils, Depths of the Earth, Foxwood Instruments, Rigaku MSCHKL, Rockland Research and Technodiamant. Additional details of the Annual Meeting may be found in the July issue of the COMPRES newsletter and at:
http://www.compres.stonybrook.edu/Meetings/2007_Annual_Meeting/index.htm

International Workshop on Synchrotron High-pressure Mineral Physics and Materials Science
December 6-7, 2007
Advanced Photon Source, Argonne National Laboratory, Chicago
Organizers: Tetsuo Irifune-GRC, Ehime University (Japan) and Yanbin Wang-GSECARS, University of Chicago.

Planning Workshops at Brookhaven National Laboratory for NSLS and NSLS II
January and February 2008
On 17 December 2007, the DOE granted Critical Decision 2 [CD-2] status to the NSLS II at Brookhaven National Laboratory. During January and February 2008, a series of workshops were held to confirm plans for the new 5-year science plan for NSLS, and lay the groundwork for new beamline installations at NSLS-II, which is scheduled for first light in 2015. Members of the COMPRES community have been active as organizers and attendees at these workshops.

At one of these workshops last month on Earth and Environmental Sciences, Dr. Lisa Miller (a colleague of Chi-chang Kao, Director of NSLS) gave a splendid presentation on plans for the transition from NSLS to NSLS-II. As part of her presentation, she focussed on the role of COMPRES at the synchrotrons at

Brookhaven. Additional details may be found at: http://www.bnl.gov/ls/workshops.asp.

SNAP/COMPRES Meeting at Oak Ridge National Laboratory
April 13-15, 2008
A Joint Meeting of SNAP [Spallation Neutrons at Pressure] and COMPRES was held at the Spallation Neutron Source [SNS] of ORNL from April 13-15. See details of program at:
http://www.compres.stonybrook.edu/Meetings/2008-04-13-SNAP/FINAL_ProgramSNAP-COMPRES.doc
Meeting concluded with a guided tour of the new SNAP beamline by Chris Tulk who oversaw the design and construction on behalf of the project team, which also included John Parise, Russell Hemley and Ho-kwang Mao.

Future Directions in High Pressure Research
National Synchrotron Light Source
May 21, 2008.
As part of the 2008 Joint NSLS-CFN Users' Meeting, a high-pressure workshop, "Future Directions in High Pressure Research," organized by Lars Ehm, Baosheng Li, Jiuhua Chen, and Zhenxian Liu, was held on May 21, 2008. The objective of the workshop was to review recent state-of-the-art experiments at high pressure and temperature and to discuss needed capabilities for high-pressure research at the NSLS and NSLS-II. The workshop featured 15 invited speakers.

Workshop to Introduce High-Resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation.
Advance Photon Source Argonne National Laboratory
May 31 - June 1, 2008

Wolfgang Sturhahn, Jennifer Jackson, Jay Bass and Hasan Yavas convened an excellent workshop highlighting the current status and future opportunities for inelastic X-ray scattering experiments at the APS and elsewhere in the world. With sponsorship of COMPRES, there were keynote talks by practitioners from the US and overseas, with plenty of time for vigorous discussion. In addition to providing travel support for the invited speakers, COMPRES offered travel grants to 8 graduate students.

Seventh Annual Meeting of COMPRES
June 25-28, 2008
Cheyenne Mountain Resort, Colorado Springs, Colorado
Program Committee: Carl Agee, Jiuhua Chen, Steven Jacobsen, and James Tyburczy. Lili Gao and Zhu Mao served as student members.
There were 113 registered participants and many accompanying persons to enjoy this splendid site. One of the new features was a set of keynote talks focused on the mantle, geochemical evolution and the core, with speakers for each topic from both within and outside the mineral physics community. Keynote speakers included:
Rajdeep Dasgupta-Rice University William McDonough-Univ of Maryland

Louise Kellogg-UC Davis Rebecca Lange-Univ of Michigan

Justin Revenaugh-Univ of Minnesota Jie Li-Univ of Illinois

The social events of the meeting were underwritten by 9 industrial sponsors: Almax, Blake Industries, D'Anvils, Depths of the Earth, easyLab, MG63, Rockland Research, Scimed and Technodiamant. In addition, Depths of the Earth provided T-shirts for all attendees [see photo at: http://www.compres.stonybrook.edu/.

Additional details of the Annual Meeting may be found in the October 2008 issue of the COMPRES newsletter and at:
http://www.compres.stonybrook.edu/Newsletter/V7N2/NewsletterV7N2_Revised.pdf

NSLS Workshop: Advances in High-Pressure Science Using Synchrotron X-rays
National Synchrotron Light Source of the Brookhaven National Laboratory
October 4, 2008

This Workshop was held in honor of Drs. Jingzhu Hu and Quanzhong Guo and was organized by by Thomas Duffy (Princeton), Haozhe Liu (Harbin Institute of Technology), Lars Ehm (BNL), Dave Mao (Carnegie Institution of Washington), Zhenxian Liu (Carnegie Institution of Washington), and Jiuhua Chen (Florida International University). It was attended by more than 50 scientists, post-doctoral fellows, and students from the high pressure and synchrotron x-ray research fields. Financial support was provided by the Consortium for Materials Property Research in Earth Sciences (COMPRES), the Carnegie- DOE Alliance Center (CDAC), and the Harbin Institute of Technology. See additional details at:
http://shp.hit.edu.cn/Meetings/2008NSLS/Home.htm

Long-Range Planning Workshop for High Pressure Earth Sciences
Fiesta Resort Conference Center, Tempe, Arizona
March 2-4, 2009

This workshop was convened by tri-chairs James Tyburczy, Michael Brown and James van Orman on behalf of COMPRES, with support from the School of Earth and Space Exploration [SESE] of the Arizona State University. Robin Reichlin and Sonia Esperanca represented the NSF Division of Earth Sciences. [See photo in Supplemental Information].

Eighty seven scientists from thirty nine institutions gathered at the Fiesta Resort in Tempe to discuss recent scientific successes of the high pressure mineral physics community and articulate directions of our research over the next decade. This two-day workshop featured nine plenary talks and breakout discussion sessions on four themes: 1) The Deeper Reaches of the Planet:
Properties of Iron and its Alloys and the Novel Materials of the Deepest Mantle; 2) The Dynamic
Ceramic Mantle; 3) Mineral Physics and Society; 4) Enabling Cutting-Edge Science: Tools and the Accomplishments they will drive in the Next Decade of Discovery.
Participants of the workshop reviewed etrospective about how our field has impacted other subdisciplines of the earth sciences, including seismology, geodynamics and

petrology. They also discussed perspective of high pressure Earth science: what are the next major breakthroughs of our
community, and what infrastructure will be necessary to achieve them? While recognizing that incremental progress will occur, what new and different developments could occur? And, what long-standing problems might we solve? This was the second COMPRES workshop focusing on long range plan for high pressure Earth sciences. The first one "A Vision for High Pressure Earth and Planetary Sciences Research: The Planets from Surface to Center" was held on March 22-23, 2003 in Miami, Florida and led to the 2004 Report on the "Current and Future Research Directions in High-Pressure Mineral Physics."[the Bass Report]. The product that arises from this meeting will be a
new scientific plan for high-pressure Earth sciences, a document that will not only serve as a blueprint for our community as itmoves forward, but will also serve as the input of our community to a new NAS report, commissioned by NSF, on Basic Research Opportunities in the Earth Sciences (BROES). Quentin Williams will serve as Editor-in-Chief of this new report.

SMEC (Study of Matter at Extreme Conditons) Conference
Miami and Western Caribbean
March 28-April 2, 2009
This inernational conference was sponsored by HPSSA, the High Pressure Science Society of America. It was organized by the Center for the Study of Matter at Extreme Conditions (CeSMEC) at the Florida International University led by the Director Surendra Saxena and his colleagues.

Eighth Annual Meeting of COMPRES
June 19-22, 2009
Mount Washington Resort, Bretton Woods, New Hampshire
Program Committee: Jay Bass (Chair), Steve Jacobsen, and Wendy Mao. Katherine Crispin and Matt Whitaker served as student members. [See Cover Photo of this report and photo in Supplemental Information].

Attended by 109 formal participants and another two dozen accompanying guests, the meeting was one of the most important events of COMPRES. Forty two institutions including thirty six US members of COMPRES and six foreign institutions were presented. As a tradition of the annual meeting, one focus of the scientific agenda is interdisciplinary presentations. This year's keynote lectures include: "Seismic Observations of Mantle Discontinuities and their Mineral Physical Interpretation" by Arwen Deuss - Cambridge University, "Some Implications of Recent Progress in High P-T Mineral Physics for Earth's Deep Interior" by John Hernlund - University of British Columbia, "Mantle Viscosity and Climate (Really)" by Jerry Mitrovica - University of Toronto/Harvard University, "Seismically Imaging the Possible Presence of Water
in the Mantle" by Michael Wysession - Washington University, "Deep Carbon Observatory" by Alexander Goncharev - Carnegie Institution of Washington, "The

Role of Mineral Physics in the Study of Earth's Evolution” by Jun Korenaga - Yale University and “The Earth is not a Spherical Chicken” by Alex Navrotsky- University of California Davis.

New additions started from this year’s meeting are the selected graduate student talk session and the proposal writing workshop, both of which were recommended by the Grad Student Committee last year at Cheyenne Mountain annual meeting. Eight of the nineteen student participants made short presentations at the student talk session. Dr. Barbara Ransom, Program Director at the National Science Foundation presented the proposal writing workshop entitled: "Funding Your Science!". Two other Directors from NSF including Robert Detrick, the new Director of the Division of Earth Sciences attended the meeting as well. Dr. Detrick delivered an upbeat presentation on the current status and future prospects for funding of the Earth sciences.

The meeting also attracted the ten industrial sponsors: Almax, Blake Industries, D'Anvils, Depths of the Earth, easyLab, Foxwoods, Leica Microsystems, MG63, Rockland Research, and Technodiamant, four of them sent representatives to Bretton Woods.

Workshop: On-line Brillouin Spectroscopy at GSECARS: Basic Principles and Application for High Pressure Research

Advanced Photon Source, Argonne National Lab, Argonne, Illinois
September 23-25, 2009
The workshop will cover the following topics:

- fundamental aspects of Brillouin scattering
- experimental challenges of BS and XRD at high pressures and temperatures
- plenary lectures
- contributed presentations
- hands-on demonstrations
- software for data collection and analysis
- suggestions for future proposals

More than 55 people attended the workshop, which was organized by Vitali Prakapenka, Jay Bass and Stanislav Sinogeikin. [See photo in Supplemental Information].

Special Session in Honor of Alex Navrotsky at GSA Annual Meeting

Portland, Oregon
October 17-21, 2009.
At the GSA Meeting,
Gordon Brown, Abby Kavner, Nancy Ross and Glenn Waychunas convened a special session in honor of Alex Navrotsky. At the MSA Awards luncheon on October 20, Alex received the 2009 Roebling Medal and Bob Hazen received the 2009 Distinguished Public Service Award.

Workshop on Laser Heating the DAC: Where we are and where we are going.

Advanced Light Source of the Lawrence Berkeley National Laboratory
December 12-13, 2009
The workshop was organized by Simon Clark and focused on the following topics:
Advances in temperature measurement
Advances in lasers and laser delivery
Updates on laser heating facilities
Advances in fixed point calibrations
Recent results pertinent to the COMPRES community

Ninth Annual Meeting of COMPRES
June 22-25, 2010
Skamania Lodge, Stevenson, Washington
[See Cover Photo of this report].

Attended by a record 125 formal participants and another two dozen accompanying guests, the meeting was one of the most important events of COMPRES. Forty two institutions including thirty six US members of COMPRES and six foreign institutions were presented. As a tradition of the annual meeting, one focus of the scientific agenda is interdisciplinary presentations. This year's keynote lectures include: "Adventures in Anisotropy in the Earth's Mantle" by Maureen Long - Yale University, "P, T, and fO2 of Mantle Melting as Determined from Basalts – Implications for Planetary Differentiation" by Cin-Ty Lee – Rice University, "Computer Simulations at the Interface of High Pressure Research and Planetary Science" by Burkhard Militzer - University of California at Berkeley, "Reaching for the Stars: Dynamic Extreme-Compression Experiments" by Jon Eggert – Lawrence Livermore National Laboratory, "Hotsheets and Cool Drips: New Views of Western US Crust and Mantle Dynamics" by Matt Fouch – Arizona State University, "Following Minerals on the Road to Oblivion" by Peter Heaney – Pennsylvania State University, and "Fluid Dynamics of Planetary Interiors" by Jon Arnou- University of California Los Angeles.

New additions started from this year's meeting are the selected graduate student talk session and the Jobs in Academic Research workshop/break-out session, both of which were recommended by the Grad Student Committee at the Cheyenne Mountain annual meeting. Eight of the nineteen student participants made short presentations at the student talk session. A panel in cluding Chi-Chang Cao, Charlie Prewitt, Tom Duffy, Bin Chen, Abby Kavner, and Joh Eggert held an open forum with students "Advising Grad Students on Search for Faculty Jobs or Research Posts". Program Directors Sonia Esperanca from gave an upbeat presentation on the current status and future prospects for funding of the Earth sciences.

The meeting also attracted the ten industrial sponsors: Almax, Blake Industries, D'Anvils, Depths of the Earth, easyLab, Foxwoods, Leica Microsystems, MG63, Rockland Research, and Technodiamant, four of them sent representatives to Skamania.

Workshop on Computational Infrastructure For Mineral Physics: A Community Consultation Workshop.

August 29-31 2010

University of Minnesota Supercomputer Center

Organized by Renata Wentzcovitch and Artem Oganov, on the topics of:

- The role of computations in high-pressure mineral physics
- The requirements for state-of-the-art computations
- Should a COMPRES facility be proposed?
- What kind of facility would serve the needs of the community?
- How much would such a facility cost?
- Are there open source codes used by a sufficient number of people such that a request of funds for their permanent support is justified?
- How would tutorials be arranged and funded?

Workshop on 4-Dimensional Studies in Extreme Environments (4DE): A High-Pressure Beamline Workshop for the National Synchrotron Light Source II (NSLS II)

April 29-30, 2010

National Synchrotron Light Source (NSLS), Brookhaven National Laboratory

Organized by Donald J Weidner and Lars Ehm on the following topics:

- Characteristics of NSLS II
- Timetable for NSLS II
- Scientific agenda of 4DE beamline
- Instrumentation of 4DE beamline
- Open discussion and solicitation of participation

Workshop on Time-Resolved X-ray Diffraction and Spectroscopy at Extreme Conditions (TEC): A High-Pressure Beamline Workshop for the National Synchrotron Light Source II (NSLS II)

June 15-16 2010

National Synchrotron Light Source (NSLS), Brookhaven National Laboratory

Organized by Alexander Goncharov and Vitali Prakapenka on the following topics:

- Characteristics of NSLS II
- Timetable for NSLS II
- Scientific agenda of TEC beamline
- Instrumentation of TEC beamline
- Open discussion and solicitation of participation

Workshop titled Lujan Workshop: Applications of Neutron Scattering to Materials and Earth Sciences

December 11, 2010
University of California at Berkeley
Organized by H R (Rudy) Wenk and Hongwu Xu

This workshop is intended for graduate students, postdocs and junior researchers in earth sciences and other sciences with an interest in applying neutron scattering to studies of synthetic and natural materials. Topics included:

Introductions to neutron scattering techniques (diffraction and spectroscopy)
Applications to materials and Earth sciences.
Data analysis tutorials for data collected at four Lujan instruments - HIPPO, SMARTS, NPDF and FDS.

Workshop titled "Dynamic Phenomena under Extremes"

January 24 – 28 2011
University of Texas at Austin
Organized by Jung-fu Lin, Alexander Goncharov, and Vitali Prakapenka

This workshop aimed at bringing together scientists with expertise in various disciplines for in-depth discussions on experiments and theory of dynamic extreme pressures, temperatures, magnetic field and strain rates. Topics included:

Thermomechanical and electromagnetic extremes: Shock and static experiments
Melting at high pressure: experiments and theory
Material properties and synthesis under static and dynamic conditions
Strength, Rheology, and Viscosity
Thermally activated reaction dynamics
Structural Changes
Transport properties: viscosity, thermal conductivity, diffusion
Bonds, phonons, electrons and spin dynamics
Non-equilibrium crystallization

A.4 COMPRES Membership

This consortium, which was founded in May, 2002, is committed to support and advocate research in materials properties of Earth and planetary interiors with a particular emphasis on high-pressure science and technology, and related fields. COMPRES, which derives its primary financial support from the National Science Foundation, is charged with the oversight and guidance of important high-pressure laboratories at several national facilities, such as synchrotrons and neutron sources. These have become vital tools in Earth science research. COMPRES supports the operation of beam lines, the development of new technology for high-pressure research, and advocates for science and educational programs to various funding agencies.

COMPRES is community based. Educational and not-for-profit US Institutions with research and educational programs in high-pressure research in the science of Earth materials are eligible to become members, and each institution is entitled to one vote in the decision process. The membership defines policy and charts the future of the consortium. Other organizations and non-US institutions are eligible to be affiliated members with a non-voting representative to all COMPRES business meeting.

As of February 2010, there were 54 U. S. institutions which were members of COMPRES and 32 affiliate institutions overseas. In the past year, one new U. S. institution has become a member of COMPRES: Washington University St. Louis, with Phil Skemer, Elector.

In addition, new one overseas institution became affiliate members of COMPRES;

Institute for Earth's Crust, Irkutsk (Russia): Peter Dorogokupets, Representative

This brings the list of foreign members to 39.

COMPRES US Member Institutions

Institution	Elector	Alternate
Argonne National Laboratory	Wolfgang Sturhahn	Ercan Alp
Arizona State University	Thomas Sharp	James Tyburczy
Auburn University	Jianjun Dong	
Azusa Pacific University	Donald Isaak	
Brookhaven National Laboratory	Lars Ehm	Markus Hücker
California Institute of Technology	Jennifer Jackson	Paul Asimow
Carnegie Institution of Washington	Ronald Cohen	Yingwei Fei
Case Western Reserve University	James Van Orman	Nancy Chabot
Colorado College	Phillip Cervantes	
Columbia University	David Walker	Taro Takahashi
Cornell University	William Bassett	Zhongwu Wang
Delaware State University	Gabriel Gwanmesia	Al Sameen Khan
Florida International University	Jiuhua G. Chen	Surendra Saxena
Harvard University	Sarah Stewart-Mukhopadhyay	Richard O'Connell
Indiana University at South Bend	Henry Scott	Jerry Hinnefeld
Johnson Space Center , NASA	Kevin Righter	John Jones
Lawrence Berkeley National Laboratory	Simon Clark	Corwin Booth
Lawrence Livermore National Laboratory	Daniel Farber	
Los Alamos Natoional Laboratory	Dana Dattelbaum	Jianzhong Zhang
Louisiana State University	Bijaya Karki	
Massachusetts Institute of Technology	San-Heon (Dan) Shim	Robert van der Hilst
New Mexico State University	Boris Kiefer	
Northern Illinois University	Mark Frank	Jonathan Berg
Northwestern University	Steven Jacobsen	Craig Bina
Ohio State University	Wendy Panero	Michael Barton
Princeton University	Thomas Duffy	Frederik Simons
Rensselaer Polytechnic Institute	Liping Huang	Bruce Watson
Smithsonian Institution	Elizabeth Cottrell	Jeffrey Post
Stanford University	Wendy Mao	Jonathan Stebbins
Stony Brook University	Michael Vaughan	John Parise
Texas A&M University	Caleb Holyoke	
Texas Tech University	Yanzhang Ma	Valery Levitas
University of Arizona	Robert Downs	Michael Drake
University of California at Berkeley	Hans-Rudolph Wenk	Raymond Jeanloz

University of California at Davis	Charles Lesher	Alexandra Navrotsky
University of California at Los Angeles	Abby Kavner	Donald Isaak
University of California at Riverside	Harry Green	Stephen Park
University of California at San Diego	Guy Masters	
University of California at Santa Cruz	Quentin Williams	Elise Knittle
University of Chicago	Dion Heinz	Mark Rivers
University of Colorado at Boulder	Joseph Smyth	Hartmut Spetzler
University of Hawaii at Manoa	Murli Manghnani	Li Chung Ming
University of Illinois at Urbana-Champaign	Craig Lundstrom	
University of Louisville	George Lager	
University of Maryland at College Park	Andrew Campbell	John Tossell
University of Michigan	Rebecca Lange	Youxue Zhang
University of Minnesota	Renata Wentzcovitch	Tony Withers
University of Missouri - Kansas City	Michael Kruger	Ray Coveney
University of Nevada at Las Vegas	Oliver Tschauner	Pamela Burnley
University of New Mexico	Carl Agee	David Draper
University of Texas at Austin	Jung-fu Lin	Stephen P. Grand
University of Washington	Michael Brown	
University of Wyoming	David Anderson	
Virginia Polytechnic Institute and State	Nancy Ross	Ross Angel
Washington University St. Louis	Philip Skemer	
Yale University	Shun-ichiro Karato	Kanani Lee

COMPRES Foreign Affiliates

Institution	Representative
Australian National University Canberra (Australia)	Hugh O'Neill
Bayreuth Universitat (Germany)	David Rubie
Chinese Academy of Science (China)	Changqing Jin
China University of Geosciences of Wuhan (China)	Zhenmin Jin
Ecole Normale Supérieure de Lyon (France)	Jan Matas
Ehime University (Japan)	Tetsuo Irifune
Eidgenossische Techniche Hochschule Zurich (Switzerland)	Carmen Sanchez-Valle
GeoForschungsZentrum Potsdam (Germany)	Hans-Joachim Mueller
Harbin Institute of Technology (China)	Haozhe Liu
Institut de Physique du Globe Paris (France)	Guillaume Fiquet
Institute for Earth's Crust, Irkutsk (Russia)	Peter Dorogokupets
Institute of Experimental Mineralogy, Chernogolovka (Russia)	Yuriy Litvin
Jilin University (China)	Xiaoyang Liu
Macquarie University Sydney (Australia)	Tracy Rushmer
Max-Planck Institute for Solid State Research, Stuttgart (Germany)	Paul Balog
National Cheng Kung University (Taiwan)	Jennifer Kung
Novosibirsk State University (Russia)	Elena Boldyreva
Okayama University (Japan)	Eiji Ito
Peking University (China)	Qiong Liu
Royal Institution of Great Britian, The (United Kingdom)	Paul McMillian
Ruhr-Universitat Bochum (Germany)	Sumit Chakraborty
Seoul National University (Korea)	Haemyeong Jung
Tel Aviv University	Moshe Pasternak
Tohoku University, Sendai (Japan)	Eiji Ohtani
Universitat Frankfurt am Main (Germany)	Bjorn Winkler
Universite Blaise Pascal (France)	Denis Andrault
Universite de Poitiers (France)	Jacques Rabier
Universite des Science et Technologies de Lille (France)	Paul Raterron
Universite Paul Sabatier (France)	Jannick Ingrin
University College London (United Kingdom)	David Dobson
University of Calgary (Canada)	Sytle Antao
University of Cambridge	Michael Carpenter
University of Edinburgh (United Kingdom) University of Manchester (United Kingdom)	Geoffrey Bromley

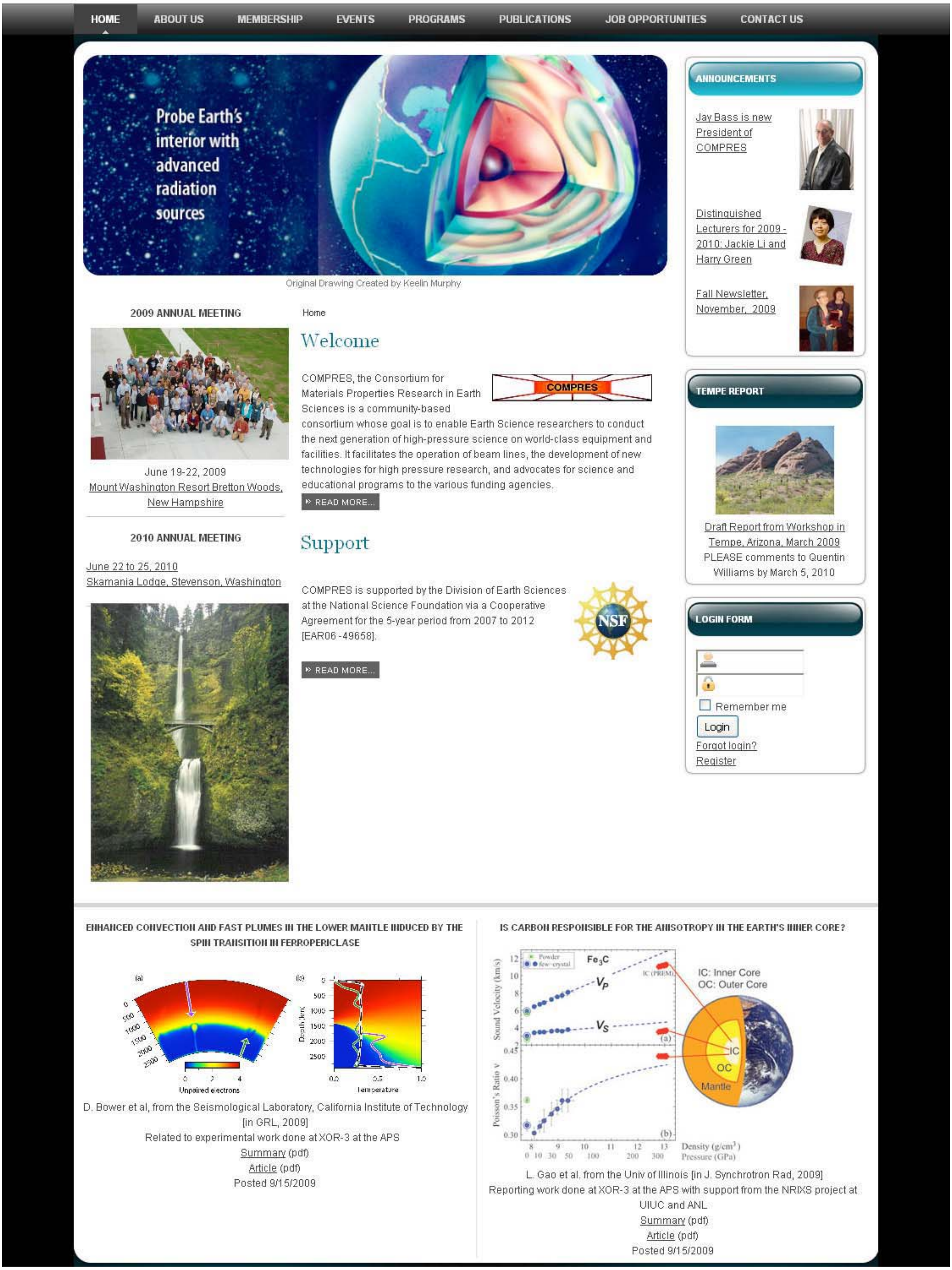
	Alison Pawley
University of Wales at Aberystwyth (United Kingdom)	Takehiko Yagi
University of Western Ontario (Canada)	Martin Wilding
Vrije Universiteit (The Netherlands)	Rick Secco
Yonsei University (Korea)	Wim van Westrenen
Yonsei University (Korea)	Yongjae Lee

A.5 Information Technology and Communications

Website

A more professional appearance of the COMPRES website is now "live" at www.compres.us. This new website has been designed by a consulting company in Stony Brook, based on advice and guidance of a special subcommittee chaired by Quentin Williams and including Tom Duffy and Nancy Ross. The website now becomes easier for readers to browse and for the webmaster to maintain. The motivation for seeking a new design and format came from comments of the Infrastructure Development Committee and the Executive Committee in December 2008. The COMPRES central office was strongly urged to engage a professional website design firm, and to make the website easier for our staff and volunteers to maintain. Steve Hurst and Chong-Hwey Fee of the UIUC Central Office have been maintaining the website since June 2010 with oversight by the President of COMPRES and the Executive Committee.

See new website at:
www.compres.us



Science Highlights on the Home Page of COMPRES website

In 2008, we introduced a new feature on the Home Page reporting recent "Science Highlights" from research published based on work performed at COMPRES-supported beamlines at the NSLS or the ALS, or on infrastructure development projects. See http://www.compres.us/index.php?option=com_content&task=blogcategory&id=45&Itemid=118

New science highlights are installed each month, based on items received by the Central Office. Please send your latest highlight and to Jay Bass.

A general overview of COMPRES

- COMPRES staff contact information
- Contact information for COMPRES the Facilities, Infrastructure Development and Executive Committees.
- Information about institutional and affiliate membership with application forms
- Links to synchrotron and neutron source web sites, including instructions for applications for beam time.
- Links to information on past and upcoming meetings.
- Publication lists for COMPRES and links to list for associated organizations [e.g., GSECARS], including:

  EOS Article "The Future of High-Pressure Mineral Physics" by Liebermann on behalf of COMPRES—4 October 2005

  Annual Reports for NSF from Years #1-5 of COMPRES I [2002 to 2007] and COMPRES II [2008 to 2010].

  Minutes of the Executive Committee

  Monthly Messages from COMPRES President

  "Current and Future Research Directions in High-Pressure Mineral Physics-The Bass Report [August 2004]

- The quarterly COMPRES Newsletters
- Education and Outreach.
- The COMPRES Image Library, described in the Education and Outreach section of this report

[link at: http://www.compres.us/index.php?option=com_joomgallery&func=viewcategory&catid=9&Itemid=94

The COMPRES Central Office envisions the future role of the web site as that of an electronic Central Office that supports all the functionality necessary to enable the Consortium to serve the community's research and educational needs. This includes automation of the entire process needed to apply to perform an experiment at a facility and for reporting on the experiment afterwards as well as the sharing of experimental results.

Other Electronic Information Technology Services

- **List servers:** The initial list server is now operational that reaches hundreds of the members of the COMPRES community. Additional lists will be established during the coming months that serve the broader high pressure community.
- **People database:** Contact information for people involved in COMPRES. Since 2004, this was made available online through a browser-based form
- **Online Forms for meeting registration:** This offers online registration for meetings and workshops.
- **Videoconferencing:** The Central Office has a license for GoToMeeting.COM to provide support for video conferences of the Executive Committee, the two Standing Committees, and other uses of the COMPRES community. This service is used regularly for bi-weekly Executive Committee meetings, and other meetings as required.

Quarterly Newsletters

Starting in November 2002, COMPRES has published a quarterly newsletter with information and announcements of interest to the COMPRES community, in the broadest sense.

These newsletters are edited by Jiuhua Chen [now at the Florida International University] and may be found on the COMPRES web site at http://www.compres.us/index.php?option=com_content&task=view&id=49&Itemid=96See COMPRES Home Page for the latest issue for November 2009.

COMPRES newsletters are resuming in 2010, after a hiatus during the transition of the Central Office from Stony Brook to University of Illinois Urbana-Champaign.

In addition to a column in the quarterly COMPRES newsletter, the President of COMPRES has sent a Monthly Message to the COMPRES community using the listserv distribution, beginning in October 2003 [see link at: http://www.compres.us/index.php?option=com_docman&task=cat_view&gid=39&Itemid=.55
The purpose of these monthly messages from the President is to keep the COMPRES community informed of recent developments as well as activities of the Executive and Standing Committees. These Monthly Messages are also sent to the Program Directors of the Division of Earth Sciences at the NSF.

A.6 Publications of COMPRES in 2008-2009

[BEAMLINE OR INFRASTRUCTURE PROJECT GIVEN IN CAPS BELOW]

2009

Aksoy, R., Selvi, E., Knudson, R., Ma, Y (2009), High pressure x-ray diffraction study of titanium disulfide, *J. Phys.: Condens. Matter*, *21*(025403).X17 DAC

Al-Khatatbeh, Y., K.K M. Lee, and B. Kiefer (2009), High-pressure behavior of TiO2 as determined by experiment and theory, *Physical Review B: Condensed Matter and Materials Physics 79, 134114* ALS

Amiguet, E., Patrick Cordier, Paul Raterron (2009), Deformation of Diopside Single Crystals at Mantle Pressure 2: TEM characterization of dislocation microstructures, *European Journal of Mineralogy, (in press).*MAC NSLS

Bower, D. J., M. Gurnis, J.M. Jackson, and W. Sturhahn (2009), Enhanced convection and fast plumes in the lower mantle induced by the spin transition in ferropericlase, *Geophys. Res. Lett.*, *36, L10306* Nuclear Resonant

Campbell, A. J., Danielson L., Righter K., Seagle C. T., Wang Y., and Prakapenka V. B. (2009), High pressure effects on the iron-iron oxide and nickel-nickel oxide oxygen fugacity buffers., *Earth Planet. Sci. Lett.*, *286, 556-564*.MAC ASU

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Chen, B., H.Z. Zhang, K.A. Dunphy-Guzman, D. Spagnoli, M.B. Kruger, D.V S. Muthu, M. Kunz, S. Fakra, J.Z. Hu, Q.Z. Guo, and J.F. Banfield (2009), Size-dependent elasticity of nanocrystalline titania, *Physical Review B: Condensed Matter and Materials Physics 79(12), 125406* ALS

Chen, B. G. L. L., K.; Wang, Y.; Li, J. (2009), In situ investigation of diapirism as a core formation mechanism using high-pressure synchrotron X-ray radiography, *Abstract, 2009 AGU Fall Meeting*.MAC ASU

Choi, C. L., K.J. Koski, S. Sivasankar, and A.P. Alivisatos (2009), Strain-Dependent Photoluminescence Behaviour of CdSe/CdS Nanocrystals with Spherical, Linear and Branched Topologies, *NANO Letters*, *9(10) 3544-3549* ALS

Ciezak, J. (2009), The high-pressure characterization of energetic materials, *Propell. Explos. Pyrot., in press*.U2A DAC (X17 DAC)

Ciezak, J. (2009), The high-pressure characterization of energetic materials: 1-methyl-5-nitramino-1H-tetrazole, *Propell. Explos. Pyrot., in press*.U2A DAC (X17 DAC)

Ciezak, J. (2009), The high-pressure characterization of energetic materials: 2-methyl-5-nitramino-2Htetrazole *Propell. Explos. Pyrot., in press*.U2A DAC (X17

DAC)
Ciezak, J., Dandekar, D. (2009), Compression and associated properties of boron carbide, *Shock Compression of Condensed Matter, in press*, *AIP, New York*.U2A DAC (X17 DAC)
Couvy, H., Jiuhua Chen and Vadym Drozd (2009), Compressibility of nanocrystalline forsterite, *Phys Chem Minerals (in press)*.MAC NSLS
Diedrich, T. M., F.C.; Leinenweber, K.; Sharp, T.G. (2009), The Effect of Small Amounts of H2O on Olivine to Ringwoodite Transformation Growth Rates and Implications for Subduction of Metastable Olivine, *Chemical Geology*, *262*, pp. 87-99.MAC ASU
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Li, B. (2009), On the characteristics of lateral heterogeneities with thermal and chemical origins in pyrolite lower mantle, *Progress Natural Science (in press)*.MAC NSLS
Li, L., Liping Wang, Michael T. Vaughan (2009), An Exploratory Study of the Viscoelasticity of Phase-Transforming Material, *Phys. Earth Planet. Interiors, in press*, *174, 174-180* MAC NSLS
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Structral Phase Transition of Y2O3/Eu3+ Nanotubes under High Pressure, *Joint AIRAPT-22 and HPCJ-50 International Conference on High Pressure Science and Technology, Tokyo, Japan, p. 67* U2A DAC

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Liu, Q., Wei Liu, Matthew Whitaker**, Liping Wang and Baosheng Li (2009), Ultrasonic study of fayalite-spinel phase transition at high pressure, *Am. Min. (submitted)*.MAC NSLS

Liu, W., Jennifer Kung, Baosheng Li, N. Nishiyama and Yanbin Wang (2009), Elasticity of Wadsleyite at 12 GPa1073K. , *Phys Earth Planet Interi.* , *174 98-104* MAC NSLS

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Lord, O. T., M.J. Walter, R. Dasgupta, D. Walker, and S.M. Clark (2009), Melting in the Fe-C system to 70 GPa, *Earth and Planetary Science Letters*, *284, 157-167* ALS

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Pravica, M., E. Romano, S.N. Tkachev and Z. Liu (2009), High pressure infrared study of 1,3,5,7-cyclooctatetraene (COT), *Journal of Physics., accepted*.U2A DAC

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A.7 Education and Outreach

During the past five years, COMPRES has worked with other organizations to promote inquiry-based education and outreach as nationwide collaborations between scientists, educators, materials developers, government agencies and other stakeholders.
Glenn Richard and William Holt at Stony Brook, and Michael Hamburger at Indiana University are currently PIs on an NSF grant entitled "Collaborative Research: Map Tools for EarthScope Science and Education". This project is aimed at the development of a suite of mapping tools and curriculum materials to enable the research and educational communities to work with EarthScope and other geological, geodynamic and geophysical data.

COMPRES maintains a searchable image library which is available on the web from its home page [see link at: http://www.compres.stonybrook.edu:8080/COMPRESImageLibrary/index.html.

This is designed to make images available to the academic community for education and research. This Library contains graphic images drawn from COMPRES meetings and workshops, with notes for referencing and appropriate attribution. We encourage members of the COMPRES and wider community to take advantage of this resource and to contribute to its growth.

New outreach initiatives for 2008-2010

Teaching Mineral Physics across the Curriculum

In collaboration with David Mogk from Montana State University, we are beginning to work with our community to develop a module for "Teaching Mineral Physics across the Curriculum." This module will be part of the "On the Cutting Edge" project which Mogk supervises as part of the Science Education Research Center of Carleton University.

Discussion of this new educational initiative was pursued at the long-range planning workshop in Tempe, Arizona [March 2-4, 2009]during the breakout session on
"Educational Opportunities: What can Mineral Physics deliver to K-16 Education?" which is being led by Pamela Burnley and Gabriel Gwanmesia. Dave Mogk also attended the 2009 Annual Meeting of COMPRES and gave a short presentation on this project and interacted with many members of our community. [See photo in Supplemental Information].

Bob Liebermann has been serving as coordinator between the COMPRES community and Mogk's project, with technical and scientific advice from Glenn Richard.

To date, contributions to this module have been received from Alex Navrotsky, Abby Kavner, Pamela Burnley, and Artem Oganov and several other people are working on developing special items on multi-anvil apparatus and use of synchrotron X-radiation facilities for research in mineral physics.

Distinguished Lecturer Program

COMPRES has established a distinguished lecture series, starting in Year #2. This was on the successful models of other organizations, such as the Mineralogical Society of America.

We proposed to select two outstanding scientists and lecturers and offer to send them to U. S. academic institutions to give a COMPRES-sponsored lecture. All travel expenses are provided by COMPRES.

For 2010-2011 James Tyburczy organized the lecture series. The resources allocated to the Distinguished Lecturer series was increased. By more extensive advertizing in EOS and Earth [the successor to Geotimes], we hoped to attract invitations from more undergraduate liberal arts & sciences colleges and community colleges, which may be less familiar with the field of mineral physics. It was also decided to cover all expenses for the lecturers, rather than asking host institutions to cover local expenses. In the current year, COMPRES received 28 requests for lecturers, a record number, and a larger fraction of those requests were received from undergraduate institutions with no mineral physicist on the faculty. Although the cost of the lecture series has increased to ~$750 per visit, we have been highly successful in reaching our target audience with the Distinguished Lecture Series.

The Distinguished Lecturers for COMPRES in 2010-2011 were:

Wendy Panero, Ohio State University visited

- West Chester University (PA)
- Lafayette College
- James Madison University
- Chapman College
- Harvey Mudd College
- Pomona College
- Carleton College
- University of Minnesota at Duluth

James van Orman, Case Western Reserve University visited

Illinois State (Normal, IL)
Indiana U South Bend
Miami U (Ohio)
Vanderbilt
Louisiana State University
Univ of Houston
College of Wooster (Ohio)

Enhancing Diversity in the Geosciences

Under the auspices of the NSF program for "Opportunities for Enhancing Diversity in the Geosciences" [OEDG], a team of Liebermann, Gwanmesia and Ehm submitted a proposal in December 2008 for a new Masters of Science Program in Geosciences Instrumentation at Stony Brook University.

`This new MS Program in Geosciences Instrumentation is proposed to build on the development of a consortium of professors from Historical Black Colleges and Universities [HBCUs] and the National Synchrotron Light Source [NSLS] of the Brookhaven National Laboratory [BNL]. This consortium [INCREASE: Interdisciplinary Consortium for Research and Educational Access in Science and Engineering] is an organization to promote research in HBCUs and other minority-serving institutions [MSIs], involving utilization of national user facilities, such as the NSLS at BNL; see http://increase.nsls.bnl.gov/. and http://www.nsls.bnl.gov/newsroom/news/2008/08-HBCU_Workshop.htm.

This MS program in Geosciences will be modeled after the existing program for Master of Science in Instrumentation in the Department of Physics & Astronomy at Stony Brook University, and will include both formal courses in Geosciences and Physics &

Astronomy and internship research at the beamlines operated by COMPRES at the NSLS of BNL. [Consortium for Materials Properties for Research in Earth Sciences http://www.compres.stonybrook.edu/]. This new OEDG program will also be complimentary to the existing OEDG program led by Gilbert Hanson of the Department of Geosciences at Stony Brook.

Partners in this new initiative will include: (1) Center for Inclusive Education at Stony Brook University, which is the lead institution for the SUNY-wide Alliance for Graduate Education and the Professoriate funded by the NSF-see website at: http://www.sunysb.edu/agep/ and its Summer Research Institute http://www.stonybrook.edu/agep/Summer_Research_Institute/; (2) the Office of Educational Programs at the Brookhaven National Laboratory http://www.bnl.gov/education/;
and its Science Undergraduate Laboratory Internship program http://www.bnl.gov/education/programs/suli.asp; (3) the Research Experience for Undergraduates summer program of the Mineral Physics Institute of Stony Brook University http://www.mpi.stonybrook.edu/SummerScholars/;

The goal of this new program is to recruit undergraduate students from underrepresented groups into the graduate program in Geosciences at Stony Brook, to educate them via formal course and research to the M. S. degree, and to position them for employment in national user facilities.

Principal Investigator: Robert Liebermann, COMPRES and Stony Brook University
Co-Principal Investigators:
Gabriel Gwanmesia, Delaware State University and Stony Brook University
Lars Ehm: Brookhaven National Laboratory and Stony Brook University

This December 2008 proposal was declined, but the PIs are planning to revise the proposal and submit it to a new GeoEd Program in the NSF Directorate of Geosciences in March 2010.

A.8 Management and Organization

Executive Committee

The Executive Committee is comprised of the Chair and four elected members, each elected by the Electorate. The responsibilities of the Executive Committee include oversight of activities, meetings, and workshops, educational and outreach programs, and coordination with the Grand Challenge programs. At all meetings of the Executive Committee, the presence of a simple majority of its members then in office shall constitute a quorum for the transaction of business.

The elected chairs of the Standing Committees on Facilities and Infrastructure Development serve as non-voting advisors to the Executive Committee.

The appointed President attends all meetings of the Executive Committee, as a non-voting member.

A statement of the Polices and Procedures for the COMPRES Executive Committee and Standing Committees can be found at:

http://www.compres.us/index.php?option=com_content&task=view&id=25&Itemid=59

Current members and affiliation (term of service)

Thomas Duffy, **Chair [2010-2013]**
Przemek Dera, Member 2010-2013
James Tyburczy, Member 2008-2011
James van Orman, **Vice Chair, 2010-2012**; Member 2009-2012
Nancy Ross, Member 2010-2013

Facilities Committee

The Facilities Committee oversees the community facility program. It evaluates the effectiveness of the service delivered by the community facilities. It coordinates between facilities (such as between beamlines) so as to maximize the community's effectiveness in using these facilities. This committee will consider the community's needs and recommend changes in the levels of support of all possible community facilities. It will formulate policies for evaluation of user proposals for accessing COMPRES community facilities.Elected by Electorate.

Current members and affiliation (term of service)

Wendy Panero, **Chair [2009-2011]** Member 2006-2012
Andrew Campbell, Member 2008-2011
Jennifer Jackson, Member 2010-2013
Wendy Mao, Member 2009-2012
Yanbin Wang, Member 2008-2011

Infrastructure Development Committee

The Infrastructure Development Committee reviews infrastructure development projects that are supported by COMPRES. It has the responsibility to assure that these projects serve the needs of the community. The committee will recommend whether a project should continue or not, and what changes are needed to better meet the needs of the community. It will also evaluate proposals by the community for new development projects and make recommendations concerning funding.

Current Members and affiliation (term of service)

Pamela Burnley, Chair 2010-2012, Member 2010-2013
Thomas Sharp, Member, 2006-2010
Steven Jacobsen, Member 2008-2011

Abby Kavner, Member 2009-2012
Jie Li . Member 2008-2011
Oliver Tschauner, 2010-2013

Advisory Council

Members and affiliation (term of service)
Edward Garnero**,** Arizona State University, Member 2008-2011
Peter Heaney, Pennsylvania State University, Member 2009- 2012
Chi-Chang Kao**,** Brookhaven National Laboratory, member 2003-2011
Louise Kellogg, University of California at Davis, Member 2007-2013 (2 terms)
Peter van Keken, University of Michigan, Member 2010-2013
Andrew Jephcoat, Diamond synchrotron and Cambridge University, 2009-2012

On 22 June 2010, the Advisory Council met with the Executive Committee just prior to the start of the Ninth Annual COMPRES Meeting in Skamania Lodge, Stevenson WA. The Advisory Council heard talks by the President, and the chairs of all committees. At the end of the annual meeting, the advisory council gave a list of recommendations to the Executive Committee.

Finally, we would like to welcome the new members of the Advisory Council for three-year terms commencing June 2010:

Peter van Keken from the University of Michigan

Operation of the COMPRES Central Office

The Central Office of COMPRES is located at the University of Illinois in the Natural History Building.

The Central Office staff includes Jay Bass, the President of COMPRES and Chong-Hwey Fee, Administrative Coordinator, both of whom are supported by the COMPRES Cooperative Agreement with the NSF. Ms Fee succeeds Ms. Emily Vance, who held the equivalent position at Stony Brook.

The administrative operation of COMPRES is also supported by Steve Hurst of the Geology Department.

Professor Jiuhua Chen of Florida International University in Miami continues to edit the COMPRES Newsletter from FIU.

President of COMPRES

The President of COMPRES acts as the Principal Investigator of the Cooperative Agreement and the Chief Administrative Officer of the consortium. He/she is appointed by the Executive Committee, in consultation with the congnizant NSF Program Director, and serves at the pleasure of the Executive Committee.

From August 2003 to January 2010, Robert Liebermann has served as the President of COMPRES. In May 2008, in consultation with the Executive Committee expressed his plans to step down from this position, as early as September 2009 and not later than February 2010.

The Executive Committee appointed a Search Committee for a new President in June 2009; the Search Committee was initially chaired by David Walker and included Abby Kavner, Harry Green, Guy Masters, and Russell Hemley as members. Walker later recused himself and Kavner was appointed chair and John Parise added as a member.

In November 2009, the Executive Committee offered the position to Jay Bass of the University of Illinois at Urbana-Champaign. Bass accepted this offer and became the President on January 1, 2010. Liebermann agreed to stay on as Past President until June 2010 to assist in the transition. In June 2010, the Central Office of COMPRES and the Cooperative Agreement will move to the University of Illinois at Urbana-Champaign.

New COMPRES Central Office

The new COMPRES central offices will be located in the Geology Department of the University of Illinois Urbana-Champaign (UIUC). The Geology Department at UIUC is part of the School of Earth, Society and Environment (SESE). The Geology Department of UIUC is providing in-kind support of the COMPRES Central Office that is necessary for COMPRES operations. UIUC is providing adjoining newly-renovated office space for the President and an Administrative Assistant to form a coherent COMPRES Central Office. Dr. Steven Hurst of SESE will be performing IT support year-round, website maintenance, and assistance in handling IT/computer requirements at the COMPRES Annual Meeting. Scott Morris and Ms Marsha Hatchel will be made available to provide in-house assistance on handling financial and proposal-related aspects of operating COMPRES.

A.9 President's Narrative

2010 has been a busy and productive year for COMPRES. Most of this progress is highlighted in Sections A, B and C of this Annual Report. I include in this narrative some additional news and highlights.

Perhaps the most significant 2 events have been 1) transfer of the COMPRES Central office to University of Illinois, and 2) A change in the management of the West Coast Synchrotron Facility (beamline 12.2.2 at the Advanced Light Source) from Raymond Jeanloz and Simon Clarke (UC Berkeley) to Quentin Williams (UC Santa Cruz). With this change in leadership, the productivity of the beamline has continued on its upward trajectory, and it has made significant progress toward building a stable, robust laser-heating facility that was a top priority for the Earth Sciences user community.

In January-May 2010 I made approximately 8 trips to Stony Brook to work with Bob Liebermann to learn about running the COMPRES organization, to visit facilities at the National Synchrotron Light Source (NSLS), and to attend town hall meetings at NSLS. At these tornhall meetings news and announcements were made about were made about the NSLS II, a replacement for the NSLS that is under construction. In February, a call for proposal for beamline development proposal at the NSLS-II was announced with a deadline of August, 2011.

In November 2009 Bass visited the Spring 8 synchrotron in Japan. Bass inspected and took part in inelastic x-ray scattering experiments. Prior to the synchrotron visit, Bass toured the facilities at foreign affiliate Tohoku University in Sendai Japan.

In June 2010 Bass and Liebermann attended the Joint Annual Meeting in Washington DC and hosted a booth describing COMPRES and it's Educational/Outreach activities.

In June Bass visited the Geophysical Laboratory of the Carnegie Institution of Washington in northwest DC. Bass gave two talks. He discussed COMPRES business with COMPRES members at CIW. I met with Bob Hazen and colleagues (Yingwei Fei and Ron Cohen) to learn about their plans for a "Deep Carbon Observatory." Hazen and Russell Hemley are the PIs on a proposal to the Sloan Foundation to develop the concept and plans for a 10-year initiative in this field. See further details at:
http://dco.gl.ciw.edu/

In May 2010 Bass attended the Spring AGU meeting in Toronto. New Fellows of the AGU from the mineral physics community were Jay Bass, Donald Dingwell, Kei Hirose and Frederic Ryerson. Fellows took part of the awards ceremony.

A.10 Annual Program Plan and Budget Request for Year #4

In preparation for the submission of the Annual Progress Report and Annual Program Plan and Budget to NSF in February, 2011, the Executive Committee developed a process that involved the COMPRES community and the two elected Standing Committees for Community Facilities and Infrastructure Development Projects.

In September 2010, the two Standing Committees asked the project directors of each of the subawards to submit annual progress reports for Year #3 and program plans and budget requests for Year #5 by November 1, 2010. The Infrastructure Development Committee also issued a call to the COMPRES community for proposed new initiatives for technological projects that would contribute to the COMPRES mission, with a deadline of November 1, 2010.

Following receipt of the requested information, the Standing Committees evaluated the progress reports and budget requests via a series of email exchanges and teleconferences, culminating in meetings of the Committees at the Fall 2010 AGU Meeting in San Francisco. Each of the Standing Committees gave oral reports on their deliberations to the Executive Committee at the Fall AGU Meeting, and then submitted their written report, with evaluations of progress and recommendations for funding in Year #5, to the Executive Committee. In the case of the Infrastructure Committee, this report included recommendations for initial funding of new projects and community workshops.

Two of the Infrastructure Development projects submitted in 2010 presented compelling cases for immediate funding of their initiatives. These were the HEETDAC project by Quentin Williams and Rudy Wenk, which requested funding for continued support of a scientific staff member at the ALS beamline 12.2.2. Funds were needed to complete a resistance heating project, and to sort out personnel decisions that became critical due to budgetary restrictions from the Year 4 allocation by COMPRES. The other project that applied for a mid-year start was an Education and Outreach proposal by Pamela Burnley of University of Nevada Las Vegas. In order to hire an available post-doc who would be extremely well suited for this project, mid-year immediate funding was needed. COMPRES therefore made a decision to reallocate available resources to start these two projects mid-year.

In January 2010, the Executive Committee met via video and teleconference on four occasions to discuss the reports of the Standing Committees and to formulate recommendations for an Annual Program Plan and Budget for Year #4. Following these meetings, the new President, Jay Bass prepared a budget plan which was discussed, revised, and approved unanimously by the Executive Committee. The budget summary is given in Section D below, with detailed NSF 1030 budget forms and budget justifications given in Section E.

B. Community Facilities

B.1 X-ray Diamond-anvil Facilities at the National Synchrotron Light Source
[PIs: Thomas Duffy, Princeton University, and Donald Weidner, Stony Brook University]
2009 COMPRES Annual report for beamlines X17C and X17B3
November 2009 – November 2010

Science Overview

From January 2009 – October 2010, 62 publications (peer reviewed, conference publications, and theses) resulting from work at X17C and X17B3 have been recorded (Appendix). These include 5 PhD theses and 1 M.S. thesis. The May/June 2010 edition of *Synchrotron Radiation News* focused on high-pressure research and included an article by Lars Ehm et al showcasing high-pressure research at X17C and X17B3. A summary of the wide range of research topics covered at the beamline is given below.

High-Pressure Structures and Phase Transitions

The apatite family of calcium phosphates is an important class of minerals that are of interest in many subfields of geology and geochemistry. One potential environmental application of these phases is the remediation of lead contamination in soils. *Fleet et al* (2010) studied structural changes in lead fluorapatite, $Pb_{10}(PO_4)_6F_2$, by powder x-ray diffraction up to 9 GPa. Rietveld structural refinements were performed and the results used to show how the response to compression of the Pb-endmember differs significantly from that of calcium apatites.

ABO_4 compounds form a number of different fundamental structure types such as monazite, zircon, and scheelite. $BaCrO_4$, which is isostructural with the mineral barite ($BaSO_4$), was studied to 25 GPa using both Raman spectroscopy and x-ray diffraction to address outstanding questions about phase transitions and compressibility in this system (*Huang et al*., 2010). A new monoclinic phase, BaCrO4-II, was found to be stable above 9 GPa and this phase has not been identified in the ABO_4 system before.

The high-pressure behavior of Y_2O_3 was studied to better understand the sequence of structural phase transitions in rare earth sesquioxides (*Halevy et al.,* 2010). Previous reports of phase transitions in this material are mutually inconsistent, and it was shown in this work that Y_2O_3 adopts the same sequence of phases with pressure (cubic→ monoclinic→hexagonal) as other lanthanide sesquioxides. The volume change and equation of state for each phase was also determined.

Pyrochlores at high pressure

Zhang et al (2010) have demonstrated a new method to detect and quantitatively measure pressure-induced atomic disordering in pyrochlore oxides. This discovery provides new insight on the formation of defects at extreme conditions and reveals a possible mechanism for photochemical reactions in these oxides. X-ray diffraction data collected on $La_2Zr_2O_7$ at X17C show that defects originating from the cation and anion sites in the pyrochlore structure have different influences on individual diffraction peaks. Using the Rietveld refinement method, it was concluded that anion defects formed below 5 GPa and cation antisite defects dominated above 10 GPa. An anomalous lattice expansion was confirmed in the oxide at 10 GPa by x-ray diffraction.

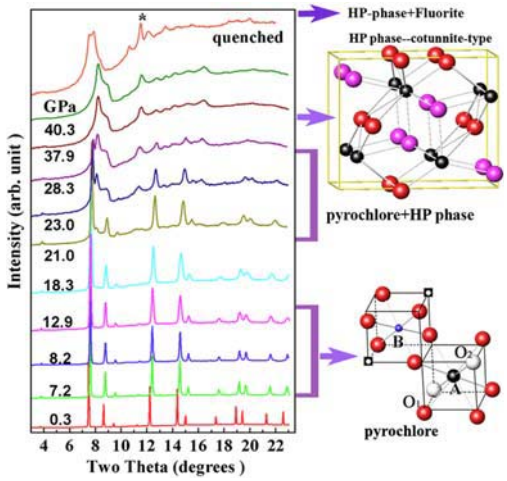

Fig. 1. Selected XRD patterns of $La_2Zr_2O_7$ at different pressures. Below 21 GPa, the structure is pyrochlore. A distorted cotunnite-type high-pressure structure starts to form after 21 GPa and the phase transition is complete after 37.9 GPa.The quenched sample is a mixture of the high-pressure phase and defect fluorite (peak marked with a star is from the gasket).

Nanomaterials

Nanocrystalline minerals are of interest in diverse areas including studies of fault gouge, phase transitions in subducting slabs, and environmental geochemistry. In experiments carried out at both X17B3 and X17B2, the compressibility of nanocrystalline forsterite was examined over a range of P-T conditions (*Couvy et al*., 2010). Nanocrystalle forsterite is more compressible than bulk material and the difference is attributed to a weakening of the elastic properties at grain boundaries and triple junctions and their more significant contribution to the behavior of the nanocrystalline sample.

The role of particle size on phase transition pressure is another topic that has attracted much interest with most studies showing that the transition pressure increases with decreasing particle size for many minerals and other phase. *Zhu et al* (2010) examined how the phase transformation from maghemite to hematite varies with particle size. Contrary to most other materials, particles size does not affect the transition pressure in this system as both nano- and bulk γ-Fe_2O_3 transform to hematite beginning from 16 GPa.

Other work on nanomaterials at X17-DAC investigated pressure-induced amorphization in one-dimension TiO_2 nanoribbons (*Li et al.* 2010), and the structural and luminescence properties of Y_2O_3 nanotubes (*Zhu et al.*, 2010).

Non-Linear Pressure Effects in Perovskite Manganites

The $RE_{1-x}A_xMnO_3$ (RE= rare earth and A = Ca, Sr, Ba) mixed valence perovskite system exhibits complex and intriguing properties and an understanding of the basic physics of these materials has still not been realized. It has been found that a strong coupling exists among the lattice, spin, and electronic degree of freedom that is manifested by complex phase diagrams. The properties of manganites depend strongly on subtle changes in the structure and chemistry of the system induced by changing the RE or A site ion size. Modification of the structure by cation substitution may alter the system in unpredictable ways.

High-pressure resistivity and x-ray diffraction measurements were conducted on $La_{0.85}MnO_{3-\delta}$ to ~6 GPa and ~7 GPa, respectively (Chen et al., 2010). At low pressures the metal-insulator transition temperature (T_{MI}) increases linearly up to a critical pressure, P* ~ 3.4 GPa, followed by reduction of T_{MI} at higher pressure. Analysis of the bond distances and bond angles reveal that a bandwidth increase drives the increase of T_{MI} below P*. The reduction of T_{MI} at higher pressures is found to result from Jahn-Teller distortions of the MnO_6 octahedra. The role of anharmonic interatomic potentials was explored.

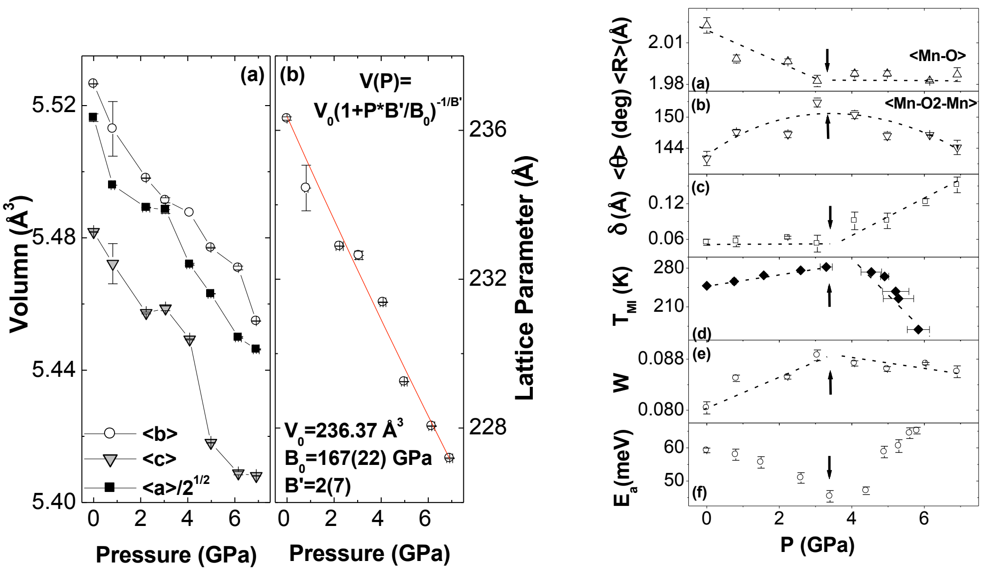

Fig. 2. Left: Lattice parameters of $La_{0.85}MnO_{3-\delta}$ as a function of pressure. **Right:**. Pressure dependence of structural and electronic parameters.

Beamline Overview, 2009-2010

Since June 2007, a multi-institution management team has led X17-DAC. The management team is headed by PIs Donald Weidner (Stony Brook) and Thomas Duffy (Princeton). The other members of the management team are: Mark Rivers (Chicago), Lars Ehm (NSLS/SBU) Alex Goncharov (Carnegie), Jiuhua Chen (FIU), and Sanjit Ghose (NSLS-II). Chi-chang Kao has been removed from the management team due to his departure from NSLS. Sanjit Ghose has been added to the management team.

Stony Brook University serves as the funding host for the project. The management team, beamline staff, and technical support staff hold telephone conferences on an as-needed basis.

Beamline Scientists

Sanjit Ghose left his position at X17-DAC on Dec. 31, 2009 to become project scientist for the powder diffraction beamline at NSLS-II. We advertised for a replacement and received 17 applications. 3 candidates were interviewed by the search committee (Ehm, Weidner, Duffy). Xinguo Hong, who has extensive synchrotron and high-pressure experience (CV in appendix), was offered the position by mid-March. Unfortunately, the process of transferring his visa from his current employer (BNL) to Stony Brook took an unusually long time, and Hong was not able to begin work at X17 until June 21, 2010. As a result, we operated for about 6 months in 2010 with only a single beamline scientist (Dr. Zhiqiang Chen). During this period, both beam lines ran smoothly for all users' experiments and some development projects also advanced (with the assistance with S. Ghose). Other projects were necessarily delayed. Since mid-June 2010, we have been working to incorporate and train X. Hong fully in the beamline operations. Returning to full staffing has enabled beamline development work to increase, and this trend should continue in the future.

Other Key Personnel

Lars Ehm (BNL/SBU) is a Research Assistant Professor at the Mineral Physics Institute at Stony Brook University and the National Synchrotron Light Source at Brookhaven National Laboratory. He provides on-site scientific and technical support to the high-pressure program at X17 at no cost to COMPRES. Lars is also playing a central role in the construction and operation of the new facility-operated beamline X17A.

Sanjit Ghose (BNL/NSLS-II) continued to devote 10% of his time to X17 under an MOU with the NSLS-II. This MOU has now expired, but Sanjit is continuing to donate his time informally. Sanjit has led a number of important development projects: testing and set-up of PE flat-panel detector, design and installation of a new universal detector mount, and general assistance with computers, communications, and controls.

Beamline operations in 2009-2010

The diamond anvil cell X-ray (X17-DAC) facilities at the National Synchrotron Light Source (NSLS) are located on a superconducting wiggler beamline and consist of two stations (X17C and X17B3) and a sample preparation/spectroscopy laboratory. The X17C beamline is a side station that runs 100% of the time, amounting to a maximum of 81 days for each of the three cycles during the year. The X17B3 beamline operates 33% of the time in dedicated mode with an additional 33% available in shared mode when the X17B2 (multi-anvil) station is running. This nominally provides a maximum of 54 days per cycle. Both X17C and X17B3 beamline are available for energy dispersive (EDXD) and monochromatic (ADXD) experiments. The major beamline characteristics are described in the Appendix. Currently all funding for the X17-DAC effort is provided by the NSF through COMPRES.

The X17 beamlines are NSLS Facility Beamlines with a Contributing User agreement with COMPRES. The NSLS is responsible for the operation of the beamline (optics, safety systems, etc.) while COMPRES is responsible for operation of the experimental stations. 50% of the beamtime is given to general users (GU) and 50% of the available beamtime (CU) is assigned to COMPRES. All proposals are first submitted through the proposal system at NSLS to compete for GU time. CU time may be assigned to proposals without a sufficiently high rating to obtain GU time, to increase the number of days for a successful GU proposal, or for use by beamline staff.

The table below provides an overview of the number of proposals received in 2009 and 2010. During Nov 2008-Nov.2010, X17C had more than 100 person-visits representing 20 separate universities and institutes while X17B3 had ~25 person-visits representing 10 separate universities and institutes. Details of the number of proposals, beamtime assignments, and total usage are provided in the Appendix. The X17 facility remains oversubscribed. The number of user groups has remained relatively steady for the last few years, and 4 new user groups have been working at X17-DAC in 2010.

	2009		2010	
	X17C	X17B3	X17C	X17B3
# proposals	48	18	55	24
# days requested	296	187	304	103
#days beamtime available *	210.73	120.66	195	100
Oversubscription	1.40	1.55	1.56	1.03
Funding **				
NSF	30	13	26	14
DOE	10	1	14	3
DOD	3	0	2	0
Foreign	9	4	16	7

Table I. Proposal statistics for 2009 and 2010.

Beamtime Losses

In 2010, NSLS has experienced continued problems with the refrigeration system for the superconducting wiggler. As a result, we lost beamtime for about 27 days this year. A new cooling system for the wiggler has been ordered and installation is expected during the winter shutdown. In addition,

Beamline Upgrades

X17C

Improved Energy Calibration for Mono beam

Drift of mono beam (~30.49 keV) at X17c can occur due to heat load on the double Laue monochromator. An effort to improve the energy calibration for the monochromatic beam was therefore initiated and tested. We perform calibrations using a CeO2 standard at multiple distances whose separations are accurately known into order to constrain the x-ray energy. The calibration is then cross-checked against other standard materials (e.g. Au). The energy calibration for the two standard is in agreement to better than 0.1%.

Sample Stage

The sample stages at X17C, X17B3, and ruby system were improved with new kinematic baseplates.

Radial X-ray Diffraction

A new panoramic DAC cell was purchased and used for the first time in 2010-II. Angle dispersive diffraction in a radial geometry can now be carried out routinely at the beamline.

X17B3

Since January 2010, our efforts at X17B3 have focused on 1) Total Scattering PDF measurements, and 2) redesign and upgrade of the beamline. With the effort of the beam line scientists, the number of proposals for PDF experiments is significantly increased. This specific technique at X17B3 has attracted more users even from outside US.

Figure 3. PE Flat Panel detector mounted on newly designed detector bench.

Amorphous Si Flat Panel Detector

An amorphous Si flat panel detector (Perkin Elmer XRD 1621) was received in Dec. 09 (Fig. 3). This is a high-energy digital imaging detector with 15 Hz frame rate optimized for use at ~80 keV. It also features exceptional dynamic range and point spread function. A computer with special specifications to accommodate fast and high volume data was obtained. Sanjit Ghose is setting up EPICS controls to remotely operate the new instrument using Mark Rivers's AreaDetector software. The commissioning of the detector ha started and the first user group will use the detector in October 2010. Based on our initial tests, the detector will work very well for powder diffraction experiments at 30 keV for high Q experiments (> 28 $Ang.^{-1}$) at 80 keV. The major drawback is the charge accumulation and decay issue and we have made considerable progress already in developing a data accumulation strategy to minimize this. A preliminary performance report on the detector prepared by Sanjit Ghose is presented in the appendix.

Computers and Communications

Two new controller computers for each beamline (X17C and X17B3) have been setup and tested (with assistance of K. Baldwin, SBU). A complete switch-over from the old system will occur during the 2010 winter shutdown.

High Energy Beam Transport and Shielding

A new X-ray transport tube with internal lead shielding was designed and mounted. This will reduce scattered background for all experiments (white, 30 keV, 80 keV). (Fig. 3.)

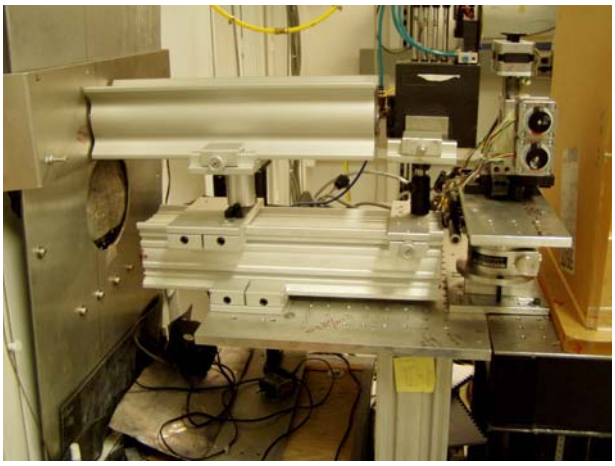

Fig. 4. The new x-ray beam pipe at X17B3.

KB Mirrors

A new mirror box (Fig. 4) to accommodate the new layout at X17B3 has been designed and constructed through the Stony Brook machine shop. This will enable us to house the mirrors in an inert gas.

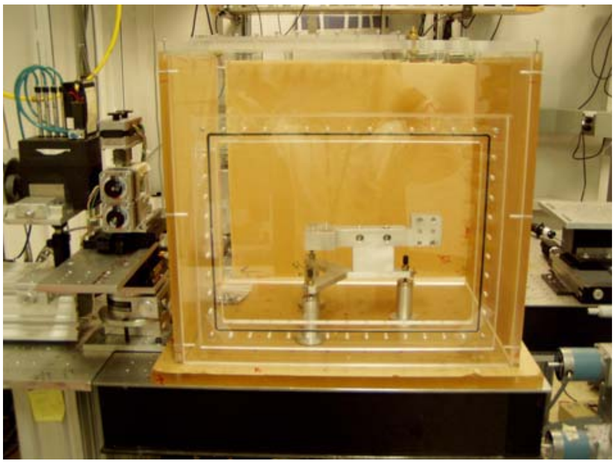

Fig. 54. The new KB mirror box at X17B3

Universal Detector Stage

A new detector bench has been designed and installed at X17B3 (Fig. 3). This system allows us to accommodate any type of detector (including the new PE) and to have X/Y/Z translation to adjust according to the size of the detector and beam center. The system was designed by Sanjit Ghose and fabricated by the machine shop at NSLS. The new table was installed and partially tested in August, 2010.

X-Ray Mirror Development

A new multi-layer lateral-gradient mirror for high energy DAC experiments is being developed for X17B3 by Sanjit Ghose. The goal is to provide the first capability to focus 80 keV energy for high-pressure experiments anywhere in the world. This will provide a unique capability for high Q experiments at high pressure. Eventually, an energy tunable monochromator will be installed at X17B3. The project serves as a test for NSLS-II development and the mirrors are being built at the NSLS-II fabrication facility. The new multi-layer optics will have the same size as the currently use Pt-coated mirrors and therefore allow the use of the same mirror bender configuration.

Laser Heating System

The following developments were realized in the last year.

The new interlock system for the X17B3 class IV laser heating system was installed, tested, and approved (Feb. 10).

A laser heating meeting was held in March 2010 attended by Ehm, Weidner, Duffy, Hong, Ghose, Chen, Goncharov, and Prakapenka to outline and plan the further steps for bringing the facility into operation.

The Fiber Laser (100W, 532nm) and NSLS-approved shutter has been mounted and tested in X17B3.

The laser heating system was set-up on a portable optical breadboard (Fig. 6). After initial tests, further modifications are now in progress.

A new spectrometer and CCD detector (Princeton Instrumenst) for temperature measurement has been obtained.

A temporary Safety Operation Procedure (SOP) for the Laser Heating System has been updated and approved by both BNL and NSLS safety personnel. The portable optical breadboard for laser beam focusing is allowed to be aligned inside X17B3 hutch by using the proper PPE and Al sheet enclosure around.

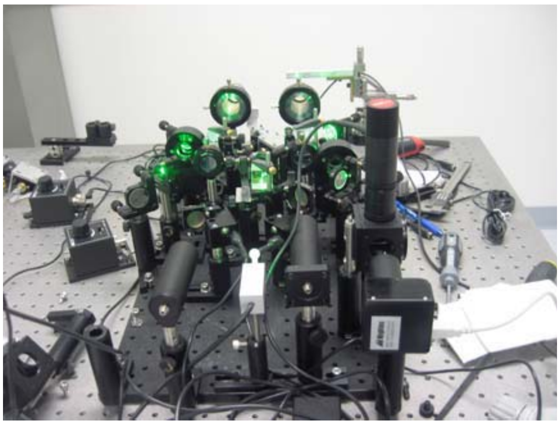
Fig. 6. The new setup for the laser bread board.

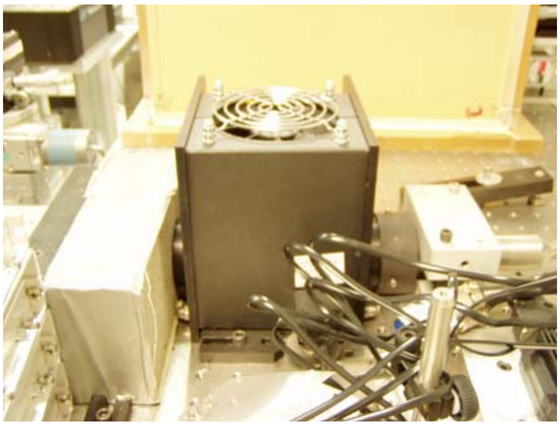

Fig. 7. IPG fiber laser (1066nm, 100W)
Fig. 8. The laser external shutter (middle) with the blocks (left) and laser head (right)

- **High-Pressure Laboratory**

The sample preparation lab and Ruby Raman System were highly used by more than 50 users from six beamlines (X17C, X17B3, U2A, X14A, X27A and X7A) affiliated with COMPRES and NSLS. According to DOE regulations, the lab safety procedures have been updated (sharp container, chemical bar code, waste removal and 3B class laser review) to maintain a safe and efficient environment.

Diamond Anvil Cells

The variety of DACs available to staff and users has been augmented. Over the last year we added:

3 symmetric DACS (Princeton)
1 panoramic DAC (Princeton)
1 plate DAC for high-P total scattering measurements (Almax)
1 short piston DAC (Princeton)

EDM machine

A new, improved EDM machine (Hylozoic) was ordered but has not yet been received.

Ruby System

A 250-mW, 532-nm laser (Ventus, Laser Quantum) was purchased for the Raman/ruby system along with the required notch filter (Semrock). The new laser will allow us to make more precise ruby fluorescence measurements relative to our Melles Griot laser, and allows for development of a mciro-Raman system in the future. A new spectrometer and CCD detector (Princeton Instruments) was also obtained for the ruby/Raman system. Due to the high usage rate of the ruby spectrometer during beam cycles, incorporation of the new equipment will be carried out during the winter shutdown.

Microscope

Our Leica stereomicroscope was improved by the addition of a new objective lens to provide longer working distance for diamond anvil cell sample loading operations.

Mail-in Gas Loading at APS

In July 2010, we had our first users taking advantage of the new mail-in service for gas loading at the COMPRES/GSECARS gas loading system (UCLA group – Kavner/Tolbert; UWO group -- Shieh)

- **Research Projects**

Both the beamline scientists at X17 have initiated new research projects this year. Z. Chen has worked on X-ray diffraction studies of CdS . He has gained experience in using the GSECARS gas loading system in this project. X. Hong has become involved in collecting and analyzing radial x-ray diffraction data at X17C. Hong was awarded beamtime to carry out XAFS studies on germanate glasses at GSECARS in Nov. 2010. Hong also carried out x-ray scattering measurements of glass at X17C.

- **Outreach, Safety, and Community**

A new web page for X17-DAC was constructed, and is linked from both the COMPRES and NSLS home pages. The web page can be viewed at: http://geoweb.princeton.edu/research/MineralPhy/X17/index.html

A first draft of a new user manual for X17C has been released and posted on our webpage.

A special issue of *Synchrotron Radiation News* highlighting high-pressure research included an article by L. Ehm et al. entitled "High-Pressure Research at NSLS".

A poster presentation entitled "Recent upgrades of X17 Beamlines for NSLS" by Hong et al. was made at the 16th Pan-American SRI Conference at Argonne National Laboratory in September, 2010.

The beamline scientists made several trips to work with scientists at other institutions. These included trips to HPCAT (Hong) to work on improved beamline operations and resistive heating techniques, and two trips to the Geophysical Laboratory to work on laser heating with A. Goncharov (Hong and Chen) and to work on internal resistive heating with C.S. Zha (Hong).

Our safety and training documentation for users was revised and improved.

Spring School March 14.-18. 2011 with hands-on training at the NSLS beamlines X17B2, X17B3, X17C and U2A . Compres , JPSI and Photon-Science Division have committed funding for the workshop (I will elaborate in the next version a bit)

Planned Activities for COMPRES II – Year 5 (June 2011 – May 2012)

We are planning the following beamline improvements in COMPRES II year 5.

1. Integrate Perkin Elmer detector fully into X17B3 operations; develop mirrors for focusing 80 keV x-rays.

2. Our software for single-crystal x-ray diffraction is outdated and no longer working. P. Dera has agreed to visit X17 and install his single crystal software at our beamline and assist us in getting it running. This will enable us to carry out single-crystal diffraction experiments using both white and energy dispersive radiation. The restricted angular range for the detector at X17C may limit the ability to carry out angle dispersive single-crystal experiments in some cases, so we will also develop and continue to offer energy dispersive single-crystal experiments.

3. We will improve the studies of structural phase transition and polyamorphism of non-crystalline materials under high pressure and temperature, such as amorphous and liquids, using both energy dispersive and angle dispersive x-ay diffraction. Our users

have observed first-order amorphous-amorphous transitions, e.g.(Sen et al Phys. Rev. Lett.. 97: 025504 (2006)). Ultimately, we would like to extend this research to high temperature using resistive heating and laser heating techniques. Our beamline scientisit, X. Hong, has extensive knowledge and experience on the structure and simulation of liquid, amorphous and glass materials.

4. The new beamline scientists, management team, and support staff will focus on further improvements and streamlining of beamline operations to enhance the user experience. We expect to realize significant improvements in mechanical design throughout the facility, beamtime usage and management, high-pressure lab equipment, and software and computer support. Specifically, we will replace some of our worn-out stages, mounts and mirrors, develop an improved clean-up pinhole system for reduced gasket signal, and streamline our alignment and set-up procedures.

5. We will work on developing improved capabilities for resistive heating. X. Hong has received training in resistive heating techniques from C. Zha (Carnegie) and S. Sinogeikin (HPCAT). We will develop both external and internal heating techniques.

6. The commissioning of the laser heating system is progressing and will be complete before the next budget commences. Tasks to be completed include: Development of EPICS controls, construction of laser enclosure, final safety approval, and purchase of new components: glassy carbon mirrors, long translation stage, breadboard.

We require further investment in equipment infrastructure at X17. Our current equipment base is far older and less advanced than those found at the third generation facilities. *We cannot continue to attract users unless our equipment base is steadily upgraded and improved in the coming years.*

Budget for COMPRES II – Year 4 (June 2010 – May 2011)

NSLS X17 DAC Budget -- COMPRES II, year 4 June 1, 2010 - May 31, 2011		
Item		**Requested Amount**
Salaries	$	100,238
Fringe Benefits, 39%	$	39,093
Travel		
Domestic	$	3000
Foreign	$	1500
Materials and Supplies	$	18,000
Computer	$	8000
Services		
Brookhaven	$	6206
Equipment repair	$	5150
Stony Brook	$	17,226
Equipment	$	54,000
Total Direct Costs	$	198,413
Indirect Costs, 26%	$	51,587
Total Direct and Indirect	**$**	**304,000**

Note: the amount we received for this year was low compared to previous years because we had only 1.5 FTE on staff compared to our normal manpower of 2.0 FTE. Note that in year 2, we received $445k and in year 3, we received $383k.

ARRA Expenditures – total received: $219,500

Equipment Purchased

Perkin Elmer	Flat Panel Detector	$ 114,507
Princeton Instruments	Spectrometers and CCDs	$ 55,028
Laser Quantum	532 nm Laser	$ 9345
Hylozoic	EDM Machine	$ 8650
Almax	Plate DAC	$ 9810
Princeton University	DACs	$ 7250
RT Technologies	Laser Shutter	$ 2330
NSLS machine shop	Detector Bench	$ 14,000

Total Expended $ 220,920

Appendix 1. X17-DAC Publications (2009-2010)

<u>2010 X17-DAC Publications (26 Total)</u>

(Includes peer-reviewed papers, conference reports, and theses; through October 15, 2010)

<u>In press</u>

Ciezak, J., The high-pressure characterization of energetic materials: 2-methyl-5-nitramino-2H-tetrazole, *Propell. Explos. Pyrot.*, in press (2010).

Fan, D., M. Ma, W. Zhou, S. Wei, Z. Chen, and H. Xie, X-ray diffraction study of arsenopyrite at high pressure, *Physics and Chemistry of Minerals*, in press, 2010.

Gao, P., Z. Chen, T. A. Tyson, T. Wu, K. H. Ahn, Z. Liu, R. Tappero, S. B. Kim, and S.-W. Cheong, High pressure structural stability of multiferroic hexagonal ReMnO3, arXiv:1010.0653v1., 2010.

<u>Published</u>

Chen Z., Tyson, T.A., Ahn K.H., Zhong Z., Hu, J., Origin of the non-linear pressure effects in perovskite manganites: Buckling of Mn–O–Mn bonds and Jahn–Teller distortion of the MnO_6 octahedra induced by pressure, *Journal of Magnetism and Magnetic Materials*, **322**, 3049-3052 (2010).

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Couvy, H., Chen, J., Drozd, V., Compressibility of nanocrystalline forsterite, *Physics and Chemistry of Minerals*, **37**, 343-351, (2010).

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Fleet, M. E., Liu, X., Shieh, S. R., Structural change in lead fluorapatite at high pressure, *Phys. Chem. Mineral.*, **37**, 1-9 (2010)

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Halevy, I., Beeri, O., Hu, J., Sc-strengthened commercial purity aluminum under high pressure, *J. Mater. Sci.*, **45**, 589–592 (2010).

Halevy, I., Carmon, R., Winterrose, M. L., Yeheskel, O., Tiferet, E., and Ghose, S., Pressure-induced structural phase transitions in Y_2O_3 sesquioxide*, J. Phys. Conf. Series,* **215**, 012003 (2010).

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Zhang, F.X., Lang, M., Liu, Z., and Ewing, R.C., Pressure-induced disordering and anomalous lattice expansion in $La_2Zr_2O_7$ pyrochlore, *Physical Review Letters*, **105**, 015503 (2010).

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Zhu, H., Ma, Y., Yang, H., Zhu, P., Du, J., Ji, C., and Hou, D., Ultrastable structure and luminescence properties of Y_2O_3 nanotubes, *Solid State Communications*, **150**, 1208-1212. (2010).

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2009 X17-DAC Publications (39 Total)

(Includes peer-reviewed papers, conference reports, and theses)

Aksoy, R., E. Selvi, R. Knudson, and Y. Ma (2009), A high pressure x-ray diffraction study of titanium disulfide, *J. Phys.: Condens. Matter*, *21*, 025403.

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Appendix II

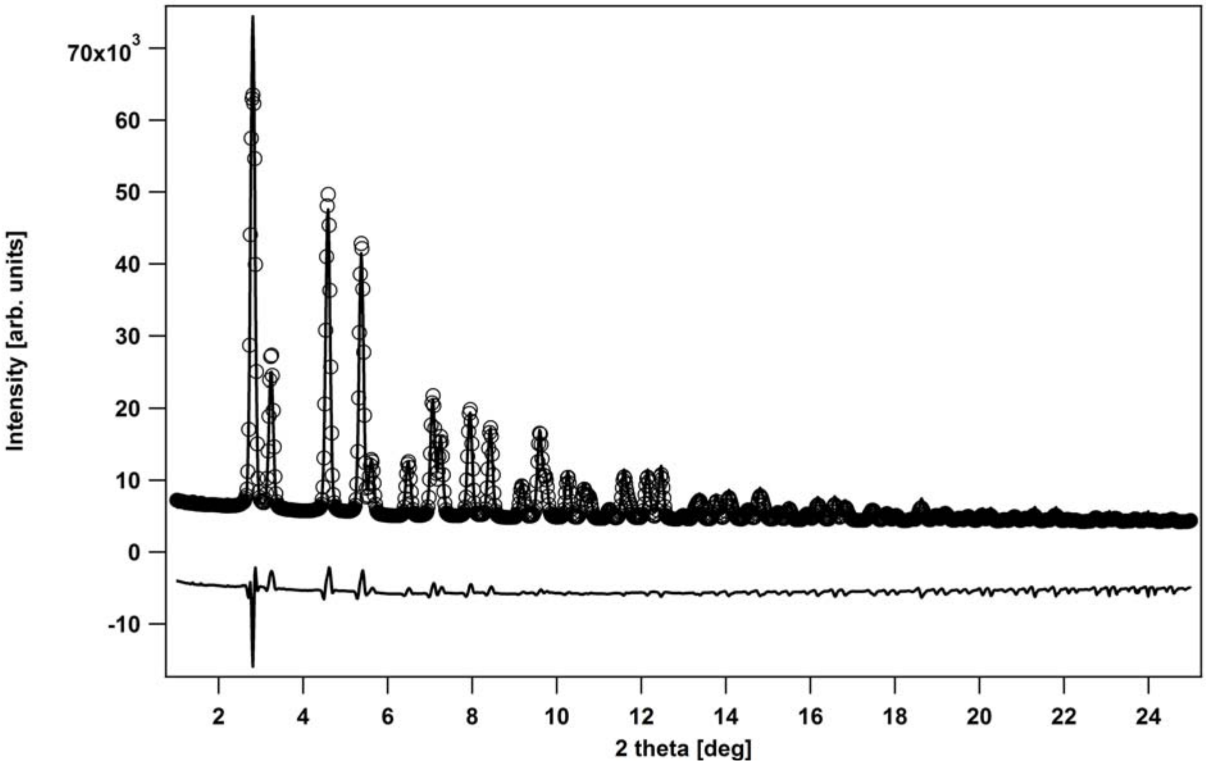
Detector Evaluation for Powder Diffraction at X17DAC facilities of NSLS

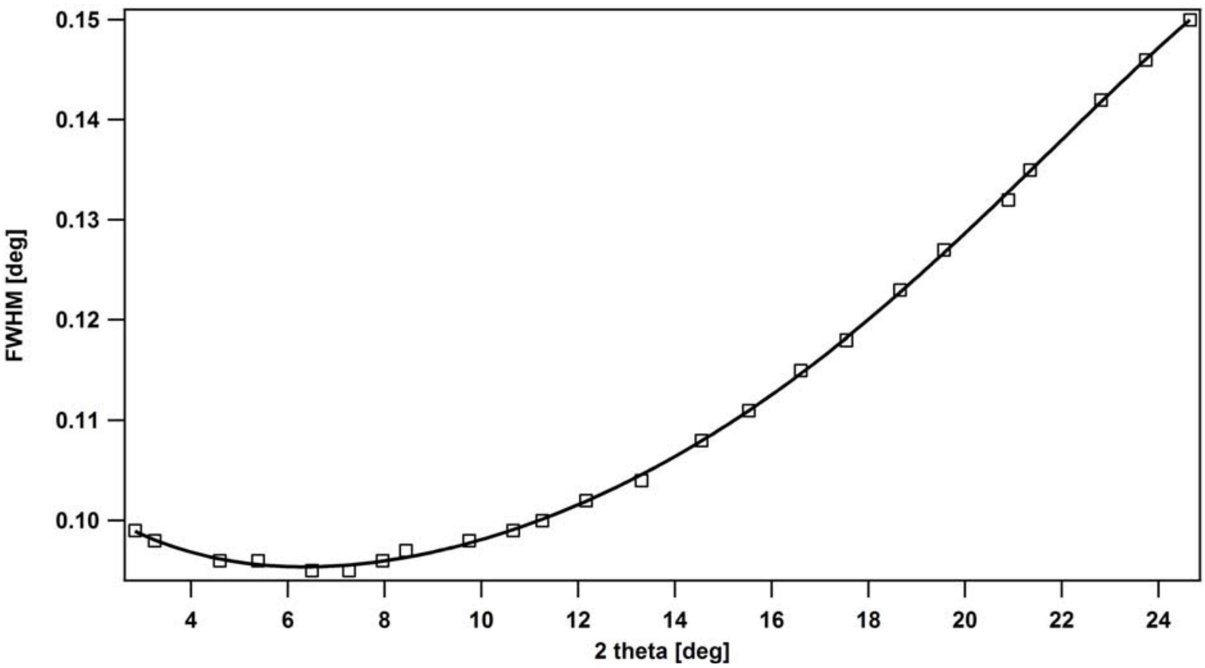
X17DAC facilities have been using three types of Area Detectors such as Rayonix 165 CCD, MAR345 Image Plate and the new a-Si PE, for High Energy (30 & 80 keV) Powder Diffraction experiments.
Here is a comparison of these three types of Area Detectors in terms of their functionality and requirement at X17DAC facilities.

Specs	CCD(Rayonix 165)	IP(MAR345)	a-Si (PE)
Sensor	45 µm, Gd_2O_2S:Tb	207 µm, BeFBr:Eu	a-Si, 500µm CsI
Pixel size(µm)	100	100	200
No. of pixels	2K x 2K	3K x 3K	2K x 2K
Point Spread	Significant(~ 3 pixel)	Significant(~ 3 pixel)	Negligible(<< 1 pixel)
Active Area(mm)	165 Diameter	345 diameter	410 x 410
Frame Rate(Hz)	~0.1	~.01	15/30
Read out/reset time(s)	0.13/.03	108	1-2
Dynamic range(bits)	16	16	16
Optimum Energy (keV)	~ 20	~20	~80
Working Temp. (^oC)	-80	ambient	Ambient
Noise level	moderate	low	moderate
Spatial distortion	moderate	low	Low
Mode of operation	shutter	shutter	shutterless
Cost ($)	250K	110K	120K

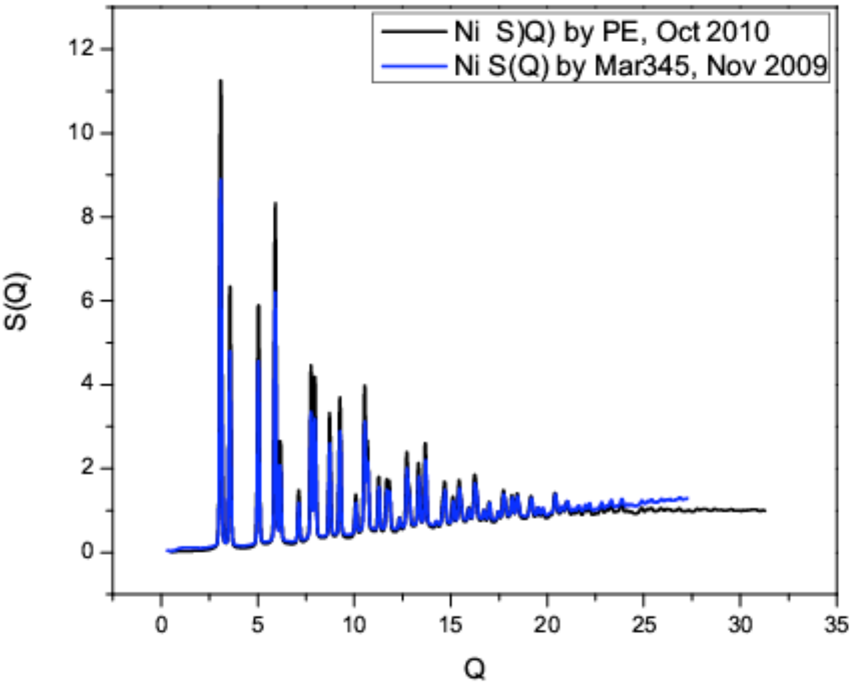
Tests Data and results from PE detector and Data Quality comparison with Mar345 IP

Resolution over Active range of 2theta using 80 keV beam energy at X17B3 and data collected from CeO2 standard. Fits are using Rietvelt method.

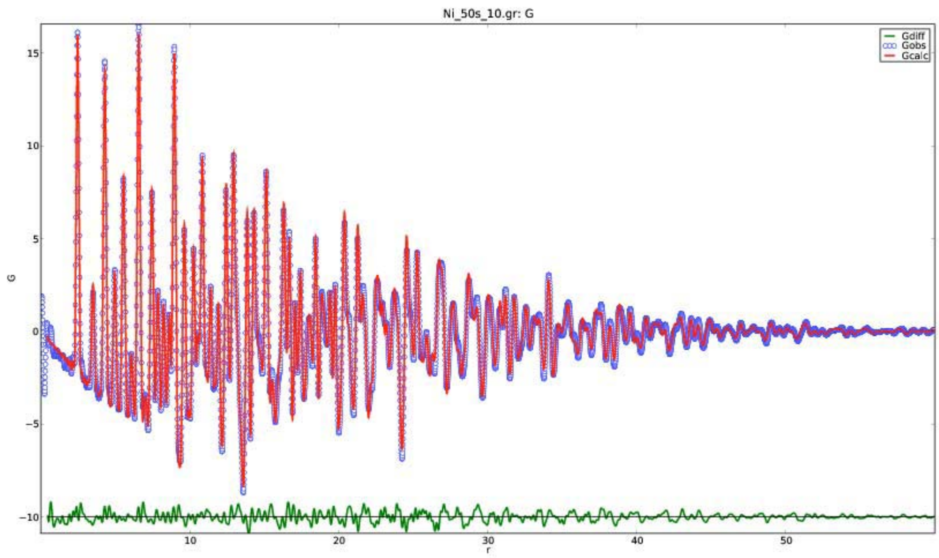




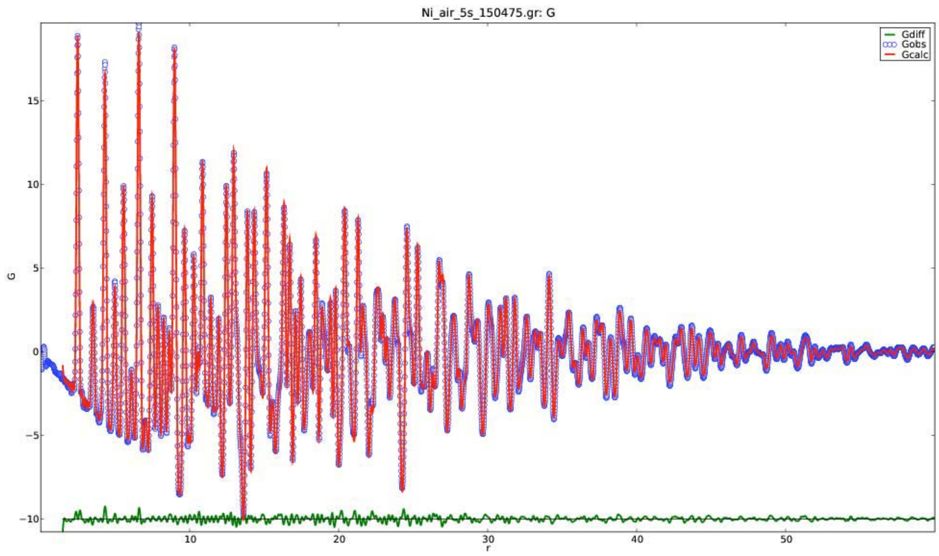
Comparison of PDF data collected with Ni (NIST) standard



G(r) vs r with MAR345 Image Plate



G(r) vs r with a-Si PE Detector



Ni_air_5s_150475.gr: G
Gdiff
Gobs
Gcalc
G
r
15
10
5
0
−5
−10
10
20
30
40
50

Appendix III. Xinguo Hong Curriculum Vitae

Name: Xinguo Hong, Ph. D.

Address: Beamline Scientist, Mineral Physics Institute, Stony Brook University X17DAC, NSLS, Bldg 725, Brookhaven National Laboratory, Upton, NY 11973-5000

Tel: (631) 344-6117 or 4066 (office), (607) 262-6050 (cell); FAX: (631)344-3238;
Email : xhong@bnl.gov; xinguo.hong@gmail.com

Education:

1. **Ph.D. (1992.10-1994.8):** In physics. Institute of Physics, Chinese Academy of Sciences (CAS), Beijing, China
2. **M.Sc (1986.9-1989.7):** In Physics. Wuhan University, China
3. **B.Sc (1982.9-1986.7):** In Physics. Wuhan University, China

Employment:

2010.7-present: Beamline Scientist, X17DAC, Mineral Physics Institute, Stony Brook University; Mailing address: NSLS, Bldg 725, Brookhaven National Laboratory, Upton, NY 11973-5000

2009.6-2010.06: BNL employee in the Life and Environmental Sciences Division, National Synchrotron Light Source (NSLS), Brookhaven National Laboratory (BNL)

2007.2-2009.6: Visiting Staff Scientist of MacCHESS, CHESS, Cornell University

2006.1-2007.2: Research associate, GSECARS, Consortium for Advanced Radiation Sources, University of Chicago, Chicago, Illinois 60637, USA

2004.10-2005.12: Research associate, worked at GSECARS, APS, for Hawaii Institute of Geophysics and Planetology, School of Ocean Earth Science and Technology, University of Hawaii.

2002.4-2004.10: Associate professor,
Beijing Synchrotron Radiation Facility (BSRF), Institute of High Energy Physics, Chinese Academy of Sciences

2001.5-2002.4: JSPS (Japan Society for the Promotion of Science) Invitation Fellowship Program for Research in Japan

1999.5-2001.4: JSPS International Fellowship for postdoctoral research
1998.2-1999.4: Research associate (Wissenschaftlicher Mitarbeiter): At Institute of Physical Chemistry, Philipps-University of Marburg, Germany.

1996.5-1998.1: Post-doctoral Research associate: Institute of Physical Chemistry and Electrochemistry 1 of University Karlsruhe (TH), Germany.

A) 10 Key Publications (* corresponding author):

Xinguo Hong*, Matt Newville, Vitali B. Prakapenka, Mark L. Rivers and Stephen R. Sutton , Review of Scientific Instruments 80 (7), 073908 (2009).
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B) Selected Publications

Xinguo Hong*, Matt Newville, Vitali B. Prakapenka, Mark L. Rivers and Stephen R. Sutton , Review of Scientific Instruments 80 (7), 073908 (2009).
M. Freeman, M. Seaman, S. Rits-Volloch, Xinguo Hong, Y. Huang, D. Ho and B. Chen, accepted by "Structure" on September 29, 2010, in press.
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`Appendix IV: Overview of Beamline Characteristics

X17C

Angle Dispersive Diffraction Experiments

Monochromator	Sagittally bent Si Laue crystals
Beam energy	tunable 20 keV to 40 keV
Focusing optic	K-B mirror
Primary beam size	0.090 mm x 0.090 mm
Focused beam size	0.025 mm x 0.020 mm
Detector	Rayonix SX-165

Energy Dispersive Diffraction Experiments

White beam E range	20 keV to 100 keV
Focusing optic	K-B mirror
Primary beam size	0.070 mm x 0.070 mm
Focus beam size	0.025 mm x 0.020 mm
Detector	Canberra Ge solid state detector

X17B3

Angle Dispersive Diffraction and High Energy X-Ray Scattering Experiments

Monochromator	Sagittally bent Si Laue crystals
Beam energy tunable	30 keV/ 80 keV
Focusing optic	K-B mirror (not for 80 keV)
Primary beam size	0.10 mm x 0.08 mm
Focused beam size	0.015 mm x 0.010 mm
Detector	MAR345 Image Plate/ Rayonix SX-165

Energy Dispersive Diffraction Experiments

White beam E range	20 keV to 100 keV

Focusing optic	K-B mirror
Primary beam size	0.10 mm x 0.080 mm
Focus beam size	0.010 mm x 0.010 mm
Detector	Canberra Ge solid state detector

High-Pressure Laboratory

Our high-pressure sample preparation lab (Rm 1-140) houses equipment for DAC sample preparation and includes an EDM (electric drilling machine), mechanical drilling machine, high-resolution optical microscopes, electrical work station, sample loading tools, DAC tools, standard samples, pressure media and pressure indicators. A simple system for cryogenic loading of liquid pressure media such as argon is also available.

Room 1-134C contains a spectrometer for pressure calibration by ruby fluorescence spectrum. This system includes an adjustable Ar laser (usually set to 488nm) and spectrometer, which can be used to determine quasi-hydrostatic pressures up to ~80-100 GPa. All of these lab facilities are open to every user in NSLS working on high-pressure experiments.

Appendix V: 2010 Beamline Proposals and Usage

X17c

Jan-Apr 2010

PI Name	Affiliation	Title	Fundings
Michael Kruger	University of Missouri Kansas City	High Pressure XRD Study of Rare-earth Pyrochlore Titanates	NSF
Changqing Jin	Chinese Academy of Sciences Institute of Physics	Pressure induced structure evolution of novel strongly correlated perovskitesystem AMO3 (M=Cr,Fe,Mn)	NSF of China
Maining Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature	NSF of China
Maik Lang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE
Wei Liu	SUNY @ Stony Brook	Elasticity across the OEN to HP-CEN Phase Transformation for Orthoenstatite	NSF
Thomas Duffy	Princeton University	Quasi-hydrostatic compression of pyroxenes and olivines	NSF
Thomas Duffy	Princeton University	Strength of Metals at High Pressure	NSF, DOE
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides	DOE
Wendy Panero	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals	NSF
Bingbing Liu	Jilin University	PRESSURE-INDUCED AMORPHIZATION AND POLYAMORPHISM IN TiO2 NANOMATERIALS	NSF of China
Trevor Tyson	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: HighPressure XRD Measurements	DOE
Jennifer Ciezak	Army Research Laboratory	Elastic-Plastic Deformation of Superhard Materials	DOD
Peter Mao	California Institute of Technology	Diffraction topography screening of flight-candidate CZT detectors for NuSTAR	NASA
Xi Liu	University of Peking	Elasticity Study on the CAS phase up to lower mantle conditions	NSF of China
George Amulele	Yale University	Water solubility studies in lower mantle perovskites by x-ray diffractionmeasurements	NSF
Lauren Borkowski	SUNY @ Stony Brook	High pressure behavior of [CH3NH2CH3][Co(CHO2)3]	NSF
Ryan Kerrigan	University of Maryland	Magnesite decarbonation and growth of fibrous talc through hydrothermalreactions: kinetics, textures and global carbon cycle	NSF
Itzhak Halevy	Nuclear Research Center	TITANIUM AND TI-ALLOYSFOR IMPLANTSAND BIOCOMPATIBLE ENDOPROSTHESIS UNDER PRESSUREAND TEMPERATURE	DOE

May-Aug 2010

PI Name	Affiliation	Title

Cheng Ji	Texas Technical University	Crystal structure and compressibility of La2Mg16Ni alloy under high pressure
Itzhak Halevy	Nuclear Research Center	Crystallographic aspects in Anharmonic Phonons in BCC Iron at High Temperature
Maining Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature
Wendy Panero	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals
Matthew Armentrout	University of California Los Angeles	Equation of state and phase stability of iron silicate at high pressures and temperatures
Lauren Borkowski	SUNY @ Stony Brook	High pressure behavior of [CH3NH2CH3][Co(CHO2)3]
Miao Xie	University of California Los Angeles	High Pressure Studies Of Ultra-Incompressible, Superhard Metal Borides
Dongbin Hou	Texas Technical University	High pressure synchrotron X-ray diffraction study of NiS2 up to 50 Gpa
Michael Kruger	University of Missouri Kansas City	High Pressure XRD Study of Magnesium substituted Tricalcium Phosphate and Hydroxyapatite
Andrew Campbell	University of Maryland	High pressure, high temperature equations of state of metal-oxide pairs
Sean Shieh	University of Western Ontario	Nitrogen-doped Carbon Nanotubes Under High Pressures
Maik Lang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences
Hongyang Zhu	Texas Technical University	Pressure Induced Phase Transition of Nanocrystalline and Bulk Maghemite (γ-Fe2O3) to Hematite (α-Fe2O3)
Changqing Jin	Chinese Academy of Sciences Institute of Physics	Pressure induced structure evolution of novel strongly correlated perovskitesystem AMO3 (M=Cr,Fe,Mn)
Yanzhang Ma	Texas Technical University	Shear induced phase transforation at high pressures
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides
Trevor Tyson	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: HighPressure XRD Measurements
Thomas Duffy	Princeton University	Strength of Metals at High Pressure
Dawei Fan	Chinese Academy of Geological Sciences	The PVT equation of state of the dominant rock-forming minerals of eclogite
George Amulele	Yale University	Water solubility studies in lower mantle perovskites by x-ray diffractionmeasurements

Sept-Dec 2010

PI Name	Affiliation	Title
Maining Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature
Paul Calderone	SUNY @ Stony Brook	Effects of high pressure on formate-based Metal-Organic Frameworks

Wei Liu	SUNY @ Stony Brook	Elasticity across the OEN to HP-CEN Phase Transformation for Orthoenstatite
Wendy Panero	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals
Lauren Borkowski	SUNY @ Stony Brook	High pressure behavior of [CH3NH2CH3][Co(CHO2)3]
Lauren Borkowski	SUNY @ Stony Brook	High pressure studies of [DABCO][V6O14]•H2O
Dongbin Hou	Texas Technical University	high pressure X-ray diffraction study of rhenium disulfide (ReS2)
Michael Kruger	University of Missouri Kansas City	High Pressure XRD Study of Bismuth Layered Compounds and Silver Tantalate
Andrew Campbell	University of Maryland	High pressure, high temperature equations of state of metal-oxide pairs
Maik Lang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences
Changqing Jin	Chinese Academy of Sciences Institute of Physics	Pressure induced structure evolution of novel strongly correlated perovskitesystem AMO3 (M=Cr,Fe,Mn)
Itzhak Halevy	Nuclear Research Center	Pressure-Induced Structural Phase Transitions in RE2O3 Sesquioxide
Trevor Tyson	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: HighPressure XRD Measurements
Thomas Duffy	Princeton University	Strength of Metals at High Pressure
Thomas Duffy	Princeton University	Static compression of Bi12SiO20: Comparison with Shock Compression Data
Sean Shieh	University of Western Ontario	Nitrogen-doped Carbon Nanotubes Under High Pressures
Dawei Fan	Chinese Academy of Geological Sciences	The PVT equation of state of the dominant rock-forming minerals of eclogite
George Amulele	Yale University	Water solubility studies in lower mantle perovskites by x-ray diffractionmeasurements

X17B3

Jan-Apr 2010

PI Name	Affiliation	Title
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides
Jiuhua Chen	Florida Internationa l University	Study of Spin State Transition in amorphous FeS using XES
Andrew Campbell	University of Maryland	High pressure, high temperature equations of state of metal-oxide pairs
Sanda Botis	University of Western Ontario	High-pressure study of potential REE-carriers into the lower mantle
Zhongying Mi	University of Western Ontario	High pressure high temperature DAC study
Sean Shieh	University of Western	Strength Study on NaCl and KCl to Megabar Pressure

	Ontario	

May-Aug 2010

PI Name	Affiliation	Title
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides
Paul Calderone	SUNY @ Stony Brook	Effects of high pressure on formate-based Metal-Organic Frameworks
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides
Hongyang Zhu	Texas Technical University	Phase transformation of phosphor under high pressure
Qiang Zhou	Jilin University	Research on structure of superhard B-C material and its high pressure behavior
Lars Ehm	SUNY @ Stony Brook	Pressure induced phase transitions in ferroic materials Investigation of dimensionality of phase transition mechanisms

Sept-Dec 2010

PI Name	Affiliation	Title
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides
Lars Ehm	SUNY @ Stony Brook	Pressure induced phase transitions in ferroic materials Investigation of dimensionality of phase transition mechanisms
Bingbing Liu	Jilin University	PRESSURE-INDUCED AMORPHIZATION AND POLYAMORPHISM IN TiO2 NANOMATERIALS
Eran Sterer	NRCN, Nuclear Research Center, Negev, isreal	systematic high pressure amorphization study of Ln(1/3)Ln'O(3)
Ilkyoung Jeong	Pusan National University	Investigation on an evolution of local structure of relaxor ferroelectrics under high pressure
Matthew Johnson	GlaxoSmithKline	Characterization of Amorphous-Phase Pharmaceuticals Using PDF

X17B3 Schedule
2010-I

Form #	PI Name	# days	Beam Time
	80keV Mono Setup	2	03/01(12:00)-03/03(12:00)
	Beamline Upgrade		03/03(12:00)-04/(12:00)

	Lars Ehm	4	4/16(12:00)-4/23(12:00)
14251	Trevor Tyson	4	4/23(12:00)-4/27(12:00)

X17B3 Schedule
2010-II

Form #	PI Name	# days	Beam Time
	80keV Mono Setup	2	06/04(12:00)-06/06(12:00)
	Beamline Upgrade		06/06(12:00)-07/02(12:00)
	Indepent Day Shutdown		07/02(12:00)-07/10(12:00)
	wiggler maintainance		07/02(12:00)-07/10(12:00)
	Lars Ehm	4	4/16(12:00)-4/23(12:00)
14251	Trevor Tyson	4	4/23(12:00)-4/27(12:00)

X17B3 Schedule
2010-III

Form #	PI Name	# days	Beam Time
	Mono Setup	1	09/02(12:00)-09/03(12:00)
	Beamline Upgrade		09/03(12:00)-09/13(12:00)
	X17A Installation		09/13(12:00)-10/07(12:00)
	Beamline Upgrade		10/07(12:00)-10/20(12:00)
16986	Lars Ehm	4	10/21(12:00)-10/25(12:00)
17528	Matthew Johnson	1	10/28(12:00)-10/29(12:00)
14251	Trevor Tyson	3	10/29(12:00)-11/01(12:00)
16994	Ilkyoung Jeong	4	11/01(12:00)-11/05(12:00)

X17C Schedule 2010-
I

Proposal	PI Name	X17C	Assigned Time
	Beamline Setup	3.16	1/20(8:00)-1/23(12:00)
	Zchen	2	1/23(12:00)-1/25(12:00)
15670	Lauren Borkowski	1.5	1/27(0:00)-1/28(12:00)
15461	Jennifer Ciezak	3	1/29(12:00)-2/1(12:00)
	Beamline Maintainance	2	2/1(12:00)-2/3(12:00)
14975	Trevor Tyson	4.75	2/3(12:00)-2/8(6:00)
	NSLS Maintainace		NSLS Maintainace
15745	Itzhak Halevy	4	2/9(12:00)-2/13(12:00)
15657	George Amulele	2	2/13(12:00)-2/15(12:00)
	NSLS Maintainace		NSLS Maintainace
	Beamline Maintainance	1.5	2/17(0:00)-2/18(12:00)
15731	Sean Shieh	4	2/18(12:00)-2/22(12:00)
	NSLS Maintainace		NSLS Maintainace
13131	Michael Kruger	4	2/25(12:00)-3/1(12:00)
15710	Ryan Kerrigan	3	3/1(12:00)-3/4(12:00)
14797	Wendy Panero	3.75	3/4(12:00)-3/8(6:00)
	NSLS Maintainace		NSLS Maintainace
13269	Maining Ma	3	3/9(12:00)-3/12(12:00)
14198	Wei Liu	3	3/12(12:00)-3/15(12:00)
	NSLS Maintainace		NSLS Maintainace
15650	Xi Liu	5	3/17(12:00)-3/22(12:00)

	NSLS Maintainace		NSLS Maintainace
14895	Bingbing Liu	4	3/25(12:00)-3/29(12:00)
	NSLS Maintainace		NSLS Maintainace
	Qiliang Cui	5.25	3/31(0:00)-4/5(6:00)
	NSLS Maintainace		NSLS Maintainace
14246	Thomas Duffy	3	4/6(12:00)-4/9(12:00)
14241	Thomas Duffy	3	4/9(12:00)-4/12(12:00)
13191	Changqing Jin	3	4/12(12:00)-4/15(12:00)
	Beamline Maintainance	1	4/15(12:00)-4/16(12:00)
15730	Andrew Campbell	3	4/16(12:00)-4/19(12:00)
	NSLS Maintainace		NSLS Maintainace
	Yanzhang Ma	4	4/22(12:00)-4/26(12:00)
13333	Maik Lang	4	4/26(12:00)-4/30(12:00)

X17C Schedule 2010-
II

Form #	PI Name	# days	Beam Time
	ADXD		
15670	Lauren Borkowski	2.75	04/30 (12:00)-05/03(6:00)
	wiggler maintainance		05/27(12:00)-05/31(12:00)
16287	Paul Calderone	2	06/02(12:00)-06/04(12:00)
15730	Andrew Campbell	3	06/04(12:00)-06/07(12:00)
16345	Michael Kruger	4	06/10(12:00)-06/14(12:00)
	Beamline upgrade	3	06/15(12:00)-06/18(12:00)
15710	Ryan Kerrigan	3	06/18(12:00)-06/21(12:00)
14975	Trevor Tyson	5	06/21(12:00)-06/26(12:00)

13269	Maining Ma	3.5	06/26(12:00)-07/01(12:00)
	Zhiqiang Chen	1	07/01(12:00)-07/02(20:00)
	wiggler maintainance		07/11(00:00)-07/15(12:00)
13333	Maik Lang	4	07/15(12:00)-07/19(12:00)
16295	Matthew Armentrout	2	07/20(12:00)-07/22(12:00)
14797	Wendy Panero	4	07/22(12:00)-07/26(12:00)
14846	Hongyang Zhu	2	07/26(12:00)-07/29(12:00)
16219	Yanzhang Ma	4	07/29(12:00)-08/02(12:00)
15657	George Amulele	3	08/05(12:00)-08/08(12:00)
13191	Changqing Jin	3	08/08(12:00)-08/11(12:00)
16330	Sean Shieh	4.75	08/11(12:00)-08/16(6:00)
EDXD	Zhiqiang Chen	3	08/17(12:00)-08/20(12:00)
16493	Itzhak Halevy	3	08/20(12:00)-08/23(12:00)
16309	Miao Xie	2	08/25(10:00)-08/27(12:00)
14246	Thomas Duffy	3	08/27(12:00)-08/30(12:00)

X17C Schedule 2010-
III

Form #	PI Name	# days	Beam Time
	Jinfu Shu	4	09/02(12:00)-09/06(12:00)
	ADXD Setup	4	09/06(12:00)-09/10(12:00)
15670	Lauren Borkowski	2.75	09/10(12:00)-09/13(6:00)
	X17A Installation		09/13(12:00)-09/29(12:00)
	X17A Backup		09/30(12:00)-10/06(12:00)
14797	Wendy Panero	3.75	10/07(12:00)-10/11(6:00)
16983	Dawei Fan	3	10/12(12:00)-10/15(12:00)

17163	Thomas Duffy	3	10/15(12:00)-10/18(12:00)
14198	Wei Liu	2	10/20(12:00)-10/22(12:00)
13269	Maining Ma	3	10/22(12:00)-10/25(12:00)
15730	Andrew Campbell	3	10/28(12:00)-10/31(12:00)
16955	Michael Kruger	3	10/31(12:00)-11/03(12:00)
13191	Changqing Jin	4.75	11/03(12:00)-11/08(6:00)
17034	Sanda Botis	3	11/09(12:00)-11/12(12:00)
17013	Sean Shieh	3	11/12(12:00)-11/15(12:00)
17058	Dongbin Hou	4	11/18(12:00)-11/22(12:00)
16287	Paul Calderone	1	11/22(12:00)-11/23(12:00)
	X17C upgrade	2	11/23(12:00)-11/25(12:00)
13333	Maik Lang	4	11/25(12:00)-11/29(12:00)
14246	Thomas Duffy	3	12/01(12:00)-12/04(12:00)

Summary of Beamtime Usage for 2010

	2009		2010		Jan-Apr 2010		May-Aug 2010		Sept-Dec 2	
	X17C	X17B3	X17C	X17B3	X17C	X17B3	X17C	X17B3	X17C	X
# proposals	48	21	56	17	18	6	20	6	18	
# days requested	296	187	286	78	85	25	100	26	101	
#days beamtime available *	210.73	120.66	181	70	65	25	60	20	56	
Oversubscription	1.4	1.55	1.58	1.11	1.3	1	1.67	1.3	1.8	
Funding										
NSF	30	13	28	6	7	2	10	3	11	
DOE	10	1	14	6	4	1	6	3	4	
Foreign	9	4	12	4	4	2	4	1	4	
DOD	3	0	1	0	1	0	0	0	0	
NASA	0	0	2	1	0	1	1	0	1	
Industry	0	0	0	1	0	0	0	0	0	
Other	0	0	0	1	0	0	0	0	0	

*** Due to the cooling system problem of the X17C wiggler, X17 DAC beamlines lost ~10 days of 2010-II and ~20 days of 2010-III**

Appendix VI: 20009 Beamline Proposals and Usage

X17C

Jan-Apr 2009

PI Name	Affiliation	Title	Fundings	# of Days Requested	# of Days by NSLS
M. Lang	U. Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	7	3
Trevor Tyson	NJIT	High Pressure Structural Measurements of Manganites	NSF	6	5
Y. Ma	Texas Tech Univ., TX	X-ray diffraction meausurement of PbMoO4 at high pressures	DOE	5	0
T. Duffy	Princeton	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	3	0
Matthew Whitaker	SUNY @ Stony Brook	Investigation of Physical Properties of Iron /Light-Element Alloys at High Pressure and Temperature	NSF	4	2
Jennifer Ciezak	Army Research Laboratory	High Pressure Crystallographic Analysis of N2/H2 mixture	DOD	5	4
Ryan Kerrigan	University of Maryland	Hydrothermal reactions kinetics and fibrous mineral development in a non-equilibrium KFMASH	NSF	5	0
Michael Kruger	University of Missouri	High Pressure XRD Study of Rare-earth Pyrochlore Titanates	NSF	6	5
Lyci George	FIU	High Pressure- Temperature Experiments and Phase Diagram of Hydrides	NSF CDAC	4	4
W. Panero	Ohio State University	Solubility of two component systems at high-pressures and temperatures	NSF	4	4
M. Lang	U. Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	5	0
Lars Erm	SUNY@Stony Brook	Investigation of the structural changes on different length scales during the pressure induced phase	NSF	5	0
Changqing Jin	Chinese Academy of Sciences	Pressure induced structure evolution of novel strongly correlated perovskite system AMO3 (M=Cr,Fe,Mn)	Foreign NSF,China	6	6
T. Duffy	Princeton	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	6	0
Itzhak Halevy	Nuclear Research Center	The crystallographic and magnetic ordering of the tetragonal REM2X2 under High-Pressure.	DOE	5	0

May-Aug 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS
Wendy Panero	Ohio State University	Solubility of two component systems at high-pressures and temperatures	NSF	5	3
Maik Lang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	6	4
Trevor A. Tyson	New Jersey Institute of Technology	High Pressure Structural Measurements of Manganites	NSF	6	0
Bingbing Liu	Jilin University	HIGH PRESSURE STUDY OF C60 NANOMATERIALS	Foreign NSF,China	7	0
Qiliang Cui	Jilin University	high pressure Synchrotron Radiation studies on AlN,BCN, C3N4	Foreign NSF,China	10	0
zhiqiang chen	SUNY @ Stony Brook	High pressure effects on crystal structure and electrical transport properties of Cadmium Sulfide	NSF	4	3
Jennifer Ciezak	Army Research Laboratory	High Pressure Crystallographic Analysis of N2/H2 mixture	DOD	4	3
Lauren Borkowski	SUNY @ Stony Brook	High pressure behavior of metal organic framework materials	NSF	2	2
Lyci George	Florida International University	High pressure- temperature phase diagram of some slected hydrides	DOE NSF	4	0
Ryan Kerrigan	University of Maryland	Hydrothermal reactions kinetics and fibrous mineral development in a non-equilibrium KFMASH	NSF	4	0
Sanjit Ghose	SUNY @ Stony Brook	Structural Phase Transition of Cryolite (Na3AlF6) at high pressures and temperatures	NSF	6	3
Andrew Campbell	University of Maryland	Equations of state of metal-oxide pairs	NSF	3	3
Matthew Whitaker	SUNY @ Stony Brook	Investigation of Physical Properties of Iron/Light-Element Alloys (FeS, FeS2,FeSi, Fe3P)	NSF	6	2
Changqing Jin	Chinese Academy of Sciences	Pressure induced structure evolution of novel strongly correlated perovskite system AMO3 (M=Cr,Fe,Mn)	Foreign NSF,China	3	3
Yanzhang Ma	Texas Technical University	X-ray diffraction meausurement of PbMoO4 at high pressures	DOE	4	3
Itzhak Halevy	Nuclear Research Center	The crystallographic and magnetic ordering of the tetragonal REM2X2 under High-Pressure.	DOE	5	0
Michelle Weinberger	Carnegie Institution of Washington	High Pressure studies of resistively heated transition metal diborides	DOD NSF	5	4
Thomas Duffy	Princeton University	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	6	4

Sept-Dec 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS
Trevor Tyson	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: High Pressure XRD Measurements	NSF	6	0
Z Chen	Stony Brook University	High pressure effects on crystal structure and	NSF	6	0

		electrical transport properties of Cadmium Sulfide			
Andrew Campbell	University of Maryland	Equations of state of metal-oxide pairs	NSF	4	3
Ryan Kerrigan	University of Maryland	Hydrothermal reactions kinetics and fibrous mineral development in a non-equilibrium KFMASH	NSF	3	0
Thomas Duffy	Princeton University	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	5	3
Itzhak Halevy	Nuclear Research Center	The crystallographic and magnetic ordering of the tetragonal REM2X2 under Temperature and High-Pressure.	DOE	5	0
Wendy Panero	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals	NSF	5	3
Wei Liu	SUNY @ Stony Brook	Elasticity across the OEN to HP-CEN Phase Transformation for Orthoenstatite	NSF	4	4
Maining Ma	Chinese Academy ofSciences	Effect of water on properties of olivine at high pressure and high temperature	Foreign	7	4
Z Chen	Beam Line	Beamline Maintainance	NSF COMPRES	3	0
Dongbin Hou	Texas Technical University	High pressure synchrotron X-ray diffraction study of NiS2 up to 50 GPa	NSF	4	2
Hongyang Zhu	Texas Technical University	Phase transformation of phosphor under high pressure	NSF	5	0
Changqing Jin	Institute of Physics Chinese Academy of Sciences	Pressure induced crystallography evolution of itinerant system compounds	Foreign	6	3
Changqing Jin	Institute of Physics Chinese Academy of Sciences	Pressure induced structure evolution of novel strongly correlated perovskite system AMO3 (M=Cr,Fe,Mn)	Foreign	18	9
Maik Lang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	7	3
Christopher DeVreugd	Virginia Tech	High Energy Synchrotron X-ray diffraction on electric field cooled NBT-10BT	NSF	3	0
Bingbing Liu	Jilin University	HIGH PRESSURE STUDY OF C60 NANOMATERIALS	Foreign NSF,China	4	0

X17B3

Jan-Apr 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS
Trevor Tyson	New Jersey Institute of Technology	Diffuse Scattering in Multiferroic Materials	NSF	5	5
Lars Ehm	SUNY @ Stony Brook	Investigation of the structural changes on different length scales during the pressure induced phase	NSF	5	0
Li Li	SUNY @ Stony Brook	Investigation of cation ordering in silicate and aluminate spinels	NSF	4	3
Hu Cao	Virginia Polytechnic Institute and State University	High resolution synchrotron x-ray diffraction of nanotwins in (1-x)Pb(Mg1/3Nb2/3)-xPbTiO3 crystals	DOE NSF	7	5
Maining Ma	Graduate University of	Effect of water on properties of olivine	Foreign	4	3

	Chinese Academy of Sciences	at high pressure and high temperature	NSF,China		
Ryan Rich	Texas Christian University	High pressure effects of	NSF	5	0
Lars Ehm	SUNY @ Stony Brook	Structure and stability of calcite-type carbonates at high-pressure and temperature	NSF	4	0

May-Aug 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS
Yongjae Lee	Yonsei University	High Pressure Powder Diffraction Studies of Zeolites	Foreign KOSEF	5	0
Lars Erm	SUNY@Stony Brook	Structure and stability of calcite-type carbonates at high-pressure and temperature	NSF	0	0
Parise John	SUNY @ Stony Brook	FexSy nano-structures and chemistry - from laboratory samples to spreading centers	NASA	4	3
Xi Liu	Peking University	Elasticity of bioapatite at ambient temperature	Foreign NSF,China	4	0
Duffy Thomas	Princeton University	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	6	3
Chih-Ming Lin	Nation Hsinchu University Taiwan	The physical properties of the FeSe and Mse under high-pressure by x-ray diffraction method	Foreign	30	0
Lars Ehm	SUNY @ Stony Brook	Investigation of the structural changes on different length scales during the pressure induced phase transitions in ATiO3 (A=Ca,Ba,Sr,Pb) perovskites	NSF	5	3
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides	NSF	6	4
Alexander Goncharov	Carnegie Institute Washington	X-ray diffraction combined with the laser heating set up	NSF COMPRES	7	0
Liang Luo	Virginia Polytechnic Institutey and State Universit	The electric field dependence of crystals structures for BNT-10BT by hig resolution synchrotron radiation XRD	NSF	5	0

Sept-Dec 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS
Bingbing Liu	Jinlin University	PRESSURE-INDUCED AMORPHIZATION AND POLYAMORPHISM IN TiO2 NANOMATERIALS	Foreign NSF,China	5	0
Qiliang Cui	Jinlin University	In situ high pressure XRD studies on metal sesquioxides and molybdenum trioxide hydrates	Foreign NSF,China	10	0
Lowell Miyagi	Univ of California @ Berkeley	Texture, and Lattice Strain Development in NaMgF3 Post-Perovskite	Foreign CDAC	4	3
Sean Shieh	Univ of Western Ontario	High-Pressure Study on Nitrogen-doped Carbon Nanotubes	Foreign Canada	4	0
Lars Ehm	Stony Brook University	High pressure	NSF	5	0
Li Li	Stony Brook University	Investigation of cation ordering in silicate	NSF	3	3

		and aluminate spinels			
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides	NSF	6	4

2009 – X17C, X17B3 User Schedule

X17C Schedule

January-April 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS
Sanjit Ghose	Beam line	ADXD Setup	NSF COMPRES	6	0
Z. Chen	Beam line	Beamline development	NSF COMPRES	3	0
M. Lang F. Zhang	U. Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	7	3
Trevor Tyson	NJIT	High Pressure Structural Measurements of Manganites	NSF	6	5
Y. Ma	Texas Tech Univ., TX	X-ray diffraction measurements of $PbMoO_4$ at high pressures	DOE	5	0
T. Duffy	Princeton	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	3	0
Matthew Whitaker	SUNY @ Stony Brook	Investigation of Physical Properties of Iron /Light-Element Alloys at High Pressure and Temperature	NSF	4	2
Jennifer Ciezak	Army Research Laboratory	High Pressure Crystallographic Analysis of N_2/H_2 mixture	DOD	5	4
Ryan Kerrigan	University of Maryland	Hydrothermal reactions kinetics and fibrous mineral development in a non-equilibrium KFMASH	NSF	5	0
Ghose & Chen	Beam line	Beamline development	NSF COMPRES	4	0
Michael Kruger	University of Missouri	High Pressure XRD Study of Rare-earth Pyrochlore Titanates	NSF	6	5
Lyci George	FIU	High Pressure- Temperature Experiments and Phase Diagram of Hydrides	NSF CDAC	4	4
W. Panero	Ohio State University	Solubility of two component systems at high-pressures and temperatures	NSF	4	4
Sanjit Ghose	Beam line	Beamline development	NSF COMPRES	3	0
M. Lang F. Zhang	U. Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	5	0
Lars Erm	SUNY@Stony Brook	Investigation of the structural changes on different length scales during the pressure induced phase	NSF	5	0
Changqing Jin	Chinese Academy of Sciences	Pressure induced structure evolution of novel strongly correlated perovskite system AMO_3 (M=Cr,Fe,Mn)	Foreign NSF,China	6	6
Ghose & Chen	Beam line	EDXD Setup	NSF	5	0

			COMPRES		
T. Duffy	Princeton	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	6	0
Itzhak Halevy	Nuclear Research Center	The crystallographic and magnetic ordering of the tetragonal REM2X2 under High-Pressure.	DOE	5	0
Ghose & Chen	Beam line	Beamline development	NSF COMPRES	2	0

May-August, 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# by
S. K. Ghose Z. Chen	Beam Line	ADXD Setup	NSF COMPRES	4	
Wendy Panero	Ohio State University	Solubility of two component systems at high-pressures and temperatures	NSF	5	
Maik Lang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	6	
Trevor A. Tyson	New Jersey Institute of Technology	High Pressure Structural Measurements of Manganites	NSF	6	
Bingbing Liu	Jilin University	HIGH PRESSURE STUDY OF C60 NANOMATERIALS	Foreign NSF,China	7	
Qiliang Cui	Jilin University	high pressure Synchrotron Radiation studies on AlN,BCN, C3N4	Foreign NSF,China	10	
zhiqiang chen	SUNY @ Stony Brook	High pressure effects on crystal structure and electrical transport properties of Cadmium Sulfide	NSF	4	
Jennifer Ciezak	Army Research Laboratory	High Pressure Crystallographic Analysis of N2/H2 mixture	DOD	4	
Lauren Borkowski	SUNY @ Stony Brook	High pressure behavior of metal organic framework materials	NSF	2	
Lyci George	Florida International University	High pressure- temperature phase diagram of some selected hydrides	DOE NSF	4	
Ryan Kerrigan	University of Maryland	Hydrothermal reactions kinetics and fibrous mineral development in a non-equilibrium KFMASH	NSF	4	
Sanjit Ghose	SUNY @ Stony Brook	Structural Phase Transition of Cryolite (Na3AlF6) at high pressures and temperatures	NSF	6	
Andrew Campbell	University of Maryland	Equations of state of metal-oxide pairs	NSF	3	
Matthew Whitaker	SUNY @ Stony Brook	Investigation of Physical Properties of Iron/Light-Element Alloys (FeS, FeS2,FeSi, Fe3P)	NSF	6	
Changqing Jin	Chinese Academy of Sciences	Pressure induced structure evolution of novel strongly correlated perovskite system AMO3 (M=Cr,Fe,Mn)	Foreign NSF,China	3	
Yanzhang Ma	Texas Technical University	X-ray diffraction measurements of PbMoO4 at high pressures	DOE	4	
S. K. Ghose Z. Chen	Beam line	EDXD Setup	NSF COMPRES	3	
Itzhak Halevy	Nuclear Research Center	The crystallographic and magnetic ordering of the tetragonal REM2X2 under High-Pressure.	DOE	5	

Michelle Weinberger	Carnegie Institution of Washington	High Pressure studies of resistively heated transition metal diborides	DOD NSF	5	
Thomas Duffy	Princeton University	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	6	

September – December, 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Da by NSL
Z Chen	Beam Line	ADXD Setup	NSF COMPRES	4	0
Z Chen	Beam Line	Sample test and Beamline development	NSF COMPRES	3	0
Trevor Tyson	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: High Pressure XRD Measurements	NSF	6	0
Z Chen	Stony Brook University	High pressure effects on crystal structure and electrical transport properties of Cadmium Sulfide	NSF	6	0
Andrew Campbell	University of Maryland	Equations of state of metal-oxide pairs	NSF	4	3
S Ghose	Beam Line	Beamline Maintenance	NSF COMPRES	3	0
Ryan Kerrigan	University of Maryland	Hydrothermal reactions kinetics and fibrous mineral development in a non-equilibrium KFMASH	NSF	3	0
Thomas Duffy	Princeton University	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	5	3
Itzhak Halevy	Nuclear Research Center	The crystallographic and magnetic ordering of the tetragonal REM2X2 under Temperature and High-Pressure.	DOE	5	0
Wendy Panero	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals	NSF	5	3
Wei Liu	SUNY @ Stony Brook	Elasticity across the OEN to HP-CEN Phase Transformation for Orthoenstatite	NSF	4	4
Maining Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature	Foreign	7	4
Z Chen	Beam Line	Beamline Maintenance	NSF COMPRES	3	0
Dongbin Hou	Texas Technical University	High pressure synchrotron X-ray diffraction study of NiS2 up to 50 GPa	NSF	4	2
Hongyang Zhu	Texas Technical University	Phase transformation of phosphor under high pressure	NSF	5	0
Changqing Jin	Institute of Physics Chinese Academy of Sciences	Pressure induced crystallography evolution of itinerant system compounds	Foreign	6	3
Changqing Jin	Institute of Physics Chinese Academy of Sciences	Pressure induced structure evolution of novel strongly correlated perovskite system AMO3 (M=Cr,Fe,Mn)	Foreign	18	9
Maik Lang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	DOE	7	3
S Ghose	Beam line	Beamline development	NSF COMPRES	2	0

X17B3 Schedule

January – April, 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS	# A
Sanjit Ghose	Beam line	80KeV Setup	NSF COMPRES	4	0	
Trevor Tyson	New Jersey Institute of Technology	Diffuse Scattering in Multiferroic Materials	NSF	5	5	
Lars Ehm	SUNY @ Stony Brook	Investigation of the structural changes on different length scales during the pressure induced phase	NSF	5	0	
Li Li	SUNY @ Stony Brook	Investigation of cation ordering in silicate and aluminate spinels	NSF	4	3	
Sanjit Ghose	Beam Line	Sample test and beamline development	NSF COMPRES	3	0	
Hu Cao	Virginia Polytechnic Institute and State University	High resolution synchrotron x-ray diffraction of nanotwins in (1-x)Pb(Mg1/3Nb2/3)-xPbTiO3 crystals	DOE NSF	7	5	
Sanjit Ghose	Beam Line	Beamline development	NSF COMPRES	3	0	
Sanjit Ghose	Beam Line	30 keV Setup	NSF COMPRES	4	0	
Maining Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature	Foreign NSF,China	4	3	
Ryan Rich	Texas Christian University	High pressure effects of	NSF	5	0	
Lars Ehm	SUNY @ Stony Brook	Structure and stability of calcite-type carbonates at high-pressure and temperature	NSF	4	0	
Alexander Goncharov	Carnegie Institute Washington	Beamline development for Laser heating system	NSF COMPRES	7	0	
Sanjit Ghose	Beam Line	Beamline development for Laser heating system	NSF COMPRES	3	0	

May-August, 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS	# Days Assignec
Sanjit Ghose Z. Chen	Beam line	30KeV Setup	NSF COMPRES	4	0	2
Yongjae Lee	Yonsei University	High Pressure Powder Diffraction Studies of Zeolites	Foreign KOSEF	5	0	2
Lars Erm	SUNY@Stony Brook	Structure and stability of calcite-type carbonates at high-pressure and temperature	NSF	0	0	2
Parise John	SUNY @ Stony Brook	FexSy nano-structures and chemistry - from laboratory samples to spreading centers	NASA	4	3	3
Xi Liu	Peking University	Elasticity of bioapatite at ambient temperature	Foreign NSF,China	4	0	2

Duffy Thomas	Princeton University	Quasi-hydrostatic compression of pyroxenes and olivines	NSF	6	3	3
Chih-Ming Lin	Nation Hsinchu University Taiwan	The physical properties of the FeSe and Mse under high-pressure by x-ray diffraction method	Foreign	30	0	2
Sanjit Ghose Z. Chen	Beam line	80KeV Setup	NSF COMPRES	3	0	2
Lars Ehm	SUNY @ Stony Brook	Investigation of the structural changes on different length scales during the pressure induced phase transitions in ATiO3 (A=Ca,Ba,Sr,Pb) perovskites	NSF	5	3	4.75
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides	NSF	6	4	5
Alexander Goncharov	Carnegie Institute Washington	X-ray diffraction combined with the laser heating set up	NSF COMPRES	7	0	5

September – December, 2009

PI Name	Affiliation	Title	Funding	# Days Requested	# Days by NSLS	# Days Assigned
M Vaughan	X17B2 Beam line	Beamline Maintain ace	NSF COMPRES	2	0	2
Z Chen	Beam line	30 KeV Beamline Setup	NSF COMPRES	5	0	4.75
M Vaughan	X17B2 Beam line	Beamline Maintain ace	NSF COMPRES	1	0	1
Bingbing Liu	Jilin University	PRESSURE-INDUCED AMORPHIZATION AND POLYAMORPHISM IN TiO2 NANOMATERIALS	Foreign NSF,China	5	0	3
Qiliang Cui	Jilin University	In situ high pressure XRD studies on metal sesquioxides and molybdenum trioxide hydrates	Foreign NSF,China	10	0	4.5
Lowell Miyagi	Univ of California @ Berkeley	Texture, and Lattice Strain Development in NaMgF3 Post-Perovskite	Foreign CDAC	4	3	3
Sean Shieh	Univ of Western Ontario	High-Pressure Study on Nitrogen-doped Carbon Nanotubes	Foreign Canada	4	0	3
S Ghose	Beam line	80KeV Beamline Setup	NSF	4	0	4
Lars Ehm	Stony Brook University	High pressure	NSF	5	0	3.5
M Vaughan	X17B2 Beam line	X17B2 maintain ace	NSF COMPRES	1	0	1
Li Li	Stony Brook University	Investigation of cation ordering in silicate and aluminate spinels	NSF	3	3	3
Trevor Tyson	New Jersey Institute of Technology	Temperature Dependent Total Scattering Measurements on Multiferroic Oxides	NSF	6	4	3.5
S Ghose	Beam line	Beamline Development For Laser Heating	NSF COMPRES	5	0	3.75

Summary of Beamtime Usage for 2009

	Jan-Apr 2009		May-Aug 2009		Sept-Dec 2009	
	X17C	X17B3	X17C	X17B3	X17C	X17B3
# proposals	15	7	17	7	16	7

# days requested	99	58	97	74	100	55
#days beamtime available *	84.73	51.91	60	32.75	66	36
Oversubscription	1.17	1.18	1.62	2.26	1.52	1.53
Funding **						
NSF	9	6	11	4	10	3
DOE	4	1	4	0	2	0
DOD	1	0	2	0	0	0
Foreign	2	1	3	3	4	4

* Available beamtime includes all beam setup, maintenance and development besides beamtime for users.
** Some proposals are supported by more than one funding.

Total for 2009

	2009	
	X17C	X17B3
# proposals	48	21
# days requested	296	187
#days beamtime from NSLS	210.73	120.66
Oversubscription	1.40	1.55
Funding		
NSF	30	13
DOE	10	1
DOD	3	0
Foreign	9	8

B.2 Infrared Diamond-anvil Facilities at the National Synchrotron Light Source
[PIs: Russell Hemley and Zhenxian Liu, Geophysical Laboratory, Carnegie Institution of Washington]

Diamond-anvil cell infrared facility at the National Synchrotron Light Source

2010 (year #4) Annual Report

[Zhenxian Liu, Russell J. Hemley, Geophysical Laboratory, Carnegie Institution of Washington]

Overview

The diamond anvil cell infrared beamline at the National Synchrotron Light Source (**NSLS-U2A**) is an integrated and dedicated facility for the measurement of far- to near-infrared spectra of materials from ambient to ultrahigh pressures at variable temperatures by coupling synchrotron infrared microspectroscopic techniques, Raman scattering, and visible spectroscopy with diamond- and moissanite-anvil cell methods. The presence of an IR beamline together with x-ray facilities for high-pressure experiments is one of the unique features of the NSLS for general users. We continue to broaden our user base, and provide convenient access for users from the COMPRES community. In addition, we promote our users' research projects on problems relating to high-pressure geoscience and planetary science, complemented by studies in materials science, condensed matter physics, chemistry, and biology (many of which are generated by the COMPRES community). The major beamline upgrades during the period of 2009-2010 provided by the support of COMPRES and CDAC have significantly improved the beamline performance and made the beamline operations more user-friendly. It also ensures that this unique facility is supplied/maintained with cutting-edge instrumentation.

I. Selected Scientific Highlights for 2010

a. ***Pyrochlore under Pressure***

Pyrochlore, $A_2B_2X_6Y$, is an isometric mineral structure with over 500 different compositions and a wide range of applications, from radiation resistant nuclear materials to being fast ionic conductors. Its properties change dramatically depending on composition and the degree of ordering on the cation sites and of the anion vacancies. However, the quantitative analysis of disordering at high pressure has always been a challenge. Researchers from the University of Michigan and the Geophysical Laboratory have demonstrated a new method for quantitatively measuring the degree of pressure-induced atomic disordering in pyrochlore oxides ($La_2Zr_2O_7$) using synchrotron x-ray diffraction (NSLS-X17C), synchrotron infrared spectroscopy (**NSLS-U2A**) and Raman scattering techniques. The research team, with the support of scientists from the diamond anvil cell x-ray facility at the National Synchrotron Light Source (NSLS) have found that the disordering on the cation and anion sites has different influences on the individual diffraction peaks and through careful analysis, their contributions to the diffraction intensities can be quantitatively distinguished. Using the Rietveld method, the research team demonstrated that anion disordering occurs first at pressures below 5 GPa and cation anti-site defects dominate above 10 GPa. An anomalous lattice expansion was confirmed in the lanthanum pyrochlore at 10 GPa by using x-ray diffraction, Raman scattering, and infrared absorption measurements, in experiments where the pressure medium contained some water. Such anomalous lattice expansion is attributed to the first report, in this study, of the incorporation of water into the structure. Water intercalation in pyrochlore oxides may be common during the process of either pressurization or ion irradiation, and is mainly caused by the cation anti-site defects that result from disordering. In addition, $La_2Zr_2O_7$ is a catalyst which can split water during photon irradiation. The photochemical reaction may be closely related to the formation of anion disordering and the formation of Frenkel defects.

Zhang, F.X., M. Lang, Z. Liu, and R. C. Ewing, Pressure-Induced Disordering and Anomalous Lattice Expansion in $La_2Zr_2O_7$ Pyrochlore, *Phys. Rev. Lett.*, **105**, 015503 (2010).

b. ***Low-Temperature Infrared Reflectivity of CH_4: Application to Hydrocarbon Lakes on Titan***

Methane is abundant on icy bodies in the solar system including Pluto and Triton, as identified in observational spectra from characteristic absorption bands at around 1.7 and 2.3 μm. The physical state of CH_4 and other hydrocarbons in the solar system, however, cannot simply be interpreted from the positions of absorption bands alone. On the other hand, reflectance spectroscopy provides one of the few direct observations of outer solar system bodies for probing their surface compositions. Recent discoveries of lakes on Titan, Saturn's largest moon, from the *Cassini* mission come from interpreting a compelling combination of low-lying and flat surfaces measured by Radar and corresponding dark features observed by infrared (IR) reflectivity. It was thought that the Titan's surface is near the triple point of methane and models of Titan's methane cycle are therefore analogous to the Earth's hydrologic cycle, where rain and clouds of methane exchange with solid and liquid methane on the surface. However, interpretation of recent and forthcoming mission observations of planetary bodies requires laboratory-based reflectance spectroscopy of planetary ices and liquids at relevant temperatures, especially to distinguish states of surface phases. Using intense synchrotron infrared radiation at **NSLS-U2A**, researchers from Northwesten University and the Geophysical Laboratory studied the reflectivity of solid (single crystal) and liquid CH_4 at temperatures from 50-100 K. At conditions below the critical pressure, co-existing states of vapor and liquid CH_4 were observed at temperatures down to 94 K. Upon crystallization below 94 K, a dramatic increase in reflectance of CH_4 was observed at the diamond-sample interface (R_{sd}). Whereas the position of characteristic absorption bands of CH_4 are insensitive to the phase state, darkening of liquid CH_4 in reflectance is consistent with Titan's observed dark surface features, which may represent large polar lakes forming seasonally through exchange with clouds and rain of methane where Titan's surface temperatures are within a few degrees of the triple point of methane.

Adams, K.A., S.D. Jacobsen, S.-M. Thomas, Z. Liu, M. Somayazulu, and D.M. Jurdy, Visible and near infrared reflectivity of solid and liquid methane: application to hydrocarbon lakes on Titan, *Planetary and Space Science, special volume "Titan through Time: Formation, Evolution, and Fate".*

c. ***Effect of H_2O on Upper Mantle Phase Transitions in $MgSiO_3$***

The mantle X-discontinuity, usually assigned to positive seismic velocity reflectors in the 260~330 km depth range, has proved difficult to explain in terms of a single mineralogical phase transformation in part because of its depth variability. The coesite to stishovite transition of SiO_2 matches deeper X-discontinuity depths but requires 5~10% free silica in the mantle to match the observed impedance contrast. The orthoenstatite (OEn) to high-pressure clinoenstatite (HPCen) transformation of $MgSiO_3$ also broadly coincides with depths of the X-discontinuity but requires chemically depleted and orthoenstatite-rich lithology at a depth near 300 km in order to match observed seismic impedance contrast. On the basis of high-pressure synchrotron infrared spectroscopy, X-ray diffraction, and Raman spectroscopy, we show that just 1300 ppm variation of H_2O content in $MgSiO_3$ can displace the transition of low-pressure clinoenstatite (LPCen) to HPCen by up to 2 GPa, similar to previous quench experiments on the OEn to HPCen phase transition, where about 30–45 km (1.0–1.5GPa) of deflection could occur per 0.1 wt% H_2O. If the mantle X-discontinuity results from pyroxene transitions in a depleted harzburgite layer, the depth of the mantle X-discontinuity could serve as a potentially sensitive indicator of water content in the upper mantle due to the strong influence of minor amounts of water on the transformation boundary. This study also demonstrates that synchrotron-based IR at the **NSLS-U2A** is highly suitable for studying the behavior of mantle silicates containing relatively low concentrations of water (10's to 100's of ppm by weight). Further synchrotron-IR studies can be carried out on other OH-bearing mantle phases to study hydrogen bonding at pressure and applied to interpretation of mantle velocity structure in potentially hydrous regions of the mantle.

Jacobsen, S.D., Z. Liu, T.B. Ballaran, E.F. Littlefield, L. Ehm, and R.J. Hemley, Effect of water on high-pressure phase transitions in MgSiO3-clinoenstatite: implications for estimating the mantle water content at 270-330 km from the depth of the X-discontinuity, *PEPI*, online first, (2010).

d. Xenon-Hydrogen Mixtures Yield Novel Compound at High Pressure

The high-pressure chemistry of rare gases is of great geochemical interest as well as being important to fundamental chemistry of understanding the nature of bonding in van der Waals compounds. In the course of investigating the Xe-H_2 system at high pressure, researchers from Geophysical laboratory and the Advanced Photon Source discovered a class of compounds with stoichiometry ranging from $Xe(H_2)_7$ to $Xe(H_2)_8$, along with the first experimental verification of bonding states in such materials. A combination of Raman and synchrotron infrared (**NSLS-U2A**) spectroscopic measurements along with synchrotron x-ray diffraction experiments showed that at 5 GPa, a hexagonal phase forms, which may be described as a tripled unit cell of solid hydrogen intercalated with xenon atoms. However, the presence of two separate Xe-Xe distances in the structure suggests the formation of Xe_2 dimers, in which the Xe-Xe distance is 3.875 A, which is close to the Xe-Xe distance in solid Xe at 5 GPa. At higher pressures, additional hydrogen is taken up by the structure, which suggests a composition of $Xe(H_2)_8$ above 5.7 GPa. Synchrotron infrared measurements also show that the material remains an insulator up to 255 GPa. Studies of the electron density maps show a surprising spread of electron density from the Xe_2 pairs toward the surrounding array of H_2 molecules. It is proposed that this spread of electron density is a signature of the depopulation of the highest occupied and fully filled Σ^* molecular orbital of the Xe_2 pair produced at high pressure. However, there is no indication at present of a transfer of electron density into the Σ^* orbital of the H_2 molecule which could lead to its dissociation. This suggests an interaction between Xe_2 dimers and H_2 molecules, which could lead to different bonding modes at higher pressures or different compositions in the Xe-H_2 system.

Somayazulu, M., P. Dera, A.F. Goncharov, S.A. Gramsch, P. Liermann, W. Yang, Z. Liu, H.K Mao and R.J. Hemley, Pressure-Induced Bonding and Compound Formation in Xenon-Hydrogen Solids, *Nature Chem.*, **2**, 50 (2010).

e. Effects of Pressure Media on Pressure-Induced Phase Transitions in Natrolite

Zeolites are hydrated framework alumosilicates which comprise an important class of low-density materials. Their frameworks are composed of corner connecting of TO4 (Si, Al, Ge, Ga, ...) tetrahedra which yield cavities and channels of molecular dimensions. Exchangeable non-framework cations occupy the cavities and channels along with absorbed water molecules at ambient conditions. As such, a plethora of structural studies have been carried out as a function of framework type, composition, and/or temperature in order to understand their relationship to catalytic, molecular sieving, and ion-exchange properties. In recent years, there has also been significant interest in pressure-induced structural and chemical changes in zeolites. Researchers from Yonsei University and Geophysical Laboratory have systematically studied the structural phase transitions in natrolite as a function of pressure and different hydrostatic media using micro-Raman scattering and synchrotron infrared (**NSLS-U2A**) spectroscopy. It was found that natrolite undergoes two reversible phase transitions at 0.86 and 1.53 GPa under pure water pressure medium. These phase transitions are characterized by the changes in the vibrational frequencies of four- and eight-membered rings related to the variations in the bridging T-O-T angles and the geometry of the elliptical eight-ring channels under pressure. Concomitant to the changes in the

framework vibrational modes, the number of the O-H stretching vibrational modes of natrolite changes as a result of the rearrangements of the hydrogen bonds in the channels caused by a successive increase in the hydration level under hydrostatic pressure. Similar phase transitions were also observed at relatively higher pressures (1.13 and 1.59 GPa) under an alcohol-water pressure medium. Furthermore, no phase transition was found up to 2.52 GPa if a lower volume ratio of the alcohol-water to natrolite was employed. This indicates that the water content in the pressure media plays a crucial role in triggering the pressure-induced phase transitions in natrolite.
Liu, D., W. Lei, Z. Liu, Y. Lee, Spectroscopic Study of the Effects of Pressure Media on High-Pressure Phase Transitions in Natrolite, *J. Phys. Chem. C,* online first, (2010).

II. Beamline Developments

It was an exciting period from June 2009 to October 2010 in terms of the major beamline developments and upgrades taking place at NSLS-U2A. The equipment funds supported by COMPRES, Carnegie/DOE Alliance (CDAC), and University of Nevada, Las Vegas (UNLV) became available in June 2009, which allowed the construction and operation of the new side station at U2A to proceed on schedule. In addition, the COMPRES supplemental equipment funds boosted other beamline upgrades originally planned for the next few years. The detailed status regarding these projects is described as below:

1. ***Construction, commission, and operation of the new side station at the U2A beamline***
   High flux and high brightness synchrotron infrared (IR) radiations are required for high-pressure experiments using a diamond anvil cell (DAC). However, the performance of an IR beamline is highly dependent on beam travel distance from the source spot to the end station. Diagnostic tests have shown that performance at the U2A beamline is significantly lower (by a factor of two) than the other IR beamlines of the NSLS in the mid-IR and much worse in the far-IR due to the considerable distance (~15 meters) between the U2A end station (spectrometer/microscope) in the hutch and the synchrotron source. This limitation poses problems for experiments that require the highest spatial resolution (e.g., IR mapping of samples down below 5 μm or the diffraction limit). As we pointed out in our previous year's annual report, we were able to raise sufficient funds to start the side station construction in 2009. Founded by COMPRES, CDAC, and UNLV, a new side station has been constructed in December, 2009, and became operational in January 2010. The side station includes a Bruker Vertex 80v FTIR spectrometer and a Bruker Hyperion 2000 IR microscope ideally for the mapping of natural samples (e.g., solid and fluid inclusions in thin section), heterogeneous charges from high-pressure experiments, as well as laser heated samples in situ at very high pressure in diamond anvil cells. The distance from the synchrotron source to the side station is only ~3 meters, which effectively eliminates the problems of beam divergence and image distortion.

   

   Newly constructed U2A side station.

   It is important to point out that all the developments on the side station project have been done in a very short period of time. An optical table has been installed in November 2009 and the Bruker 80v FTIR spectrometer and Hyperion-2000 IR microscope were delivery and installed in

December 2009. We were able to couple the vacuum synchrotron beam delivery system and the FTIR spectrometer during the NSLS winter shutdown and commissioned the complete system right after the synchrotron beam came back in early January. As a result, no scheduled user beam time was affected due to the construction. Instead, many users (most of them from the COMPRES community) took the advantage of the side station as soon as it became available in January 2010 and an up to date list of those user's institutions is shown as below:

Army Research Laboratory
Brookhaven National Laboratory
Carnegie Institution of Washington
Florida International University
Graduate University of Chinese
Academy of Sciences, China
Jilin University, Changchun, China
Kobe University, Japan
Montclair State University
New Jersey Institute of Technology
Northwestern University
Ohio State University
SUNY-Stony Brook
University of Arizona
University of Chicago
University of Michigan
University of Nevada-Las Vegas
University of Saskatchewan, Canada
University of Tennessee
Yale University
Yonsei University

Current development at the side station is focused on building additional custom IR microscopes dedicated to far-IR experiments at high pressure or low-T and high-P experiments in the range from far- to near-IR. These IR microscope systems will be completed in year #4. The side station project will be fully completed in 2011 with an onsite small ruby system and enclosure surrounding all the instruments on the optical table (see the budget request for permanent equipment in year #5).

2. ***Compact cryostat***
   The combined high-pressure and low-temperature techniques are very important to address a broad range of problems in planetary sciences (see the second scientific highlight as an example). Such capabilities could also attract a lot of users. The new cryostat from Cryoindustries with a compact design for accommodating standard symmetric DACs was purchased with the COMPRES supplemental equipment funds and was delivered in February 2010. The cryostat was immediately tested right away and the first user experiment took place on March 10, 2010 (user group from the Ohio State University). The experiments conducted with the cryostat demonstrate that the performance of the cryostat is well above the specifications and much more user friendly. Thus, the combined cryostat and standard symmetric DACs provide a way for general users to routinely and reliably perform *in situ* high pressure and low temperature IR studies at U2A beamline. In addition, this cryostat is also shared by all DAC facilities at the NSLS.
3. ***Laser upgrade for the Raman/IR Microscope system***
   The U2A beamline has integrated synchrotron FTIR spectroscopy, Raman scattering as well visible spectroscopy together with DAC techniques for all users to conduct spectroscopic studies under extreme conditions. In order to replace the Ar^+ laser (more than 14 years old and running with a refurbished tube) and take the advantage of the solid-state laser techniques, three DPSS lasers (532 nm 646, and 785 nm) and sets of filters/beamsplitters have been purchased, delivered, and installed in the micro-Raman system (available since June 2010). Preliminary tests have shown that fluorescence from most of type-IIa diamond anvils is substantially reduced with red laser excitation. This will make the *in situ* Raman and IR measurements available for the same sample in a DAC at same pressure. An additional microscope for combined Raman/IR measurements at high pressure and variable temperatures (10~1000 K) with slide stage was added as well. These improvements make the switch between Raman and IR systems more efficient and user friendly. Most of these upgrades are supported by the COMPRES supplemental equipment funds.
4. ***New sample preparation station***
   The sample preparation lab at X17C shared by all the NSLS DAC users is not sufficient to accommodate this number of users since all three DAC beamlines are running at the same time. With the COMPRES supplemental equipment funds, we purchased a Leica microscope for sample loading and an EDM machine for gasket drilling. All the items have been delivered, tested, and installed in the U2A hutch. These tools became available for all users in September 2010.
5. ***CO_2 laser heating system***

The ability to generate high pressure and high temperature is crucial for the COMPRES user community to address a range of problems on mineral physics/chemistry related to the Earth's interior. High-pressure and temperature >1000 K are essential for infrared studies of Earth and planetary materials. CO_2 laser heating techniques combined with DACs are the best approach to creating such extreme conditions for studying the water solubility in lower mantle minerals. We are continuing to make progress on the CO_2 laser heating system during the period of 2009-2010. Major progress has been made on the laser interlock system, which been installed by the NSLS interlock group to comply with the laser safety requirements at BNL. In addition, an entire new temperature calibration system including a spectrometer with an OMA-InGaAs detector from Princeton Instruments has been purchased with the COMPRES supplemental equipment funds, which has been installed and fully tested. We will focus on the process of getting the safety operation procedure (SOP) approved by the BNL laser officer during the NSLS winter shutdown and move the whole system into the commissioning phase.

IV. The Fraction of Beam Time on the IR Beamline Available to the Community Next Year

Under the current NSLS Contributing User arrangement, 50% of the beam time is allocated to U2A for General Users (GU time). Currently, the COMPRES community is the dominant user group in this category. Unfortunately, the current situation on the beamline staff support at NSLS-U2A can't be sustained and the number of available days for general users must be reduced from 50% to 25% next year due to the lack of beamline staff support and number of ongoing beamline developments/upgrades. The remaining 75% of contributing user (CU) beam time is allocated by COMPRES and Geophysical Laboratory, Carnegie Institution of Washington including the following categories:

a) The first portion of the CU beam time is allocated by COMPRES being dedicated to support research by members of the COMPRES community through proposals vetted by the NSLS General User program. The NSLS User Administration provides the CU group proposed here with the ratings of all proposals for a beam time cycle, so that these ratings may be honored in decisions on requests;
b) The second portion of the CU beam time will be utilized by the beamline scientist and postdoc for beamline improvements/upgrades to keep the beamline state of the art as well for carrying out their research projects. The remaining CU beam time goes to Geophysical Laboratory for development projects and users supported by its grants, such as CDAC and EFree. These beam time is commensurate with the support of the beamline from those grants.

VI. Users (including collaborating groups) and Beam Time Usage

(June 1, 2009—August 31, 2010)

User name	Affiliations	Project	Dates of the experiments	GU Days allocated for the cycle

T. Strobel	Geophysical Lab	Infrared Spectroscopy of novel a H2+SiH4 compound (proposal # 14273)	Jun. 4-5, 2009 Jun. 6-7, 2009	2 CU beam time
M. Pravica S. Tkachev E. Romano	University of Nevada	Infrared studies of cyclooctatetraene at high-pressure (proposal #11925)	Jun. 10-11, 2009	2
W. Han	CFN, Brookhaven National Lab	High-pressure IR Study gases storage in boron nitride nanotubes (proposal # 11755)	Jun. 12, 2009	CU beam time
S. Garimella	CeSMEC, Florida International University	High-Pressure studies on group VI metal hexacarbonyls (proposal #14088)	Jun. 23-25, 2009	3
M. Lang F. Zhang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High-Pressure: A Novel Approach in Geosciences (proposal # 13333)	Jun. 28-30, 2009	3
J. Smedley	Brookhaven National Lab	Characterization of Impurities in Diamond (proposal # 11735)	Jul. 1, 2009	1
M. Weinberger J. Cizark	Army Research Laboratory	Elastic-Plastic Transformation of Ultrahard Materials (proposal # 13891)	Jul. 14-15, 2009	2
Y. Lee D. Seoung Y. Lee	Yonsei University Korea	High-Pressure Powder Diffraction Studies of Zeolites (proposal # 14035)	Jul. 17-19, 2009 Jul. 20, 2009	3 CU beam time
Y. Wang	SUNY @ Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application (proposal # 14806)	Jul. 22, 2009	CU beam time
W. Han	CFN, Brookhaven National Lab	High-pressure IR Study gases storage in boron nitride nanotubes (proposal # 11755)	Jul. 23-24, 2009	2
H. Liu	National Taiwan Normal University	Infrared studies of strongly correlated systems at high-pressure (proposal # 10871)	Aug. 17-21, 2009 Aug. 22, 2009	5 CU beam time
K. Otsuka G. Amulele	Yale University	In situ measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR (proposal # 11707)	Aug. 24-26, 2009	3
X. Chen	Geophysical Lab	High-pressure optical spectroscopy of hydrogen-based electron materials (proposal # 12535)	Aug. 27-30, 2009	4
S. Tkachev	University of Nevada	Infrared studies of cyclooctatetraene at high-pressure (proposal #11925)	Sep. 10-11, 2009	CU beam time
Y. Wang	SUNY @ Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application (proposal # 14806)	Sep. 14-18, 2009	5
S. Tkachev	University of Nevada	Infrared studies of cyclooctatetraene at high-pressure (proposal #11925)	Sep. 21-24, 2009	CU beam time
W. Han	CFN, Brookhaven National Lab	High-pressure IR Study gases storage in boron nitride nanotubes (proposal # 11755)	Sep. 25-26, Oct. 1-2, 2009	CU beam time 2
J. Smedley	Brookhaven National Lab	Characterization of Impurities in Diamond (proposal # 11735)	Oct. 5, 2009	1
D. Reaman J. Pigott	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals (proposal #14797)	Oct. 8-9, 2009	2
Q. Cui	Jilin University	high pressure infrared studies on molybdenum trioxide hydrates MOO3.xH2O (x= 1/3, 1/2,1, 2) (proposal #14867)	Oct. 10-14, 2009	CU beam time
M. Ma	Graduate University of	Effect of water on properties of olivine at high pressure and high temperature (proposal	Oct. 15-16, 2009	2

	Chinese Academy of Sciences	#13269)		
C. Seagle T. Strobel	University of Chicago	Optical Properties of Tin at High Pressures and Temperatures (proposal # 14822)	Oct. 19-22, 2009	4
C. Lui	Columbia University	Probing the Electronic Structure of Graphene Nanoribbons by Infrared Photoconductivity (proposal #14783)	Oct. 28-29, 2009	2
T. Tyson P. Gao	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: IR Measurements (proposal # 14969)	Nov. 1-4, 2009 Nov. 5-6, 2009	4 CU beam time
G. Amulele K. Otsuka	Yale University	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements (proposal # 14936)	Nov. 8-9, 2009 Nov. 15, 2009	3
G. Yang	Instrumentation department, BNL	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe (proposal #14165)	Nov. 10-12, 2009	2
K. Otsuka G. Amulele	Yale University	In situ measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR (proposal # 11707)	Nov. 12-14, 2009	3
M. Lang F. Zhang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High-Pressure: A Novel Approach in Geosciences (proposal # 13333)	Nov. 16, 2009 Nov. 17-20, 2009	1 CU beam time
Z. Liu	Geophysical Lab	Coupling the new side station with the synchrotron source	Jan. 5-25, 2010	CU beam time
Y. Wang	SUNY @ Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application (proposal # 14806)	Jan. 19-20, 2010	2
T. Strobel Yoku	Geophysical Lab	Infrared Spectroscopy of novel high-pressue low-temperature H2O+H2 clathrate phases (proposal # 14131)	Jan. 26-27 Jan. 28-29 2010	2 CU beam time
J. Cizark	Army Research Laboratory	Elastic-Plastic Transformation of Ultrahard Materials (proposal # 13891)	Jan. 31- Feb. 1, 2010	2
Yongjae Lee D. Seoung Moon Lee	Yonsei University Korea	High-Pressure Powder Diffraction Studies of Zeolites (proposal # 14035)	Feb. 2-4, Feb.5, 2010	3 CU beam time
G. Amulele K. Otsuka	Yale University	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements (proposal # 14936)	Feb. 16-19 Feb. 20, 2010	4 CU beam time
W. Han	CFN, Brookhaven National Lab	High-pressure IR Study gases storage in boron nitride nanotubes (proposal # 11755)	Feb. 24-27, 2010	4
W. Panero J. Pigott	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals (proposal # 14797)	Mar. 2-3, 2010 Mar. 4, 2010	2 CU beam time
Y. Wang	SUNY @ Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application (proposal # 14806)	Mar. 8-10, 2010	3
K. Otsuka G. Amulele	Yale University	In situ measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR (proposal # 11707)	Mar. 15-19, 2009	5
M. Ma	Graduate	Effect of water on properties of olivine at high	Mar. 24-25,	2

	University of Chinese Academy of Sciences	pressure and high temperature (proposal #13269)	2010	
B. Liu Q. Li	Jilin University	Pressure-Induced Amorphization and Polyamorphism in TiO2 Nanomaterials (proposal # 14895)	Mar. 29-31, 2010	3
G. Yang	Instrumentation department, BNL	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe (proposal #14165)	Apr. 6-9, 2010	4
T. Tyson P. Gao	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: IR Measurements (proposal # 14969)	Apr. 12-17, 2010	6
M. Lang F. Zhang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High-Pressure: A Novel Approach in Geosciences (proposal # 13333)	Apr. 25-27, 2010	3
Y. Wang	SUNY @ Stony Brook	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application (proposal # 14806)	May 27-29, 2010	3
M. Pravica M. Galley	University of Nevada Las Vegas	Far- and mid- IR high pressure studies of detonation products (proposal #16214)	Jun. 5-6, 2010	2
J. Musfeldt	University of Tennessee	Pressure-induced switching of the Jahn-Teller axis in Cu(pyz)F2(H2O)2 by synchrotron infrared spectroscopy (proposal #16236)	Jun. 27-Jul. 1, Jul. 1, 2010	5 CU beam time
M. Lang F. Zhang	University of Michigan	Phase Transitions in Minerals Induced by Ion Beams and High-Pressure: A Novel Approach in Geosciences (proposal # 13333)	Jul. 12-13, Jul. 14, 2010	2 CU beam time
L. Wang	SUNY @ Stony Brook	Incorporation of water in nominally anhydrous mantle minerals (proposal #16328)	Jul. 15-16, 2010	2
M. Ma	Graduate University of Chinese Academy of Sciences	Effect of water on properties of olivine at high pressure and high temperature (proposal #13269)	Jul. 18-19, 2010	2
M. Pravica N. Velisavljevic	UNLV LANL	Far- and mid- IR high pressure studies of detonation products (proposal #16214)	Jul. 22-24, Jul. 25, 2010	3 CU beam time
D. Reaman J. Pigott	Ohio State University	Elasticity and mechanism of water incorporation deep Earth minerals (proposal #14797)	Jul. 26-27, Jul. 28, 2010	2 CU beam time
G. Yang	Instrumentation department, BNL	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe (proposal #14165)	Jul. 29-31, 2010	3
H. Okamura	Kobe University	High pressure IR studies of strongly correlated electron materials (Proposal #16191)	Aug. 4-7, Aug. 8-11, 2010	4 CU beam time
G. Amulele K. Otsuka	Yale University	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements (proposal # 14936)	Aug. 12-14, 2010	3
Yongjae Lee D. Liu D. Seoung Moon Lee T. Kim	Yonsei University Korea	High-Pressure Powder Diffraction Studies of Zeolites (proposal # 14035)	Aug. 15-16, Aug. 17, 2010	2 CU beam time
K. Otsuka	Yale University	In situ FTIR measurements on hydrogen	Aug. 18-20,	3

G. Amulele		solubility and speciation in olivine and magnesiowüstite at high pressures and temperatures (proposal # 16326)	Aug. 21, 2010	CU beam time
T. Tyson P. Gao	New Jersey Institute of Technology	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: IR Measurements (proposal # 14969)	Aug. 23-26, 2010	4
H. Feng	Montclair State University	Examination of Organic Contaminants (PAHs) in Passaic River Sediments Using Synchrotron-UV-FTIR Techniques (proposal #16418)	Aug. 27-28, Aug. 29, 2010	2 CU beam time

VII. General Users Proposals Submitted through the NSLS PASS System for Beamtime Request at U2A: January 1, 2010—December 31, 2010

From	Title	PI	Date submitted
13819	Elastic-Plastic Transformation of Ultrahard Materials January - April 2010	X9114	09/09/2009
11755	High-pressure IR Study gases storage in boron nitride nanotubes January - April 2010	23205	09/25/2009
14806	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application January - April 2010	W7325	09/29/2009
11707	In situ measurements on hydrogen solubility and speciation in (Mg,Fe)O and olivine using synchrotron FTIR January - April 2010	J7501	09/29/2009
14131	Infrared Spectroscopy of novel high-pressue low-temperature H2O+H2 clathrate phases January - April 2010	N7993	09/29/2009
14165	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe January - April 2010	23876	09/29/2009
14936	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements January - April 2010	N7833	09/29/2009
14895	PRESSURE-INDUCED AMORPHIZATION AND POLYAMORPHISM IN TiO2 NANOMATERIALS January - April 2010	J7454	09/30/2009
14797	Elasticity and mechanism of water incorporation deep Earth minerals January - April 2010	X6885	09/30/2009
13333	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	J7513	09/30/2009

January - April 2010

14969	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: IR Measurements	T5969	09/30/2009	January - April 2010
15680	Infra-red spectroscopy mapping of boron and nitrogen in natural diamonds	P5481	09/30/2009	January - April 2010
14035	High Pressure Powder Diffraction Studies of Zeolites	U7560	09/30/2009	January - April 2010
13269	Effect of water on properties of olivine at high pressure and high temperature	N7293	10/02/2009	January - April 2010
13333	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences	J7513	01/07/2010	May - August 2010
16188	Far- and mid- IR high pressure studies of HMX	P5534	01/20/2010	May - August 2010
16214	Far- and mid- IR high pressure studies of detonation products	P5534	01/23/2010	May - August 2010
16236	Pressure-induced switching of the Jahn-Teller axis in Cu(pyz)F2(H2O)2 by synchrotron infrared spectroscopy	M7156	01/25/2010	May - August 2010
14806	Biomacromolecule imprinting and immobilization with self-assembled monolayers for sensor application	W7325	01/28/2010	May - August 2010
13269	Effect of water on properties of olivine at high pressure and high temperature	N7293	01/29/2010	May - August 2010
14936	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements	N7833	01/29/2010	May - August 2010
16328	Incorporation of water in nominally anhydrous mantle minerals	W7206	01/29/2010	May - August 2010
16326	In situ FTIR measurements on hydrogen solubility and speciation in olivine and magnesiowüstite at high pressures and temperatures	J7501	01/29/2010	May - August 2010
16395	Study gas storage in boron nitride nanostructures by high-pressure IR and Raman	23205	01/31/2010	May - August 2010

16191	High pressure IR studies of strongly correlated electron materials May - August 2010	A8613	02/01/2010
16418	Examination of Organic Contaminants (PAHs) in Passaic River Sediments Using Synchrotron-UV-FTIR Techniques May - August 2010	F5980	02/01/2010
14969	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: IR Measurements May - August 2010	T5969	02/01/2010
14797	Elasticity and mechanism of water incorporation deep Earth minerals May - August 2010	X6885	02/01/2010
14035	High Pressure Powder Diffraction Studies of Zeolites May - August 2010	U7560	02/01/2010
14165	Synchrotron infrared microspectroscopy and photoluminescence investigation of CdZnTe and CdMnTe ▪	23876 May - August 2010	02/01/2010
13819	Elastic-Plastic Transformation of Ultrahard Materials September - December 2010	X9114	05/05/2010
16879	Infrared spectroscopy of N2/H2 mixtures subjected to high pressures September - December 2010	X9114	05/05/2010
16418	Examination of Organic Contaminants (PAHs) in Passaic River Sediments Using Synchrotron-UV-FTIR Techniques September - December 2010	F5980	05/25/2010
13333	Phase Transitions in Minerals Induced by Ion Beams and High Pressure: A Novel Approach in Geosciences September - December 2010	J7513	05/26/2010
13269	Effect of water on properties of olivine at high pressure and high temperature September - December 2010	N7293	05/27/2010
17039	Electronn band gap for semconducting organometallic radical compounds September - December 2010	T5503	05/27/2010
14895	PRESSURE-INDUCED AMORPHIZATION AND POLYAMORPHISM IN TiO2 NANOMATERIALS September - December 2010	J7454	05/31/2010
14936	Water solubility studies in lower mantle perovskites by Fourier transform infrared measurements September - December 2010	N7833	06/01/2010
16395	Study gas storage in boron nitride nanostructures by	23205	06/01/2010

	high-pressure IR and Raman September - December 2010		
14797	Elasticity and mechanism of water incorporation deep Earth minerals September - December 2010	X6885	06/01/2010
14969	Spin-Driven Local Distortions in Multiferroic Hexagonal ReMnO3: IR Measurements September - December 2010	T5969	06/02/2010

VIII. U2A Beamline Publications 2009-20010

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Ciezak, J., The High-Pressure Characterization of Energetic Materials: Diaminotetrazolium Nitrate (HDAT-NO3), *Propell. Explos. Pyrot.*, **35**, 24-30 (2010).

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Ciezak, J., The High-Pressure Characterization of Energetic Materials: 2-methyl-5-nitramino-2Htetrazole, *Propell. Explos. Pyrot.*, in press.

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B.3 X-ray Multi-anvil Facilities at the National Synchrotron Light Source

[PIs: Donald Weidner and Michael Vaughan, Stony Brook University]

Multi-anvil High Pressure Facilities at the National Synchrotron Light Source, Nov. 2010

Prepared by
Michael T. Vaughan
Donald J. Weidner

Available MAC beamtime. 2009-2010 has again been an exciting year at the multianvil facility at the NSLS. The 'B' portion of the superconducting wiggler beam (X17) supports three hutches, X17B1, X17B2, and X17B3. The X17B2 houses the multianvil facility and X17B3 houses a portion of the diamond anvil cell program. Together B2 and B3 are in use 2/3 of the time and can be run simultaneously. Thus the multianvil system is available 2/3 of the time that the NSLS is operating.

The B2 hutch has a white beam and a monochromatic beam that is generated by a single bounce monochromator. Thus it is possible to place two high pressure stations on the floor, each receiving beam. The shielding of the mono station has been completed, so that these two stations can now operate simultaneously. We have successfully tested the T-cup and the DT-cup in the side station and all are functioning properly. The T-cup is a 6-8 styled module with 10mm second stage anvils. We have achieved 29GPa pressure in this system with 2 mm truncations in the past. The DT-cup is a modified T-cup with continuous deformation capabilities. These two guideblocks are compressed by a V-8 Paris-Edinburgh 500 ton press frame. The DT-cup has two additional 50 ton jacks to drive the differential rams. This system is now ready for experiments.

NSLS has now commissioned X17A (no direct impact on high pressure beam time). This will be a high energy end station that can run simultaneously with the X17B line. With the completion of the A leg, some users in materials science that now use X17B1 will move to X17A. This may allow the high pressure portion of the X17B time to increase beyond the current 2/3 allocation. Furthermore, we expect to support some high pressure research on the X17A beamline using either PE or DAC style cells. However, these plans have not yet been implemented.

High accuracy stress measurements. We succeeded in developing and deploying a new diffraction detector for the white beam that can resolve differential stress to an accuracy of 10 MPa. A 10 element energy dispersive detector is being used. This detector simultaneously records diffraction spectra from the 10 detectors that are located at a fixed two theta around the transmitted beam. This allows a complete analysis of the magnitude and orientation of the stress field in the sample. This system was entirely designed by our beamline team (including Bill Durham at MIT) and is reported in a Rev. of Scientific Instruments article. In order to increase the accuracy, we restricted the slits and reduced the gauge volume. The pleasant surprise is that we can collect robust spectra in shorter data times than before. We have been able to determine stress in spectra that took 15 seconds to gather. This enables time resolved studies that were not possible before.

Activities accomplished planned from last year

We now fully operate two beamlines simultaneously in the MAC hutch. One uses a white beam, the other monochromatic; one with a DIA system, the other with a Tcup. Both have differential stress capability. We have taken delivery of a 1100 Ton (1000 Tonne) press, along with alignment stage.

NSLS II The next generation of synchrotron at Brookhaven is under construction. We continue to be engaged in the discussion but have no progress to report at this time on the status of high pressure at NSLS II.

Activities for 2010-11

We will be installing the 1100 ton press commissioning it with a DT25 guide block on the white beam this winter, with full user access by May, 2011.

Major Support Personnel

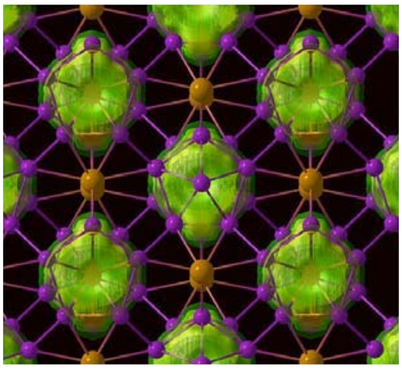
Liping Wang beam line scientist	COMPRES funds
Carey Koleda machinist	COMPRES funds
Michael T. Vaughan NSLS coordinator	MPI
Donald J. Weidner, scientist spokesperson	SUNY
Ken Baldwin, software support	MPI
William Huebsch, part time electronics	COMPRES funds

Science Highlights

Collaboration between Theoreticians and Experimentalists Made Discovery of Single Element Compound at High Pressure

Artem R. Oganov[1,2], Jiuhua Chen[3,4], Carlo Gatti[5], Yanzhang Ma[6], Yanming Ma[1,7], Colin W. Glass[1], Zhenxian Liu[8], Tony Yu[3], Oleksandr O. Kurakevych[9] & Vladimir L. Solozhenko[9]

Experimental teams led my Jiuhua Chen and Vladimir Solozhenko successfully synthesized a new phase of boron at pressures and temperatures above 12 GPa and 1800K. The sample was characterized at the NSLS using x-ray diffraction and infrared spectroscopy indicating many complex and unique features that the new phase holds. Theoretician Artem Oganov and his team employed a computational technique that they have developed for predicting crystal structures, and were able to determine the structure, which matched all experimental observations. The crystalline phase consists of two substructures. One is an icosahedron made of 12 boron atoms. The other is a simple pair of boron atoms. These two sub-substructures stack together in the same way that ions of chlorine and sodium in table salt (sodium chloride) do. Electronegativities of the B12 icosahedra and B2 pairs are so different that it causes charge redistribution and the emergence of partial ionicity in this elemental structure.



The newly discovered phase of boron consists of two substructures ─ one is a 12-atom cage, purple, the other is a two-atom dumbbell, orange. Ionic bonds form between the two substructures. This is the first time that ionic bonds have been seen in crystal structures consisting of a single element.

[1]Laboratory of Crystallography, Department of Materials [2]Geology Department, Moscow State University. [3]Center for the Study of Matter at Extreme Conditions and Department of Mechanical and Materials Engineering, Florida International University. [4]Mineral Physics Institute and Department of Geosciences, Stony Brook University. [5]CNR-ISTM Istituto di Scienze e Tecnologie Molecolari. [6]Department of Mechanical Engineering, Texas University of Technology.[7]National Laboratory of Superhard Materials, Jilin University. [8]Geophysical Laboratory, Carnegie Institution of Washington. [9]LPMTM-CNRS, Universite´ Paris Nord.

CaIrO3 deformation

The post perovskite phase of $MgSiO_3$ controls the dynamics the lower thermal boundary layer of the Earth's mantle, determining core-mantle interaction and, ultimately, giving rise to hot-spot volcanism. A combined analogue experimental and theoretical approach is the only way to determine many of its physical properties. Here we determined the relative strength of perovskite and post-perovskite: post perovskite is significantly weaker than perovskite meaning that we will have to fundamentally revisit the dynamics of the D" region at the base of the Earth's mantle.

Hunt, S.A., Weidner, D.J., Li, L., Wang, L., Walte, N.P. Brodholt, J.P. and Dobson, D.P., Weakening of $CaIrO_3$ during the perovskite-post perovskite transformation. *Nature Geoscience*, 10.1038/NGEO663, 2009.
Ammann, M.W., Brodholt, J.P., Wookey, J. and Dobson, D.P. First Principles Constraints on Diffusion in Lower Mantle Minerals and a Weak D'' Layer. *Nature*, 465, 462-465, 2010.

Elastic properties of yttrium-doped $BaCeO_3$ perovskite

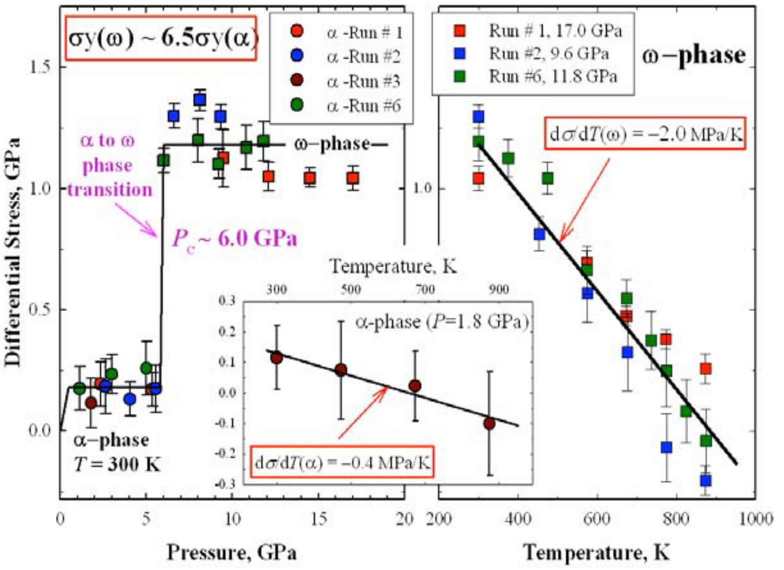
The variation of elastic properties with oxygen vacancies, a fundamental problem in solid-state science as well as in materials design and application, has not been well understood by either experiments or theory. To date, our understandings of this problem are mainly derived from first-principles calculations on aluminum-doped silicate perovskite. These studies suggested that, with an atomistic-scale vacancy-forming mechanism for Al substitution, $2Al^{3+} + V_O \rightarrow 2Si^{4+}$, the silicate perovskite containing oxygen vacancies (V_O) would have elastic bulk moduli that are up to 35% smaller than those for a defect-free counterpart. However, there is so far no direct experimental prove on materials with well-characterized vacancy-forming mechanism.

The cerate perovskite is a member of the ceramic $A^{2+}B^{4+}O_3$ perovskite. Numerous measurements under rigorously controlled conditions on these ceramic materials have yielded data essential to gaining quantitative understanding of the defect equlibria and the effects of oxygen vacancies on ionic transport. In this family of perovskite, the tetravalent B cations can be Ti, Ce, Zr, or Sn, and the divalent A cations can be Ca, Sr, and Ba. A number of trivalent rare-earth elements (M = Y, Yb, Nd, Gd) have been found to substitute only for tetravalent ions, resulting in a doped series $A^{2+}(B^{4+}{}_{1-x}M_x)O_{3-0.5x}$ in which the diminished positive charge is compensated by oxygen vacancies. These doped ceramic perovskites, with the well-characterized vacancy-forming mechanisms, are ideal materials for the study of defect chemistry, ionic transport, and the effect of oxygen vacancies on the elastic properties.

We studied the elasticity of the oxygen-deficient $BaCe_{1-x}Y_xO_{3-0.5x}$ perovskite with x = 0.00 and 0.15 using ultrasonic interferometry and synchrotron x-ray diffraction. Our results show that the presence of 2.5% oxygen vacancy has no measurable effect on the elastic bulk modulus. The shear modulus, however, decreases by approximately 5% in $BaCe_{0.85}Y_{0.15}O_{2.925}$ perovskite. The differences between Y^{3+} doped cerate and Al^{3+} doped silicate suggest that the effect of oxygen vacancy on the elastic properties could be system-dependent. In $BaCe_{1-x}Y_xO_{3-0.5x}$ perovskite, for example, the substitution of Y^{3+} for Ce^{4+} and formation of oxygen vacancies cause a decrease in the unit-cell volume, whereas an opposite trend is revealed by both experiments and theoretical calculations for the substitution of Al^{3+} into Mg-silicate perovskite. This comparison points to a crystal-chemistry difference of the atomistic-scale substitution between the two systems. Another area of importance is the distribution of oxygen vacancies within the structures of the parent compounds, which has not been well characterized for both silicate and cerate perovskite. In other cases, such as $LaGeO_3$-based oxygen-deficient perovskites, oxygen vacancies tend to be trapped around dopant ions (such as Y^{3+} in $BaCe_{1-x}Y_xO_{3-0.5x}$) to form vacancy-cation clusters. Thus the dopant ions may be in a reduced coordination by oxygen (pentagonal or tetrahedral coordination). It can also be expected that when the oxygen vacancy concentration exceeds a certain threshold, vacancy-vacancy interaction may become predominant. These structural mechanisms as well as their complex interactions may eventually lead to different behaviors of bulk modulus as a function of oxygen vacancy concentration.

This work was conducted by J. Zhang, Y. Zhao, H. Xu (Los Alamos National Laboratory), B. Li, D.J. Weidner (Stony Brook University), and A. Navrotsky (UC Davis) at beamline X-17B2 of National Synchrotron Light Source, Brookhaven National Laboratory and has been published in *Applied Physics Letters* (Vol. 90, 161903-1-3, 2007).

Enhancement of Yield Strength in Zirconium Metal through High-Pressure Induced Structural Phase Transition



Most materials have a certain intrinsic strength related to atomic bonds, which need to be broken and reformed when the dislocation moves. Pure and ductile metals typically have low yield strength due to weak metallic bonding, making it fundamentally important to find and understand the strengthening mechanisms. Although the yield strength of crystalline materials as a function of pressure (*P*) and temperature (*T*) has been documented previously, the changes of yield strength associated with the *P*-*T* induced structural phase transitions have to date not been well studied, both experimentally and theoretically, which impedes our current understanding of the mechanisms underlying the phase-transition driving plasticity and ductility.

We conducted *in-situ* deformation studies on ultra-pure zirconium metal using synchrotron x-rays under high *P*-*T* conditions. With a well-known and also commonly used method of peak-profile analysis, we determined the differential strain and hence yield strength in polycrystalline zirconium samples under the applied stress. We observe a high-pressure phase-transition induced strengthening with more than 6-fold abrupt increase in yield strength at the transition pressure of P_c = 6 GPa, from 180 MPa in the low-pressure phase of α-Zr to 1180 MPa in the high-pressure phase of ω-Zr (Figure 1). To our knowledge, this represents the most significant enhancement in yield strength among the known strengthening techniques, such as quenching, alloying, forging, and grain size reduction, for pure metals. Our findings also support the theoretical modeling and physics arguments of plastic deformation; the high-*P* phase transition induced enhancement in yield strength can be interpreted by: (1) soft metallic bonding in α-Zr *vs.*

strong covalent bonding of ω-Zr; (2) relatively easy sliding over smooth close-pack sheets in α-Zr *vs.* bumpy corrugation in slip plane for the open structure in ω-Zr atomic layers; and (3) large population of $(10\bar{1}1)_{hcp}$ twins and basal stacking faults in α-Zr *vs.* repulsive nature of the preferred grain orientations and related microscopic defects such as vacancies and dislocation loops in the ω-Zr, which would present strong resistance to plastic flow in the high-pressure phase of zirconium. Our finding unveils a new route for the materials strengthening and is expects to provide new prospects for the understanding of the mechanisms underlying the phase-transition driving plasticity and ductility.

This work was conducted by scientists of Los Alamos National Laboratory at beamline X-17B2 of National Synchrotron Light Source, Brookhaven National Laboratory and has been published in *Applied Physics Letters* (Y. Zhao and J. Zhang, Vol. 91, 201907-1-3, 2007).

High-pressure, temperature deformation experiments using the *in-situ* x-ray facility at X17B at NSLS S. Karato, Yale.

We have conducted a series of deformation experiments on minerals in the Earth's deep interior under high-pressure and temperature conditions. The experimental studies involve three components: (1) development of a new type of deformation apparatus, (2) applications of x-ray facilities at X-17B at NSLS, and (3) the development of a theoretical model to interpret x-ray diffraction data.

In 2004, we started this series of work in collaboration with Don Weidner's group at Stony Brook University who has developed all the x-ray facilities needed for this work. In this study, we apply differential stress to a sample under high-pressure and temperature using a newly designed apparatus (RDA (rotational Drickamer apparatus)), and measure stress and strain using *in-situ* x-ray facility at NSLS. The new theory is used to interpret x-ray diffraction data in terms of stress level and its distribution. The maximum pressure and temperature range explored so far is P to ~22 GPa and T to ~2200 K. Using this technique, we have determined (1) the pressure dependence of creep strength of water-free olivine to P~10 GPa and T~1900 K, (2) obtained the creep strength data for wadsleyite and ringwoodite (to P~22 GPa, T~2200 K). These results help understand the stability of the deep continental roots, the energy dissipation associated with deep slab deformation.

Simultaneous Ultrasonic Interferometry and X-radiation Measurements at X17B2 of NSLS to 20 GPa 1773K Baosheng Li

Ultrasonic Group of Mineral Physics Institute at Stony Brook University

We have developed techniques to conduct simultaneous ultrasonic interferometry, X-ray diffraction and X-ray imaging measurement on solid and liquids at high pressure and high temperature. A series of experiments on minerals relevant to the Earth's deep interior as well as other functional materials under high-pressure and temperature have been performed and unprecedented data have been obtained. It is worth noting that similar techniques implemented at other synchrotron facilities around the world have all used X17B2/NSLS as a model experimental set-up. The greatest advantage of the current setup is that a combined analysis of the ultrasonic velocity and X-ray diffraction data on crystalline materials provides a unique means to determine the thermalelasticity with a direct determination of pressure using the sample itself. These techniques can also be applied to (1) reliably determine the density equation of state for glass/amorphous materials through the measurements of ultrasonic velocities with direct sample length measurements (e.g., see data on ZrW_2O_8 published in ***Appl. Phys. Lett***. 93, 191904, 2008, doi:10.1063/1.3023049), (2) establish absolute pressure scales, and (3) conduct in-situ investigation on time-dependent processes such as phase transformation and melting. The newest development has enabled us to conduct these measurements up to 20 GPa in pressure and 1773 K in temperature.

Summary of Beamtime Usage

Total number of users, including assistants, but not beamline staff: 53
Total number of days of beam available:
Total number of days of beam used: 79.13
Total number of runs: 155
Number of PI's granted beamtime: 27 (see table, below)

PI	PI Institution	Proposal	Dates scheduled	actual
Botez, Cristian	UT El Paso	15098-Temperature-resolved HP studies of the superprotonic phase transition in the fully-hydrogen-bonded solid acid RbH_2PO_4	2/25-27	2/25-26 (1.15 days)
Burnley, Pamela	UNLV	16382-In-situ X-ray diffraction study of quartz deformation using the D-DIA apparatus	2/13-2/15	3/25-27 (2.08 days) 9/11`-13 (2.06 days)
Bystricky, Michal	Universite Paul Sabatier	11672-Rheology of polyphase mineral aggregates at mantle (P,T) conditions	4/2-5; 10/5-9	4/2-4/4 (1.62 days) 10/5-9 (4.08 days)
Bystricky, Michal	Universite Paul Sabatier	16426-Rheology of polyphase olivine-enstatite aggregates at mantle (P,T) conditions	10/4-9	10/5-9 (4.08 days)
Dai, Lidong	USB from China	16145-Electrical conductivity of quartz crystal and its polymorph at HT&P	7/27-30	
Dobson, David	UCL	17043-Thermal diffusivity of perovskite – post-perovskite analogues	10/19-22	10/19-22 (1.28 days)
Durham, William	MIT	14080-High-temperature, low stress creep rheology of olivine-righ rocks	4/7-12; 7/22-26; 11/1-5	2/18-21; (3.67 days) 4/6-4/14 (7.83 days) 7/22-25; (3.25 days) 11/1-5 (3.96 days)
Girard, Jennifer	FIU	14986-Determination of the water effect on the olivine plasticity at upper-mantle conditions	2/10-12; 6/1-4 (moved to ?); 10/9-11; 10/12-13	2/9-15 (6.09 days) 10/9-13 (2.90 days)

Gwanmesia, Gabriel	DSU	11608-Elasticy of pyrope-almandine-grossular garnet solid solution series at HP&T using ultrasonic interferometry in conjunction with synchrotron radiation	6/29-7/2	6/29-7/2 (2.95 days)
Holyoke, Calib	Texas A&M	14229-Dislocation creep of orthopyroxene aggregates	2/12-2/15; 6/4-8; 10/13-16	6/4-6/14 (7.62 days) 10/13-16 (2.08 days)
Hunt, Simon	UCL	16244-Rheology and the development of crystallographic texture and seismic anisotropy in hollandite-structured $KAlSi_3O_8$	8/5-8	6/28-29 (1.0 day); 8/5-8 (3.03 days) 9/2-5 (2.87 days)
Karato, Shun	Yale	13156,15413-Plastic deformation and deformation microstructure of transition zone minerals	4/27-5/3, 11/19-23	4/27-28 (6.96 days) 11/19-23
Li, Baosheng	USB	14168-Sound velocity measurements on metals at HP&T	3/12-15; 3/16-17	3/14-17 (2.52 days)
Li, Li	USB	14739-Attenuation of materials at HP&T	7/14-17	7/14-17 (3.06 days)
Lin, Zhijun	LANL	15555-Hith P-T and large volume study of inorganic-organic hybrid compounds with nearly zero thermal expansion	3/6-8	
Liu, Wei	USB	14198-Elasticity across the OEN to HP-CEN phase transformation for orthoenstatite	3/11-3/12; 10/30-11/1	3/11-14 (3.29 days) 3/18-22 (4.36 days) 10/30-11/1 (2.3 days)
Liu, Xi	U. Peking	15650-Elasticity study on the CAS phase up to lower mantle conditions	3/20-3/22	
Long, Hongbo	USB	15739-Deformation of garnet at HP&T	4/7-4/9	2/18-21 (3.67 days) 9/5-11 (5.87 days)
McCormack, Richard	UCL (student)	16450-Deformation systematic of perovskite and	10/16-18	10/16-18 (2.08 days)

		post-perovskite analogues		
Petrykin, Valeriy	J. Heyrovsky Inst. (Chech)	16216-Search for new multicomponent sulfide materials using combination of solution and HP syntheses	none	
Qian, Jiang	US Synthetics	14728-Melting of brazing filler metal (Palcusil) under high pressure	3/27-29 (declined)	3/27-3/29 (1.42 days)
Raterron, Paul	CNRS, Lille	16321-Investigation of upper-mantle rheology: HP experiments and micromechanical modeling	6/10-14 (declined)	
Tsakalakos, Thomas	Rutgers	16833-Thermokinetic origins of sintering in nanocrystalline materials by in-situ HP&T synchrotron energy dispersive . . .	11/6-8 (transferred from X17B1)	11/5-7 (2.18 days)
Whitaker, Matthew	Ehime U., Japan	16290-Acoustic velocities and thermoelastic properties of iron/light-element alloys at HP&T	7/17-19; 7/20-22	7/18-22 (3.71 days)
Woerner, William	USB (student)	16464-HP synthesis of oxynitride photocatalysts	8/17-19	8/8-11 (2.97 days)
Woerner, William	USB (student)	15707-Synthesis of Zn)-rich $(Ga_{1-x}Zn_x)(N_{1-x}O_x)$ photocatalysts: i=an *in situ* study at HP&T	3/30-4/1	3/30-4/2 (1.89 days)
Xu, Hongwu	LANL	15723-High P/T synchrotron –ray diffraction study of ankerite and kutnahorite	2/27-3/3;6/15-17; 10/22-25	2/26-3/2 (4.23 days) 3/22-23 (0.28 days) 10/22-28 (4.39 days)
Xu, Jianmei	China U of Geosciences	15671-Elastic property of lherzolite from North China Craton under HP&T	3/17-20; 10/28-30	10/28-30 (1.75 days)
Yu, Xiaohui	LANL	16350-Stress and strain measurements of nano diamond, diamond/MWCNT and diamond/SiC/WMCNT composite under HP&T	6/17-22	6/15-23 (7.9 days)
Yu, Xiaohui	LANL	15422-Carbon nanotube reinforced metal/veramics with improved mechanical, electrical, and thermal properties	3/2-5	cancelled

Weidner	USB	D-Tcup on monochromatic side station commissioning (done in conjunction with other experiments)	2/21-25 (2.79 days) 3/17-25 1.14 days) 4/2-4/14 (4.4 days) 6/16 (0.21 days) 8/5 (0.05 days)

Publications for X17B2 (2009 and 2010 reviewed articles)

Kawazoe, T., S. Karato, J. Ando, Z. Jing, K. Otsuka, and J. W. Hustoft (2010), Shear deformation of polycrystalline wadsleyite up to 2100 K at 14–17 GPa using a rotational Drickamer apparatus (RDA), J. Geophys. Res., 115, B08208, doi:10.1029/2009JB007096.

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B.4 West Coast Synchrotron Facilities

[PIs: Raymond Jeanloz and Simon Clark, University of California at Berkeley]

Annual (2009-2010) Report to COMPRES from Beamline 12.2.2 of the Advanced Light Source at LBNL

Q. Williams, COMPRES PI

(6/10 to present)

Summary

The last five months have seen dramatic advances in the performance, reliability and robustness of the laser-heating setup at 12.2.2; major advances in resistive heating capabilities have been made; the publication rate of 12.2.2 remains healthy; applications for beamtime are up; and user satisfaction appears to be high. New and highly anticipated infrastructure is either on site or on order: these include a new laser milling system, purchased through stimulus funds to COMPRES (on site); the availability of a new Bruker P200 CCD detector (on site, supplied by the ALS); and a gas-loading apparatus (on order, supplied by the ALS).

In short, although the year has been a turbulent one for the facility (and particularly for the staff) with changes in the COMPRES management, the ALS staffing for the beamline, and the prioritizations associated with the beamline, the current status and trajectory of the beamline and its associated infrastructure are all extremely positive. Our plan for the coming year is to build on the successes of the last year and gain experience with our enhanced infrastructure, as well as evaluate possible new initiatives as they emerge. The successes on which we plan to build include continuing improvements to the laser-heating system (which are progressively evolving towards fine-tuning) and further developing and refining our external resistive-heating capabilities (for which a new P/T record for such experiments was recently set at the ALS). Moreover, the capabilities at ALS in the domain of radial diffraction at high pressures are at the cutting-edge of current capabilities, and we (obviously) plan to continue this as a primary area of emphasis. Possible new initiatives include the development of high-P single-crystal diffraction capabilities, and increasing the multi-beamline nature of the high-pressure effort at ALS. In this last respect, a few users have taken highly effective advantage of both the BL 12.2.2 High Pressure beamline and 12.3.2, the microdiffraction beamline spearheaded by Kunz and Tamura. We fully expect the synergies between these beamlines to increase with time as users become increasingly aware of the highly complementary capabilities of these two beamlines.

Introduction:

The high-pressure operation at beamline 12.2.2 of the Advanced Light Source has made dramatic strides in the capabilities and user-friendliness of its facilities during the second half of 2010. These improvements have involved a systemic change in how business is conducted in the high-pressure operation at the ALS. Briefly, tasks that need to be conducted, improvements that need to be made, and user support assignments for the staff are identified, plans and timeframes for tasks/changes are agreed upon by all principals, and are then sequentially tracked on a weekly basis until they are accomplished. User feedback is critically important in this process: all difficulties, complaints (which have grown markedly scarcer) and recommendations are recorded and discussed, followed by a plan for improvement and a sequence of tasks being devised. As a result, the size of the task list is extensive, and varies from (for example) “find and purchase a new dichroic optic with these specs” and “label drawers and organize tools in the sample prep area” to “design and construct a slide that will mount and translate three detectors in-and-out of the x-ray beam completely reproducibly within the spatial limitations of the hutch” and “design lower thermal expansion replacements for the legs on the upper optical table, get them made, and then replace them.” Obviously, we will not describe each task in this report (which span the gamut from hardware to software to beamline organization to the website), but highlights will be emphasized. The primary message is simple: a highly systematic (and universally agreed upon) approach is taken with respect to all issues of beamline maintenance, possible improvements, user support and user feedback.

This is also an extremely exciting time in high-pressure science at the ALS. Dramatic new temperature-pressure records have been established by our external heating enterprise; and a large influx of new infrastructure is coming on-line (a new detector, a gas-loading apparatus, and a laser-mill). In short, the overarching goal of the ALS high-pressure effort to provide state-of-the-art facilities coupled with superb support for the user community is completely on-track.

The Changes:

So that all readers of this report are fully aware of the changes that took place over the last year, we provide a brief synopsis here. The changes were induced by a Report by the COMPRES Facilities Committee on the COMPRES-funded effort at the ALS, produced in conjunction with a site visit in December, 2009, and including extensive interviews with users, staff and the PI’s associated with the high-pressure effort at the ALS. The Report recommended that the COMPRES management of the beamline be changed; and, ALS management recognized in turn the need for a change in the configuration of ALS staffing at the beamline as well.

1) COMPRES Management: The PI-ship of the COMPRES effort at the ALS moved from S. Clark and R. Jeanloz at UCB to Q. Williams at UCSC, effective 6/1/10. The employment of COMPRES beamline support scientists moved from UCB Earth and Planetary Sciences to the UCSC Institute of Geophysics and Planetary Physics on this date, including visa transfers, creation of new positions, waivers

of recruitment, benefits transfers, etc. This transfer occurred while COMPRES headquarters was also moving (on the same day) from Stony Brook to Illinois, which produced a supplementary degree of complexity associated with NSF's difficulties in conducting the COMPRES transfer. As an informational note, while the inter-UC transfer was perhaps somewhat easier than a transfer between two entirely disconnected institutions, it was still (probably inevitably) a very time-consuming and bureaucratic process. For example, because of the timeframe and complexity of portions of the transfer (COMPRES funding ultimately arrived at UCSC in the last week of June—literally, the day before paychecks had to be cut--after the employments initiated on the first of June), special dispensations and approvals rose to the levels of both the Dean of Physical and Biological Sciences and the Vice Chancellor for Research at UCSC.

2) COMPRES Staff: Three staff members were on-site (Bin Chen, Selva Vennila Raju, and Jinyuan Yan) at the end of FY 09-10. COMPRES Central had funded two employees at the ALS, but three employees were hired using carry-forward funds derived from a period when the COMPRES staff positions were vacant (from the departures of Kunz and Caldwell). We understand that the carry-forward funds ran out on ca. 6/1/10. At this point, Howard Padmore, the head of the Experimental Systems Group at the ALS (under whose aegis 12.2.2 falls), who recognized the importance of the external heating effort at the 12.2.2, funded Vennila Raju for a six month span (6/1/10-12/31/10) out of ALS funds via a subcontract to UCSC.

3) ALS Staff: Jason Knight, who plays a primary technical role in the beamline, moved from 50% to 100% time in support of high pressures at 12.2.2 as of 6/1/10. Alastair MacDowell, who is a highly experienced beamline manager, now oversees the 12.2.2 high-pressure effort on behalf of the ALS. As of roughly 7/10/10 (the hiring date of his replacement on the ALS tomography beamline), he is (formally) 33% time at 12.2.2 (given the initial demands associated with the high-pressure operation, his informal effort at the beamline has been substantially larger—for example, his involvement in beamline planning and task recognition, development and assignment initiated well prior to June 1). Simon Clark does work at 12.2.2 that is in support of non-COMPRES-related studies (primarily materials science) and is spearheading the nascent high-pressure single-crystal diffraction initiative in collaboration/consultation with P. Dera and O. Tschauner.

4) Experimental Infrastructure: The Brillouin spectroscopy system that had been purchased several years ago from non-COMPRES funds by Prof. Jeanloz and installed in the high-pressure sample preparation laboratory at the ALS was shipped (at ALS's considerable expense) back to a laboratory in UCB's Dept. of Earth and Planetary Sciences. The COMPRES Facilities Committee report was highly critical of the role of this instrument in the ALS/COMPRES enterprise, it consumed significant COMPRES staff time, and it also occupied space needed for the tandem additions of the computer-controlled laser mill and the gas loading

apparatus. Hence, it was removed in June, immediately following the completion of data collection for Arianna Gleason's UCB Ph.D. thesis.

The Laser-Heating System:

The importance of establishing the ALS as a reliable and world-class high-pressure laser-heating facility was forcefully emphasized both in the CALIPSO (California High Pressure Observatory) external review committee report of January, 2007 (a committee convened by Jeanloz and Clark) and by the COMPRES Facilities Committee Report of January, 2010. Hence, the primary focus of the ALS and COMPRES staff since the change in management has been on improving the laser-heating setup.

The utility of the laser-heating system as of the start of the year was succinctly and accurately described in the latter committee's report:

> "Groups very experienced with this beamline and laser heating system report success in laser heating and x-ray imaging after 2-3 days of setup time for the laser heating system. Users expressed frustration that it is not always possible to schedule beamtime immediately after a shutdown, requiring that beamtime be spent on rebuilding of the system for laser heating experiments. Groups with less direct experience with the beamline (but ample laser-heating experience) or with less time available, report less success, often not able to collect any useful data."

Indeed, experienced users typically expected to arrive and completely realign the system from scratch, since non-systematic readjustments/realignments of the system by both users and probably staff had the cumulative effect of misaligning the system. Indeed, users routinely readjusted the system in ways that were not tracked (or trackable), and which were not guided by any principle other than adjusting a subset of the optics to improve their experimental throughput.

The new ALS staffing has, in conjunction with COMPRES personnel conducted a sequence of tasks (some of which are ongoing) that are oriented towards (1) making the system consistently reliable and user-friendly; and (2) improving the optics and software of the system so that (for example) temperature gradients are reduced and characterized. Notably, the COMPRES Facilities Committee report indicated that the laser-heating system should be reliable and user-friendly by June of 2010—we believe we have recently reached that point. In this context, it is critical to note that the transition to new management/staffing did not occur until June 1, 2010, which is when a highly systematic approach to debugging, retooling and (where necessary) repairing the system initiated. The short-term goals have hence been ensuring that the system is always aligned, or when disaligned that the misalignment can be instantly recognized and rectified; and ensuring that the system is mechanically stable. The new alignment philosophy associated with the laser-heating optical system (Fig. 1) is simple: the beam should go through (or reflect off of) the center of each optic, and each corner-turn in the optical system should be at a 90° angle. With these straightforward design principles, misalignment of an individual optical component is now easy to detect and rectify at the source of the misalignment; that is, we now avoid the situation where other portions of the optics are misaligned to compensate for a problem originating elsewhere in the optical system.

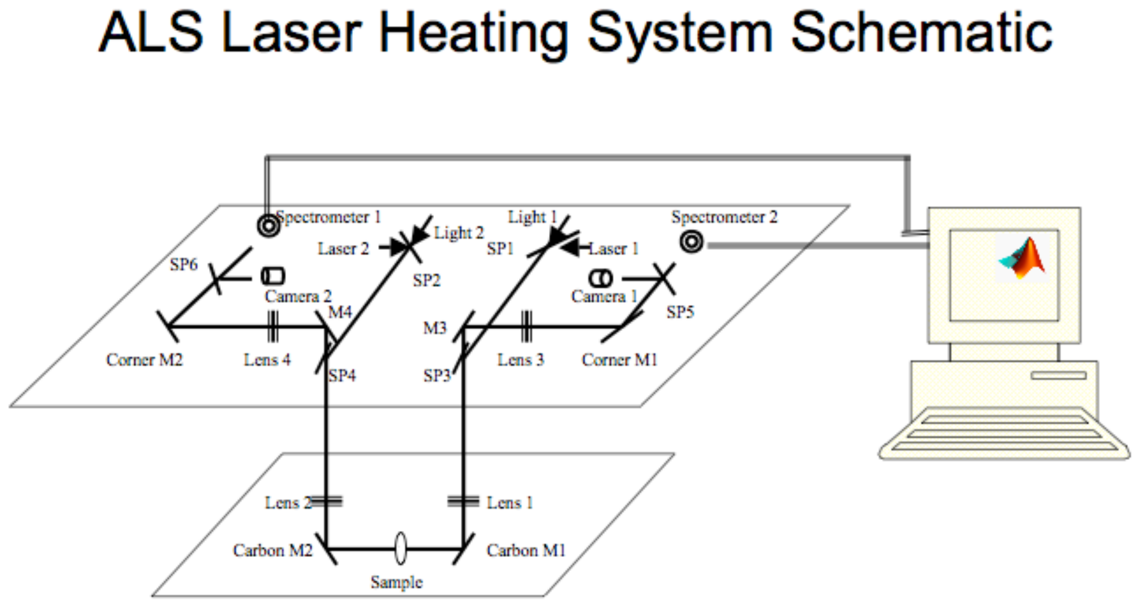


Figure 1. Schematic of the Laser-heating optical system at the ALS, with mirrors, splitters and lenses labeled; for reference, the bulk of the optics sit on an upper table in the hutch, with the sample and carbon mirrors lying above a lower table (on which the upper table is mounted.

The software associated with the laser-heating system has undergone progressive modifications, both by the beamline-associated staff and in-house programmers at the ALS. The goal here is to simply ensure that the software rapidly collects and reports data in a manner that is rapid, user-friendly and has easy access to all possible information that users might want/need. A sample screeenshot of lateral variations in temperature distribution is shown in Figure 2 – the software has been notably improved in the last several months, but is (in response to users' suggestions) under continual development.

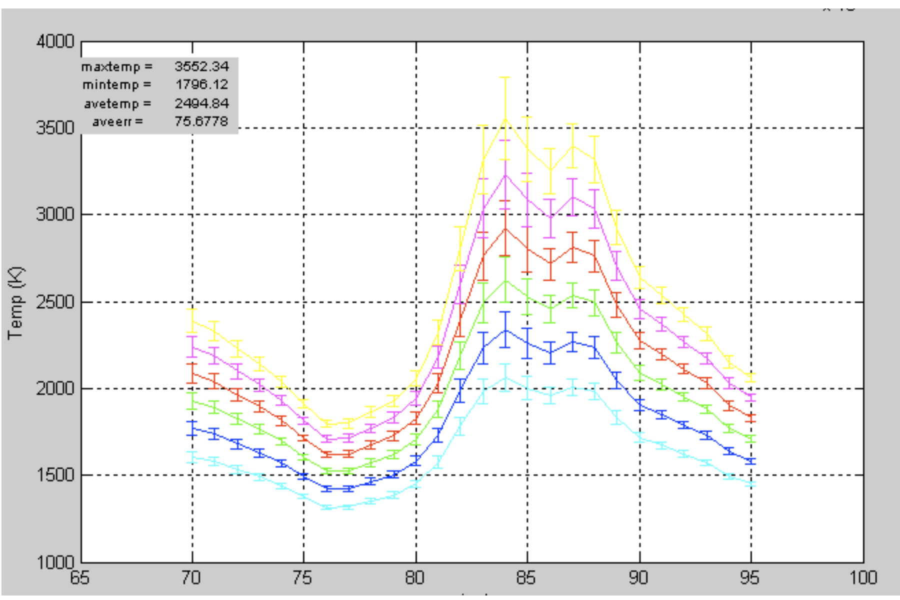


Figure 2. Screenshot of temperature gradients across a heated spot. Horizontal axis is pixel number. Increase in amplitude between 70 and 75 pixels is associated with minimal thermal emission from the sample.

With respect to mechanical stability of the system, the most involved change has been to replace the legs that hold up the upper table (on which most of the laser-heating system sits: Fig. 1). These hollow aluminum legs expanded and contracted with temperature variations in the hutch (causing sample movement of up to ~40 microns over the course of an experiment—these fluctuations were particularly extreme when the AC flipped off). These spatial variations seem to have been the cause of many prior user complaints about lack of collocation between the x-ray beam and the laser-heated spot. Other spatial variations were due to inconsistent optical alignment practices due to the wide range of people carrying out optical alignments – i.e., it helps if the optics are bolted down.

Thus, new, thicker-walled steel legs were made, filled with epoxy cement (for its thermal mass and vibration damping characteristics) , and reinstalled---replacing the legs was not a small operation, and required a couple of days of commissioning time. Since this replacement was made, the sample motion produced by temperature fluctuations has vastly decreased (~2 microns appears to be a typical deflection at this point). In addition to this change, many of the optics mounts in the system have been replaced so as to ensure that the optics are absolutely rigidly held; and, as needed, a number of optics have been replaced. Indeed, upgrading of the optical system continues, with (for example) plans to acquire specialized dichroic optics that will improve both the throughput and spectral characteristics of the thermal radiation transmitted through the system. At the same time, improved sample imaging has been a priority—again, for example, software is in the process of being written that will correlate x-ray position determination from x-ray mapping of the sample with visual imaging of the sample from GigE cameras whose acquisition is planned in the coming year.

The 4-color temperature measurement system (with which, at its initial deployment of ~10 months ago, there were some technical difficulties) has been moved off-line during this period of retooling and reconfiguring the basic laser-heating system. We are prioritizing a return to the 4-color system over the next few months (which will quite possibly run into the next fiscal year), as we fully expect that this will be a valuable complementary temperature measurement system.

We have also been engaged in characterizing new optical components for installation in conjunction with the laser-heating system. For example, pi-shapers (to flatten the peak of the beam intensity distribution and hence reduce temperature gradients) have been characterized off-line, and will likely be installed on the beamline in the coming months.

These improvements in alignment of the laser-heating system have also extended to the x-ray optics: recurrent (and justified) user complaints that gasket lines were present in experiments in which the (ca. 10 micron) x-ray beamsize should have precluded major (or any) diffraction from the gasket were recognized to be associated with misalignments/mispositionings of the x-ray beam-shaping, clean-up and guidance optics. The occasional appearance of gasket lines in experiments in which they should not occur is now treated as a symptom of misalignment, and is immediately rectified.

Net Summary: The laser-heating system has transitioned from a setup that functioned adequately for expert users (with an investment of setup time) to an apparatus that is far more in-line with what is expected from a user facility: a robust system that routinely produces data for any user.

ALS Support

The COMPRES support to the ALS enterprise helps to leverage very substantial resources from the ALS itself. These include not only the extant ALS-provided staffing (33% of Alastair MacDowell, 100% of Jason Knight), but also funding for Vennila Raju (the external heating expert at the ALS, and previously funded by COMPRES funds) from 6/1/10 to 12/31/10. Equipment purchased or accessed through ALS funding spans from a range of routine expendables at the beamline (drills, etc.) to optics (like the pi-shapers) to large-ticket items such as the gas-loading apparatus on order (ca. 180 K) and the loan of the P200 Bruker CCD (ca. 200 K). As such, the ALS high-pressure effort has had extremely robust and sizable institutional support, which in turn provides a measure of the value of the high-pressure enterprise to both the ALS and to the COMPRES user base.

The COMPRES-funded Staff

Two support personnel have been funded by COMPRES since 1/1/10 to the present: Jinyuan Yan and Bin Chen. Selva Vennila Raju was funded by COMPRES funds from 1/1/10 to 5/31/10, at which time the ALS Experimental Systems Group funded her for six months (from 6/1/10 to 12/31/10): this funding was because of her key role in developing external heating capabilities at the ALS. Each person has been engaged in a lead role for COMPRES user support: Yan is most involved in day-to-day user support at the beamline, Chen is likely to be engaged in support if laser-heating is being utilized, and

Raju is the go-to person for external heating. The staff has had emphasized to them that their jobs are, as per their job descriptions, tri-fold: user-support, research and development of capabilities on the beamline. To support their research (which can, and often is, collaborative with users), eight shifts were negotiated for usage by the staff in this last beamline cycle out of Director's Discretionary Funds. This is a direct consequence of the ALS policy that ALS staff must apply for beamtime, and was a transitional move designed to ensure that they could collect data in order to prepare competitive proposals. With respect to technique development, Yan has engaged in software development and characterization of the laser-heating system, particularly with respect to calibrations and temperature gradient measurements; Chen has been involved in off-line characterization of optical components (like the pi-shaper) for prospective installation; and Raju has been the responsible person for external heating applications (and users).

Management Details

We describe management details at some length, as major critiques of the Facilities Committee Report involved the lack of consistency in management direction and delineation of a chain-in-command at the beamline. The overarching oversight of the beamline operation is conducted by Alastair MacDowell. A weekly meeting (two hours) occurs between the COMPRES management (Williams), MacDowell, and the beamline staff, at which primary and secondary responsibility for different user groups is assigned. Contact with user groups about their needs now occurs weeks before their arrival, to make sure that the style of experiments (laser-heating, external heating, conventional diffraction, radial diffraction) that they wish to pursue has not changed since their proposal submission (a common occurrence) and that the beamline is fully prepared for their arrival. Additionally, issues arising at the beamline and a post-mortem on recent user time is discussed; if the timing works, the head user at the beamline is often asked to attend this meeting to provide their in-person advice and perspective on the beamline. Moreover, an ongoing task list has been established and updated at these meetings, which contains specific assignments spanning from the immediate to the relatively long-term (couple of months) for each beamline-affiliate. The prioritization of different tasks (and introduction of new ones) is discussed and resolved at each meeting. Ultimately, all principals agree on these assignments, priorities and tasks. Hence, we believe that the previous management problems are completely resolved: priorities are agreed upon by all principals (in conjunction with, and in the presence of, the staff), and full accord exists between the principals.

Future Directions:

While we expect a significant portion of the ALS effort over the next few months to be in the mode of continuing to enhance the performance of its laser-heating setup and ensure that we garner the expertise to take full advantage of both the new laser-milling system and the new Bruker detector that have been added to our portfolio, there has been one very major advance in capabilities and techniques on which we plan to expand. Briefly, our external heating effort achieved dramatic success with a modified Liermann-type radial diffraction cell (conducted in conjunction with the Wenk group at UCB), achieving record-setting conditions for such experiments: 40 GPa and 2000 K in an externally resistively heated cell (Figure 3). We believe that these conditions can be improved upon, and such improvements are the subject of a complementary Infrastructure Development Proposal. Hence, we view external resistive heating as a valuable and absolutely cutting-edge addition to the capabilities at the ALS—based solely on initial brief informal communications of these results, users are already expressing strong interest in these new capabilities.

28 GPa, 1300 K   40 GPa, 2000 K

Figure 3. Images of the modified Liermann cell at the ALS in radial diffraction mode during a recent high pressure, high temperature experiment. Temperatures were calibrated using Pt-Rh thermocouples, and pressures from the equation of state of iron. Image from Jane Kanitpanyacharoen (UCB).

In the longer term (beyond the few month timeframe), we expect that such external heating will be a prominent area of emphasis for 12.2.2—and the advantages presented by the prospect of simultaneous laser-heating and external resistive heating may also become important for experiments at the ALS. Indeed, the current experimental geometry is such that simultaneous laser-heating and resistive heating could be relatively straightforward to achieve, and the advantages of such an approach (including smaller temperature gradients, larger laser-heated spots and greater hot spot stabilities) may well provide the motivation necessary to make such experiments feasible (if not entirely routine) at the ALS.

A second area that has been emphasized by multiple prominent users of the ALS is the proximity and complementary character of 12.2.2 and 12.3.2—the microdiffraction beamline run by Martin Kunz (the former COMPRES staff member at 12.2.2) and Nobumichi Tamura. The scientific motivations for this interaction is simple: synthesis and high P/T characterization of samples can be conducted at 12.2.2, followed by detailed chemical and structural imaging of the quench products at 12.3.2. Indeed, results of a joint study at 12.2.2 and 12.3.2 generated one of our high-profile papers of the last year (Friedrich et al., PRL, 2010, on rhenium nitrides), and the prospect for future studies along these lines has the prospect of providing an additional valuable scientific niche for the ALS. The organization and time-scheduling procedures at the ALS render getting joint/simultaneous time on two beamlines quite feasible (with the natural caveat that the beamtime proposal is rated highly), and we hence view future closer collaborations/user interactions with 12.3.2 (and perhaps other stations around the ring) as a natural area of expansion over the next several years.

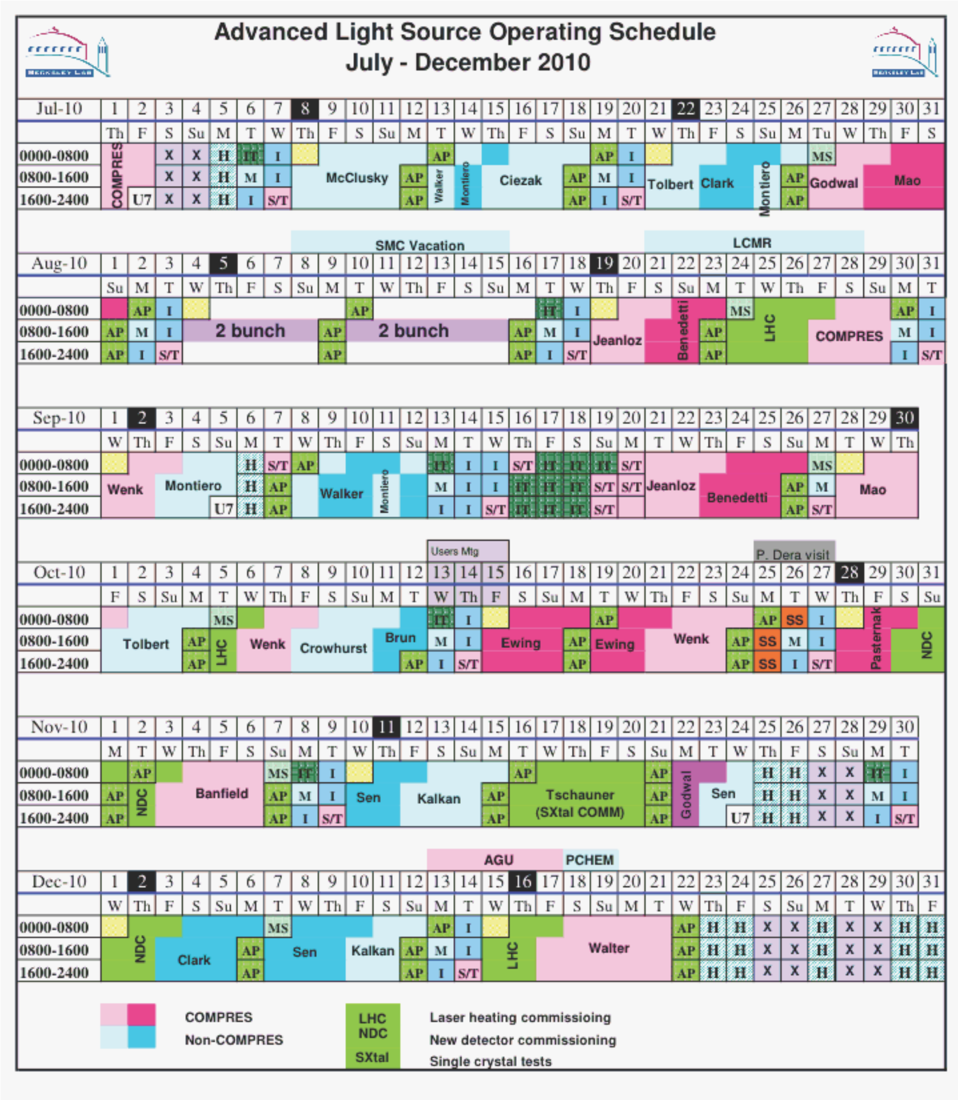
Finally, a collaborative effort between S. Clark, P. Dera (GSECARS) and O. Tschauner (UNLV) is working towards establishing high-pressure single crystal diffraction capabilities at 12.2.2. Significant commissioning time is being dedicated to this project (see Appendix 1: 14 shifts allocated in late November), and Dera will be installing his custom software that is designed to utilize a standard 2-D detector to collect single crystal diffraction data in early November at the ALS. Presuming that this effort is successful (and the analogous effort at the APS is, so there appear to be no fundamental impediments), the degree to which this effort is attractive to new and existing COMPRES users at the ALS will dictate how much COMPRES employees engage with this effort over the next year.

Output and Oversubscription

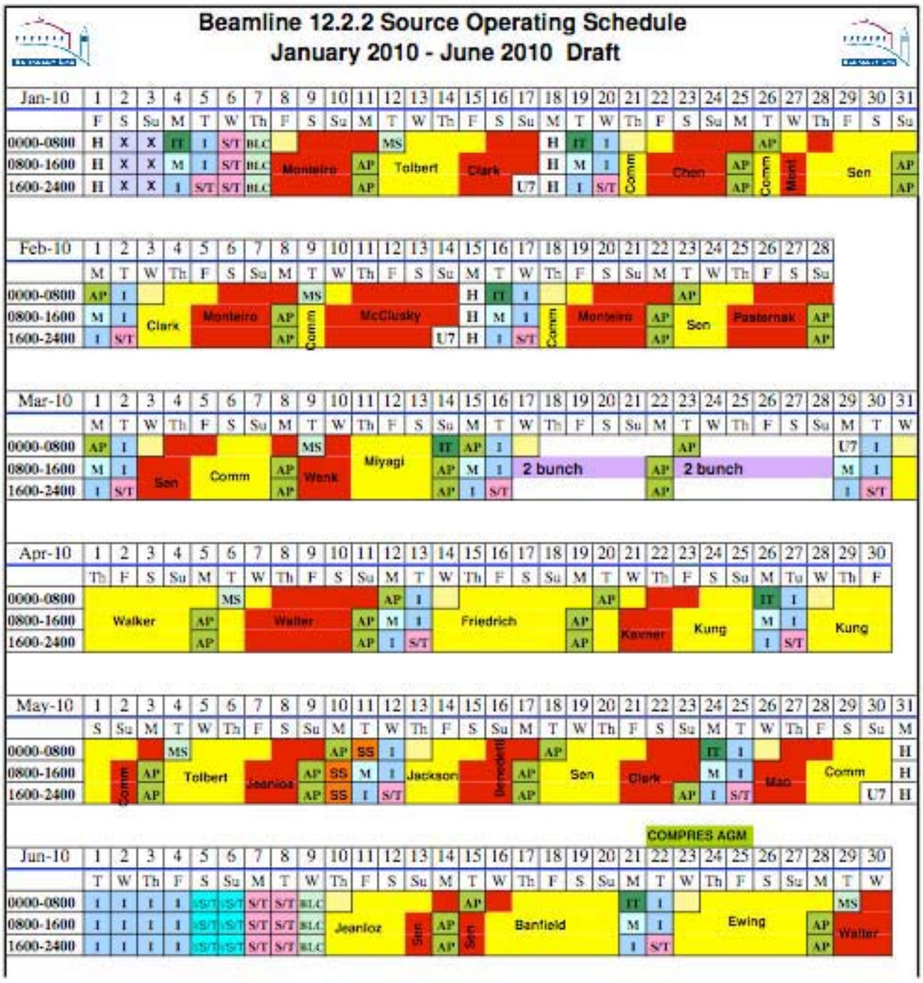
As shown in Appendix 2, the scientific output of 12.2.2 continues to be at a notably higher level than in the mid-part of the decade: 18 refereed publications (most of them by COMPRES-affiliated groups) have been published to date in calendar year 2010 (see Appendix 2), and we fully expect that this calendar year will become the most productive year in 12.2.2's history. These include a Science paper and a PRL paper.

Our oversubscription rate for the last beamtime cycle for which statistics are available (July-December 2010: the January-June 2011 cycle scheduling is undergoing final revisions as of the writing of this report) involved 657 shifts requested, when the availability was 252, for a 2.6:1 requested-to-available beamtime ratio (Appendix 3). Because the beamline was progressively becoming more user-friendly (and particularly the laser-heating apparatus), COMPRES management requested that the allocated number of shifts per group be reduced, and more groups be awarded smaller blocks of time. In effect, groups no longer should have had to use beamtime to optimize the laser-heating system. The onset of this shift in philosophy is detectable between the Jan.-June 2010 and the July-Dec. 2010 allocations (Appendix 3), and we expect that this trend should continue (and indeed be enhanced) into the future.

Ultimately, COMPRES-affiliated users received over 150 of the 252 allocated shifts or ~60% of shifts in the July-Dec. 2010 cycle, which is historically a reasonably representative value for the percentage of COMPRES user time at 12.2.2 (which typically varies from 50-70%). For reference, the last Memorandum of Understanding between COMPRES and the ALS required that the COMPRES Approved Program (AP) receives 35% of the beamtime at 12.2.2. There have been discussions of renegotiation of this MOU between COMPRES and the ALS, but such a renegotiation has not been viewed as an urgent priority at this time. For reference, there is a clear recognition within the ALS management that the COMPRES AP is unique among the AP's at the ALS, as (in contrast to all other AP's) time is only allocated through the proposal system on a competitive basis for the COMPRES PI (or PI's).



Appendix 1a: Final Schedule for Jun-Dec. 2010. COMPRES users are (for the most part) in pink or red. Note that Walker (Sept. 9-11) is a COMPRES user despite his time being blue, as is Tschauner (Nov. 16-20) despite being in green. The COMPRES slot (Aug. 27-29) was negotiated between QW and Bob Schoenlein out of Director's Discretionary Funds as seed time for COMPRES researchers' experiments so that they would be in a position to submit competitive proposals for future beamtime. The different shades of pink for COMPRES are solely so that juxtaposed COMPRES beamtimes can be distinguished from one another. User time was somewhat reduced during this period due to the need to have commissioning time for the Laser Heating system and for the new Bruker P200 CCD detector.



Appendix 1b. Schedule for Jan-Jun 2010. Despite the “Draft” label, this is (with the exception of one-for-one timeswaps between users) essentially the final schedule. In this case, colors are only meant to distinguish one group’s beamline from another.

Appendix 2.
12.2.2 -- 2010 Publications in the ALS Data Base through 10/24/10 and graph of long-term publication rates, COMPRES user publications denoted by C-

C- Al-Khatatbeh, Y., K.K.M. Lee, and B. Kiefer, "Phase relations and hardness trends of ZrO_2 phases at high pressure ," Physical Review B: Condensed Matter and Materials Physics 81(21), 214102 (2010). (12.2.2)

C- Armentrout, M.M., and A. Kavner, "Incompressibility of osmium metal at high pressures and temperatures," Journal of Applied Physics 107(9), 093528 (2010). (12.2.2)

C- Chen, Bin, A.E. Gleason, J.Y. Yan, K.J. Koski, Simon Clark, and Raymond Jeanloz, "Elasticity, strength, and refractive index of argon at high pressures," Physical Review B: Condensed Matter and Materials Physics 81, 144110 (2010). (12.2.2)

C- Friedrich, A., B. Winkler, L. Bayarjargal, E.A. Juarez-Arellano, W. Morgenroth, J. Biehler, F. Schroeder, J. Yan, and S.M. Clark, "In situ observation of the reaction of tantalum with nitrogen in a laser heated diamond anvil cell," Journal of Alloys and Compounds 502, 5-12 (2010). (12.2.2)

C- Friedrich, A., B. Winkler, L. Bayarjargal, W. Morgenroth, E.A. Juarez-Arellano, V. Milman, K. Refson, M. Kunz, and K. Chen, "Novel Rhenium Nitrides," Physical Review Letters , 105(8):085504 (2010). (12.2.2,12.3.2)

C- Godwal, B.K., S. Speziale, S.M. Clark, J. Yan, and R. Jeanloz, "High pressure equation of state studies using methanol-ethanol-water and argon as pressure media," Journal of Physics and Chemistry of Solids 71, 1059-1064 (2010). [Proceedings of study of matter at extreme conditions, 2009, (Miami, FL, 3/28/2009-4/2/2009)](12.2.2)

C- Godwal, B.K., S. Speziale, M. Voltolini, R. Wenk, and R. Jeanloz, "Postcotunnite phase of the intermetallic compound $AuIn_2$ at high pressure," Physical Review B: Condensed Matter and Materials Physics . (12.2.2)

C- Grocholski, B., S. Speziale, and R. Jeanloz, "Equation of state, phase stability, and amorphization of SnI_4 at high pressure and temperature," Physical Review B: Condensed Matter and Materials Physics 81, 094101 (2010). (12.2.2)

Hanna, G.J., and M.D. McCluskey, "Equation of state and refractive index of argon at high pressure by confocal microscopy," Physical Review B: Condensed Matter and Materials Physics 81(13), 132104 (2010). (12.2.2)

C- Hou, Dongbin., Yanzhang Ma, Jianguo. Du, Jinyuan. Yan, Cheng. Ji, and Hongyang Zhu, "High pressure X-ray diffraction study of ReS_2," Journal of Physics and Chemistry of Solids, 71, 1571-1575 (2010) . (12.2.2)

C- Juarez-Arellano, E.A., B. Winkler, L. Bayarjargal, A. Friedrich, V. Milman, D.R. Kammler, S.M. Clark, J. Yan, M. Koch-Müller, F. Schröder, and M. Avalos-Borja, "Formation of scandium carbides and scandium oxycarbide from the elements at high-(P,T) conditions," Journal of Solid State Chemistry 183, 975-983 (2010). (12.2.2)

C- Lord, O.T., M.J. Walter, D.P. Dobson, L. Armstrong, S.M. Clark, and A. Kleppe, "The FeSi phase diagram to 150 GPa," Journal of Geophysical Research-Solid Earth 115, B06208 (2010). (12.2.2)

C- Miyagi, L., W. Kanitpanyacharoen, P. Kaercher, K.K.M. Lee, and H.R. Wenk, "Slip Systems in $MgSiO_3$ Post-Perovskite: Implications for D " Anisotropy," Science 329(5999), 1639 (2010). (12.2.2)

Oh, J.E., P.J. Monteiro, S.S. Jun, S.S. Choi, and S.M. Clark, "The evolution of strength and crystalline phases for alkali activated ground blast furnace slag and fly ash based geopolymers ," Cement and Concrete Research 40(2), 189-196 (2010). (12.2.2)

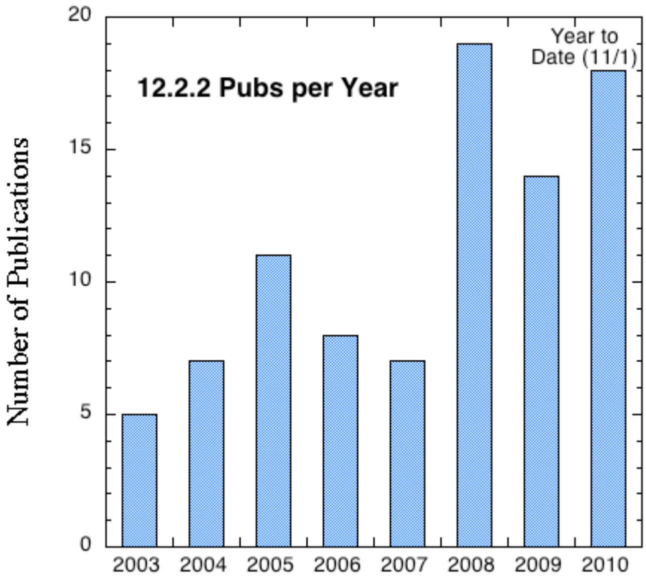
Veprek, S., S.M. Clark, and S.G. Prilliman, "Elastic moduli of nc-TiN/a-Si_3N_4 nanocomposites: Compressible, yet superhard ," Journal of Physics and Chemistry of Solids 71(8), 1175-1178 (2010). [Proceedings of Study of Matter at Extreme Conditions, (Miami, Florida, 3/28/09-4/2/09)](12.2.2)

C- Wicks, J.K., J.M. Jackson, and W. Sturhahn, "Very low sound velocities in iron-rich (Mg,Fe)O: Implications for the core-mantle boundary region," Geophysical Research Letters, 37, L15304, doi:10.1029/2010GL043689 (2010) (12.2.2)

C- Yan, J., J. Knight, M. Kunz, S.V. Raju, B. Chen, A.E. Gleason, B.K. Godwal, Z. Geballe, R. Jeanloz, and S.M. Clark, "Characterization of X-ray diffraction of beamline 12.2.2 at the Advanced Light Source," Journal of Physics and Chemistry of Solids 71, 1179-1182 (2010). [Proceedings of study of matter at extreme conditions 2009, (Miami, Fl, 3/28/2009-4/2/2009)](12.2.2)

C- Zhuravlev, K.K., J.M. Jackson, A.S. Wolf, J.K. Wicks, J. Yan, and S.M. Clark, "Isothermal Compression behavior of (Mg,Fe)O using neon as a pressure medium," Physics and Chemistry of Minerals 37(7), 465 -474 (2010). (12.2.2)

Theses:
Gleason, A.E., "Elasticity of Materials at High Pressure," Ph.D. thesis, University of California, Berkeley, CA, 2010, Advisor Raymond Jeanloz.(12.2.2)



Appendix 2, Figure A. Refereed publications for beamline 12.2.2 in the ALS database since 2003.

Appendix 3. User Applications for the June-Dec. 2010 Beamline Cycle (Not for Distribution Beyond COMPRES Committees)

ALS Shifts Allocation (July 2010 – December 2010)

C	GU	Investigator	Title	BL	Shf Req	Alternate Beamlines	Other Beamlines
12		Wenk, H	Simultaneous high-pressure and ?temperature investigation of texture development in polycrystalline $MgSiO_3$ perovskite	12.2.2	12		
	15	Kalkan, B	Is there really a polyamorphic phase transition in SnI_4?	12.2.2	15		
27		Walter, M	Water in the Deep Earth	12.2.2	15		
45		Ewing, R	Phase Transitions Induced by Simultaneous Exposure to Relativistic Ion Beams and High Pressure	12.2.2	18		
	24	Ciezak, J	High-Pressure Crystallographic Analysis of Nitrogen/hydrogen mixtures	12.2.2	9		
	42	Tolbert, S	High pressure studies of ultra-incompressible, superhard metal borides	12.2.2	18		
	51	Crowhurst, J	In situ x-ray diffraction study of the decomposition products of a high nitrogen content precursor	12.2.2	9		
	72	Sen, S	Pressure and temperature induced structural and topological changes in molecular chalcogenide glasses	12.2.2	20	21	
54		Wenk, H	Investigation of Texture Memory and Variant Selection during Phase Transformations in Uranium	12.2.2	9		
72		Paz-Pasternak, M	Search for a Mott-Hubbard transition in NiO, NiI_2 and $NiCl_2$	12.2.2	21	18	
	90	Weinberger, M	In situ high pressure X-ray diffraction of new green energetic materials	12.2.2	18		
90		Walker, D	X-ray Absorption Contrast Images of Binary Chemical Reactions	12.2.2	21	18	
105		Mao, W	Structural studies of 3d transition metal compounds at high pressure	12.2.2	48	~~18~~ 15	
120		Benedetti, L	Melting curve of graphite from ambient pressure to ten gigapascals	12.2.2	18	15	
135		Jeanloz, R	Platinum and iron phase boundaries in the laser heated diamond anvil cell	12.2.2	27	15	
	105	Friedrich, A	Formation and structure of binary transition metal carbides, -nitrides, and -borides at extreme-(P,T) conditions	12.2.2	18	15	
147		Banfield, J	Determining interfacial free energy of iron oxyhydroxide nanoparticles in various surface environments using synchrotron X-ray diffraction	12.2.2	21	Alternate Beamline 1: 11.3.1 for Beamline: 12.2.2 Shifts Req: 21 Entire Prog: 12	
		McCluskey, M	X-ray diffraction of ZnO, MgZnO, and CdZnO under pressure	12.2.2	12		
		Godwal, B	High-Pressure Elasticity and Stability of Osmium: An Analog for Iron in Earth's Core	12.2.2	12	Alternate Beamline 1: 9.0.1 Shifts for Cycle: 12 Shifts for Entire Program:	

ALS Shifts Allocation (July 2010 – December 2010)

	Investigator	Title	BL		Shf Req		Alternate Beamlines	Other Beamlines
	Godwal, B	Angle Dispersive X-ray Diffraction Studies on GaCMn3 under High Pressure	12.2.2		12			
	Monteiro, P	Effect of pressure on the structure of calcium silicate hydrates	12.2.2		25			
	Godwal, B	High pressure high temperature Angle dispersive X-ray diffraction (ADXRD) studies on Intermetallic Compound Auln2.	12.2.2		9			
	Raju, S	Study of thermal equation of state of Dilute magnetic semiconductors	12.2.2		21			
	Kung, J	Searching perovskite to post perovskite transition in (Ca,Sr)SnO3 at high pressure and high temperature	12.2.2		18			
	Chen, B	Elasticity and Structural Stability of Natural and Commercial Silicate Glasses at High Pressures	12.2.2		12			
	Gleason, A	The fate of iron-hydroxides at very high densities; structural and spectroscopic studies of goethite (FeOOH) and jarosite KFe3(OH)6(SO4)2.	12.2.2		21			
	Geballe, Z	Wet vs. dry post-spinel transition in resistive and laser heated diamond anvil cells	12.2.2		15		Alternate Beamline 1: 1.4.4 Shifts for Cycle: 9 Shifts for Entire Program:	1.4.3
	Lipinska-Kalita, K	Hybrid Glass*]Nanocrystal Composites at High*]Pressures	12.2.2		32			
	Crowhurst, J	In situ x-ray diffraction study of novel uranium compounds formed under extreme conditions of pressure and temperature	12.2.2		3			
	Braun, A	Influence of mechanical pressure on the proton conductivity of the Y-substituted barium zirconate proton conductor at elevated temperatures	12.2.2		15			
	Monteiro, P	Effect of pressure on the crystal structure of organic/inorganic Calcium Silicate Hydrates nanocomposites	12.2.2		8			
	Godwal, B	High pressure high temperature Angle dispersive X-ray diffraction (ADXRD) studies on Intermetallic Compound Auln2.	12.2.2		12		Alternate Beamline 1: 9.0.1 Shifts for Cycle: 12 Shifts for Entire Program:	
	Lee, K	Solidus Determination of Hydrous Pyrolite at Lower Mantle Conditions	12.2.2		16			1.4.3
	Godwal, B	High Pressure High Temperature X-ray Diffraction and melting Curve Studies on Osmium	12.2.2		9			
	Manghnani, M	Melting relationships and density of Fe-Ni based alloys and melts at high P-T: Implications for the Earth's core	12.2.2		24			
	Chan, S	Study of the size effect on bulk modulus of cerium oxide nanoparticles by X-ray diffraction under high pressure	12.2.2		18			

ALS Shifts Allocation (July 2010 – December 2010)

	Investigator	Title	BL		Shf Req		Alternate Beamlines	Other Beamlines
	Lipinska-Kalita, K	Compressibility and Structure of Ion Conductive Ceramics from the NaSICON Family for Low Cost Biodiesel Production	12.2.2		12			
	Yan, J	The composition effect of Gillespite on phase transition	12.2.2		9			
	Gleason, A	Phase Transitions of alpha-FeOOH Above 50 GPa Using X-ray Diffraction	12.2.2		4			
	Lu, T	Elasticity and Strength of Transparent Micro- and Nano-ceramics	12.2.2		21			
Totals					657			
Goal								

Appendix 3. Beamline proposals for the July-December 2010 cycle with numbers of shifts requested. The C and GU designations on the top portion of this figure (right hand side) indicate the number of shifts allocated on a preliminary basis to COMPRES users versus General Users. In many instances, since laser-heating was becoming more routine and hence extended user set-up time was no longer necessitated, beamline allocations were substantially reduced below those requested. When scheduling constraints were finalized, allocated beamtime extended to 6 shifts for Godwal on the first display item (see Appendix 1).

C. Infrastructure Development Projects

C.1 Multi-anvil cell assembly project
[PIs: Kurt Leinenweber, Thomas Sharp and James Tyburczy, Arizona State University]

Multi-Anvil Cell Assembly Development Project

Kurt Leinenweber, Thomas G. Sharp, James A. Tyburczy (Arizona State University)
Yanbin Wang (GSECARS, University of Chicago)

Introduction

The multi-anvil cell assembly development project has existed as an infrastructure development project since the inception of COMPRES. The purpose of the project is to develop multi-anvil cell assemblies and then make them readily available to any laboratory with a multi-anvil press. A series of cell assemblies of different sizes and pressure/temperature capabilities have been developed, using both preexisting and new materials and techniques. These cell assemblies involve many components with complex shapes and compositions, that need to fit together and function as a successful working high-pressure cell. All of these components – the pressure medium, gasketing, thermocouple, thermal insulation, furnace, and sample container – are specially made and are not generally available “off the shelf.” This presents a requirement that a significant amount of development is necessary to achieve “first pressure” in a new laboratory. Our project has made it possible for many laboratories, both new and established, to achieve predefined pressure/temperature conditions readily, and to quickly set about pursuing the research that their laboratories were created for.

Since the beginning, a parallel purpose of the project has been to provide a way for users to readily obtain data on a synchrotron beam line. A series of cell assemblies that are based on the standard designs described above, but are modified to allow the passage of x-ray beams, have been simultaneously developed, and used for in-situ studies by groups who have applied for and received beam time on a synchrotron.

We strongly believe that this project is providing a useful service to the high pressure community, and are seeking to continue this project in the new COMPRES. The standard assemblies are provided to the community, and the cost recovery from these assemblies keeps that part of the project going. Our funding request is for the purposes of developing new abilities and techniques, both in the area of new cell assemblies and capabilities, and for strengthening the overall quality and success of the existing assemblies. A stronger and more integrated focus on beam line development is enabled by the inclusion of Yanbin Wang, from the University of Chicago beam line GSECARS, as a new PI on the project. We will pursue further beam line developments with this beam line as well as beam line X17B at the National Synchrotron Light Source in Brookhaven. And we will continue to follow the needs of the community and the suggestions and advice of the COMPRES committees in formulating new ideas and in choosing new directions.

Cell Designs for Conventional Pressure/Temperature Experiments

The most visible effect on the community and the most widely distributed activity in the project is the provision of multi-anvil cell designs for conventional multi-anvil synthesis and phase equilibria experiments. We have a broad series of cell assemblies, and they are in widespread use in various laboratories around the world. In cases where the assemblies and their materials are well-established and people are completely happy with them, the project is simply self-sustaining by the cost recovery from the assemblies. The COMPRES development will be focused on developing and improving the capabilities of the assemblies where needed.

One area of this need is higher temperature. It is inevitable, we have found, that research groups will desire assemblies that go beyond the pressure and temperature capabilities that exist – they naturally encounter the limits as they pursue their research objectives. One such area is in the achievement of higher temperatures. We currently lack higher temperature capabilities at lower pressures (pressures below 15 GPa and temperatures above 1200 °C to 1500 °C). We need to develop cell assemblies specifically to reach temperatures of 2000 °C and above in the lower pressure ranges. This effort was impeded recently by problems with the lanthanum chromite supply from Japan, but these problems appear to have recently been solved with new formulations, and we will use COMPRES funding to test the new formulas and develop higher-T assemblies for lower pressure melting experiments, glass syntheses and others. The higher pressure 10/5 and 8/3 assemblies have much greater temperature capabilities already (in excess of 2200 °C) but even higher temperatures are still useful and a temperature limit of 3000 °C will be sought by eliminating melting components such as Al_2O_3 and the ZrO_2 cement from the assemblies. Another advantage of these extended temperature capabilities is that they will simultaneously represent a longer time capability at the current limit, where the temperatures of 2200 °C and above are only achievable for a matter of minutes.

Another area is larger volume. The synthesis of large samples requires large-volume assemblies that are specialized for this purpose. We have developed 18/12 and 25/15 assemblies recently for this purpose, but they are not routine to fabricate yet and some development of ceramic techniques (extrusion of zirconia, porous mullite octahedra) are still needed to make an inexpensive off-the-shelf version that can be maintained by cost of sales.

Finally, the COMPRES development funding will be used to address the problem of "underperforming" assemblies. A current example is our G2 box furnace assembly, a Stony Brook design that has drifted downward in its pressure capabilities for unknown reasons. We suspect a change in the zirconia ceramic or some other systemic issue. In this regard, we need to note that in a project such as this, we need to be very realistic about the actual capabilities, success rates, and overall expectations of assemblies. It is one thing to claim a capability or success rate within your own laboratory, but quite another to provide assemblies to others and claim such capabilities, because the capabilities will be quickly brought to the test.

Improved multi-anvil cells for in-situ x-ray diffraction

The first 10 years of this project were characterized by a strong and increasing interaction with beam lines, particularly the GSECARS beam line where many of the assemblies were calibrated, and beam line versions tested and used, in the large-volume press (LVP) at Sector 13, but also with beam line X17B at NSLS, where various DIA assemblies and materials were tested. We now wish to go beyond our previous involvement and develop a truly optimized set of assemblies that are capable of very clear beam access to the sample as well as optimal pressure and temperature capabilities with high success rates. We intend to have a set of assemblies that are comparable in performance to the "planar" assemblies that are used in Japan. In order to pursue this objective, we have included Yanbin Wang, from the GSECARS beam line, as a PI on the new version of this project.

Our current beam line assemblies are based on thermally insulating porous mullite pressure media (specially developed for our project) and either equatorial MgO windows (the 14/8 and 10/5 equatorial assemblies) or rhenium heaters with laser-cut windows (the 10/5 and 8/3 windowed assemblies). Recent re-designs of the windows have allowed more open x-ray access. However, the x-ray beam still has to pass through pyrophyllite gaskets and mullite or MgO/spinel pressure media. We will test offline and then introduce online new designs with boron epoxy and/or boron nitride beam paths through these components. This will bring the absorption levels far lower and allow good access to a wide energy range. It should not affect the temperature capabilities or success rates of the experiments.

We will also work on careful dimensioning of the assemblies and specially made sample/standard capsules that will provide full access to the sample and standard with positioning reliably within the beam window. This is important to the rapid success of users who bring their projects to the beam line.

Success at the beam line depends on careful offline testing combined with significant online experience. In developing these assemblies, we will perform the offline tests at ASU, including furnace testing and post-run sectioning to check the sample positioning, before putting the assemblies to online use. Beam time is very precious and should be spent collecting data for the scientific objectives, so the primary testing should be done offline to the extent possible. We can also perform detailed absorption calculations and simulations of spectra in order to ensure that the scientific objectives are attainable with our assemblies.

Other areas of online development will be in ultrasonics, deformation, and electrical conductivity experiments, and each of these objectives is described in the relevant sections.

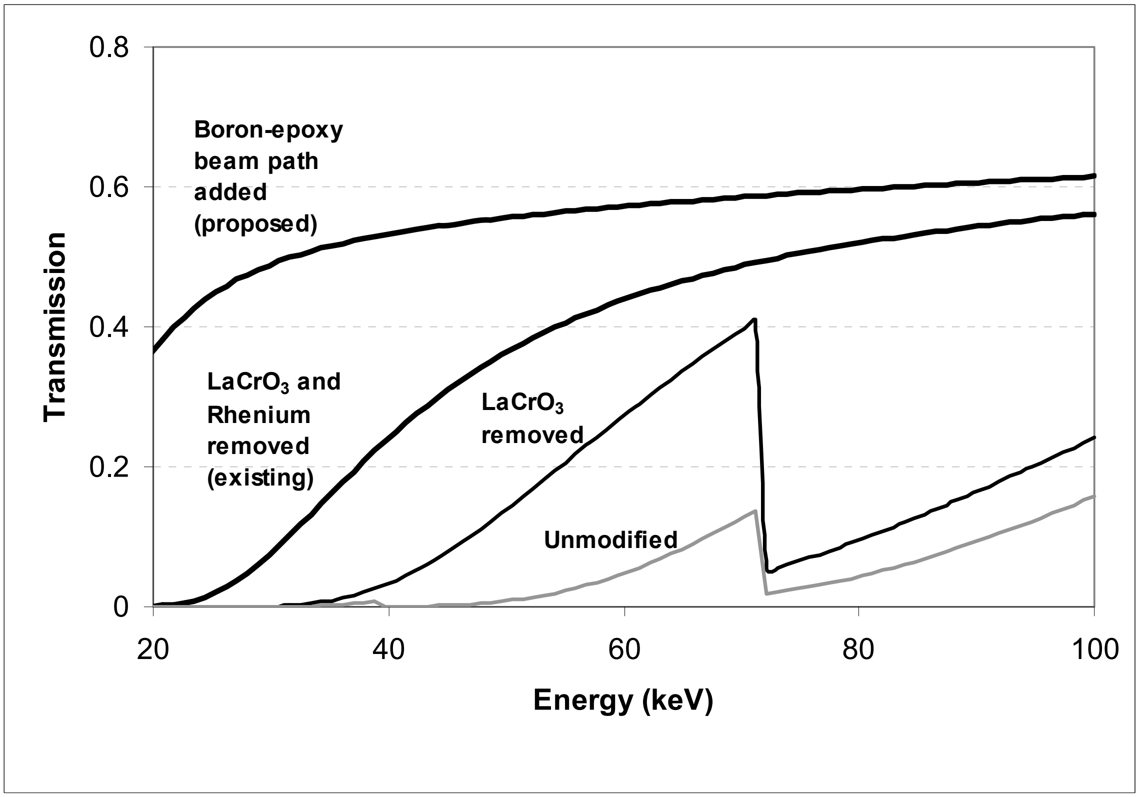


Figure: X-ray transmission curves for various versions of the 10/5 assembly, showing the current existing beam line assembly, and the proposed assembly with the addition of boron-epoxy beam paths through the octahedron and gasket.

Improved sample encapsulation

In the first phase of this project, we have often left it to the end users to encapsulate their samples, simply providing the assemblies with an empty space or "hole" where the sample and its capsule are intended to go. However, despite the complex and sample-specific nature of encapsulation in general, there are several standard ways to encapsule samples, and there are cost and other benefits in providing some of these to the community. For instance, precious metals are a significant cost and are not available in small pieces that would be needed for these experiments. It would be useful to develop a technique of precisely and cleanly cutting precious metal capsules into the precise lengths needed for multi-anvil experiments, allowing various compositions to be supplied in small, single-run quantities and eliminating the commitment that is usually needed to acquire precious metal tubing for sample encapsulation. We would work partly with Depths of the Earth, Inc. on this issue. Machined capsules, such as boron nitride, MgO, molybdenum, etc. are also a specialty item that some laboratories would prefer to have access to a supply of. And, single crystal capsules (MgO, forsterite, etc.) are of great and continuing interest to several groups using the COMPRES cells. Some of this has already been pursued by our project but we would like to make this a more standard and fully realized part of the project. Also, the discussion among different groups of encapsulation techniques for various types of samples will be a very useful one to have, and the actual procurement and development of such capsules will provide a concrete basis for such a discussion.

For the beam lines, the development of low-Z capsules, such as titanium, for in-situ hydrothermal experiments will be potentially very useful and will be pursued as part of this project.

Ultrasonics

The performance of ultrasonic measurements in situ is an objective of many groups, because of its application in comparing mineralogical models to seismic studies of the Earth. We will help to develop ultrasonic assemblies to provide to interested research groups. An ultrasonics setup at the beam line is currently targeted. Ultrasonic studies at the beam line are especially desirable because of the ability to measure pressure in-situ and to make a direct measurement of the sample length in real time, which enters into the calculation of the ultrasonic wave velocities. We intend to add ultrasonics assemblies to our list of standard assemblies available off the shelf. We will work with ultrasonics researchers such as Julien Chantel (sp?) at Bayreuth and others to design the assemblies, test them offline, and then use them at the beam line. The ultrasonics equipment will stay at the beam line for outside users to access for their own research.

Deformation

Several forays into D-DIA research have been made by this project, including the use of mullite spheres or cubes as pressure media (Durham, Burnley) and the fabrication of provisional assemblies for D-DIA work (Holyoke). ASU does not have a DIA or D-DIA for testing, but will develop full D-DIA assemblies in consultation with D-DIA experts such as Pamela Burnley and with both the NSLS beam line and the GSECARS beamline, both of which have well-established D-DIA capabilities.

We have also been involved in helping with the new deformation 6-8 device at GSECARS with the Lesher group, and will assist with this project and develop new cell assemblies for that device as well.

Electrical Conductivity

We are currently working on a 14/8 *in-situ* electrical impedence cell assembly based on the drawings in Scarlato et al. (2004). This assembly will be available to the community after testing in electrical conductivity measurements.

Pressure Standards

It would be a significant service to the community to provide pressure standards to the community for high temperature fixed-point pressure calibrations. High-purity glasses and crystalline phases used for calibrations include SiO_2, Mg_2SiO_4, $MgSiO_3$, $CaGeO_3$, $ZnSiO_3$ and others. High accuracy can be obtained by using mixtures of the target phases, such as a mixture of coesite and stishovite for locating the coesite-stishovite transition near 9 GPa. This reduces the kinetic issues, acting as a selfcontained reversal, and also minimizes the problem of large volume changes associated for example with the direct transformation of SiO_2 glass to stishovite, which can affect the pressure measurement. We will use the COMPRES project to obtain or synthesize high-purity materials that we can distribute to the community, thus providing a uniform set of pressure standards. Some of the samples can be made in large quantities in the belt apparatus at Diamond Innovations in Ohio (a division of Sandvik) and we have a collaborative relationship with this group, and will pursue the synthesis of large quantities of high-pressure phases of these pressure standards for community use.

Triage

We have provided and will continue to provide triage assistance for groups in distress – this includes situations where unexpected urgent difficulties have arisen, sudden beam time needs, etc. Costs of these are generally covered by the groups, but sometimes they also involve rapid developments that are of general interest to the community, for instance to quickly replace failing components with new designs, and the COMPRES development project is used in cases such as this.

Cell Assemblies for 5000 T press

In the event that COMPRES develops a 5000 Ton press for use by the high pressure community, we will assist that effort by developing larger cell assemblies for the press. Our largest cell assembly is currently 25 mm on the octahedral edge (octahedron/truncation sizes 25/15), but the methods used in that assembly are scaleable, and we can build even larger assemblies. On the large press at Ehime, in the synthesis of nanopolycrystalline diamond aggregates for anvils, octahedra/truncation sizes of up to 38/22 have been used to 15 GPa (Futoshi Idobe, pers. comm..), and we would develop similarly large assemblies using our injection-molded octahedron formulas.

Table 1 – Laboratories and Investigators involved in the COMPRES Multi-Anvil Cell Development project through the continuing use of high-pressure COMPRES cell assemblies.

Institution	Location	Contact(s)
Argonne National Laboratories	Lemont, IL	Tamas Varga
Arizona State University	Tempe, AZ	Kurt Leinenweber
Australian National University	Canberra, Australia	Robert Rapp
Bayerishches Geoinstitut	Bayreuth, Germany	Dan Frost
Brookhaven National Laboratories	Brookhaven, NY	Liping Wang
Brown University	Providence, RI	Stephen Parman, Geertje Ganskow
California Institute of Technology	Pasadena, CA	Jed Mosenfelder
Carnegie Institution of Washington, Geophysical	Washington, D.C.	Valerie J. Hillgren, Li Zhang

Laboratory		
Case Western Reserve University	Cleveland, OH	James Van Orman, Katherine Crispin
China University of Geosciences	Wuhan, China	Zhenmin Jin
Chinese Academy of Sciences	Beijing, China	Changqing Jin
Columbia University, Lamont-Doherty Earth Observatory	Palisades, NY	David Walker, Wei Du
Delaware State University	Dover, DE	Gabriel Gwanmesia
Florida International University	Miami, FL	Jiuhua Chen, Helene Couvy
GFZ Helmholtz-Zentrum Potsdam	Hamburg, Germany	Monika Koch-Muller, Hans J. Mueller
Institute for Geowissenschaften, Universität Frankfurt	Frankfurt, Germany	Alan Woodland
IPGP	Paris, France	James Badro
Jilin University	Changchun, China	
Los Alamos National Laboratories	Los Alamos, NM	Jianzhong Zhang
Lawrence Livermore National Laboratories	Livermore, CA	Julien Siebert
Massachusetts Institute of Technology	Cambridge, MA	William B. Durham, Nathaniel Dixon
NASA Johnson Space Center	Houston, TX	Kevin Righter, Lisa Danielson
National Cheng Kung University	Tainan, Taiwan	Jennifer Kung
Northern Illinois University	DeKalb, IL	Heather Watson
Stony Brook University	Stony Brook, NY	Baosheng Li, Hongbo Long, Li Li
Texas A&M University	College Station, TX	Caleb Holyoke
Toshiba Tungaloy America	Itaska, IL	Ron Pang
Yale University	New Haven, CT	Kazuhiko Otsuka, Justin Hustoft, George Amulele, Shun-ichiro Karato
Yanshan University	Qinhuangdao, China	Dongli Yu
University College London	London, England	Edward Bailey
University of Amsterdam	Amsterdam, The Netherlands	Wim van Westrenan
University of Arizona	Tucson, AZ	Kenneth Domanik
University of California at Davis	Davis, CA	Charles Lesher, Alisha Clark, Lara O'Dwyer Brown
University of Chicago,GSECARS	Argonne, Illinois	Yanbin Wang, Zhicheng Jing
University of Colorado	Boulder, Colorado	Joseph Smyth
University of Hawaii	Honolulu, HI	Murli Manghnani
University of Michigan	Ann Arbor, MI	Jie Li
University of Minnesota	Minneapolis, MN	Shenghua Mei, Tony Withers
University of New Mexico	Albuquerque, NM	Laura Burkemper, Carl Agee, Karen Hutchins,

		Stephen Elardo
University of Western Ontario	London, Ontario, Canada	Richard A. Secco

Table 2: Multi-anvil assemblies developed by the COMPRES project

Assembly name	Peak pressure	Status	Proven temperature	Design
8/3	25 GPa	Available	2319 °C	Rhenium furnace
10/5	20 GPa	Available	2000 °C	Rhenium furnace
14/8 "G2"	13 GPa	Available	1200 °C	Graphite box furnace
14/8 step heater	15 GPa	Available	1400 °C	Graphite/$LaCrO_3$ step furnace
18/12	9 GPa	Available	1500 °C	Graphite box furnace
25/15	5 GPa	Available	1500 °C	Graphite box furnace
8/3 window assembly in-situ	25 GPa	Available	2200 °C	$LaCrO_3$ sleeve and rhenium furnace with windows
10/5 window assembly *in-situ*	20 GPa	Available	2200 °C	$LaCrO_3$ sleeve and rhenium furnace with windows
10/5 equatorial assembly *in-situ*	20 GPa	Available	1700 °C	TiB_2+BN straight furnace, MgO equatorial window, mullite octahedron.
14/8 "G2" *in-situ*	13 GPa	Available	1200 °C	Graphite box furnace, forsterite sleeve
14/8 equatorial assembly *in-situ*	15 GPa	Available	1500 °C	TiB_2+BN step furnace, MgO equatorial window, mullite octahedron

Table 3: New multi-anvil assemblies in development by the COMPRES project in the near term

Assembly name	Target pressure	Proposed availability	Target temperature	Possible Design
8/3 higher T	25 GPa	Summer 2012	3000 °C	LaCrO3 furnace
10/5 higher T	20 GPa	Fall 2012	3000 °C	LaCrO3 furnace
10/4 in-situ XRD and ultrasonics	20 GPa	Spring 2012	2000 °C	Equatorial window, TiB2 + BN furnace
Improved x-ray access assemblies (8/3, 10/5, 14/8)		Spring 2012		Boron epoxy and/or BN x-ray beam paths added to existing assemblies
14/8 higher T	15 GPa	Spring 2012	3000 °C	LaCrO3 furnace
14/8 in-situ XRD and ultrasonics	15 GPa	Summer 2012	1400 °C	Graphite/$LaCrO_3$ step furnace
14/8 electrical conductivity	15 GPa	Fall 2011	1400 °C	Graphite/$LaCrO_3$ step furnace
18/12 lower power consumption assembly	25 GPa	Spring 2011	1800 °C	Porous mullite octahedron
25/15 lower power consumption assembly	20 GPa	Spring 2011	1800 °C	Porous mullite octahedron
6 mm D-DIA assembly	9 GPa	Summer 2011	1200 °C	Graphite furnace, with alumina deformation inserts

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C. 2 High-resolution Inelastic X-ray Scattering at High P & T: A New Capability for the COMPRES Community

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- **As of 1 January 2010 when he assumed his position as President of COMPRES, Jay Bass is no longer a Co-PI on this project.**
- **Ercan Alp is the responsible PI on this project since Wolfgang Sturhahn has left his position at the APS and moved to the Jet Propulsion Laboratory.**

2010 Report & 2011 Planned Activities
High-resolution Inelastic X-ray Scattering extreme conditions of pressure and temperature:
A Unique Capability for the COMPRES Community

Report Summary

We report here on the activities to date of Year 4 of a five-year infrastructure development project on High-resolution Inelastic X-ray Scattering at high P and T. The full three-year proposal was submitted in 2006 to COMPRES, and it was funded for the full term with the possibility of continued funding beyond this time period. In 2009, we have asked an extension. We include here a description of activities to date, planned activities for the coming year, and a budget request for an extension of the project.

High-resolution inelastic x-ray scattering (IXS) techniques provide the Earth and Planetary Science community with unique opportunities for new and exciting results on the properties of materials at high pressure and temperature conditions. Our infrastructure development project is aimed at outreach to the COMPRES community on the capabilities and use of these techniques and at creating state of the art IXS techniques for characterizing the properties of materials under the high-PT conditions of planetary interiors.

We are pursuing the development of two related techniques: Nuclear Resonant Scattering (NRS), which provides information on electronic, vibrational, and elastic properties, such as the density of states and sound velocities, and momentum-resolved IXS which directly gives the dispersion relation of low-energy collective excitations to provide directional information on vibrational and elastic properties, such as the elastic tensor and sound velocities. Both methods are in many ways ideally or even uniquely suited for addressing a number of important geophysical questions.

During our infrastructure development project, the fulltime postdoctoral researcher (Dr. Hasan Yavas) finished his term and left APS. He was hired to build the PETRA-III Inelastic X-Ray Scattering beamline in Hamburg, Germany. We have hired a new postdoctoral fellow, a recent graduate from UIUC Geology Department, Dr. Lili Gao. Along the lines to support the goals laid out in the original proposal text, we initiated high pressure experiments at the new IXS beam line (sector 30-ID) of the Advanced Photon Source and improved the experimental capabilities of the NRS and IXS beam line (sector 3-ID) to enhance its performance in high-pressure research. In particular, Sector 3–ID-C momentum-resolved IXS instrument has been converted for high-pressure measurements by adopting a new tandem focusing system, reducing the beam size to under 18 micrometers with high efficiency. Immediately following this development, the high-pressure research activity at this station picked up, to the point where we are planning to upgrade this instrument specifically for high-pressure research within the context of the APS Upgrade proposal.

We have engaged in outreach activities, e.g., three presentations at the COMPRES annual meeting in June 2010 and international conferences to broadly disseminate information on applications of NRS and IXS to understand Earth materials.

In particular, we accomplished the following tasks:

1. Hired a fulltime postdoctoral researcher (Dr Lili Gao) in October 2010,
2. Provided support for generating of user proposals for sectors 3-ID and 30-ID by COMPRES members,
3. Created new high-pressure capabilities at for IXS at 3-ID by implementing tandem focusing of toroidal and K-B mirrors,
4. Developed a new DAC set-up for sound anisotropy measurements, and an adaptor for panoramic DAC gas-loading,
5. A new panoramic membrane cell has been designed, and ordered.

Currently, Dr. Lili Gao is involved with helping users to install CONUSS and PHOENIX programs, including troubleshooting, helping a number of graduate students from University of Texas, University of Michigan, MIT, Caltech, and Princeton. She maintains and improves two high-pressure research programs: PRESSURE SCALE and FTIEOS. She has designed, built and integrated a beam absorber into station 3-ID-B as part of the beamline component last year; ans she is building another beam absorber for station 3-ID-C. She is also assisting Ercan Alp to upgrade the Mössbauer Spectroscopy laboratory, by separating the two existing systems so they now function independently, designing and implementing the new setup dedciated to DAC’s, setting up computer control of the new Mössbauer setup.

During the last year, we have explored the possibility of reducing the size of the x-ray beam at the momentum-resolved IXS station in sector 3-ID. Hasan's contributions were crucial in this effort. We were able to obtain a 17x20 μm^2 spot size (prior 150ö150 μm^2) with the highest spectral flux density of any IXS beam line in the world, as shownin Figure 1. This success will enable high-pressure studies using momentum-resolved IXS at 3-ID. Even though not immediately apparent to some COMPRES users, the effort of Hasan Yavaş was important for our future growth potential, e.g., by increasing the total amount of beam time available.

1.Performance details:

On the instrumental side, we now offer routine use of the capability of x-ray diffraction with the nuclear resonance scattering experiments in sector 3-ID-B. We now extend a dedicated high-pressure set-up in Sector 3-ID-C station for momentum-resolved IXS measurements. The COMPRES members now routinely apply the HERIX spectrometer at Sector 30-ID-C for momentum-resolved IXS measurements. Finally, the MERIX instrumentat 30-ID-B station is receiving requests for resonant inelastic x-ray scattering under high pressure. At least, three such proposals have been submitted. I think, it will be fair to recognize that the COMPRES activities related to inelastic x-ray scattering is growing in its reach and depth. Experiments above 1 Mbar hove become routine. More and more, we see "difficult" samples with very low iron concentrations are being measured. Polycrystalline samples to measure longitudinal sound velocities are being brought in, with good results, as seen in Figure 2. New areas in RIXS are being explored.

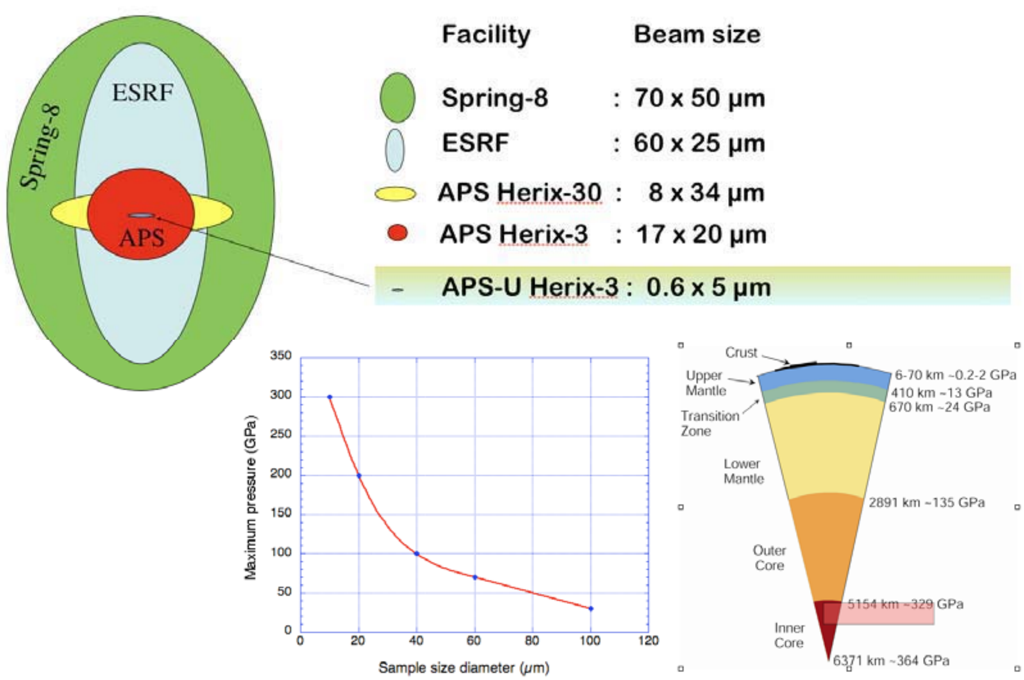


Figure 1. Comparison of full-focus beams size for all momentum-resolved IXS instruments in the world, which is a total of 4. Both instruments at the APS represent a unique opportunity for the COMPRES community, especially for experiments above 1 Mbar.

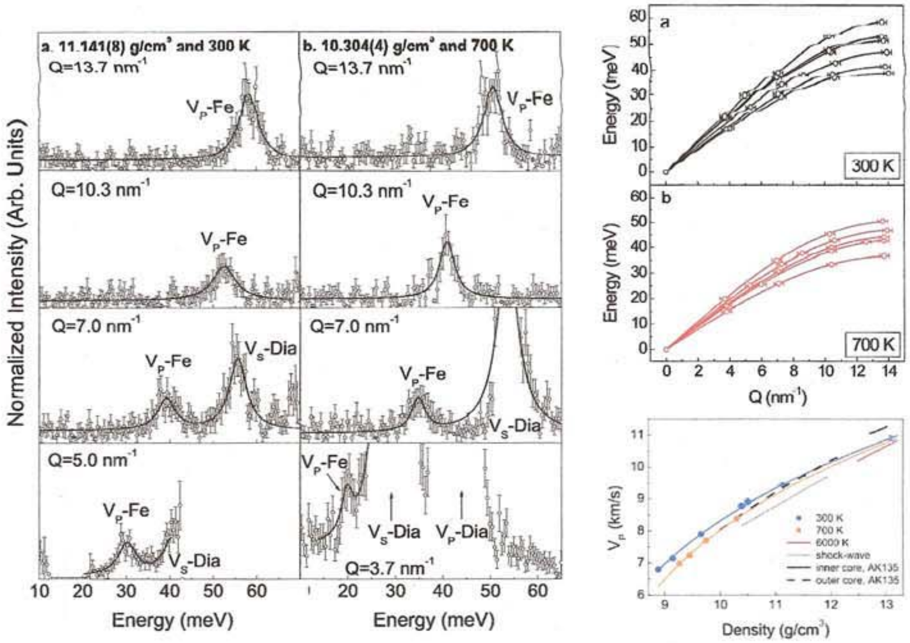
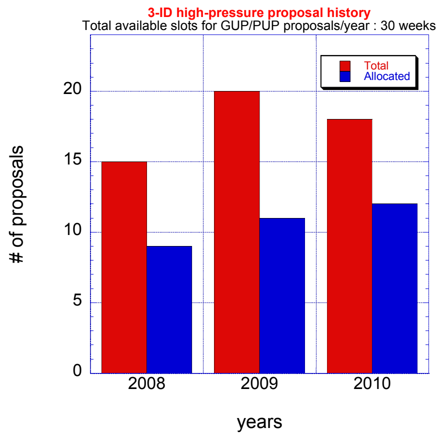


Figure 2. The new capability at Sector 3-ID-C IXS instrument is used to measure the phonon dispersion curves of hcp-Fe at high P-T. On the right, (a), ρ = 11.141 g/cm3 at 300 K, corresponding to 105 GPa; (b), ρ = 10.304 g/cm3 at 700 K, corresponding to 67 GPa. Blue and orange lines: modeled V_P at 300 K and 700 K from the IXS results, respectively. On the left, top, 4-analyzer results for phonon frequencies at different momentum-transfer points inside the Brilloulin Zone obtained at two different temperatures, and bottom, V_P –ρ relation of hcp-Fe in Earth's core. (Z. Mao, submitted to Nature)

Generation User Proposals (GUP) to APS

In the time period of 2008-2010, we have seen an increase in the number of proposals submitted, as well as a significant increase in beam time allocations. 12 independent research groups from 10 COMPRES member institutions submitted a total of 53 proposals to 3-ID and 17 proposals to 30-ID.



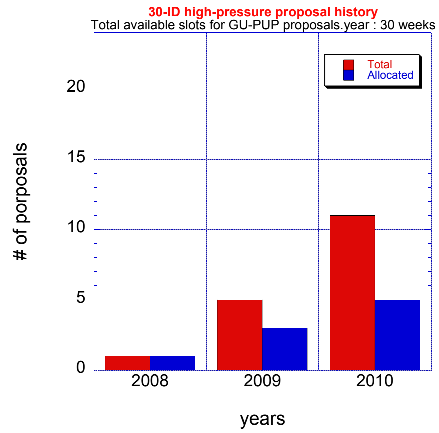


Figure 3. The historical development of high-pressure related research proposals submitted through the APS General User Proposal system. Allocation of the 2010 submitted proposals include the estimates for the next cycle.

Table 1. The general user proposal entry summary for high-pressure related activities in dedicated inelastic x-ray scattering beamlines of 3-ID and 30-ID.

Years	3-ID Allocated	3-ID Submitted	30-ID Allocated	30-ID Submitted
2008	9	15	1	1
2009	11	20	3	5
2010	12	18	5	11
Total	**32**	**53**	**9**	**17**

Of these proposals 32 (= 60 %) and 9 (= 53 %) were granted beam time at 3-ID and 30-ID, respectively (see Figure 1). These percentages are above average and demonstrate a relatively higher success rate for COMPRES proposals. In almost all proposals granted beam time, students at graduate or undergraduate levels participated actively. The high success rate of proposals by COMPRES members demonstrates that Dr. Hasan Yavas and now Dr. Lili Gao worked well with many of the PIs to develop effective proposals that were very competitive for beam time.

Details about proposals that were submitted but not allocated beam time are considered confidential information by the APS and cannot be distributed in cross-institutional reports.

Table 2: COMPRES affiliated universities and research organizations that were allocated beamtime in 2009-2010 period (or will be in 2011-1 period), many of them repeatedly.

Affiliation	PI	Student
Caltech	J. Jackson	Yes
Princeton	T. Duffy	Yes
MIT	S. Shim	Yes
U. Texas-Austin	J.F. Lin	Yes
ORNL	O. Delaire	Yes
Stanford	W. Mao	Yes
Carnegie Institute of Washington	Y. Ding	Yes
Washington University St. Louis	J. Schilling	Yes
University of Chicago	N. Dauphas	Yes
U. of Hawaii	M. Mangahni	Yes
UNLV	A. Cornelius	Yes
UIUC	J. Li	Yes

3. Publications (Second half of 2009-2010) :

Jennifer M. Jackson, Wolfgang Sturhahn, Oliver Tschauner, Michael Lerche, and Yingwei Fei, Geophysical Research Letters, 36, L10301 (2009)
Behavior of iron in (Mg,Fe)SiO3 post-perovskite assemblages at Mbar pressures

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4. Planned Activities

We consider the APS Upgrade as an opportunity to optimize the inelastic x-ray scattering instruments for high-pressure studies. This optimization process has already started. The lessons learned in the last decade dealing with high-pressure researchers determined the basic philosophy many of the significant changes planned. Thus, the involvement of COMPRES community through the existing ID projects will provide a bigger return in the long run for this community. The planned upgraded layout for 3-ID is given in Fig. 4.

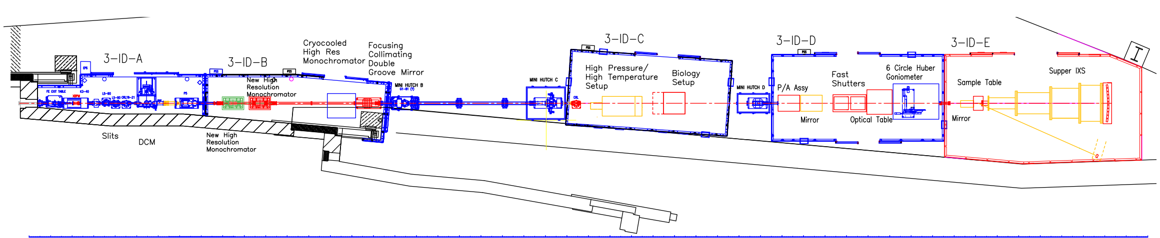

Figure 4. The proposed upgrade of 3-ID beamline will have two dedicated stations optimized for high-pressure research, 3-ID-C and a newly added 3-ID-E (shown in red). The former will house the high-pressure/high-temperature set-up with the added capability of low-temperature for magnetism under high-pressure, and valence/spin state determination for iron-bearing minerals. The latter will house the new IXS instrument with 5 micron focusing, increase number of analyzers from 4–to-8, increased momentum transfer range, from 32 to 59 nm^{-1}, and built-in x-ray diffraction and single crystal orientation capability.

In the extension of our infrastructure development project, we will continue the outreach effort to the COMPRES community by assisting interested groups in design, preparation, execution, and evaluation of their high-resolution IXS experiments. In this context, we make CONUSS package available for nuclear forward scattering (NFS) data evaluation, PHOENIX package for nuclear resonant inelastic scattering measurements (NRIXS), as well as FitEoS for equation of state.

We intend to organize a workshop in May 2011, in connection with the APS User Meeting, to introduce the high-resolution IXS and its applications for studying planetary interiors with emphasis on attracting graduate students and young scientists. For those who wish to perform experiments in the near term, we will assist the COMPRES community in the preparation of proposals for beam time.

Another area we are involved in improving this year is the in-situ XRD capability, in combination with the IXS spectrometer in 3-ID-C station. A separate COMRES-ID proposal has been submitted for the special, low-profile detector (A. Alataş from ANL, and J.F. Lin of U. of Texas). The added diffraction capability will provide us with structural confirmation as well as with an equation-of-state.

For NRIXS experiments, our current laser system needed replacement with a fiber laser. While we have acquired a new one with the APS funds, it turns out that we need a second one for two-sided heating. This is due to special unpolarized nature of the fiber laser. Furthermore, for high-pressure melting experiments, we need faster temperature readout than what the current spectrometer is capable of. In collaboration with Jennifer Jackson (Caltech) we have designed a new system, which is ready to be installed. This system relies of blackbody radiation profile to measure limited number of wavelengths, and fitting the data to a temperature, all the necessary optics and data acquisition tools are in place. The system will be installed in January 2011. We expect to push the temperature readout time to a few Hz.

We are also installing web-based cameras for remote-access and classroom access. This will provide COMPRES PI's to observe the experiments from their labs, participate the experiments in a more meaningful way, as well as demonstrate to the students who are not taking part in the experiment itself for that particular run period. If successful, we may plan, for limited experiments, remote-access operations for data collection, and on-line data evaluation. This should further expand the experimental domain in the COMPRES community.

C.3 Postdoc for DAC gas-loading system at GSECARS-APS

[PI: Mark Rivers, GSECARS and University of Chicago]

COMPRES Infrastructure Development Project for a post-doctoral position for the gas-loading system at APS

Year 2 Progress Report
Mark Rivers
Sergey Tkachev
University of Chicago

The COMPES Infrastructure Development Committee funded the capital equipment costs (~$85,000) of a gas-loading system at the APS. GSECARS contributed the design and construction effort to build the system. The system began operation in February 2008 and has been running with minimal downtime since then. The system works extremely well, with the only significant problems being some failures of the commercial compressor. We have in-house technical support (Guy Macha) to repair such problems, and the mean time to repair has typically been 1 day.

The COMPRES system at the APS is available for use by any member of the COMPRES community, regardless of whether they are performing experiments at GSECARS, at another APS sector, at another synchrotron, or in their home laboratory. The problem for some members of the COMPRES community is that they need to load cells, but cannot afford the time or money to travel to APS.

GSECARS has provided the support (training and supervision) for any users who come to the APS to use the system. This is a substantial time commitment for our staff, but one which we can manage with our existing staffing level. We do not, however, have the staff to be able to handle a "mail-in" service to load cells for users; we rely on users to do most of the work once they have been trained.

This COMPRES project funds 50% of a post-doc to reside at the APS. This person is responsible for loading cells that are sent to the APS by users who do not travel here. The other part of this person's salary and responsibilities will be covered by GSECARS.

Dr. Sergey Tkachev began in this post-doc position in the second week of June, 2010. He has performed an excellent job, providing both mail-in service for the COMPRES community not running at the APS, and hands-on assistance for users who come to the APS to load cells when running on any of the beamlines here.

The following table summarizes the mail-in service in the 5 months since Sergey began.

University Name Number of DACs loaded
UCLA Miao Xie 5
Stanford Shibing Wang 2
University of Michigan Maik Lang 3
Ohio State University Wendy Panero 1

A total of 11 diamond-anvil cells have been loaded for 4 user groups with the new COMPRES supported mail-in service.

In addition to this mail-in service, there have been 54 users who have loaded cells with Sergey's assistance since June 7, 2010 at the APS. They have loaded a total of 154 cells, an average of about 1 per day in the 5 months since Sergey started.

The following is a description of the mail-in service, as presented at 2010 COMPRES Annual Meeting:

• Mail-in service is available only for diamond anvil cells (DACs) that are being used for experiments at locations other than the APS.
o Users who wish to load cells for experiments at the APS, including GSECARS, HPCAT and other APS beamlines, are expected to load the cells themselves.
o Training and assistance will be provided by the staff from the beamline where the experiment will be conducted.
• Potential users must contact Sergey (tkachev@cars.uchicago.edu, 630-252-0430) to discuss the technical and scheduling requirements prior to sending the cells to the APS.
o At this time we are providing mail-in service only for Ne and He gases in the standard symmetrical (Princeton) DAC
o For all other type of DACs and gases the available options should be discussed directly with Sergey.
• Cells must be shipped with appropriate packaging that can also be used to return the cells.
o A prepaid shipping label must be included for returning the cells to you.
o Cells containing any hazardous materials must be not be shipped directly to GSECARS, but rather to the hazardous materials receiving building at Argonne.
o Contact Sergey or Nancy Lazarz (lazarz@cars.aps.anl.gov) for details.
• We will make every effort to load the cells with the requested gas at the desired pressure.
o However, COMPRES and GSECARS cannot guarantee that the cell will be successfully loaded.
o The loading process also entails some risk of damaging the cell or diamonds. Users accept this risk, and agree not to hold COMPRES or GSECARS, or any of their staff, liable for any damage that may occur.

• Mail-in service is available only to staff and visitors at COMPRES member institutions in the United States, with shipping to and from US locations only.

C.4 A new collaborative facility for **high-**pressure melt property characterization at the **Advanced Photon Source**

[PIs: Yanbin Wang, GSECARS and University of Chicago and Guoyin Shen, Carnegie Institution of Washington]

COMPRES
Infrastructure Development
First Year Progress Report
Yanbin Wang, Guoyin Shen
November 1, 2010

A new facility for melt property characterization at high pressure using synchrotron radiation

Introduction

This component of the COMPRES Infrastructure Development program was aimed at establishing a new user facility at the Advanced Photon Source for liquid and melt property studies. By combining expertise and resources at GSECARS and HPCAT, we have completed a Paris-Edinburgh (PE) Press setup at 16-BM-B. We plan to open the facility to general users starting in June 2011. In January 2011, a beamtime call with technical details will be sent to COMPRES community.

The need for a user facility for high-pressure liquid/melt property studies at synchrotron sources

Structural and related physical properties of non-crystalline materials, i.e., glasses, liquids, and melts at high pressure are of fundamental importance in physics, materials science, earth science, and industrial applications. Generally, there are two basic approaches in studying these properties. One is the diamond anvils cell (DAC), laser heated or externally heated, the other is the large-volume press (LVP) with resistive heating. The two techniques are complementary. The DAC is capable of generating multi-megabar pressures, with sample volumes usually smaller than 10^{-3} mm^{-3}. Experiments are generally conducted using monochromatic radiation, with an area detector

to record intensities. Large background is almost always present, due to Compton scattering of the diamonds. Subtraction of such background is feasible but a challenging task especially for low scattering materials such as oxides and silicates. The LVP is capable of generating stable and homogeneous temperatures. Due to the solid pressure media used, energy-dispersive x-ray diffraction (EDXD) is the preferred technique, which can exclude scattering contributions from the media. Diffraction signals are collected at 10 - 15 fixed two-theta angles and are then combined in Q space to construct a complete spectrum for structural analysis. Contributions from incoherent (Compton) scattering are removed based on theoretical predictions, and relative intensity variation from the synchrotron source is modeled using the Monte Carlo approach based on redundant intensity backgrounds at different two–theta angles. The PE press (an LVP system) at 16-BM-B is the only facility in the world aimed at "complete" liquid/melt property characterization by combining x-ray diffraction (for structural characterization), absorption (density), radiographic observation (viscosity), and ultrasonic interferometry (elasticity) measurements.

We began constructing this system in early 2010, by combining the PE press purchased by GSECARS (with a pressure control system designed and built in-house) and the EDXD diffraction setup at HPCAT. The hutch is equipped with a large Huber rotation stage, which allows accurate 2θ angle control up to almost 40°, with finely collimated white radiation as the source.

Progress made to date

Several silicate melts have been studied to test the capability of the facility. Yamada et al. (2010) studied albite and anorthite to 6 GPa and 2000 K, and compared the results with previous studies. For albite, based on the position of the first strong diffraction peak (FSDP), it appears that the aluminous silicate network undergoes an intermediate range ordering and shrunk by ~18% compared to the structure of glass at 1 atm. These data also indicate that the T-O-T (where T represents Si and/or Al) bound angle, which is the linkage of the Si-O and Al-O polyhedra, is the most responsible for densification. Yamada et al (2010) found that the T-O-T peak near 3 $Å^{-1}$ in the radial distribution function $G(r)$ splits into two peaks (Fig. 1), suggesting a differentiation of the bond angle at high pressure. This work has been accepted for publication.

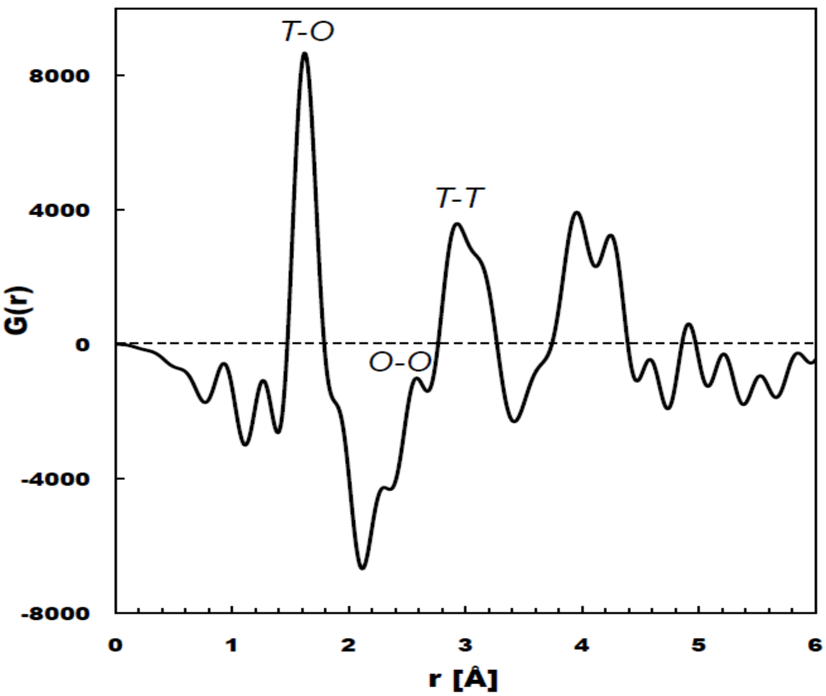

Figure 1. Reduced radial distribution function for Structure factor for liquid $NaAlSi_3O_8$ at 5.3 GPa and 1873 K. *T* in figure represents the atoms of Si and Al.

Sakamaki et al. (2010) studied the melt system along the jadeite (Jd) – diopside (Di) join. Preliminary data (Fig. 2) shows evolution of the first strong diffraction peak (FSDP) as a function of pressure and temperature for three melt compositions: Jd100, Jd50Di50, and Di100. Systematic variation indicates strong composition influence on the compressibility of the melts.

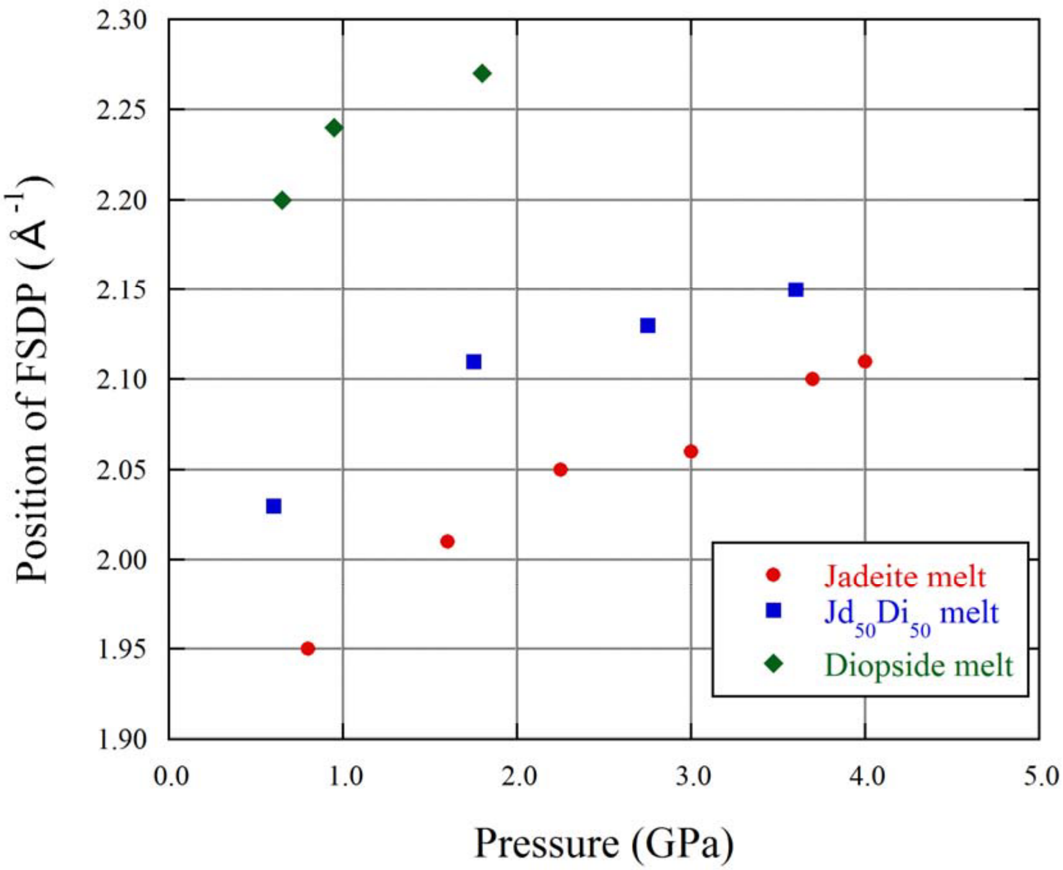

Figure 2. FSDP of melts along the Jd-Di join as a function of pressure.

Kono et al (2010) tested ultrasonic setup with the PE press. With crystalline MgO as the testing sample, high quality acoustic signals were recorded at high pressure. This project is now moving towards high temperature, and we hope to be able to measure acoustic wave velocities for melts in about one year of time from now.
Mei et al (2010) used the PE system for measuring the structure of MgSiO3 glass up to 9 GPa. The goal is to check any structural signature at around 7 GPa where a clear softening in sound velocity was observed by Brillouin spectroscopy. The PE cell results do not shown an obvious structural change. However, detail analysis is still in progress.
Pravica et al (2010) recently published their results on phase transitions of an energetic material, based the newly established PE facility at 16BM-B. The relatively large volume in the PE cell is the key for the successful phase diagram mapping on this low Z material.
Lipp et al from LLNL studied high pressure melting with the PE system. With the white beam radiography capability, the morphology of the sample upon melting can be monitored and the onset of melting can be determined. It is found that the pressure may change during melting. The in situ x-ray diffraction with EDXD from some standard materials can be used for pressure determination.

User involvement

From the beginning this facility attracted many outside users as well as local users. Several users from Japan are particularly instrumental in assisting us to develop a user-friendly facility. We have benefitted greatly from collaboration from the Geodynamics Research Center (Ehime Univ., Japan). Drs. T. Inoue, A. Yamada, and Y. Kono made multiple visits in the last two years. The PE system has been used by several HPCAT users from Lawrence Livermore National Laboratory (Drs. Evans, Lipp) and University of Nevada at Las Vegas (Drs. Pravica, Galley).

Future developments

<u>Future developments will include the following:</u>

(1) Densitometry with monochromatic X-ray absorption: the density measurement is a significant challenge for equations of state of melts. The flexibility between white beam and monochromatic beam setup on the same experimental table will also greatly enhance the accuracy of MA-EDXD data normalization by providing the sample density in-situ.

(2) High-pressure X-ray tomography or white beam radiography: the excellent angular access of PEC can also benefit the studies for 3D or 2D textures and volumetric properties of liquid and amorphous phases under pressures. A full 3D tomography is not possible for a portable PEC due to the intrinsic design but a partial 3D pictures or 2D projection of the x-ray transmission images still have a great potential for the application. Through radiographic images, viscosity of melts can be measured by the falling-sphere method, for example.

(3) Ultrasound velocity measurement combined with X-ray radiography and scattering measurement: precise measurement of travel distance is a key prerequisite for successful sound velocity measurement, which is difficult for liquid samples under pressure. With the white beam radiography capability of PEC described above, the exact liquid dimension through which the ultrasound travels can be measured within micro to sub-micrometer precision. Simultaneous or subsequent measurement of X-ray scattering intensities may provide a unique combination of in-situ techniques to study equations of state and structures at the same time.

(4) Angle dispersive powder diffraction: the accurate and wide angular accessibility of current PEC setup can be applied for structure refinement of crystalline phases under pressure with monochromatic beam.

Publication:

Akihiro Yamada, Yanbin Wang, Toru Inoue, Wenge Yang, Changyong Park, Tony Yu, Guoyin Shen (2010) High-pressure X-ray diffraction on the structure of liquid silicate using a Paris-Edinburgh type large volume press. *Rev. Sci. Instrum.*, in press.

Pravica, M., J. Galley, C. Park, H. Ruiz, and J. Wojno. (2010). A high pressure, high temperature study of 1,1-diamino-2,2-dinitro ethylene. *High Pressure Res.*, (20 Oct 2010 on-line).

Abstracts and presentations:

Changyong Park, Curtis Kenney-Benson, Tony Yu, Qiang Mei, Tatsuya Sakamaki, Guoyin Shen, and Yanbin Wang (2010) Potential applications of Paris-Edinburgh cell with synchrotron white X-rays at HPCAT 16BM-B for high-pressure mineral physics, AGU Fall Meeting, 2010.

Changyong Park, Qiang Mei, Guoyin Shen, Wenge Yang, Curtis Kenney-Benson, Tony Yu, Tatsuya Sakamaki, Yanbin Wang, Akihiro Yamada, Toru Inoue (2010) Structure of Amorphous Solids and Liquids under High-Pressure with White-Beam EDXD and Paris-Edinburgh Cell at the APS 16BM-B, Conference on Synchrotron Radiation Instrumentation (SRI2010), Sept. 2010, Argonne, Illinois.

Tatsuya Sakamaki, Yanbin Wang, Tony Yu, Changyong Park, Guoyin Shen (2010) In situ X-ray experiments on the structure of jadeite-diopside melt at high pressure by Paris-Edinburgh press, AGU Fall Meeting, 2010.

Wang, Yanbin (2010) New applications of in-situ synchrotron x-ray techniques for studies of earth and planetary materials at high pressure and temperature, Goldschmidt Conference, June, 2010, Knoxville, TN.

Tony Yu, Yanbin Wang, Changyong Park, Jonathan Stebbins, Guoyin Shen (2010) Energy-Dispersive X-ray Diffraction Investigation of Amorphous Lithium Borate Structure: A Demonstration of the Paris-Edinburgh Cell Setup at 16BM-B at the APS, AGU Fall Meeting, 2010.

C.5 A Mössbauer spectroscopy facility for the high-pressure community at the Advanced Photon Source

[PIs: Ercan Alp and Wolfgang Sturhahn, Argonne National Laboratory; Jie Li, University of Michigan; J. Jackson, California Institute of Technology; Jun-Fu Lin, University of Texas; Dennis Brown, Northern Illinois University]

Progress report for COMPRES proposal
"A Mossbauer Spectroscopy Facility for the High Pressure Community"

Ercan Alp[1], Wolfgang Sturhahn[1,] Jie Li[2], Jennifer Jackson[3], Jung-Fu Lin[4], D. E. Brown[5]

1) Argonne National Laboratory, 2) University of Michigan, 3) California Institute of Technology, 4) University of Texas at Austin, 5) Northern Illinois University

The proposal offered setting-up a specialized Mossbauer spectroscopy facility for high-pressure experiments. We have decided to make maximum use of the existing components, and use the available money to add new capabilities. Below is a summary of activities so far for the period of June-October, 2010.

First, we have separated the controls of the two existing Mossbauer drives, so that high pressure-set-up can be a dedicated system. Secondly, we have acquired micrometer-resolution x-y-z stages to mount the DAC in front of the Mossbauer parent radioactive source. This point source currently has strength of approximately 3 mCi, and we are in the process of renewing it with a 10 mCi source, coincident with the completion of the high-pressure set-up. We are now in the process of motorizing these stages. All the required components, the VME crate, OSM control boards, Step-Pak motor drivers, and data input scalers are in place. We are waiting for the control computer to be installed to start the data acquisition with micro-positioning. Figure 1 shows the current progress in the lab.

Second, we have designed a new panoramic membrane diamond-anvil cell (PM-DAC) that is compatible with nuclear resonant inelastic scattering and nuclear forward scattering experiments in the beamline and in the laboratory. This cell is currently in the manufacturing stage, and we expect to receive it in February 2011. We hope to be able to offer such PM-DAC's to the COMPRES community so that they can concurrently take data in the Mossbauer lab as well as at the 3-ID beamline. Figure 2 shows the details of this new DAC.

Third, we worked on the idea of using reliable software for data analysis in the energy domain, as well as in the time domain. After studying the available commercial software, the initial decision is to stay with CONUSS, and make it readily available at the Mossbauer lab, as well as for researchers to take home. To demonstrate the capability, we provide three examples from the data taken in our Mossbauer Laboratory at Argonne National Laboratory. The data shown in Figure 3 contains analysis of the fitting to Fe_2O_3, $Mg_{0.87}Fe_{0.13}SiO_3$, and a meteorite sample that fell to Chicago area in 2002. We plan to offer this program in the lab, in the same computer where data is collected, as well as at the beamline, using the same format for input files.

We have hired a post-doctoral research associate helping with the progress of this proposal, Dr. Lili Gao, who has started on October 2010.

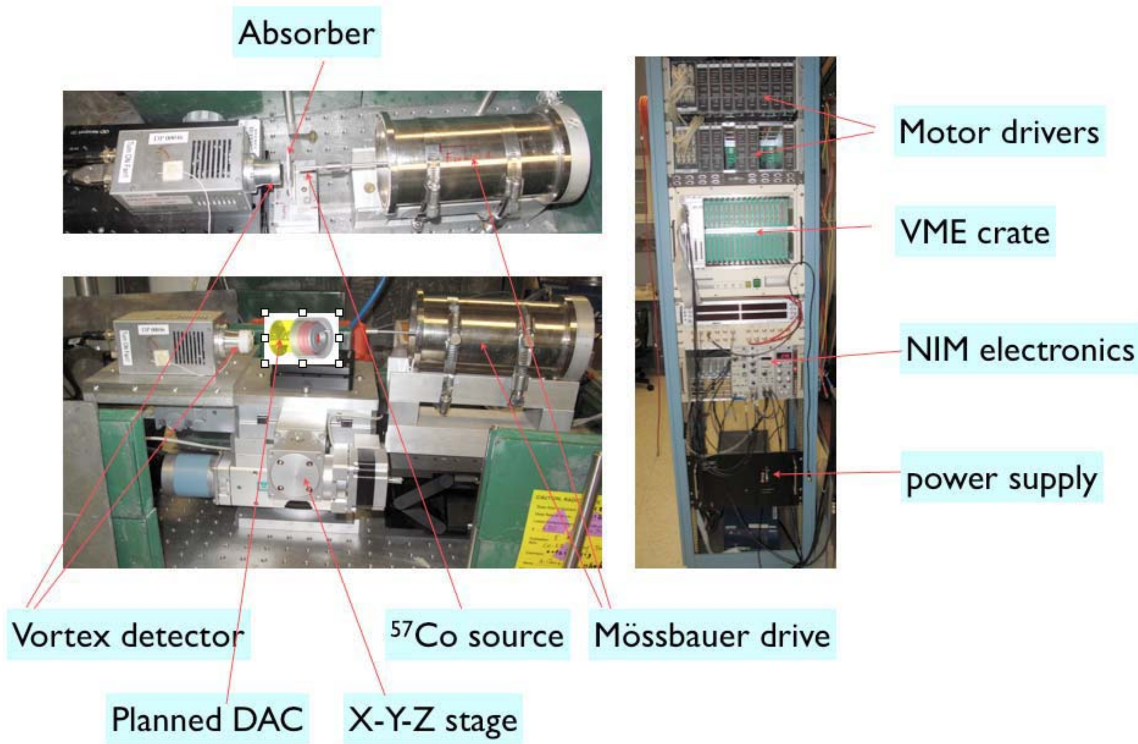

Figure 1. Top: The system before modification, Bottom: The current system modified for PM-DAC, side: Control electronics and motion control equipment rack

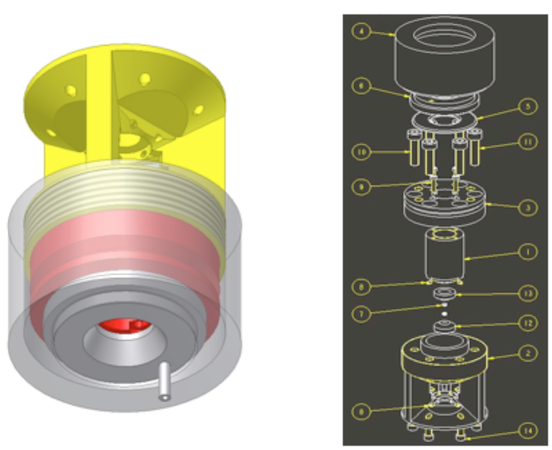

Figure 2. The panoramic membrane DAC, design based on original Mao cell, modified to accommodate a membrane.

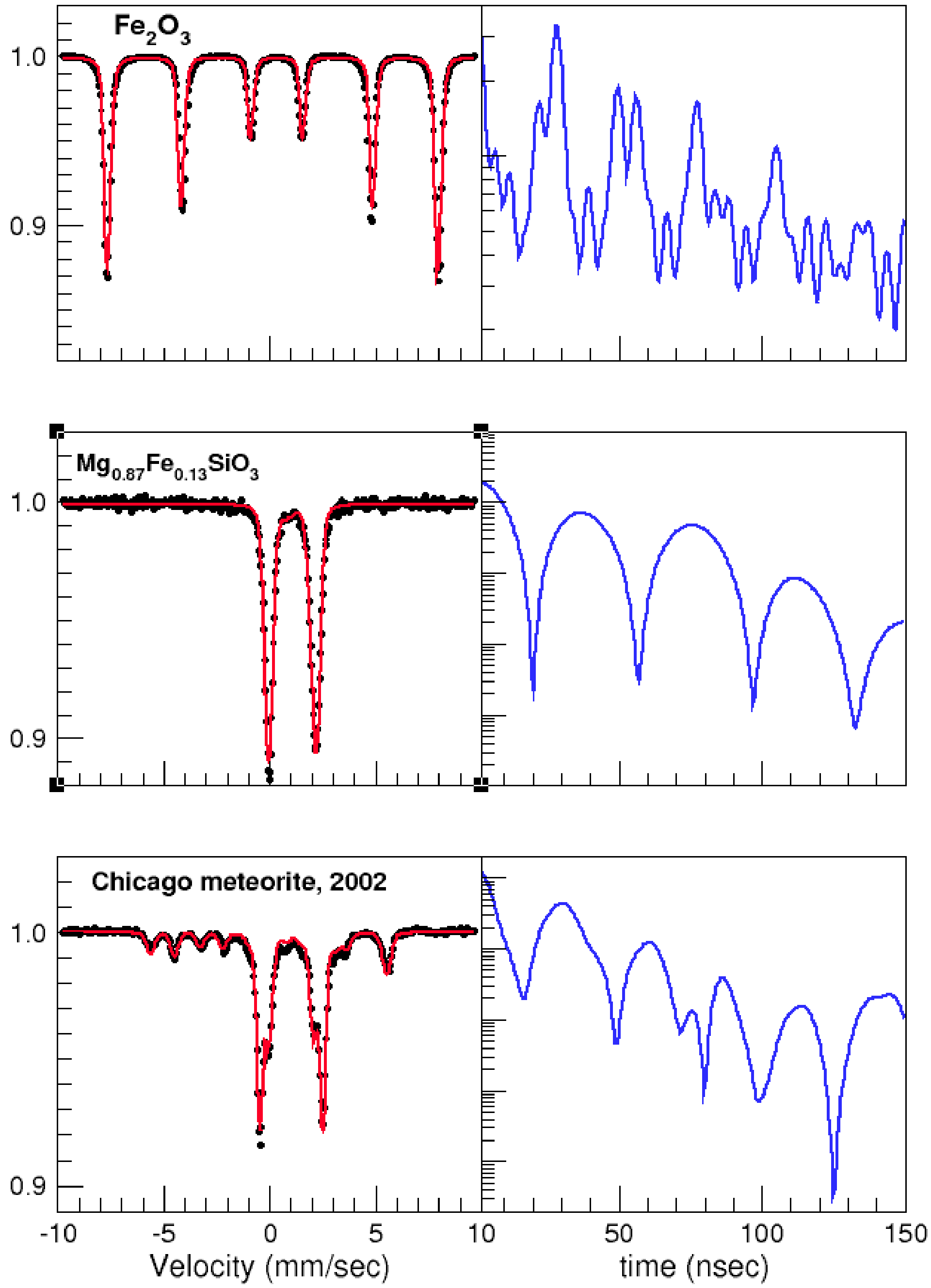

Figure 3. The Mossbauer spectra taken in the laboratory, analyzed with CONUSS software in the energy domain (figures on the left), and time spectra predicted (figures on the right) using the same parameters for three different samples of geophysical interest. The possibility to predict the synchrotron Mössbauer spectrum provides an additional advantage to prepare the experiments ahead of time, and be more economical with the limited time available at the beamlines.

C.5 Heating Externally to Extreme Temperatures in the Diamond Anvil Cell (HEETDAC):

A COMPRES Infrastructure Development Proposal

P.I.'s Q. Williams and R. Wenk

Summary

Recent developments using a modified Liermann-type cell at the Advanced Light Source have resulted in the shattering of past records for the pressure and temperature range of an externally heated diamond anvil cell in radial diffraction geometry. This cell has accessed the pressure/temperature range up to 40 GPa and 2000 K. The current design of the cell allows for significant refinements of its thermal characteristics, and given some effort will achieve significantly higher temperatures. The high pressure limits of this assembly have yet to be explored. The goal of this Infrastructure Development Project is to optimize the design and probe the performance limits of this external-heating apparatus and make its design (and hence capabilities) accessible to the broader COMPRES community. Simultaneous laser-heating with external heating will also be developed to determine whether this synergy can produce substantially larger sized and lower thermal gradient laser-heated spots. The ALS set-up is well-suited for this work and preliminary results look promising. To achieve these goals, we request salary funding for 4 months for Researcher Selva Vennila Raju, who has been the driving force behind the ALS external heating effort. She will spearhead the design improvements and community distribution aspects of this project.

Introduction

The importance of external resistance heating within the diamond anvil cell has long been recognized (e.g., Schiferl, 1987; Bassett et al., 1993)—the advantages of such heating include the notable stability of the thermal environment and lack of temperature gradients within the sample chamber. Indeed, the importance of these advantages has led to continuing design developments in such cells (e.g., Petitgirard et al., 2009; Liermann et al., 2009): however, these cells were utilized to only 1273 and 1100 K, respectively. Indeed, the canonical wisdom is that such experiments are limited to temperatures below ~1400 K or so, due to the instability of diamond anvils relative to graphite at high temperature conditions. This is certainly the case in environments that are even slightly oxidizing. However, based on the results we describe below, we believe that the limitation on anvil stability in environments that are designed to be highly reduced entirely hinges on the kinetics of the solid-state reversion of single crystal diamond to graphite—a physical process that is quite poorly constrained, but allows for external heating to be conducted under markedly higher temperature conditions.

Results

Over the last eight months, the Wenk group at UCB and the high-pressure group at the ALS have utilized a modified Liermann-type externally heated cell in a radial diffraction geometry to achieve conditions previously thought impossible in such a device. Leading this initiative are Lowell Miyagi (formerly UCB, now at Yale), Jane

Kanitpanyacharoen, Jason Knight and Vennila Raju. Figure 1 shows the pressure-temperature history of three experiments on iron and its alloys and wustite, with temperatures produced by Pt-Rh thermocouples embedded next to the anvils, and pressures derived from the equations of state of iron or iron oxide. Two experiments involved purely external heating over several hours, while the third combined external heating with laser heating (to 2300K). The goal was to record *in situ* texture development at high P and T (some inverse pole figures are shown).

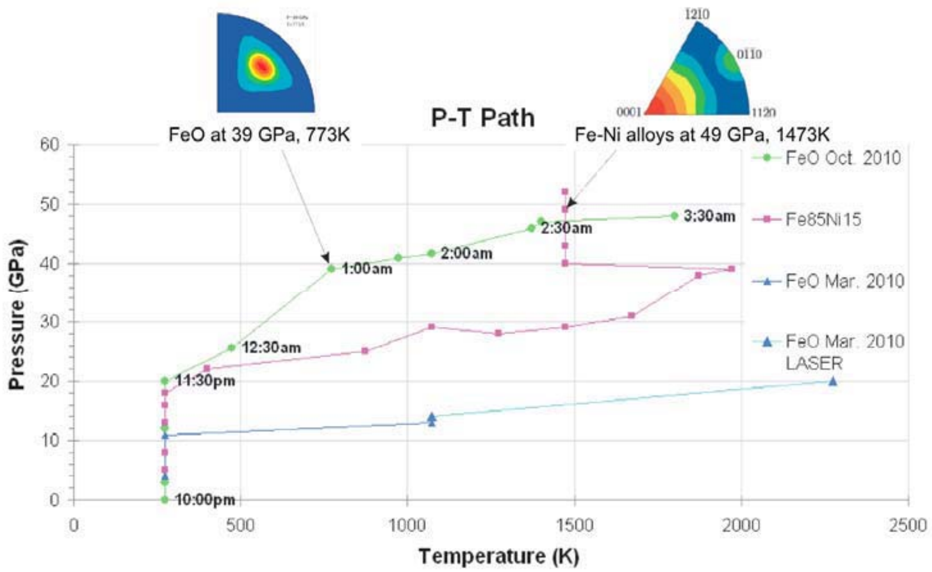

Figure 1. Pressure-temperature histories of multiple radial diffraction experiments; experiments on an $Fe_{85}Ni_{15}$ alloy reached a maximum temperature of 1950 K at 39 GPa, before the experiment ended at 52 GPa and 1450 K; that on FeO reached 48 GPa and 1773 K. Figure from Jane Kanitpanyacharoen (UCB).

Why were these experiments so successful at reaching extreme conditions? A key observation is that the means by which the diamonds were mounted involved their complete juxtaposition with the graphite heater (they were, in fact, pressed through the heater) (Figure 2). Hence, the diamonds (which survived these experiments) were directly juxtaposed with a large-scale oxygen getter (the graphite furnaces), which in turn was stabilized by a constant rapid flow of argon. A plausible interpretation is that no oxygen-related decomposition of the diamonds could initiate, as they were plausibly present in an entirely reduced environment. Thus, the kinetics of diamond reversion to graphite in the solid-state in an anoxic environment plausibly modulates the upper stability limit of diamond anvils under these conditions. Regardless of the precise physical origin of this dramatic extension of the thermal stability range of externally heated diamond anvil cell experiments, the key point here is that this new capability markedly enhances the range of science that can be conducted using this apparatus. These include potentially utilizing the externally heated diamond cell to study topics as diverse as interrogating the kinetics of mantle phase transitions, exploring the deformation mechanisms of mantle materials, and conducting petrologic experiments at mid-mantle conditions. Indeed, this extended range means that a large portion of the pressure-temperature domain occupied by multi-anvil presses can now be accessed by externally heated diamond cells (Fig. 3).

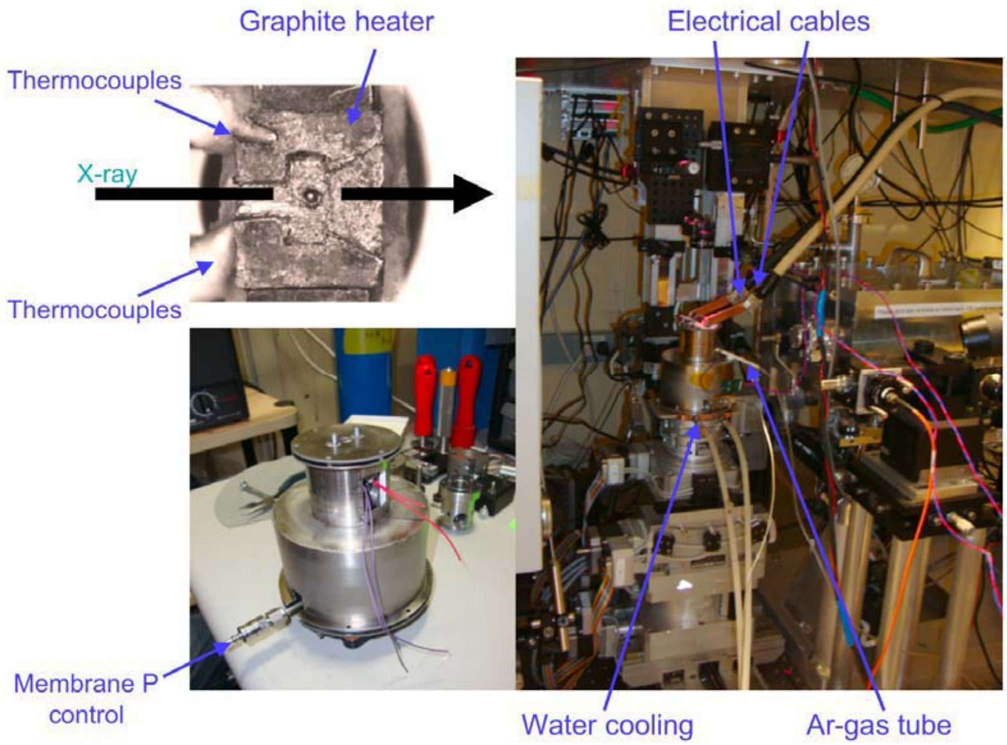

Figure 2. (Upper left) Image of the lower half of the diamond and cell juxtaposed with the graphite heater and thermocouples (the diamond is visible as the small circle in the center); (Lower left) The apparatus at ambient conditions showing the feedthrough for the membrane pressure control system; (Right) Image of the apparatus prior to a heating experiment.

Improvements and New Directions

The notable aspect of this apparatus is that there are a number of possible ways to prospectively improve its performance. At the simplest level, the water cooling associated with the system needs to be improved to access extreme conditions: the heat flow from the apparatus is such that at the highest temperature conditions, there were legitimate concerns that either the leads or portions of the apparatus might access a eutectic (and melt) or irreversibly deform. Similarly, the thermal shielding associated with the system needs to be markedly enhanced (Fig. 4): substantial radiative losses occurred at the highest-pressure conditions. Furthermore, the current system is designed for radial diffraction experiments: relatively modest geometric modifications could be made to adapt it for axial diffraction applications. The key aspect of each of these changes is that they could be accomplished in a relatively short timeframe: we view 6 months as a perfectly reasonable timeframe for conducting a sequence of moderate design modifications to the system, conduct a sequence of tests to characterize the effectiveness of these changes (including calibration runs on materials with reasonably well-constrained melting curves), and document the detailed design of the system (and each design modification) for access by, and distribution to, the broader COMPRES community. This is, we believe, the type of advancement in capabilities for the high-pressure community that COMPRES was designed to spearhead—and holds the prospect of placing the U.S. high-pressure geosciences enterprise in a clear world leadership role in external heating at high pressures.

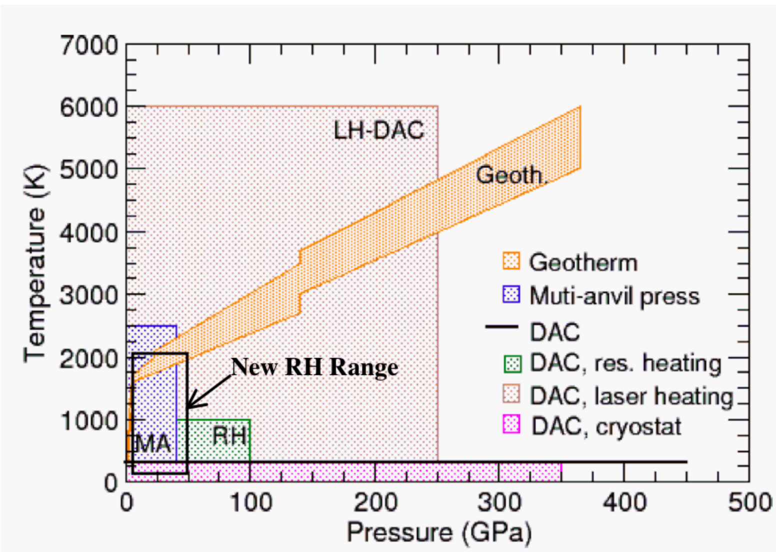

Figure 3. Pressure-temperature ranges of different experimental techniques; green box denotes a (slightly conservative) estimate of prior resistive heating capabilities; the black box denotes the new range already demonstrated at the ALS (Figure modified from S. Sinogeikin's modification of G. Shen's figure).

Additional development possibilities will also be probed during the period of funding: the configuration at ALS beamline 12.2.2 is particularly amenable to simultaneously laser-heating within a resistively-heated cell because of the ideal geometry of laser beam, X-ray and DAC axis in radial diffraction (Miyagi et al. 2008). Substantial prospects hence exist to both access higher temperature conditions, but also (and perhaps more importantly) to access higher temperatures with markedly minimized temperature gradients, and larger laser-heated spots—a configuration that could prove particularly valuable for (for example) accurate high-pressure and temperature melting studies, or characterization of solid-solid phase boundaries.

This project will be a coordinated effort between the ALS 12.2.2 beamline team and the UCB group on campus. Close collaboration will be maintained with Lowell Miyagi and Peter Liermann (now at DESY) who spear-headed resistive heating for radial diffraction geometry.

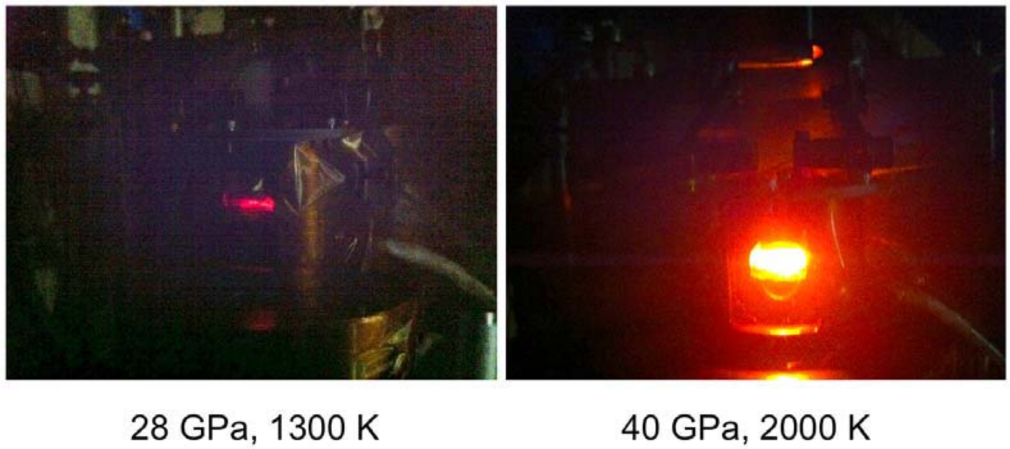

Figure 4. Images of the apparatus during a high-pressure, high-temperature experiment.

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C.6 Mineral Physics Educational modules for advanced undergraduates and graduate students

Pamela Burnley, High Pressure Science and Engineering Center and Department of Geosciences, University of Nevada Las Vegas

I propose that COMPRES assemble a group of web-based educational modules for a course entitled "Introduction to Mineral Physics". Although the modules would be designed to function as part of a full semester course, each module would also be able to stand alone. The modules would be targeted at entry level graduate students and advanced undergraduate students. The materials would be designed to be compatible with common distance learning platforms. Potential users would include COMPRES members teaching "bricks and mortar" classes at their own institutions, COMPRES members teaching in a distance education setting, mineralogy teachers interested in including supplementary material in their mineralogy class, undergraduates doing independent study projects and graduate students and colleagues in other subdisciplines who wish to brush up on a mineral physics topic. The modules would reside on the COMPRES web site and or on the SERC web site. The existence of the modules would facilitate the creation of graduate distance education courses in mineral physics that could serve mineral physics graduate students nationwide. The creation of such courses would address current problems faced by faculty in state universities where rising minimum enrollments are making it difficult to teach a suitable graduate course to incoming students.

Module Format:
Each module would cover a week's worth of material for a 3 credit hour class.

1. Learning outcomes for module
2. Introductory overview (text with figures)
3. Reading list or pdfs of relevant readings if copyrights can be obtained.
4. Short lectures (Powerpoint with voice)
5. Homework sets:
    a. Exercises, if possible using existing web resources and programs (e.g. RRUFF, VESTA)
    b. Problems with full solutions
    c. Problems with answers only
    d. Essay questions
6. Video virtual tours of relevant facilities, for example:
    i. a Multi-anvil lab
    ii. a synchrotron
    iii. a DAC lab
    iv. a Raman lab
    v. a shock lab
7. Lists of reference works, web based compilations etc.
8. Test questions with solutions (available on request for faculty only)

Possible Modules (suggestions welcome):

Structure and chemistry of Earth's interior
Introduction to high pressure techniques
  - Temperature measurement
  - Pressure calibration and pressure scales

In depth look at shock wave studies
In depth look at LVP & DAC techniques
Introduction to tensor math – stress, strain and elasticity
Plastic Deformation at high pressure
Diffusion and other transport properties
Raman & IR spectroscopy
Brillouin spectroscopy
Mossbauer spectroscopy
Thermodynamics at high pressure
  - EOS
  - Thermal expansivity & Heat capacity
  - Solution calorimetry of high pressure phases
  - Phase equilibria

Phase Transformations
Synchrotron diffraction techniques
Neutron diffraction

Time line:

January – May 2011
  - Gather content and create 4 modules:
    1. Structure and chemistry of Earth's interior
    2. Introduction to high pressure techniques
       - Temperature measurement
       - Pressure calibration and pressure scales
    3. In depth look at shock wave techniques and studies
    4. In depth look at LVP & DAC techniques and studies
  - Get feedback on module content from expert practitioners and teaching faculty
  - Investigate formats and smoke test modules
  - Package modules for distribution

C.6 Workshop Proposals for Year #5 of COMPRES II

During Years #1-4, COMPRES has supported 9 workshops in two categories:
a. Cultivate and expand the user base for national laboratory facilities.
b. Nurture new funding initiatives.
See list of those from 2007-2009 in Section A.3 above.

In Year #5, we request funding for additional workshop and cite two examples below, for which funding has already been approved by the Executive Committee on the recommendation of the Infrastructure Development Committee. We anticipate funding an additional 4-6 workshops in 2010.

COMPRES Nanofabrication in the DAC and FIB Techniques
Carnegie Institution of Washington

Organizer:
Yingwei Fei
fei@gl.ciw.edu
Scope and goals of the summer school

Particpants will get lectures on the theory and practice of the Focused Ion Beam technology for preparing micro-specimens of samples for high-pressure research. Hands-on practicum will be performed using the newly installed FIB at the Carnegie Institution of Washington.

Workshop "Evolutionary crystal structure prediction using the USPEX code: discovery of new materials and mineral phases"
Organizer: Artem R. Oganov (Stony Brook, USA)
Steering committee: Artem R. Oganov (Stony Brook, USA), Renata M. Wentzcovitch (U. Minnesota, USA), Andriy O. Lyakhov (Stony Brook, USA), Salah E. Boulfelfel (Stony Brook, USA).
Proposed dates and venue: 5 – 8 September 2011, Stony Brook (USA).

Rationale and outline: Prediction of the atomic structure of matter is crucial for understanding the physics and chemistry of materials [1], yet until recently was thought to be impossible [2]. A series of recent methodological developments [3-7] helped to make this problem tractable and demonstrated numerous successes. This direction of research is creating a scientific and technological revolution in our times. Among the existing methods, the most widely used one is the evolutionary algorithm USPEX [6,7], implemented in the same-name freely distributed code (http://han.ess.sunysb.edu/~USPEX). USPEX has outperformed all the other methods in a recent blind test of inorganic crystal structure prediction [1]. Today, the USPEX code is utilized by nearly 200 researchers worldwide and has resulted in major advances – such as the discovery of a transparent phase of sodium, partially ionic structure of boron, and a new superhard allotrope of carbon [8-10]. The importance of the discovery of new crystal structures in geosciences is well illustrated by the recent discovery of $MgSiO_3$ post-perovskite [11-13], which has explained many anomalies of the Earth's D" layer

This workshop aims at training a new generation of computational mineral physicists and materials scientists in this area of research, and at making experimentalists aware of and be able to use the latest theoretical developments for their needs. Such interdisciplinarity will be useful for the participants, who will have an opportunity to learn from other related fields of research. The participants will have detailed tutorials on structure prediction for crystals, surfaces and nanoparticles and the USPEX code and how to analyze the rich data provided by this method using specifically developed advanced tools [14]. These tutorials will allow the students to tackle a range of problems from Earth sciences, crystallography, and surface science. There will be a plenty of time for discussions (15 minutes at the end of each talk, and informal discussions during free parts of the day). The workshop will include local excursions, beach walk and a banquet.

Venue: The workshop will be held at Stony Brook, the site of a flagship SUNY campus. Stony Brook University is one of the best public universities in America and home to the internationally renowned Mineral Physics Institute and New York Center for Computational Sciences. Stony Brook is also the center of development of the USPEX method and code, the most widely used tool for predicting the structure of materials. Located in a beautiful part of Long Island, near a myriad of beaches and relaxed historical villages, Stony Brook is the perfect place for conducting this workshop.

D Budget Request for Year #5 of COMPRES II [June 1, 2011 to May 31, 2012]

All numbers in $K

D.1 Community Facilities-operational budgets

$249	for ops	West Coast Synchrotron Facilities [Q. Williams]
$337.5	for ops	X-ray Diamond-anvil cell facilities at the NSLS [T. Duffy and D. Weidner]
$40	for equip	[Ops funds includes $42K to Princeton and $250K to Stony Brook]
$255	for ops	Infrared Diamond-anvil facilities at the NSLS [R. Hemley and Z. Liu]
$14	for equip	
$404	for ops	Multi-anvil X-ray Facility at the NSLS [D. Weidner and M.Vaughan]
$21		
$25		Beamline user housing
$0		Subawards IDC
$1270.5	for ops	Total operational budget for Community Facilities
$75	for equip	See details above

D.2 Infrastructure Development Projects

$76.1	Inelastic X-ray Scattering at High P & T: A New Capability for the COMPRES Community [E. Alp, J. Jackson]
$78.8	Multi-anvil Cell Assembly Initiative: New Developments and Production [K. Leinenweber, T. Sharp, and J. Tyburczy]
$38.7	Postdoc for Gas-Loading system at GSECARS [M. Rivers]
$61.8	Educational Modules [P. Burnley]
$60	Detector, contribution for PUP proposal with Sector 3 of the APS [A. Alatas, J-f Lin]
$90	Workshops (5 to 7 per year)
15.5	Elasticity database (1/4-time grad student) [Bass]
$0.4	Subawards IDC
$331.3	Total for Infrastructure Development projects (not including workshops)

D.3 Other COMPRES Activities

$222.5 **Other Community Activities** which includes

- $62.5 Annual Meeting ($60K subaward to Stony Brook and $2.5K at UIUC)
- $30 Travel for committees
- $18 COMPRES lecture series
- $25 Beamline housing
- $90 Workshops

$497.9 **Central Office** which includes: [all items have indirect costs incorporated]

- $438.7 Salaries and fringe benefits
- $21.2 Materials and Supplies
- $35 Travel
- $3 Website services

$723.4 Total for Other COMPRES Activities

TOTAL BUDGET REQUEST FOR YEAR #4 OF COMPRES II

$1270.5	**Operational costs for Community Facilities**
$75	**Equipment upgrades for facilities**
$331.3	**Infrastructure Development Projects**
$225.5	**Other Community activities**
$497.9	**Central Office**
$2400K	**Total of budget request**