Year 2 Annual Progress Report 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

1 March 2009

2008 Annual Meeting of COMPRES at Cheyenne Mountain Resort in Colorado

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A COMPRES Year 2: Overview

A.1 Executive Summary

In the first 18 months of COMPRES II [June 2007 to December 2008], , 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.

The management of these 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 53 U. S. institutions which are voting members of COMPRES [the Electorate] and another 33 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 year.
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]
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].

In this section of the Annual Report for Year #2, 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 #3 [June 1, 2009 to May 31, 2010]; 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.

- A new gas-loading system for diamond-anvil cells has been constructed and commissioned with COMPRES support at the GSECARS facilities at the APS by Mark Rivers and his team. The system is now "open for business" and many investigators have already taken advantage of it. Until other systems are constructed and made available to the user community at the NSLS and the ALS, COMPRES will fund a half-time postdoc at GSECARS to train users and provide mail-in service to others. See Section C.3 and photo in Supplementary Documents.

- A team from Abby Kavner's laboratory at UCLA has conducted experiments at beamline X17C of the NSLS on osmium metal, which is a proxy for iron at high P and T. See M. Weinberger et al in Section B.1.

- A team from Thomas Duffy's laboratory at Princeton has studied hydrous wadsleyite at beamline X17C of the NSLS using single-crytal X-ray diffraction and Brllouin scattering. See Z. Mao in Section B.1.

- A team from the Geophysical Laboratory has used beamline U2A to discover a metallic state of silane, a hydrogen-rich material. See X. Chen in Section B.2.

- The first shock-wave experiments at a synchrotron were conducted by a team from the Sandia National Laboratory in Los Alamos at beamline U2A of the NSLS. See R. Malone et al. in Section B.2.

- Measurements of Q and elastic dispersion at beamline X17B2 of the NSLS led to the discovery of the softening of the bulk modulus during phase transitions relevant to the Earth's mantle. See L. Li and D. Weidner in Section B.3.

- New measurements of activation volume in olivine under anhydrous conditions were conducted at beamline X17B2 of the NSLS using cell assemblies designed in collaboration with the multi-anvil cell development project at ASU. See W. Durham et al. in Sections B.3 and C.1.

- A team led by Michael Walter of the University of Bristol [UK] has studied the behavior of primary carbonatite melts using beamline 12.2.2 at the ALS. See M. Walter et al. in Section B.4.

- A team from Dan Shim's laboratory at MIT has studied the equation-of-state of $NaMgF_3$ using beamline 12.2.2 at the ALS. See J. Hustoft et al in Section B.4.

- Lisa Danielson of the NASA Johnson Space Center has performed in suit hgigh P-T experiments on the Allende meteorite at the GSECARS beamlines of the APS using cell assemblies designed in collaboration with the multi-anvil cell development project at ASU. See L. Danielson et al in Section C.1.

- A team led by Jung-Fu Lin of the University of Texas at Austin has studied the intermediate-spin state of ferrous iron in lowermost mantle post-perovskite and perovskite at beamline XOR-3 of the APS with support from the NRIXS development project at UIUC and ANL. See J-F. Lin et al in Section C.2.

- A team led by Jie Li of UIUC has studied a pressure-induced magnetic transition and sound velocities in Fe_3C at beamline XOR-3 of the APS with support from the NRIXS development project at UIUC and ANL. See. L. Gao et al in Section C.2

- A team led by Jay Bass of UIUC has studied the post-stishovite phase transition in hydrous-bearing SiL2 using the Brillouin spectroscopy system developed by COMPRES and GSECARS and installed and on the 13 BM beamline at the APS. See D. Lakshtanov et al in Section C.4.

- A new gas-loading system for diamond-anvil cells has been constructed and commissioned with COMPRES support at the GSECARS facilities at the APS by Mark Rivers and his team. The system is now "open for business" and many investigators have already taken advantage of it. Until other systems are constructed and made available to the user community at the NSLS and the ALS, COMPRES will fund a half-time postdoc at GSECARS to train users and provide mail-in service to others. See Section C.3 and photo below and in Supplementary Documents.

A.3 Meetings and Workshops

The following meetings and workshops were sponsored, at least in part, by COMPRES:

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

The Second VLab Workshop
August 5-10. 2007
Minnesota Supercomputing Institute
Organizer: Renata Wentzcovitch, University of Minnesota

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

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 2008, there were 51 U. S. institutions which were members of COMPRES and 31 affiliate institutions overseas. In the past year, four U. S. institutions have become members of COMPRES:

Stanford University: Wendy Mao, Elector; Jonathan Stebbins, Alternate Elector.

Texas A&M University: Caleb Holyoke, Elector; Andreas Kronenberg, Alternate Elector,

Harvard University: Sarah Stewart-Mukhapadhyay, Elector; Richard O'Connell, Alternate Elector

University of Texas at Austin: Jung-fu Lin, Elector; Stephen Grand, Alternate Elector.

These additions brought the the membership list to 55 U. S. institutions.
Both Georgia State University and the University of Vermont have requested that their memberships be suspending pending appointment of new faculty in mineral physics.
These actions leave COMPRES with 53 active U. S. members..

In addition, the following overseas institutions became affiliate members of COMPRES;

China University of Geosciences in Wuhan: Zhenmin Jin, Representative.

Macquarie University in Australia: Tracy Rushmer, Representative.

This brings the list of foreign members to 33.

COMPRES US Member Institutions

Institution	Elector	Alternate
Argonne National Laboratory	Wolfgang Sturhahn	Marcos Grimsditch
Arizona State University	Thomas Sharp	James Tyburczy
Auburn University	Jianjun Dong	
Azusa Pacific University	Donald Isaak	
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	Yusheng Zhao	Gary Chesnut
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	Anurag Sharma	John Schroeder
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	Jay Bass	Jie Li
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	David Kohlstedt
University of Missouri - Kansas City	Michael Kruger	Ray Coveney
University of Nevada at Las Vegas	Oliver Tschauner	Malcolm Nicol
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 University	Nancy Ross	Ross Angel
Yale University	Shun-ichiro Karato	Kanani K.M. Lee

COMPRES Foreign Affiliates

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	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)	Frank Schilling
Harbin Institute of Technology (China)	Haozhe Liu
Institut de Physique du Globe Paris (France)	Guillaume Fiquet
Institute of Experimental Mineralogy, Chernogolovka (Russia)	Yuriy Litvin
Johann Wolfgang Goethe Universitat	Bjorn Winkler
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
Royal Institution of Great Britian, The (United Kingdom)	Paul McMillian
Ruhr-Universitat Bochum (Germany)	Sumit Chakraborty
Seoul National University (Korea)	Haemyeong Jung
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 Manchester (United Kingdom)	Alison Pawley
University of Tokyo (Japan)	Takehiko Yagi
University of Wales at Aberystwyth (United Kingdom)	Martin Wilding
University of Western Ontario (Canada)	Rick Secco
Vrije Universiteit (The Netherlands)	Wim van Westrenen
Yonsei University (Korea)	Yongjae Lee

A.5 Information Technology and Communications

Web Site

Internet technology presents COMPRES with numerous options for implementing organizational services for its members and for developing an attractive and useful interface with the educational and public communities. For the mineral physics community, it can provide a centralized location for information on important events, job openings, detailed information on the organization and management of COMPRES, and streamlined systems for finding information, applying for facilities time and registering for events. It projects our organization to the world and is one of the first impressions we will make on people who are not familiar with COMPRES and its work. In order to realize the benefits that Internet technology makes possible, COMPRES has established a Web site with a new URL link address http://www.compres.us; all of the files related to the COMPRES website are still physically located on the http://www.compres.stonybrook.edu server and are being maintained by Glenn Richard, Emily Vance, and Michael Vaughan. At present, the COMPRES site provides the following information:

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.stonybrook.edu/ScienceHighlights/index.html

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

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]

  COMPRES Booth Powerpoint presentation at December 2007 AGU

  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.stonybrook.edu:8080/COMPRESImageLibrary/index.html]

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.

In collaboration with a web consulting firm on Long Island, we are revising our website, and will engage an off-campus site for hosting it in the future. Example of the new Home Page is given below; we hope to have this new site in place by May 2009.

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 acquired a host bridge to provide support for video conferences of the Executive Committee, the two Standing Committees, and other uses of the COMPRES community.

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 www.compres.us/Newsletter/. See COMPRES Home Page for the latest issue for October 2008.

In addition to a column in the quarterly COMPRES newsletter, the President of COMPRES [Robert Liebermann] has sent a Monthly Message to the COMPRES community using the listserv distribution, beginning in October 2003 [see link at: http://www.compres.stonybrook.edu/Publications/Monthly%20Messages%20from%20COMPRES%20President/Index.html]. 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.

June 2008 issue of *Elements* on “”Deep Earth and Mineral Physics.”

Jay Bass and John Parise served as Guest Editors of the most recent issue of Elements in June 2008. This issue includes fine articles on Elastic Properties by Bass, Stas Sinogeikin and Baosheng Li, on the Upper Mantle and Transition Zone by Dan Frost, on the Lower Mantle and Core by Guillaume Fiquet, François Guyot and James Badro, on Post-perovskite and the CMB by Kei Hirose and Thorne Lay, and on Rheology Studies by Shun Karato and Don Weidner. There is also a very thoughtful editorial by Bruce Watson on “Scientific Frontiers and Risky vs Safe Science.”

A.6 Publications of COMPRES in 2007-2008

[BEAMLINE OR INFRASTRUCTURE PROJECT GIVEN IN CAPS BELOW]

2007

Antao, S., I. Jackson, B. Li, J. Kung, J. Chen, I. Hassan, R. Liebermann and J. Parise (2007). High-temperature elasticity, cation disorder and magnetic transition in magnesioferrite. Phys Chem Min **34**: 345-350. MAC NSLS

Back, A., I. Halevy, I. Yaar, S. Kahane, O. Levy, E. Auster, H. Ettedgui, E. Caspi, M. Ganor, O. Rivin (2007). TDPAC study of the intermetallic compound HfB2. XII International Conference on Hyperfine Interactions, Iguazu Falls, Brazil, Aug , p. 128, (2007). X17 DAC

Bass, J., S. Sinogeikin, B. Li (2007). Elastic Properties of Minerals: A Key For Understanding the Composition and Temperature of Earth's Interior. Elements (submitted). MAC NSLS

Biswas, K., D. Muthu, A. Sood, M. Kruger, B. Chen, C. Rao (2007). Pressure-induced phase transitions in nanocrystalline ReO3. J. Phys.: Condens. Matter **19(436214)**. X17 DAC

Botez, C., J Hermosillo, J Zhang, J Qian, Y Zhao, J Majzlan, R Chianelli, C Pantea (2007). High-Temperature Phase Transitions in CsH2PO4 Under Ambient and High-Pressure Conditions: A Synchrotron X-ray Diffraction Study. J. Chem. Phys. **127(194701)**. MAC NSLS

Botez, C. C. R., Zhang J, Qian J, Zhao Y., Majzlan J, and Pantea C (2007). Evidence for a structural transition to the superprotonic phase of CsH2PO4 under high pressure. Submitted to J. Phys. Chem. MAC NSLS

Caldwell, W. A. K., M.; Celeste, R.S.; Domning,E.E; Walter, M.J; Walker, D.; Glossinger, J.; MacDowell, A.A.; Padmore, H.A.; Jeanloz, R.; and Clark, S (2007). Laser Heated Diamond Anvil Cell at the Advanced Light Source Beamline 12.2.2. Nuclear Instrumentation and Methods in Physics Research **Section A 582**: 221-225. ALS

Carpenter, M. A. B. L., R. C. Liebermann (2007). Elastic anomalies accompanying phase transitions in (CaSr)TiO3 perovskite III: experimental investigation of polycrystalline samples. Am. Min.. **92**: 344-355. MAC NSLS

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Zhang, J., Y Zhao, R Hixson, G Gray lll, L Wang, W Utsumi, S Hiroyuki, H Takanori (2008). Experimental Constraints on the Phase Diagram of Titanium Metal. J. Phys. Chem. Solids **69(10)**: 2559-2563. MAC NSLS

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2009

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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 2008-2009

Distinguished Lecturer Program

COMPRES requested $6,000 in funds to support a distinguished lecture series 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. Travel expenses are provided by COMPRES, and local subsistence expenses are to be provided by the host institutions [to be chosen on the basis of applications in response to ads in EOS and on the COMPRES website]. On the basis of 2 lecturers and 4 lecture visits each @$500 per visit, plus advertising costs and logistics, we estimated $6,000 for the first year of this new initiative.

The Distinguished Lecturers for COMPRES in 2008-2009 are:

Wendy Mao of Stanford University will visit
University of Illinois at Chicago
University of California Davis

David Walker of Columbia University will visit
University of Nevada at Las Vegas
University of Illinois at Urbana-Champaign
Case Western Reserve University
University of Tennessee at Knoxville

We plan to continue this program in 2009-2010 and have requested $8,000 for this purpose. By more extensive advertizing in EOS and Earth [the successor to Geotimes], we hope to attract invitations from more undergraduate liberal arts & sciences colleges and community colleges, which may be less familiar with the field of mineral physics.

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

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 will be 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.

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

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 can be found at:
http://www.compres.stonybrook.edu/People/Committees/ExComm%20Pol%20&%20Proc-revised%2010%20June%202004.doc

Current members and affiliation (term of service)

Quentin Williams, **Chair [2007-2010]** (831) 459-3132 (quentw@rupture.ucsc.edu)
2004-2010
Carl Agee, **Vice Chair [2008-2010]** (505) 277-1601 (agee@unm.edu) 2007-2010
Jay Bass, (217) 333-1018 (bass@hercules.geology.uiuc.edu) 2002-2009
James Tyburczy, (480) 965-2637 (jim.tyburczy@asu.edu) 2008-2011
Donald Weidner, (631) 632-8211 (dweidner@sunysb.edu) 2002-2010

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.

A statement of the Polices and Procedures for the COMPRES Facilities Committee can be found at:
http://www.compres.stonybrook.edu/People/Committees/4%20June%202004%20Pol%20and%20Proc--Fac%20Comm.doc

Current members and affiliation (term of service)

Thomas Duffy, **Chair [2007-2009]** (609) 258-6769 (duffy@princeton.edu) 2007-2010
Andrew Campbell (301) 405-4086 (ajc@umd.edu) 2008-2011
Charles Lesher (530) 752-9779 (lesher@geology.ucdavis.edu) 2006-2009
Wendy Panero (614) 292-6290 (panero.1@osu.edu) 2006-2009
Yanbin Wang, (630) 252-0425) (Wang@cars.uchicago.edu 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.

A statement of the Polices and Procedures for the COMPRES Infrastructure Development Committee can be found at:
http://www.compres.stonybrook.edu/People/Committees/June%204%202004%20Infrastructure%20Development%20Comm--Policies%20and%20Procedures%204%20June%202004.doc

Current Members and affiliation (term of service)
Thomas Sharp, **Chair [2008-2010]** (480) 965-3071 (Tom.Sharp@asu.edu) 2006-2010
Nancy Ross (540) 231-6356 (nross@vt.edu) 2003-2009
Steven Jacobsen (847) 467-1825 (steven@earth.northwestern.edu) 2008-2011
Jie Li (217) 333-3540 (jackieli@uiuc.edu) 2008-2011
Sang-Heon Dan Shim (sangshim@MIT.EDU) 2004-2010

Advisory Council
Members and affiliation (term of service)
Wang-ping Chen, University of Illinois at Urbana-Champaign [2006-2009]
Edward Garnero**,** Arizona State University [2008-2011]
Chi-Chang Kao**,** Brookhaven National Laboratory [2003-2011]-appointment renewed
Louise Kellogg, University of California at Davis [2007-2010]
William McDonough, University of Maryland [2007-2010]
Malcolm Nicol**,** University of Nevada at Las Vegas [2006-2009]

On 25 June 2008, the Advisory Committee met with the Executive Committee just prior to the start of the Seventh Annual COMPRES Meeting in Cheyenne Mountain, Colorado. The term of one of the founding members of the Advisory Council ended at Cheyenne Mountain: Guy Masters. We especially wish to thank him for their service during the formative years of COMPRES and hope that they will feel welcome to attend future annual meetings of our community.

Finally, we would like to welcome the new member of the Advisory Council for three-year terms commencing June 2008::

Edward Garnero from Arizona State University

Relationship to National Facilities

- GSECARS: COMPRES will review the high pressure facilities and assure highest service to the user community.
- NSLS: COMPRES funds Multi-anvil and Diamond-anvil facilities at NSLS. COMPRES will review the high pressure facilities and assure highest service to the user community.
- ALS: COMPRES funds Diamond-anvil facilities at ALS. COMPRES will review the high pressure facilities and assure highest service to the user community.
- ORNL: Members of the COMPRES community [J. Parise, H-k. Mao, R. Hemley and C. Tulk] have succeeded in obtaining DOE funding to build a high pressure facility at the Spallation Neutron Source that is now open for general users. COMPRES will work to build the user community and assure access to this facility.

Operation of the COMPRES Central Office

The Central Office of COMPRES is located at Stony Brook University in the ESS Building, in an office complex shared with the Mineral Physics Institute [MPI], which is directed by Donald Weidner.

The Central Office staff includes Robert Liebermann, the President of COMPRES (from September 2003) and Emily Vance, Administrative Coordinator, both of whom are supported by the COMPRES Cooperative Agreement with the NSF. Ms Vance succeeds Ms. Ann Lattimore, who retired in November 2007 following 27 years of outstanding service to the mineral physics research programs at Stony Brook University, the last 5 of which were dedicated to COMPRES.

The administrative operation of COMPRES is also supported by the following personnel who are employees of the Mineral Physics Institute of Stony Brook University: Glenn Richard, Educational Coordinator: COMPRES role: Web Manager and Education/Outreach activities. Michael Vaughan, Research Associate Professor: COMPRES role: Manager of listserv and database. Samantha Lin, Administrative Assistant: COMPRES role: Video-conferencing logistics; cooperate with Ms. Vance to provide administrative support to COMPRES activities.

In September 2007, Professor Chen moved from Stony Brook University to the Florida International University in Miami; we are pleased to report that he has agreed to continue to edit the COMPRES Newsletter from FIU.

Note:
In June 2008, the Executive Committee appointed a Search Committee to identify a successor to Robert Liebermann. Members of this Search Committee are: Abby Kavner from UC Los Angeles as Chair, Harry Green from UC Riverside, Russell Hemley from the Carnegie Institution of Washington, Guy Masters from UC San Diego, and John Parise from Stony Brook University. The new President is to take up their duties between September 2009 and February 2010.

Special Committee on Incorporation of COMPRES

In September 2007, the Executive Committee appointed a Special Incorporation Committee to explore the implications of incorporation for COMPRES. This Committee is chaired by Jay Bass and includes Michael Brown from the Executive Committee and Louise Kellogg and Guy Masters from the Advisory Council. At the Fall 2007 AGU Meeting, the Incorporation Committee met with representatives of other Earth Science consortia and centers, including:
Adam Dziewonski—IRIS
Rick Hooper-CUASHI
Meghan Miller-UNAVCO
David Simpson—IRIS

The committee report was submitted to the Executive Committee in March 2008 and may be found on the COMPRES website at:
\\sbmp80\Compres_website\Publications\Incorporation Report REV 3-08pdf.pdf

The committee concluded that there were no compelling reasons for COMPRES to incorporate at this time, but that COMPRES should reevaluate the incorporation issue periodically, especially if one or
more of the following changes occur:
(1) There is an increase in its scientific advising or lobbying activities in Washington DC.
(2) COMPRES is funded by multiple agencies. At present, all of COMPRES funding comes from the NSF EAR division.
(3) The COMPRES constituency requests that the organization not be tied to a home institution.

A.9 President's Narrative

2008 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, largely drawn from my Monthly Messages to the COMPRES community and from the President's column in the Quarterly Newsletter.

At the March 2008 Meeting of the American Physical Society in New Orleans, Boris Kiefer of New Mexico State University and I convened Focus Sessions on Earth and Planetary Materials; these sessions included invited talks by John Brodholt [University College London] and Jonathan Crowhurst [Lawrence Livermore National Laboratory]. Russell Hemley also convened a Town Hall Meeting on "Materials Physics at Gigabar Pressures" which featured invited talks by Raymond Jeanloz, David Stevenson and Richard Martin.

On March 21-23, I attended a special symposium at the Institute for Study of the Earth's Interior at Okayama University in Misasa, Japan. This symposium was sponsored by the Center of Excellence-21 program at ISEI to mark the retirement of Eiji Ito after 40 years of pioneering research in high-pressure mineral physics. In the last month of his formal employment, Ito-sensei achieved pressures of 85 Gpa in a double-stage, Kawai-type apparatus interfaced with the synchrotron at Spring-8; he thus fell a little short of his lifelong dream of reaching a megabar in a large-volume, multi-anvil apparatus.

Among the invited speakers at this international symposium were George Cody, Kei Hirose, Albrecht Hofmann, Trevor Ireland, Eiji Ito, Ian Jackson, Shun Karato, Jung-Fu Lin, Dan McKenzie, Bjorn Mysen, David Rubie, Andrew Steele and Michael Zolensky.
It was a special pleasure for me to contribute to the Ito Symposium and to toast Ito-sensei at the banquet in his honor. One of his many contributions to high-pressure mineral physics is having his Uniaxial Split-Sphere Apparatus-5000 in Misasa serve as the model for similar apparatus at the University of Alberta, Bayreuth Geoinstitut, and Stony Brook University.

At the meeting of the European Geosciences Union in Vienna, Austria, three members of the COMPRES community were honored:

a. Brian Evans was awarded the 2008 Louis Néel Medal.
b. Richard O'Connell was awarded the 2008 Augustus Love Medal.
c. Artem Oganov was awarded the Research Excellence Medal of the European Mineralogical Union.

These distinctions, in addition to recognizing their significant achievements, bring honor and visibility to the community of mineral and rock physicists throughout the world.

On May 29-30, I attended the Joint Assembly in Ft Lauderdale, Florida where I had the pleasure of honoring the following new AGU Fellows from mineral physics at the Honors Ceremony and Banquet:

Patricia Dove from Virginia Tech
Greg Hirth from Brown University
Tetsuo Irifune from Ehime University in Japan
Renata Wentzcovitch from the University of Minnesota

I also attended the Union symposium on the Deep Earth convened by Andy Campbell, Jiuhua Chen and Dan Shim.

While in Florida, I took the opportunity to visit the labs of Surendra Saxena and Jiuhua Chen at the Florida International University, the only COMPRES institution in the state. Chen joined the faculty in September 2007, and he has recently replaced Saxena as the Elector for FIU. He also has agreed to continue to serve as Editor of the COMPRES newsletter, which we expect to publish twice a year in steady-state.

From June 4-6, I attended the 2008 IRIS Workshop at the Skamania Lodge on the Columbia River in Stevenson, Washington, along with 280 other scientists. There was a special session on "Integration of Seismology and Mineral Physics", with a keynote talk by Tom Duffy of Princeton University on "Hydrogen in the Upper Mantle: Are the Water-Rich Regions Red or Blue?" Skamania Lodge is an excellent venue for such meetings and COMPRES should consider booking it for 2009 or 2010.

On June 29-July 4, I attended the GRC on High Pressure at the University of New England in Biddeford, Maine. Although this year's conference was thin on geoscience, among the featured speakers were Natalia Dubrovinskaia, Chris Tulk, Baosheng Li, Jeffrey Yarger, and Leonid Dubrovinsky. This is the longest, continuous Gordon Research Conference, starting in 1955. Among the attendees in 2008 who also attended the GRC in Meriden, NH in 1968 were: Neil Ashcroft (last minute cancellation due to illness), Dattatraya Dandekar, and Bob Liebermann. Malcolm Nicol missed the 1968 meeting, but earns pride of place for his attendance at the 1966 meeting.

The Cooperative for Deep Earth Research [CIDER] hosted its summer program at the University of California Santa Barbara campus from June 22 to August 8. Among the featured mineral physics instructors in the tutorial portion of this program were Abby Kavner from UCLA, Jie (Jackie) Li from UIUC and Bob Liebermann.

On September 17-19, I attended a Workshop on Long Range Science Plan for Seismology [LRSPS] convened by IRIS in Lakewood, Colorado. More than 120 seismologists gathered for this workshop, with three attendees from other geoscience disciplines: Thorsten Becker and Louise Kellogg from Geodynamics and Bob Liebermann from Mineral Physics. The organizers used the 2004 Bass Report as a model of what the NSF-EAR was asking them to do on behalf of the seismological community.. Also, the importance of "mineral physics" data and theory was invoked many times in the LRSPS workshop. Details may be found at: http://www.iris.edu/hq/lrsps.

Quentin Williams, Wang-Ping Chen and Bob Liebermann visited the consulting firm of Lewis-Burke Associates and met with four senior members of their staff, each with specialization in different federal agencies [NSF, DOE, NASA, NIH and Education & Outreach]. Three U. S. member institutions of COMPRES are clients of Lewis-Burke: Caltech, New Mexico State University, and the University of Illinois at Urbana-Champaign. The UIUC client relationship was the springboard for obtaining the meeting.

The staff at Lewis-Burke encouraged COMPRES to be pro-active in lobbying for science funding in Washington, including at the level of the White House Office of Science and Technology Policy.

They also urged us to showcase our involvement in Education & Outreach in all our communications and publications; examples include undergraduate students who come to the beamlines at the national laboratory facilities with their professors to participate in experiments. They reminded us that all members of Congress are very well aware of the lack of young people pursuing degrees and training in science and engineering.

On October 10, Tom Sharp [Chair], Steve Jacobsen and Jie Li of the Infrastructure Development Committee visited the APS to learn the progress on various infrastructure development projects supported by COMPRES, including:

CO_2-laser heated DAC
Brillouin spectroscopy
D-DIA 30 apparatus
Gas-loading for DACs
Johnson noise
HRIXS, NRIXS and SMS at high P&T

On October 20-21, I attended a Workshop on Midterm Renewal of the Advanced Photon Source at Argonne National Laboratory as a member of the science panel for Geological, Environmental and Planetary Sciences, which is chaired by Neil Sturchio of the University of Illinois at Chicago; Russell Hemley and Steve Sutton also serve on this panel. Planning focused on the period 2009-2014, during which the APS anticipates major developments in X-ray optics and X-ray detectors, but with no upgrades to the source [that is deferred until after 2020].

In November 2008, a Special Issue of PEPI on "Frontiers and Grand Challenges in Mineral Physics of the Deep Mantle" appeared. Jung-Fu Lin, Shun Karato, Jay Bass, Eiji Ohtani and Charles Prewitt served as editors of this speciall issue which contains sets of articles on

a. Transport and Rheological Properties
b. Elasticity
c. Phase Transition and Electronic State

with each set introduced by an article by one of the editors. See Vol. 170, Issues 3-4, Nov 2008.

Mineral physics and COMPRES featured prominently in the sessions and social activities of the Fall 2009 AGU Meeting in San Francisco, California in December 2008.

a. Scientific program

The Deep Interior and Mineral Physics sessions were very well-attended.
Our compliments and thanks to Heather Watson, Program Committee representative from Mineral and Rock Physics.

b. Honors

Our congratulations to James Badro who was awarded the James B. Macelwane Medal.

c. Mineral and Rock Physics Reception

Organized by Carl Agee, Chair of the Focus Group on Mineral and Rock Physics, this

reception was once again the best attended and attracted many people from throughout the sections of Tectonophysics, Seismology, Geodesy, and Volcanology-Petrology-Geochemistry.
At the reception, the 2008 Outstanding Student Award was presented to Innokenty Kantor from the Bayerisches Geoinstitüt.

On January 16, I served on an advisory panel for the Alfred P. Sloan Foundation to consider a new 10-year initiative to understand "Deep Carbon." This initiative is an outgrowth of a workshop organized by the Geophysical Laboratory of the Carnegie Institution of Washington in May 2008, and is being led by Robert Hazen and Russell Hemley. Additional details may be found at http://www.gl.ciw.edu/sloan_deep_carbon

New faculty appointments in mineral physics in the U. S. and overseas during the past year:
We take great pleasure in noting the following new faculty appointments in mineral physics:
Daniele Antonangeli
and
Anne-Line Auzende—both at the Institut de Minéralogie et de Physique des Milieux Condensés in Paris.
There have been a large number of faculty appointments at universities in Japan in the field of mineral physics recently, including:

Norimasi Nishiyama to Ehime University
Motohiko Murakami to Tohoku University
Takao Okuchi to Okayama University
Naotaka Tomioka to Okayama University
Daisuke Yamazaki to Okayama University
Takahashi Yoshino to Okayama University

Jung-feng Zhang to China University of Geosciences (Wuhan)
Sytle Antao to the University of Calgary
Jung-Fu Lin to the University of Texas at Austin
Lars Ehm to Stony Brook University

A number of mineral physics faculty have recently announced their transition to a new academic institution, including:
Lars Stixrude from the University of Michigan to University College London in 2008.
Carolina Lithgow-Bertelloni will also join the faculty of UCL.
Kanani Lee from New Mexico State University to Yale University in June 2008.
Falko Langenhorst from Bochum to the Bayreuth Geoinstitüt in June 2008.
Artem Oganov from the ETH-Zürich to Stony Brook University in November 2008.
Agnes Dewaele from the Commissariat à l'Energie Atomique in France to Stony Brook University in February 2009.

Membership in COMPRES

In the past year, we note the following changes in institutional membership of COMPRES.

U. S. Institutions

Stanford University: Wendy Mao, Elector; Jonathan Stebbins, Alternate Elector.
Texas A&M University: Caleb Holyoke, Elector; Andreas Kronenberg, Alternate Elector,
Harvard University: Sarah Stewart-Mukhapadhyay, Elector; Richard O'Connell, Alternate Elector
University of Texas at Austin: Jung-Fu Lin, Elector; Stephen Grand, Alternate Elector.

These additions brought the the membership list to 55 U. S. institutions.
Both Georgia State University and the University of Vermont have requested that their memberships be suspending pending appointment of new faculty in mineral physics.
These actions leaves COMPRES with 53 active U. S. members..

Foreign Affiliates

China University of Geosciences in Wuhan: Zhenmin Jin, Representative.
Macquarie University in Australia: Tracy Rushmer, Representative.
This brings the list of foreign members to 33.

A.10 Annual Program Plan and Budget Request for Year #3

In preparation for the submission of the Annual Progress Report and Annual Program Plan and Budget to NSF in February, 2009, 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 2008, the two Standing Committees asked the project directors of each of the subawards to submit annual progress reports for Year #2 and program plans and budget requests for Year #3 by November 1, 2008. 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, 2008.

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 2008 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 #3, to the Executive Committee. In the case of the Infrastructure Committee, this report included recommendations for initial funding of new projects and community workshops.

In January 2009, the Executive Committee met via video and teleconference on three occasions to discuss the reports of the Standing Committees and to formulate recommendations for an Annual Program Plan and Budget for Year #3. Following these meetings, the President 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]

Diamond Anvil Cell X-Ray Diffraction Facility

2008 COMPRES Annual report for beamlines X17C and X17B3
November 2007 – November 2008

Overview

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) together with 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. Both X17C and X17B3 beamline are available for energy dispersive (EDXD) and monochromatic (ADXD) experiments. The X17B3 beamline operates 33% of the time in dedicated mode with an additional 33% available in parasitic mode when the X17B2 (multi-anvil) station is running. This nominally provides a maximum of 54 days per cycle. In 2008, the total cycle days allocated for X17C was 207 and for X17B3 68.3.

The X17-DAC facility was the first dedicated high-pressure beamline in the world, and has been a workhorse for diamond anvil cell research for more than two decades. The facility has led the way in many developments that have now spread around the world. For example, X17 was the location of the first *in situ* x-ray diffraction (xrd) experiment with double-sided laser heating; the first cryogenic high-pressure xrd experiment, the first single-crystal xrd experiment above 60 GPa, and the first x-ray diffraction experiment on an amorphous material. The X17-DAC beamline remains one of the most productive beamlines at the NSLS. Since 2002, the beamline has recorded 144 publications, including 27 in premier journals.

From January 2007 – October 2008, there are 45 publications in the NSLS publication database for X17C and X17B3. Six of these are in NSLS-defined premier journals. Thus, the facility is continuing to maintain its high level of productivity. A total of 6 Ph.D. and 1 M.S. thesis in 2007-2008 have been based on work carried out in whole or in part at X17 (Table 1)

Table 1: PhD and MS theses at X17 (2007-2008)

C. Liyanage	U. Missouri – Kansas City	PhD	2007
E. Selvi	Texas Tech University	PhD	2007
R. Aksoy	Texas Tech University	PhD	2008
Z. Chen	New Jersey Institute of Technology	PhD	2008
M. Weinberger	UCLA	PhD	2008
M. S. Lucas	Caltech	PhD	2008
L. Petruska	U. Missouri – Kansas City	MS	2008

Selected Scientific Highlights for 2008

Osmium Metal Studied Under High Pressure and Nonhydrostatic Stress

Michelle B. Weinberger[1,2], Sarah H. Tolbert[1,*], and Abby Kavner[3,*]

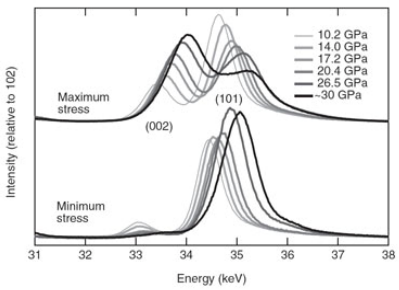
[1]*Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA 90095-1569*
[2]*Current address: Geophysical Laboratory Carnegie Institution of Washington, 5251 Broad Branch Rd N.W.. Washington DC 20015*
[3]*Department of Earth and Space Sciences and Institute of Geophysics and Planetary Physics, UCLA, Los Angeles, CA 90095-1567*

Recent attempts to correlate material hardness with other mechanical properties, particularly bulk modulus, have resulted in significant interest in osmium metal.. While the hardness of osmium is low (only 4 GPa), the modulus results have inspired interest in using osmium as a host matrix for the incorporation of small covalent atoms to make superhard materials. Our interest in osmium also stems from the potential analogy between the behavior of iron at high pressures and that of osmium at moderate pressures. Osmium has a hexagonally close-packed crystal structure, similar to that of iron at the conditions of the Earth's core. Predicted trends suggest that higher Z elements in the same periodic group mimic behavior of lower Z elements at high pressures, as long as the crystal structures are the same. Success in drawing this correlation between the mechanical properties of osmium and iron could be very useful in the ongoing quest to characterize the behavior of the Earth's core.

To elucidate the unique mechanical properties of Os, we performed non-hydrostatic *in-situ* high pressure diffraction experiments to determine its strength and deformation behavior using the COMPRES-supported beamline X17C at NSLS. Os supports a differential stress up to 10.0 GPa at 25 GPa (for the (110) plane). If the measured *t* values are considered a lower bound on the shear strength, this suggests that osmium plastically deforms less easily than any other pure metal. In addition, the data shows distinct evidence of development of lattice preferred orientation as pressure is increased (Fig. 3). At ψ=90° (minimum stress direction), the intensity of the (101) peak increases, while the intensity of the (002) peak decreases. This trend is reversed at ψ=0° (maximum stress direction) where the (002) intensity increases while (101) decreases. These changes in intensity as the sample pressure increases indicate that the sample is preferentially aligning the least strong [00l] direction with the primary stress direction.

Reference:

Michelle B. Weinberger[1,2], Sarah H. Tolbert[1,*], and Abby Kavner[3,*]
Osmium Metal Studied Under High Pressure and Nonhydrostatic Stress
Phys. Rev. Letters 100(4):045506 (2008)



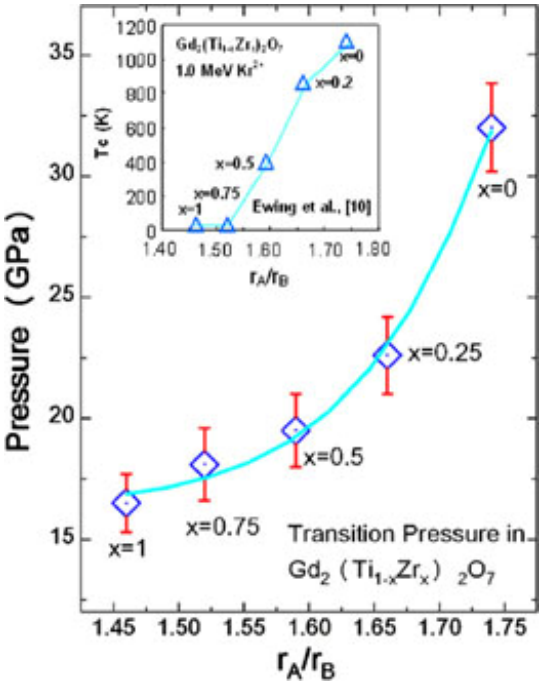
Phase stability and pressure dependence of defect formation in $Gd_2Ti_2O_7$ and $Gd_2Zr_2O_7$ pyrochlore

F. X. Zhang, J. W. Wang, J. Lian, M. K. Lang, U. Becker, and R. C. Ewing

Department of Geological Sciences, University of Michigan

Dramatically different behaviors between isostructural $Gd_2Ti_2O_7$ and $Gd_2Zr_2O_7$ pyrochlore at pressures up to 44 GPa, in which the substitution of Ti for Zr significantly increases structural stability, were observed by x-ray diffraction techniques. Upon release of pressure, the $Gd_2Ti_2O_7$ becomes amorphous. In contrast, the high-pressure phase of $Gd_2Zr_2O_7$ transforms to a disordered defect-fluorite structure. First principle calculations for both compositions revealed that the response of pyrochlore to high pressure is controlled by the intrinsic energetics of defect formation. By comparing with ion irradiation experiments, a consistent trend in the phase stability and structural transformation processes for isostructural titanate and zirconate pyrochlores at high pressures and in high radiation fields. Pyrochlore compositions that can accommodate disordering are resistant to forming an amorphous phase at high pressures or high irradiation fluxes. The response of such structures to extreme environments, such as high pressures or irradiation fields, is directly related to the energetics of the disordering process. The performance of materials in extreme environments can be much improved by a consideration of the atomic-scale disordering mechanism and energetics.

Reference: F. X. Zhang, J. W. Wang, J. Lian, M. K. Lang, U. Becker, and R. C. Ewing, Phase stability and pressure dependence of defect formation in $Gd_2Ti_2O_7$ and $Gd_2Zr_2O_7$ pyrochlore, *Phys. Rev. Lett.* 100(4): 045503, 2008



Deformation of the Lower-Mantle Ferropericlase across the Electronic Spin Transition

Jung-Fu Lin[1], Hans-Rudolf Wenk[2], Marco Voltolini[2], Sergio Speziale[3], Jinfu Shu[4], Thomas Duffy[5]

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[2]*Department of Earth and Planetary Science, University of California, Berkeley, California 94720, USA*
[3]*GeoForschungsZentrum Potsdam, Telegrafenberg, 14473 Potsdam, Germany*
[4]*Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, USA*
[5]*Department of Geosciences, Princeton University, Princeton, New Jersey 08544, USA*

We investigate the deformation of lower-mantle ferropericlase [$(Mg_{0.83},Fe_{0.17})O$] through the spin transition under non-hydrostatic conditions in a diamond cell using radial X-ray diffraction techniques at X17c of the NSLS. We observe unexpectedly lower stress and strength of ferropericlase, together with active slip systems and high elastic anisotropy. These results indicate that ferropericlase would play more dominant roles in the deformation and seismic anisotropy of the lower mantle, including subducting slabs, than what is expected by studying the high-spin ferropericlase.

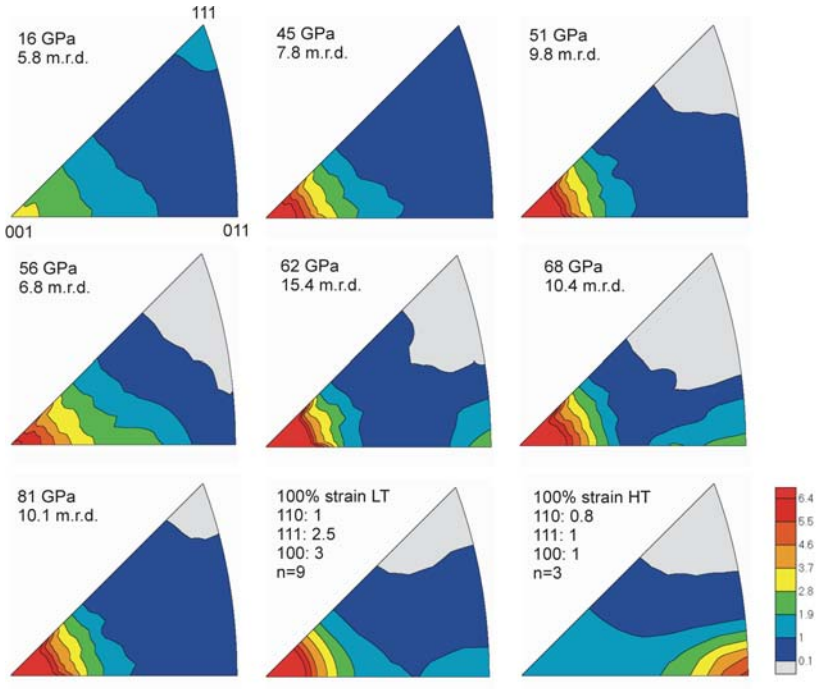

Figure: Inverse pole figures of the compression direction for $(Mg_{0.83},Fe_{0.17})O$ at high pressures in equal area projection.

Reference: J. F. Lin, H.-R. Wenk, M. Voltolini, S. Speziale, J. Shu, T. Duffy, Deformation of the lower-mantle ferropericlase across the electronic spin transition, submitted to *Proc. National Acad Sciences,* 2008.

Single-Crystal X-Ray Diffraction and Brillouin Scattering of Hydrous Wadsleyite

Zhu Mao[1], Fuming Jiang[1], Steve Jacobsen[2], Joe Smyth[3], Chris Holl[2], and Thomas Duffy[1]
[1]*Department of Geosciences, Princeton University, Princeton, New Jersey*
[2]*Department of Earth and Planetary Sciences, Northwestern University, Evanston, Illinois*
[3]*Department of Geological Sciences, University of Colorado, Boulder, Colorado*

We have used Brillouin scattering techniques to measure the elastic properties of a suite of hydrous wadselyite at ambient and high pressures. To deterimine the elastic constants, from such measurements, the Brillouin data must be combined with constraints on density and crystal orientation. For each sample, we determine the unit cell volume and orientation of the single crystal using energy-dispersive x-ray diffraction techniques at X17C. Wadsleyite, β-Mg_2SiO_4, is potentially a major hydrogen host in the Earth's transition zone (410-660 km depth) due to its large water solubility. Determination of the effect of water on the elasticity of wadsleyite can provide constraints on the water content in the earth's transition zone through comparison with seismic data. In our first study [Mao et al., *Earth Planet. Sci. Lett.*, 2008], we showed that the elasticity of wadsleyite decreases strongly with increasing water content at ambient conditions. More recently, we have measured the single-crystal elastic properties of wadsleyite, β-Mg2SiO4, with 0.84 wt.% H_2O measured to 12 GPa by Brillouin scattering and single-crystal x-ray diffraction. (*Geophys. Res. Lett.,* in press). Pressure derivatives of the aggregate bulk modulus, K_{S0}, and shear modulus, G_0, of hydrous wadsleyite are 4.1(1) and 1.4(1) respectively. These values are indistinguishable within uncertainty from those of anhydrous wadsleyite. Given that the bulk seismic velocity increase at 410-km depth in the mantle is too large for dry pyrolite (60 vol% olivine), we estimate that ~1 wt.% H_2O in wadsleyite at 410-km depth is required to reconcile seismic bulk sound velocities with a pyrolite-composition mantle by using our measured high-pressure elastic constants.

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Mao, Z, S. D. Jacobsen, F. Jiang, J. R. Smyth, C. M. Holl, and T. S. Duffy, Elasticity of hydrous wadsleyite to 12 GPa: Implications for Earth's transition zone, *Geophysical Research Letters,* in press, 2008

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Somayazulu, M., J. Shu, C. Zha, A. Goncharov, O. Tschauner, H. Mao, R. Hemley, In situ high-pressure x-ray diffraction study of H_2O Ice VII, *J. Chem. Phys.*, **128**, 064510 (2008).
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Chung, H., M. Weinberger, J. Levine, A. Kavner, J. Yang, S. Tolbert, R. Kaner, Synthesis of ultra-incompressible superhard rhenium diboride at ambient pressure, *Science*, **316**, 436 (2007).[premier]
Ehm, L., S. Antao, J. Chen, D. Locke, F. Michel, D. Martin, T. Yu, J. Parise, P. Lee, et al., Studies of local and intermediate range structure in crystalline and amorphous materials at high pressure using high-energy x-rays, *Powder Diffr.*, **22**, 108 (2007).
Zhang, F., J. Sang, U. Becker, J. Lian, J. Hu, S. Saxena, R. Ewing, Pressure-induced splitting and buckling of Cu-O chains in the low-dimensional structure of $SrCuO_2$, *J. Am. Chem. Soc.*, **129**, 13923-13926 (2007).[premier]
Zhang, Z., J. Yang, H. Rong, J. Hu, J. Su, H. Mao, Discovery of diamond in eclogite from Chinese Continental Scientific Drilling Project Main Hole (CCSD-MH) in Sulu UHPM Belt, *Acta Petrol. Sin.*, **23**, 3201-3206 (2007).

Beamline Overview 2007-2008

Management and Manpower

Management Team

Since June 2007, a multi-institution management team has led the X17-DAC effort. 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 Chi-chang Kao (Director, NSLS). 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 approximately monthly basis.

Beamline Scientists

Jingzhu Hu (18 years service at X17) and Quanzhong Guo (10 years service at X17) retired on October 1, 2008. A search committee (Tom Duffy, Lars Ehm, Don Weidner) evaluated a pool of about a dozen applicants and selected six for on-site interviews. The CVs of the two candidates who accepted offers at X17-DAC are attached. Sanjit Ghose has extensive experience in synchrotron operations and a scientific background in surface science including geological applications. He began serving as beamline scientist on October 1, 2008. Zhiqiang Chen carried out a portion of his Ph.D. research at X17C. He is a condensed matter physicist who received his Ph.D. from New Jersey Institute of Technology in 2008. He began employment as a beamline scientist on October 31, 2008.

Awards and Honors

Jingzhu Hu was awarded the 2008 Community Service Award from NSLS. This honor is bestowed by the Users' Executive Committee in recognition of service, innovation, and/or dedication to NSLS users.

Ancilliary 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 since September 2007. 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.

Beamline operations in 2007-2008

The X-17 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.

In 2007, X17C had approximately 80 person-visits representing 18 separate universities and institutes. X17B3 had 23 person-visits representing 10 separate universities and institutes.

Currently all funding for the X17-DAC effort is provided by COMPRES.

Beamline improvements completed in the June 2007-November 2008 period

X17C

With the addition of two external hard-drives, and a new back-up system for user data was set up.

With the assistance of Mark Rivers and Peter Eng (GSECARS), the KB mirror system was tested and improved. The best beam size achieved was 22 μm (H) x 8 μum (V) with a slit size 140 μm (h) x 140 μm (v) at energy of 30.493 keV and 2 mrad tilt angle. Since X17C is a side branch of the X17 beam, it has a larger apparent source size and the horizontal focusing capability is therefore limited compared with the main branch (X17B3).

Documentation of the operating and alignment procedures for beamline scientists was prepared. This document will be improved and upgraded by the new staff in the coming year. Although there was very minimal overlap in personnel, Sanjit Ghose has been trained in beamline set up, alignment, and operation. He has operated the beamline successfully on his own since October 1, 2008. Zhiqiang Chen also received some training prior to his starting date.

Motor control programs for oscillating the sample in omega during data collection were created for the first time. This is useful for reducing the effects of sample preferred orientation during data collection.

Two germanium solid-state detectors, which had been contaminated by Indium fluorescence, were repaired.

X17B3

A two-Laue monochromator with energy tunable between 29-32 keV was set up. The offset in position between 29 and 32 KeV is about 100μm. Further efforts are needed to improve the flux by optimizing crystal thickness. Shinan Qiang and Peter Takacs (Department of Instrumentation, BNL) have provided guidance on this issue.

Funds to motorize the high-energy monochromator for X17B3 have been included in the FY09 NSLS budget for beamline improvements at X17. The motorization of the monochromator would have to positive aspects:

1. Users can choose from a larger range of incident beam energies (~ 70-90 keV) for their high-energy scattering experiments at X17B3.
2. The setup time of the monochromator can be drastically reduced. Leading to more available user beamtime at X17B2 and X17B3.

Currently, it is unclear due to the budget situation at the NSLS if the requested budget will be approved.

With the assistance of Mark Rivers and Peter Eng (GSECARS), the KB mirror system was tested and improved. The smallest white beam focal spot size has been improved to 10 μm (V) x 15 μm (H), compared with ~30 μm previously. The incident beamsize defined by entrance slits size is 289 μm (H) and 119 μm (V) with tilt angle of 1.7mrad. Using monochromatic radiation (32 Kev), the focal spot size was improved to
7 μm (V) x 12 μm (H) with the entry slits size set to 360 μm (H) and 160 μm (V) and a tilt angleof 1.9mrad.

In collaboration with Kenneth Evans-Lutterodt (BNL), a kinoform lens was successfully tested at X17B3 at 30 keV to produce a vertically focused beamsize smaller than 7 μm. The next step is to set up and test a double-focusing system using a pair of kinoform lenses.

A new laser heating system has been designed. Components have been obtained and the system is currently being assembled. Testing of the system will commence in late 2008, and we expect to have the system assembled at the beamline during the first cycle of 2009.

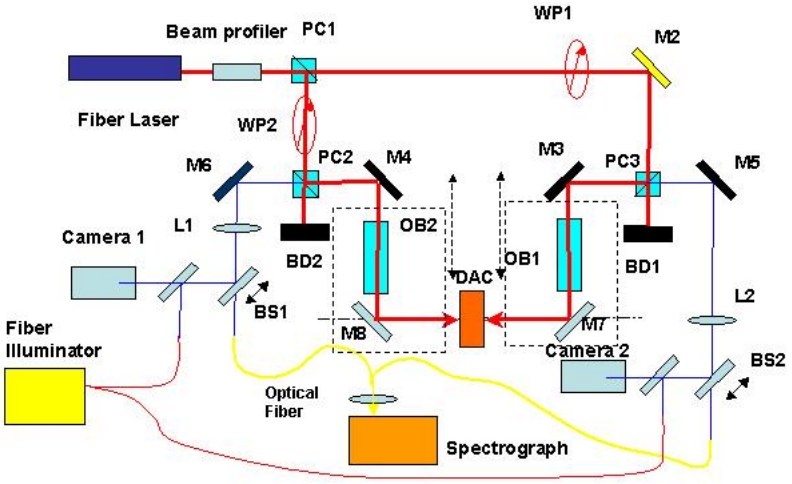

Fig. 1. Schematic for proposed redesign of laser heating system based on Fiber laser

A new area detector (Rayonix SX-165) has been ordered, and delivery is expected in early 2009. The active area of the detector is 165 mm (2048 × 2048 pixels) and it is sufficiently large for powder and single-crystal diffraction experiments in a diamond anvil cell. The readout time of 2.5 seconds is fast enough for experiments on kinetics of phase transitions and reactions. Previous generations of the 165 marccd detector system are currently in use at many dedicated high-pressure beamlines (e.g. GSECARS, HPCAT) and are very efficient and reliable. A new feature of the SX-165 marccd is the capability to partially read out the detector in milliseconds. This will facilitate studies on a time scale previously not available in high-pressure and temperature research.

Support Laboratory

Supplementary funding was requested from COMPRES to partially replace the diamond anvil cells and anvils that were returned to the Geophysical Laboratory upon Jingzhu Hu's departure. COMPRES granted the funding request for $13,434 and a set of 3 news diamond cells and related equipment (gaskets, seats, etc) has been ordered from the Princeton University machine shop with delivery expected in early to mid 2009. 6 diamond anvils have also been ordered using these fudns.

Outreach Activities

2008 was a very active year for beamline outreach as 3 workshops were held at NSLS.

Materials at High Pressure Breakout Session

On January 17-18, 2008, a breakout session on "Materials at High Pressure" was held during the joint workshop for "The NSLS-II Powder Diffraction Project Beamline" and "Materials Science Engineering Strategic Planning for NSLS and NSLS-II". This breakout session was attended by 34 people. The outcome was a white paper on "Future directions in high pressure science and instrumentation at NSLS & NSLS-II" prepared by Lars Ehm and others. This white paper formed the basis of the scientific and technical case included in the letter of intent for a high-pressure superconducting wiggler beamline at NSLS-II as discussed below.

Future Directions in High Pressure Research

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 features 15 invited speakers.

Participants of the Future Directions in High Pressure Research Workshop

The two morning sessions were focused on the Earth's mantle and core. D.Weidner, from Stony Brook University, presented the results on strain, stress, and time relationships in mantle phases at high pressure and temperature.Y. Wang, from the University of Chicago and GSECARS at the Advanced Photon Source (APS), showcased the experimental capabilities of the large volume press research at Sector 13 at APS. He showed that the different experiments could be accommodated on large press using different module designs. The benefit for the user

community of the so-called "Swiss army knife" approach was demonstrated. Professor A. Campbell, from University of Maryland, presented investigations of phase relationships at high pressure and temperature in iron alloyed with light elements, relevant for Earth's core. Furthermore, Campbell introduced a new technique for temperature measurements during laser-heated high-pressure experiments in a diamond anvil cell. Professor S.-H. Shim, from the MIT, showed how the combination of nuclear forward scattering and x-ray diffraction at high pressure and temperature could be used to understand small variations in the elasticity of the Earth's lower mantle. The morning session was concluded with two talks on the water content in the nominally anhydrous MgSiO3 perovskite. Dr. H. Watson, from Lawrence Livermore National Laboratory, and Professor O. Tschauner, from University of Nevada, Las Vegas, presented results of infrared spectroscopy data collected at the NSLS beamline U2A and were able to determine a upper limit for the water content in Earth's mantle.
The first afternoon session was devoted to materials at high pressure and variable temperature. Dr. C. Benmore (APS) opened the session with a presentation on amorphous solids at elevated pressure. He demonstrated the power of total x-ray scattering for the determination of the atomic arrangements in amorphous materials. Professor Wendy Mao, from Stanford University, talked about how the investigation of molecular compounds at high-pressure and low temperature might lead to a new high-performance hydrogen storage material. The session was concluded by Dr. R. Cohen from the Carnegie Institution of Washington. Dr. Cohen presented the capabilities of joint experimental and theoretical approaches for developing novel electromechanical materials.

The session was followed by four short talks given Dr. M. Huecker, from Brookhaven National Laboratory, Dr. Emre Selvi, from Texas Tech University, and Matthew Whitacker and Hongbo Long, from Stony Brook University.
The final session was opened by Dr. Viktor Struzhkin from the Carnegie Institution of Washington. Dr. Struzhkin gave a review of x-ray spectroscopy techniques and their potential for understanding materials at high pressure. The presentation determined the instrumentation needs for x-ray spectroscopy experiments at NSLS-II. Professor Thomas Duffy, from Princeton University, gave the final presentation of the workshop. He informed the attendees on the capabilities of the new synchrotron radiation facility and the ongoing effort of the high-pressure community to transfer the high-pressure program from the NSLS to NSLS-II.
The workshop finished with a discussion of Professor Duffy's presentation and led to an enhanced formulation of the instrumentation needs of the high-pressure community for a successful high-pressure program at NSLS-II.

Advances in High-Pressure Science Using Synchrotron X-rays

A workshop on "Advances in High-Pressure Science Using Synchrotron X-rays" was held at the National Synchrotron Light Source, Brookhaven National Laboratory, on October 4, 2008 (Appendix II). The workshop was attended by more than 50 scientists, post-doctoral fellows, and students from the high pressure and synchrotron x-ray research fields.

The workshop was divided into 4 sessions and there were 18 oral presentations. Dave Mao (Carnegie Institution of Washington), a pioneer in diamond anvil cell synchrotron x-ray diffraction studies, offered an overview lecture titled "The legacy of X17" to open the workshop. Qun Shen (Brookhaven National Laboratory) discussed the many opportunities for ground-breaking high-pressure science that will be afforded by the development of NSLS-II. Li Hua Yu

(Brookhaven National Laboratory) gave an overview of current research towards free-electron lasers. Gene Ice (Oak Ridge National Laboratory) discussed how improved source brilliance, optics and detectors will enable important new capabilities for high-pressure x-ray and neutron studies.

Kenneth Evans-Luterodt (Brookhaven National Laboratory) described the status and planned future developments of x-ray kinoform optics for high-pressure science. Alexander Goncharov (Carnegie Institution of Washington) discussed recent developments in the laser-heated diamond anvil cell with a focus on pulsed heating techniques. Other talks covered such topics as anomalous scattering at high pressures (Wenge Yang, Carnegie Institution of Washignton), combining high pressures with heavy-ion radiation (Maik Lang, Michigan), and x-ray tomography of amorphous materials under diamond anvil cell compression (Luhong Wang, Harbin Institute of Technlogy).

A number of talks focused on applications to geological sciences. Jie Li (Illinois) described her work on density and sound velocities of Fe alloys with applications to the Earth's core. Andy Campbell (Maryland) presented results on the high-pressure behavior of metal/oxygen buffer systems. There were also presentations on thermal equations of state of perovskites (Yingwei Fei, Carnegie Institution of Washington) and viscoelasticity of mantle minerals at high pressures and temperatures (Li Li, Stony Brook). Many other interesting and exciting talks were offered by distinguished experts in this field followed by fruitful discussions.

This workshop was organized in honor of Jingzhu Hu and Quanzhong Guo in celebration of their retirement after up to 18 years of dedicated service to the high-pressure community as beamline scientists at X17. Chi-chang Kao (Chairman of NSLS), Robert Liebermann (President of COMPRES), and Don Weidner (Director of the Mineral Physics Institute, Stony brook University) all made presentations to express the gratiute of the community to Drs. Hu and Guo.

The workshop was organized 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). Financial support was provided by the Consortium for Materials Property Research in Earth Sciences (COMPRES), the Carnegie- DOE Alliance Center (C-DAC), and the Harbin Institute of Technology.

We will collect papers from key contributions of these three workshops for a special issue on "Advances and Synergy of High-Pressure Science at Synchrotron Sources" to be published in the *Journal of Synchrotron Radiation* in 2009. The issue will also incorporate papers highlighting recent advances at high-pressure synchrotron facilities in Europe and Asia. As such, an international team of guest editors has been selected: H. Liu (Harbin), T. Duffy (Princeton), L. Ehm (SBU/BNL), W. Crichton (ESRF), and K. Aoki (JAEA/SPring-8).

Planned Activities for COMPRES II – Year 3 (June 2009 – May 2010)

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.

The construction, testing, and commissioning of the laser heating redesign is a major goal of the upcoming year. No funds are being requested for laser heating equipment as we anticipate being able to purchase all necessary components from existing funds.

Our software for single-crystal x-ray diffraction experiments is outdated. New software and methods for single-crystal x-ray diffraction will be implemented in the coming year.

Working with Z. Zhong (BNL), the Laue monochromator at x17c will be improved to allow for wavelength variation and improved shielding to reduce background.

The beamline scientists will initiate and carry out their own research programs at X17 focusing on high-pressure materials and earth science research.

We plan to seek external funds for purchase of a gas loading system based on GSECARS design.

The X17-DAC facility is the most productive COMPRES facility, and provides a major fraction of the total number of COMPRES publications. In order to maintain this productivity, it is absolutely essential that we have equipment and staff that are on a par with those found at 3rd generation facilities (HPCAT, GSECARS). We have hired two high-quality staff members this year. We absolutely require further investment in equipment infrastructure at X17. Our current equipment base is far older and less advanced than those found at the 3rd generation facilities. *We cannot continue to attract users unless our equipment base is steadily upgraded and improved in the coming years.* Our minimal equipment needs for the coming budget year are described below in the budget section.

The Future of the NSLS

Continued upgrades to the NSLS and the development of and transition to NSLS-II represent an enormous opportunity for the high-pressure Earth science community represented by COMPRES. We are working with our colleagues at X17B2 and U2A to take advantage of these opportunities and lead the effort to enhance and develop the capabilities for high-pressure earth science research at NSLS.

Development of X17A

In the latest 5-year plan for NSLS, it is proposed to develop a new side station, X17A, to enhance utilization of the superconducting wiggler beamline of X17. While mainly serving the materials science community, the addition of X17A will increase the share of beamtime available to the X17 end-stations, X17B2 and X17B3 and thus directly impact the amount of beamtime available for high-pressure activities.

During FY08 the project for the construction of the new facility beamline X17A progressed through the conceptual design phase and entered the pre-construction phase. The high level specifications such as energy, flight path, hutch size have been agreed upon by the design team.

The scientific mission of the beamline will be focused on X-ray total scattering experiments with an emphasis of high-throughput measurements at ambient conditions or low temperature. The desire to perform measurements at extreme conditions, e.g. high pressure and/or high temperature, has been taken into account during the design. High-pressure devices of the Paris-Edinburgh type and high temperature furnaces can be accommodated on the beamline. The final design stage is currently in progress and the start of the construction is anticipated for December 2008.

NSLS-II

NSLS-II is a proposed new storage ring at Brookhaven that promises to deliver x-rays with 10^4 times the brightness of the current NSLS. Design and engineering of the new light source is in progress and operations are expected to commence in 2015 (and the current NSLS will be decommissioned shortly thereafter). Design goals for the project include achieving spatial resolution of 1 nm and energy resolution of 0.1 meV. Current plans involve the development of 6 insertion device beamlines as part of the construction project, with additional insertion device beamlines pursued via separate Major Items of Equipment (MIE) DOE-BES funding. There will also be a number of beamlines (~20) that will be transitioned and upgraded from current NSLS beamlines. The project can accommodate up to 58 beamlines in total.

The high-pressure community has established a high-pressure working group to advocate for the development of high-pressure facilities at NSLS-II. A letter of intent for a high-pressure superconducting wiggler beamline proposed to be one of the 6 project beamlines at NSLS-II was submitted in 2008. While our proposed beamline was not selected as a project beamline by the NSLS-II Experimental Facilities Advisory Committee (EFAC), the committee stated in their response that they expect that ultimately one or more beamlines with the capabilities outlined in our LOI will "in all likelihood, be part of the fully built out complement of beamlines at NSLS-II and we look forward to working with the community in the development of one or more recast LOIs at the appropriate time." We are planning a formal response to the EFAC recommendation, and we plan to continue to work toward the development of high-pressure facilities at NSLS-II in the coming year.

Year 3 Proposed Budget
June 1, 2009 – May 31, 2010
Details of the requested budget for Year #3 and the justification for each budget category are given below in Section E of this report.

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Appendix II -- 2008 Outreach Activities

NSLS Users' Meeting workshp:
"Future Directions in High-Pressure Research"
Date: Wednesday, May 21, 2008

Organizer(s):
Lars Ehm (Stony Brook University) lars.ehm@stonybrook.edu
Jiuhua G. Chen (Florida International University) jiuhua.chen@fiu.edu
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Description:
High-pressure is used in a large variety of scientific disciplines as a parameter to modify the atomic structure of materials and to understand microscopic and macroscopic phenomena. The research topics span from the structure of earth and planetary interiors over the design and synthesis of new materials to the understanding of the collective phenomena that yield to high-temperature superconductivity. The workshop will focus on recent results on structural phase transitions, elasticity, plasticity, melts properties and new materials at high pressure and high temperature. Novel technical developments at the NSLS and other synchrotron radiation sources will be part of the presentations as well. The workshop will also emphasize on future developments and applications, beamline design and potential opportunities at NSLS-II for high pressure research.

Time	List of Speakers
9:00 a.m. - 9:10 a.m.	Welcoming Remarks -- Organizers
9:10 a.m. - 9:40 a.m.	Don Weidner, Stony Brook University "Stress - Strain - Time Relationships at High Pressure and Temperature"
9:40 a.m. - 10:10 a.m.	Yanbin Wang, University of Chicago "Large-Volume High Pressure Research at GSECARS"
10:10 a.m. - 10:40 a.m.	Andrew Campbell, University of Maryland "X-ray Diffraction Studies of Iron Alloys at High Pressures and Temperatures"
10:40 a.m. - 11:00 a.m.	Coffee Break
11:00 a.m. - 11:30 a.m.	Sang-Heon Dan Shim, Massachusetts Institute of Technology "X-ray Diffraction and Nuclear Forward Scattering Measurements of Mantle Phases up t 150 GPa"
11:30 a.m. - 12:00 p.m.	Heather Watson, Lawrence Livermore National Laboratory "Synchrotron FTIR Studies of Hydrogen in MgSiO3 Perovskite"

12:00 p.m. - 12:30 p.m.	Oliver Tschauner, University of Nevada "On the Water Content of the Lower Mantle"
12:30 p.m. - 1:00 p.m.	Lunch at Berkner Hall
1:00 p.m. - 1:30 p.m.	Chris Benmore, Argonne National Laboratory "Amorphous to Amorphous Transitions at High Pressure"
1:30 p.m. - 2:00 p.m.	Wendy Mao, Stanford University "Hydrogen Storage in Molecular Compounds"
2:00 p.m. - 2:30 p.m.	Ron Cohen, Carnegie Institution of Washington "Joint Theoretical and Experimental Studies for Developing New Electromechanical Materials"
2:30 p.m. - 3:10 p.m.	Science Snapshots
3:10 p.m. - 3:25 p.m.	Coffee Break
3:25 p.m. - 3:55 p.m.	Viktor Struhzkin, Carnegie Institution of Washington "Synchrotron Spectroscopy Methods at High Pressure"
3:55 p.m. - 4:45 p.m.	Tom Duffy, Princeton University "New Frontier in High-Pressure Research at the NSLS-II"

Advances in High-Pressure Science Using Synchrotron X-rays

A workshop in celebration of Jingzhu Hu and Quanzhong Guo

National Synchrotron Light Source, Brookhaven National Laboratory
Oct 4, 2008,

Sponsors

Organizing Committee

Haozhe Liu (Harbin Institute of Technology) Co-chair
Tom Duffy (Princeton University) Co-chair
Dave Mao (Carnegie Institution of Washington)
Lars Ehm (Stony Brook University/Brookhaven National Laboratory)
Jiuhua Chen (Florida International University)
Zhenxian Liu (Carnegie Institution of Washington)

Meeting Program

9:00 – 9:15	**Opening Session**
9:00	Opening **Tom Duffy (Princeton University)**
9:05	Welcome **Chi-chang Kao (BNL)** **Bob Liebermann (COMPRES, Stony Brook University)**
9:15 – 11:00	**Session 1** *Chair: Tom Duffy (Princeton University)*

9:15	*The legacy of X17* **Dave Mao (Carnegie Institution of Washington)**
10:00	*R & D towards X-ray free electron laser* **Li Hua Yu (BNL)**
10:30	*Some new directions for high-pressure research?* **Gene Ice (ONRL)**
11:00 – 11:20	Coffee Break
11:20 – 12:30	**Session 2** *Chair: Haozhe Liu (Harbin Institute of Technology)*
11:20	*Opportunities for high-pressure research at advanced synchrotron facilities* **Qun Shen (BNL)**
11:50	*X-ray kinoform optics for high pressure science: Status and opportunities* **Ken Evans-Lutterodt (BNL)**
12:10	*Laser heating in the DAC: New pulsed techniques and recent results* **Alex Goncharov (Carnegie Institution of Washington)**
12:30 – 13:30	**Lunch** NSLS Seminar Room
13:30 – 15:10	**Session 3** *Chair: Lars Elm (Stony Brook University)*
13:30	*Seeding the future: The high pressure program at Texas Tech University* **Yangzha Ma (Texas Tech)**
13:50	*Anomalous scattering study of crystal and amorphous materials under high pressure* **Wenge Yang (HPCAT)**
14:10	*Bridging stage from amorphous Se to crystal under compression* **Luhong Wang (Harbin Institute of Technology)**
14:30	*Combining high pressure and heavy-ion irradiation: A novel approach* **Maik Lang (University of Michigan)**
14:50 – 15:10	Coffee Break
15:10 – 17:50	**Session 4:** *Chairs: Jiuhua Chen (Florida International University)* *Zhenxian Liu (Carnegie Institution of Washington)*
15:10	*Density and sound velocity of iron-rich alloys and nature of Earth's core* **Jie Li (University of Illinois at UC)**
15:30	*Geochemical applications of high pressure, high temperature equations of state of metals and oxides* **Andy Campbell (University of Maryland)**
15:50	*Viscoelasticity of rocks at mantle P-T* **Li Li (Stony Brook University)**
16:10	*High-pressure X-ray diffraction and Raman study on $BaCrO_4$ and $SrCrO_4$*

	Sean Shieh (University of Western Ontario)
16:30	*Using X17C to study ultra-incompressible superhard materials*
	Michelle Weinberger (Carnegie Institution of Washington)
16:50	*Progress on P-V-T measurements of solids using synchrotron X-ray diffraction techniques*
	Yingwei Fei (Carnegie Institution of Washington)
17:10	*Application of synchrotron-based high-pressure techniques to understand strongly correlated transition metal oxides*
	Trevor Tyson (New Jersey Institute for Technology)
17:30	*Pressure induced phase transition in ammonia borane*
	Jiuhua Chen (Florida International University)
17:50	**Closing Remarks**
	Dave Mao (Carnegie Institution of Washington)

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

2008 Annual Report

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

Overview

U2A beamline is an integrated and dedicated facility for measurement of far- to near-infrared spectra of materials from ambient to ultrahigh pressures at variable temperatures by coupling synchrotron infrared microspectroscopic techniques with diamond- and moissanite-anvil cell methods. The presence of an IR beamline together with x-ray facilities for DAC is one of the unique features of NSLS for general users. We continue to broaden the user base, and provide convenient access for users from the COMPRES community, and promote user research projects on problems in high-pressure geoscience, complemented by studies in materials science, condensed matter physics, chemistry, and biology (many of these studies by the COMPRES community).

I. Selected Scientific highlights for 2008

a. Discovery of Metallic State of Hydrogen-Rich Material: Solid Silane

There is a great interest in electronic transitions in hydrogen-rich materials under extreme conditions. It has been recently suggested that the group IVa hydrides such as methane (CH_4), silane (SiH_4), and germane (GeH_4) might become metallic at far less pressures than expected for pure hydrogen at equivalent densities because the hydrogen is compressed in group IVa hydride compounds. Raman and infrared (both absorption and reflection) spectra of silane have been measured in diamond anvil cells up to 70 GPa. We found that SiH_4 undergoes three phase transitions before becoming opaque at 27-30 GPa. The vibrational spectra indicate the material transforms to a polymeric or framework structure in this higher-pressure range. Room-temperature infrared reflectivity data taken at U2A beamline revealed that the material exhibits Drude-like metallic behavior above 60 GPa, indicating the onset of pressure-induced metallization. Therefore, SiH_4 can be considered as the first example for the metallization of a group IVa hydride. The reported metallic state of SiH_4 was confirmed by the measurements of the electronic resistance [see, M. I. Eremets et al., Science 319, 1506 (2008)].

Chen, X. J., V. V. Struzhkin, Y. Song, A. F. Goncharov, M. Ahart, Z. Liu, H. K. Mao and R. J. Hemley, Pressure-induced metallization of silane, *Proc. Nat. Acad. Sci.,* **105**(1), 20-23 (2008).

b. Isotope Effect on Band Gap and Radiative Transitions Properties of Boron Nitride Nanotubes

The electronic structures of boron nitride nanotubes (BNNTs) are very different from those of carbon nanotubes because of the wide gap of the BN sheets compared to the zero

gap in graphite. In contrast to carbon nanotubes, whose electric properties depend on the chirality and diameter of the nanotubes, theoretical values of the direct band gap of BNNTs with a diameters more than 9.5 Å are about equal to that of h-BN (around 5.5 eV) and nearly independent of the nanotube's diameter, chirality, and wall-wall interactions. We have carried out an isotope study on the band gap and radiative transition spectra of boron nitride nanotubes (BNNTs) using both experimental and theoretical approaches. The direct band gap of BNNTs was determined at 5.38 eV, independent of the nanotube size and isotope substitution, by cathodoluminescences (CL) spectra. At lower energies, several radiative transitions were observed, and an isotope effect was revealed. In particular, we confirmed that the rich CL spectra between 3.0 and 4.2 eV reflect a phonon-electron coupling mechanism, which is characterized by a radiative transition at 4.09 eV. The frequency red shift and peak broadening due to isotopic effect have been observed using synchrotron IR spectroscopy and Raman scattering at U2A beamline. Our FTIR spectra and density functional theory calculations suggest that those radiative transitions in BNNTs could be generated by a replacement of some nitrogen atoms with oxygen.

Han, W., H. Yu, C. Zhi, J. Wang, Z. Liu, T. Sekiguchi, and Y. Bando, Bandgap Properties of Boron Nitride Nanotubes, *Nano Letter*, **8**(2), 491-494 (2008).

c. Infrared Dielectric and Vibrational Properties of Non-Stoichiometric Wüstite at High Pressure: First high-pressure far-IR reflectivity studies at U2A Beamline

Wüstite, Fe_xO, is a vacancy ridden mineral that crystallizes in the rocksalt structure. Due to its geophysical and technological importance, wüstite has attracted a wealth of theoretical and experimental investigations into its vibrational, dielectric and thermoelastic properties. Detailed theoretical investigations of wüstite often rely on comparison to thermoelastic data to corroborate their results. The far infrared (IR) reflectivity of $Fe_{0.91}O$ was investigated from 1 bar up to 33 GPa at room temperature using synchrotron Fourier transform infrared reflectivity techniques in conjunction with the diamond anvil cell (DAC) at U2A beamline. The frequency of the fundamental transverse optic (TO) mode was found to be nearly independent of pressure up to 4.6 GPa followed by an increase of the TO frequency with pressure up to the rhombohedral phase transition. In addition, a second weak mode at 583 cm^{-1} at 1 bar was well resolved and found to shift to higher frequency and increase in strength with pressure. This localized mode arises from the presence of vacancies in the crystal structure and the relative strength of this mode suggests pressure induced charge localization near the vacancy sites. The data was fit with the classical Lorentz model with the addition of a plasmon resonance. This allowed an estimation of the electrical conductivity as well as plasmon-phonon coupling energies. The pressure dependencies of the dielectric properties of wüstite have been quantified, and their pressure derivatives show a change in sign near the pressure induced rhombohedral phase transition. Classical theories relating dielectric, vibrational and elastic properties are evaluated, and in the case of the bulk modulus, the theory fails to reproduce accepted literature values.

Seagle, C.T, W. Zhang, D.L. Heinz, and Z. Liu, Far Infrared Dielectric and Vibrational Properties of non-Stoichiometric Wüstite at High Pressure, *Physical Review B.,* submitted.

d. First Gas-gun Shock Wave Experiments at a Synchrotron

Material emissivity measurements at extreme conditions can provide fundamentally important data that allow the measurement of temperature on short time scales, which is crucial for the complete characterization of dynamic compression events. For opaque materials such as metals, reflectivity measurements are necessary and must be conducted under dynamic compression in order to provide the necessary information. A gated spectrometer has been designed for real-time, pulsed infrared (IR) studies at U2A beamline, the National Synchrotron Light Source at the Brookhaven National Laboratory. A pair of 90-degree, off-axis parabolic mirrors are used to relay the light from an entrance slit to an output IR recording camera. With an initial wavelength range of 1500-4500 nm required, gratings could not be used in the spectrometer because grating orders would overlap. A magnesium oxide prism, placed between these parabolic mirrors, serves as the dispersion element. The spectrometer is doubly telecentric. With proper choice of the air spacing between the prism and the second parabolic mirror, any spectral region of interest within the InSb camera array's sensitivity region can be recorded. The wavelengths leaving the second parabolic mirror are collimated, thereby relaxing the camera positioning tolerance. To set up the instrument, two different wavelength (visible) lasers are introduced at the entrance slit and made collinear with the optical axis via flip mirrors. After dispersion by the prism, these two laser beams are directed to tick marks located on the outside housing of the gated IR camera. This provides first-order wavelength calibration for the instrument. Light that is reflected off the front prism face is coupled into a high-speed detector to verify steady radiance during the gated spectral imaging. Alignment features include tick marks on the prism and parabolic mirrors. This instrument was designed to complement single point pyrometry, which provides continuous time histories of a small collection of spots from shock-heated targets. Malone, R., D. Dolan, R. Hacking, and I. McKenna, IR Spectrometer Using 90-degree Off-axis Parabolic Mirrors, *SPIE Optics & Photonics*, Vol 7068, p. 706808, sponsored by SPIE (2008).

II. Beamline Developments 2007-2008

1. **Raman/IR Microscope system**: The micro-Raman system at U2A beamline is not only an important complementary tool with the synchrotron FTIR spectroscopy but also crucial for in situ pressure calibration at extreme conditions, e.g. diamond cell in cryostat or a resistive heating cell. The original plan is to build an independent and user-friendly Raman microscope system and upgrade the IR microscope system with the capacity of far-IR reflection with diffraction-limited spatial resolution. However, a controller for the CCD detector on the micro-Raman system was broken and the model was too old to be replaced after more than ten years operation. In this case, we decided to completely replace the whole Raman system. This has been done through the support of CDAC ($34,975 for the new spectrometer, controller, and CCD detector) and COMPRES ($13,052 for all remaining necessary optical components). The new Raman/IR system is significantly improved the beamline performance and several projects have already been achieved on this system (see the second selected scientific highlights in section I).

2. **CO_2 laser heating system:** The laser heating technique combined with DACs is crucial for the COMPRES user community to address a range of problems on mineral physics/chemistry related to Earth interior. As demonstrated before, high pressure and high temperature >1000 K extreme conditions are essential for infrared studies of Earth and planetary materials. Based on the equipment fund provided by COMPRES and feedback from the user community, we made one of our priorities is to develop and build a CO_2 laser heating technique at U2A. As first step, we purchased a CO_2 laser with outstanding power stability (<3%) from Coherent ($20K) in year #1. It's very fortunate that the NSLS strongly supports this project and provided a lab space (available in May) to locate this off-line CO_2 laser heating system. An optical table ($8047) has been purchased and moved into the lab in June.

III. Planed Beamline Upgrade 2008-2009

1. **CO_2 laser heating system:** We will continue to focus on the laser heating system and try to complete the system in May 2009. Additional accessories including a controller, a DC power supply, and a chiller for the CO_2 laser will be purchased and installed before the end of this year. After initial test of the laser, we will work with the NSLS interlock group to address the laser safety requirement at BNL. Meanwhile, we are going to setup a temporary temperature calibration system utilizing the dismissed spectrograph and CCD detector from the old Raman system (see section VIII) and a controller for the CCD detector borrowed from the NSLS. The whole system will be moved into a commissioning phase after passing through the laser shutter and interlock inspection. All the cost for the laser heating system is contained within our current equipment budget. We expect that the laser heating system based on Fiber laser at X17B3 will become available soon and we will work closely to attract and coordinate users to access both facilities.
2. **New side station at U2A beamline:** The U2A beamline has been built as the first dedicated high pressure IR beamline in the world with many unique features, such as vacuum far-IR microscopic system for measurements down to the THz region (1 THz=33 cm^{-1}), and integrated synchrotron IR/Raman/visible spectroscopy at high pressure and variable temperature (4-1000 K). Despite these features and upcoming CO2 laser heating capability, there are important limitations in the present configuration that preclude optimized performance. These limitations are becoming particularly important as the IR user community grows. The distance between the U2A beamline end station (spectrometer/microscope) and the synchrotron source spot is about 15 meters, 3-5 times longer than the other five IR beamlines at NSLS. The synchrotron beam is collimated with a parabolic mirror and delivered with several flat mirrors through a vacuum pipe system; we have found that the beam divergence, scattering, and distortion becomes significant after the so-called "collimated" beam travels more than 8 meters. As a result, the performance at U2A is significantly lower (by a factor of two) than the other beamlines in the mid-IR and much worse in the far-IR. 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). There is

increasing interest from the high-pressure community in conducting these kinds of experiments. In addition, the existing Bruker spectrometer and microscope is running for more than ten years and some parts start malfunctions from time to time.

During the past two years, an exciting opportunity has arisen to create a side station on the beamline as a result of new space that has been created next to the U2 port. A vacuum pipe for beam delivery was installed in 2006 for the gas-gun shock wave experiments. The distance from the synchrotron source to the IR system would then be only about 3 meters. This will remove the problem of beam divergence and image distortion. Ray-tracing calculations have indicated a significant improvement in spatial resolution (equivalent to U10B, which is essentially identical to the proposed side station). Thus, the proposed side station will allow measurements on high-pressure samples with the highest spatial resolution possible at a synchrotron source while also having the highest broadband IR brightness. With a new microscope coupling a newly developed IR FPA detector and FTIR instrument, the facility will be ideal for mapping 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 or moissanite anvil cells. As such, the side station would therefore complement the main beamline in the U2A hutch, with its general-purpose microscopes, vacuum capability, far-IR features, and laser spectroscopy systems. Optics is available to split the beam and allow us the option of operating both the existing and the new station alternately. Moreover, addition space will be available to accommodate the CO_2 laser heating system after removing some IR microscope systems from the hutch to the side station. This will offer the opportunity for users to perform in situ high pressure and high temperature studies using the combined laser heating and DAC techniques. The total cost for the FTIR spectrometer (Bruker Vertex 80v) will be ~$150K. We request funds in the year #3 permanent equipment budget in total amount of $100K. The rest will be raised through other sources, such as CDAC.

IV. Proposed budget for year #3 (May 1, 2009-April 30, 2010)

U2A provide more beam time to general users and contributing users in comparison to any other COMPRES supported community facilities. In view of this fact as well as the beamline upgrades needed by our user community, we request $207 K for maintaining and operating the beamline, and $100 K for beamline upgrade for the year May 1, 2009 to April 30, 2010. The budget and budget justification are given in the Detailed Budget section E below.

VII. 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. This reflects a 100% increase of available beam time to general users compared with the original PRT arrangement. Currently, the COMPRES community is the dominant user group in this category. The remaining 25% of beam time

will be allocated by COMPRES with at least half of this time being dedicated to support research by members of the COMPRES community through proposals vetted by the NSLS General User program; the NSLS User Administration will provide 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 for the 25% of beam time to be allocated by COMPRES. The remaining 25% will go to Geophysical Laboratory, Carnegie Institution for development projects and users supported by its grants such as CDAC.

VIIII. U2A Beamline Publications 2007-2008

Ciezak, J. A., T. A. Jenkins, and Z. Liu, Evidence for a high-pressure phase transition of ε-2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (CL-20) using vibrational spectroscopy, *Propellants Explos. Pyrotech. 32,* 472 - 477, 2007.

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Han, W., H. Yu, C. Zhi, J. Wang, Z. Liu, T. Sekiguchi, and Y. Bando, Bandgap Properties of Boron Nitride Nanotubes, *Nano Letter*, **8**(2), 491-494 (2008).

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Mao, Z., S. Jacobsen, F. Jiang, J. Smyth, C. Holl, D. Frost, and T. Duffy, Single-Crystal Elasticity of Wadsleyites, beta-Mg_2SiO_4, Containing 0.37-1.66 st.% H_2O, *Earth Planet Sci. Lett.*, **268**(3-4), 540-549 (2008).

Struzhkin, V., A. Goncharov, R. Caracas, H. Mao, and R. Hemley, Synchrotron Infrared Spectroscopy of the Pressure-Induced Insulator-Metal Transitions in Glassy As_2S_3 and As_2Se_3, *Phys. Rev. B: Condens. Matter*, **77**, 165133 (2008).

Malone, R., D. Dolan, R. Hacking, and I. McKenna, IR Spectrometer Using 90-degree Off-axis Parabolic Mirrors, *SPIE Optics & Photonics*, Vol 7068, p. 706808, sponsored by SPIE (2008).

Meng, Y., C. Yan, J. Lai, S. Krasnicki, H. Shu, T. Yu, Q. Liang, H.K Mao, and R. J. Hemley, Enhanced optical properties of chemical vapor deposited single crystal diamond by low-pressure/high-temperature annealing, *Proc. Nat. Acad. Sci.,* **105**(46), 17620–17625, 2008.

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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. 2008

Prepared by
Michael T. Vaughan
Donald J. Weidner

Available MAC beamtime. 2007-2008 has been an exciting year at the multianvil facility at the NSLS. We are continuing to expand the user time available by increasing access to multi-anvil experiments in time periods that were previously unavailable. The first phase is to time-share with the B3 diamond anvil cell hutch. When the new hutches were designed, the beam was split so that one part fed the B2 hutch and the other went through the hutch to the B3 station. By placing a shutter between hutches, we are able to run experiments in the B2 hutch while they can enter the B3 hutch. Currently, the B line of X17 (a high energy wiggler beamline) receives 2/3 of the total time available on the X-ray ring. Materials science uses the other 1/3. The X-17B2 multi-anvil system can use all of the 2/3 of beamtime for COMPRES research. NSLS plans to develop X17A is continuing. This will be a high energy end station that can run simultaneously with the X17B line. With the completion of the A leg, many users in materials science that now use X17B1 will move to X17A. This will 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.

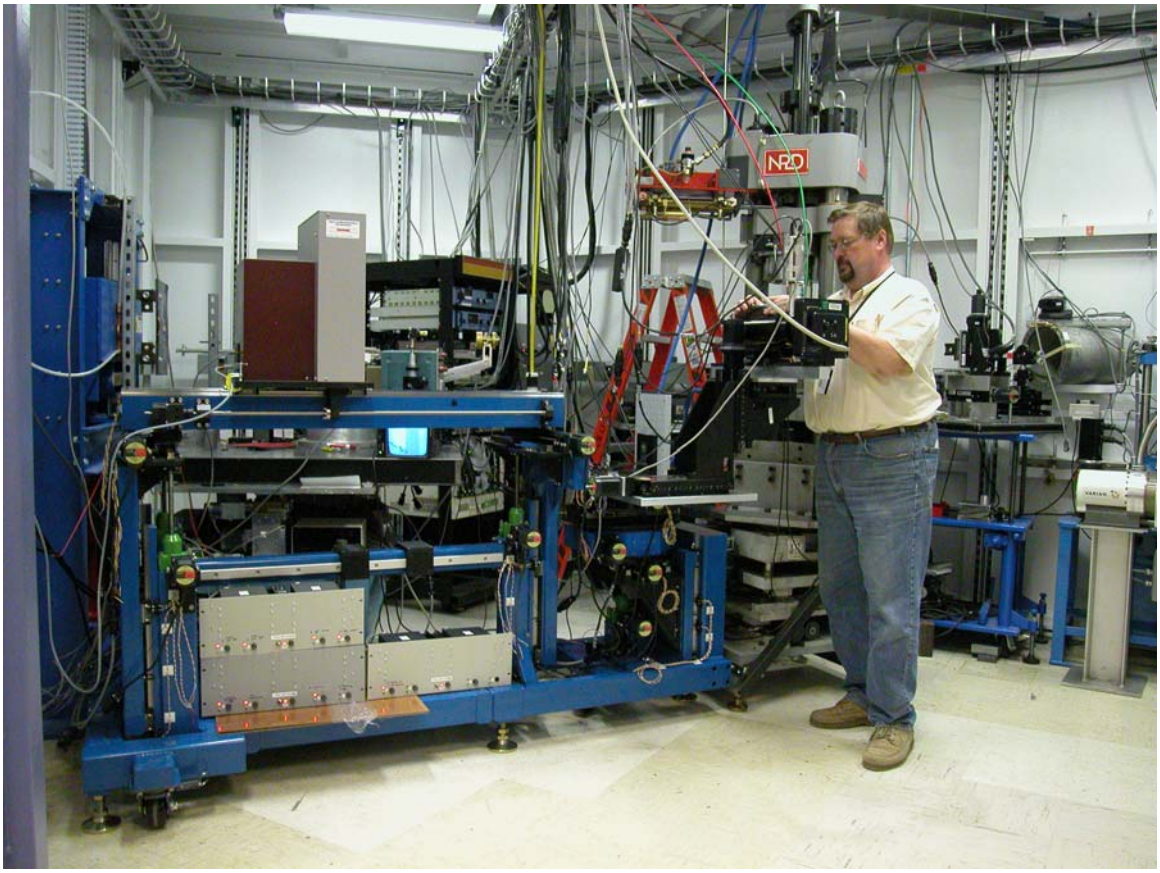
In-hutch monochromatic side station We are now near completion of a second high pressure station within the high pressure hutch. A single bounce monochromator will remove a thin slice of beam from the white beam and deliver it behind the main press to a second press equipped with a T-cup high pressure device. In January, 2009 we anticipate the installation of the T-cup system on the mono beam. Everything is in place and we expect to do the installation during the beam down time in December of this year.

High accuracy stress measurements. We have purchased a new detector and electornics (mostly from other NSF funds) for improving the accuracy of stress measurements. A 10 element energy dispersive detector has been installed and is now working. 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. A complete spectra take about 5 minutes of data collection time. We are nearly completed with the construction of a new set of conical slits that will improve the resolution of this data. We will replace our prototype conical slit with one that has better spacial resolution. We anticipate the ability to resolve 10 MPa of stress. This will bring the high pressure rheology system to a similar accuracy as the room pressure systems.

Beam time allocation We are continuing our process of beam time allocation. Now all experiments must be submitted to NSLS review panel using the NSLS review process for general users. NSLS then assigns up to 50% of the standard mode beam time on the basis of their review (this does not count parasitic time). We reserve 10% for

beamline development. We assign the remaining time following the rating of the NSLS review, but upgrading proposal that are consistent with a COMPRES agenda.

NSLS II The next generation of synchrotron at Brookhaven is nearly ready to begin construction. We have participated in planning and preparation of high pressure white papers. As a result of workshops and discussions, we submitted a Letter of Intent for a high pressure beamline at this facility. While we are not one of the project beamlines (and did not expect to be) we continue to champion high pressure at this new facility.



Installation of Monochromatic Side Station in X17B2 Hutch

Science Highlights – activities of 2007

- ***Q*** Measurements are now being made that are sensitive to the Q and dispersion of elastic properties. Using imaging as a means to measure elastic deformation, stress can be measured with a 50 millisecond exposure. This allows stress – time relations to be monitored at P and T. New results on the effect of phase transformations was published by Li in Nature (see publication list). Dobson adapted the imaging system to measure thermal diffusivity at high P and T.

Activities for 2008-9

We plan to fully operate two beamlines simultaneously in the MAC hutch. One will be white beam, the other monochromatic. One with a DIA system, the other with a Tcup. Both will have differential stress capability. This represents the culmination of many years of planning, designing, and constructing. We are currently formulating our plans to move forward beyond this.

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, electronics expert	SUNY

Other support for X17B2 2008-2009

Equipment

Stony Brook for detector	**$50,000**
NSF for detector system	**$200,000**
(includes some support for D-Tcup system)	

Personnel

Stony Brook Mineral Physics Inst	**$300,000**

Year 3 Proposed Budget
June 1, 2009 – May 31, 2010

Details of the requested budget for Year #3 and the justification for each budget category are given below in Section E of this report.

Publications in 2007-2008 for X17B2

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Carpenter, M. A. B. L., R. C. Liebermann (2007). Elastic anomalies accompanying phase

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Beamline activity

In calendar year 2008, there were 136.25 days of beam time used by X17B2, out of a total of approximately 204 Operations Days. 14 days were used by X17B2 in a mode which excluded sharing the beam with X17B3, but the remaining (122.25 days) were shared, half in parasitic mode under the control of X17B3, and half under the control of X17B2. 8½ days were used for beam line development
As in the past, every user submitted a proposal to the Light Source for review; beam time was assigned based on the quality of the proposals as expressed in the review, with the goal of maximizing access.

Number of distinct proposals submitted	26	4 proposals essentially duplicates of others submitted by same PI
Number of PIs submitting proposals	23	1 PI submitted 4 distinct proposals, 1 submitted 2
Number of PIs receiving beam time	20	3 proposals not appropriate for X17B2
Number of research groups with 4 PIs	2	7 distinct proposals in 1 group, 4 in the other
Number of research groups with 3 PIs	0	
Number of research groups with 2 PIs	2	2 distinct proposals each
Number of research groups with 1 PI	11	
Number of institutions with ≥ 15 days ea.	7	
Number of institutions with ≥ 10 < 15 days ea.	5	
Number of institutions with ≥ 5 < 10 days ea.	3	
Number of institutions with ≥ 1 < 5 days ea.	3	
Number of institutions with 0 days ea.	3	

The complete list is shown below. As this information is confidential, so this table should not appear in any public document. For most proposals, there were multiple submissions; when 0 days were assigned, usually there wasn't time available, and time was assigned in another cycle.

B.4 West Coast Synchrotron Facilities

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

Report to COMPRES from the west coast synchrotron program for year 2008

Simon Clark and Raymond Jeanloz
October 20th 2008

Summary

This has been a busy transitional year. We have reformulated our mission goals, completed the hire of three support scientists, completed the induction and training of the three scientists, renewed the COMPRES approved program at the ALS, continued our support of COMPRES users and made progress with our facilities development plan. Our refocusing of the program is already bearing fruit with demonstrated increased productivity this year. Our goal for next year is to consolidate the gains we have made with a focus on short term scientific productivity.

Activities this year

1. **Staff appointments**

   The departure of the two COMPRES beamline scientists based at the ALS gave us the opportunity to reassess the priorities and necessary skill sets required for this project. We used the Williams' report and the latest feedback from the Executive committee as the basis for our a new operating plan,

   Our highest priority for the current grant is the delivery of outstanding science as measured by scientific output. We have all of our baseline systems for x-ray diffraction with laser or resistive heating and ancillary spectroscopic measurements in place and now need to work with the COMPRES community to realize the potential of that investment. To achieve this we need to provide the highest possible level of support to COMPRES users of our facilities, and have therefore invested in several new appointments reflecting a broad spectrum of technical capabilities.

   We have hired three beamline scientists, and have managed to do this within our budget by hiring at a lower level than before and by making use of monies accrued during the search and hire process and by making purchases using alternate funds. We concluded that this is the best way to meet our new delivery mission, and it is totally in line with the increase of guaranteed COMPRES beamtime (from 20% to 35%). The previous beamline scientists

were more experienced and skilled at setting up experimental systems. Our new beamline scientists are at an earlier stage in their careers, but have the ability to support the systems that are now established, and have the drive and determination to fully exploit those systems.

We have assigned areas of special responsibility to each of them:

Jinyuan Yan	Provide general support and training for bl12.2.2 users. Provide support and training for cell alignment and loading. Take responsibility for the beamline, cell loading area and off-line ruby fluorescence area, ensuring the highest level of readiness.
Selva Vennila Raju	Provide general support and training for bl12.2.2 users who are using the resistively heated diamond anvil cells. Take responsibility for the development, maintenance and validation of the resistively heated diamond-anvil cells.
Bin Chen	Provide general support and training for bl12.2.2 users who are using the laser-heating system. Take responsibility of the laser heating system, and the high-pressure laboratory including the Brillouin and Raman systems.

In addition to this Raymond Jeanloz will continue to provide guidance and oversight, Simon Clark will provide day to day management and take responsibility for development of the laser heating system, and Jason Knight (ALS 50% assigned to beamline 12.2.2) will continue to take responsibility for hardware upgrades and maintenance and provide additional user support when required.

2. **Reorganization of high-pressure laboratory**

The high pressure laboratory has been reorganized. The cell alignment and loading equipment has been moved to a new area close to beamline 12.2.2 that is more convenient for users. The laboratory has been reclassified as a laser laboratory. The room is now restricted to use of the Brillouin and Raman systems. A fully automated laser-door interlock system is in the process of installation. This new arrangement allows us to use the Brillouin and Raman systems for routine data collection without interfering

with other users of the laboratory. Also, the cell loading is much closer to the beamline allowing users to do cell preparation while collecting data.

3. Development of resistively heated diamond anvil cells

A diamond anvil cell with an external heater has been developed for use with the Brillouin system and on beamline 12.2.2. The cell has been tested to 600^{o} C and 30 GPa. A range of fluorescent pressure markers are being evaluated. An additional $MoSi_2$ heater, potentially capable of reaching over 1000^{o} C, has been tested to temperature and is undergoing some redesign. The cell will be offered for use by COMPRES users on beamline 12.2.2 and with the Brillouin system from January 2009.

4. Development of Brillouin and Raman systems into user facilities

The Brillouin and Raman systems are fully operational. They are completing commissioning with measurements of polycrystalline systems such as argon, water and sodium chloride. Bin Chen spent a week being trained in Brillouin methods by Tom Duffy in Princeton. Sergio Speciale will visit from Potsdam in December 2008 to complete the commissioning and validation tests with Bin. From January 2009 the system will be offered for use by COMPRES user groups.

5. Upgrade laser heating system

Due to the problems that we had with staff recruitment we have not managed to make as much progress as we planned this year. A new top table has been designed and ordered, two four-color systems have been built and one is installed on beamline 12.2.2. This is currently being tested and integrated into the beamline data acquisition system. The new laser beam shaping optics have been assembled and tested offline. Two one-color systems have been installed and tested. We are now waiting for the new top table to complete the installation of all of these systems.

6. Continue the validation of our laser heating system

Validation of the laser heating system continued with measurements from resistively heated wires and foils as well as metal foils contained inside diamond anvil cells. The resistively heated wires have shown that we can accurately measure temperatures from both sides of a wire and achieve melting points

within the errors reported in the literature. Also, comparison of melting temperatures along some eutectics by Mike Walter's group from Bristol gave melting temperatures close to those measured in their laboratory and close to those in the literature.
Support a program of outstanding scientific research.

7. Support a program of outstanding scientific research.
We continued to provide a high level of support for COMPRES users. We have had a significant increase in productivity this year with two high profile publications appearing in press.

Summary of beamtime allocation process

Beamtime on beamline 12.2.2 is made available to COMPRES users as part of the COMPRES-ALS Approved Program. This guarantees a minimum of 35% of the beamtime on beamline 12.2.2 to COMPRES users.

COMPRES users apply for beamtime at the ALS using the same system as general users. These proposals are reviewed for safety, feasibility and scientific merit and ranked in priority order. COMPRES proposals are then allocated beamtime until all of the COMPRES time is allocated. Any remaining COMPRES proposals are then combined with all the other beamline proposals and the remaining beamtime is allocated in priority order. We work closely with those making beamline allocations to ensure that every promising COMPRES proposal has a maximum chance of getting beamtime, either under the COMPRES umbrella or as part of the general-user community.

Summary of proposed activities for next year

For next year we have six main goals:
1. Complete the training of our beamline scientists

Training of our staff is well underway. They have completed all mandatory ALS training and specific training in their areas of chief responsibility. Bin Chen has been concentrating on the Brillouin system so far and will have completed additional training in laser heating early in the New Year. Cross training will then begin to ensure that all of our support scientists can provide support on all of our systems.

2. **Complete the development of the Brillouin and Raman systems into user facilities**

The Brillouin and Raman systems are working well for polycrystalline samples in diamond anvil cells. We aim this year to add additional motorized alignment systems and remote viewing systems to make the alignment of the system as straight forward and safe as possible. As the user program ratchets up we intend to commission a resistively heated diamond cell with the Brillouin and Raman systems and start planning for the addition of laser heating.

3. Upgrade laser heating system.
We aim to complete the upgrades started last year. We will:

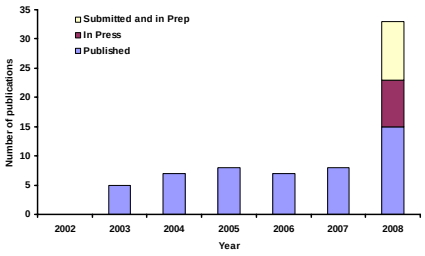
a. Install a new larger top table with improved stability
b. Install two four color temperature measurement systems
c. Install two one color temperature measurement systems
d. Install pellicle beam splitters to reduce the number of ghost images.
e. Develop new temperature determination software to automatically utilize all temperature measurement systems in parallel.
f. Improve temperature stability by installing a two loop temperature feed back system using both the laser power and light emitted from the sample to control the temperature on both sides.
g. Complete the commissioning and validation of this whole system.

4. Continue validation of on-line laser heating system.
We plan to continue the validation of the temperature measurement further measurements from resistively heated wires and metals held in diamond anvil cells.

5. Commission resistive heating cell.
The resistively heated diamond anvil cell is working up to 600^{o} C. We aim this year to extend that maximum temperature up to around 1000^{o} C. This will involve addition of secondary internal (close to the diamond) heating systems. We have two that we are developing at the moment using $MoSi_2$ and Pt wire heaters.

6. **Support a program of outstanding scientific research.**
We will continue to provide the current high level of support for COMPRES users of the beamline and the off-line Brillouin and Raman systems.

Summary of publications



High-pressure publications from the ALS have shown a dramatic increase this year. We attribute this in part to our readjustment of the skill set of our user support team. Most of these publications are due to COMPRES users. A list of publications for this year is contained in Appendix 5.

Appendix 5: List of ALS high-pressure publications for this year

COMPRES

S.A. Parry, A.R.Pawley and S.M.Clark, **An infrared spectroscopic study of 10-Å phase to 10 GPa, and comparison to talc** *American Mineralogist*, **92**, 525 - 531 (2007).

M. Kunz, W. A. Caldwell, L. Miyagi and H.-R. Wenk **In situ laser heating and radial synchrotron X-ray diffraction in a diamond anvil cell** *Review of Scientific Instruments* **78**, 063907 (2007).

W.A. Caldwell, M. Kunz, R.S. Celestre, E.E. Domning, M.J. Walter, D. Walker, J. Glossinger, A.A. MacDowell, H.A. Padmore, R. Jeanloz and S.M. Clark, **Laser Heated Diamond Anvil Cell at the Advanced Light Source Beamline 12.2.2** *Nuclear Instrumentation and Methods in Physics Research, Section A* **582** 221-225 (2007).

K. Catalli, S.-H. Shim and V.B. Prakapenka, **A crystalline-to-crystalline phase transition in Ca(OH)2 at 8 GPa and room temperature** *Geophysical Research Letters* **35**, L05312, doi:10.1029/2007GL033062 (2008).

D.V.S. Muthu, B. Chen, B.A. Cook, and M.B. Kruger, **Effects of sample preparation on the mechanical properties of AlMgB14,** *High Pressure Research* **28** 63-68 (2008).

A.E .Gleason, S. Parry, A.R. Pawley, R. Jeanloz and S.M. Clark, **P-V-T equation of state for Talc and 10A phase: implications for water transport into the Earth**, *Am. Min.* **93** 1043-1050 (2008).

J. Yan, P. D. Adams, R. J. Angel, N. L. Ross, M. Rivers, J. B. Parise and S. M. Clark, **The Development of an Automated Data Analysis System for powder diffraction data collected using an area detector** *High Pressure Research*, **28** 293-298 (2008).

S. Speziale,. R. Jeanloz, S.M. Clark, S. Meenakshi, V. Vijayakumar, A.K. Verma, R.S. Rao and B.K. Godwal, **Axial ratio anomalies and Electronic Topological Transitions in Cd0.80Hg0.20 at High Pressures**, *J. Physics and Chemistry of Solids*, **69**, 2325-2331 (2008).

J.M. Zaug, A.K. Soper and S.M. Clark, **The pressure-dependent structures of amorphous red phosphorus and the origin of the first sharp diffraction peak**, *Nature Materials* doi:10.1038/nmat2290 (2008).

B.K. Godwal, S. Speziale, S.M. Clark, J. Yan and R. Jeanloz, **Electronic Phase Transition and Amorphization in AuIn2 at High Pressure**, *Phys. Rev. B.* **78**, 094107 (2008).

M.J. Walter, G.P. Bulanova, L.S. Armstrong, S. Keshav, J.D. Blundy, G. Gudfinnsson, O.T. Lord, A.R. Lennie, S.M. Clark, C.B. Smith and L. Gobbo, **Primary carbonatite**

melt from deeply subducted oceanic crust, *Nature* **454** 622-625 doi:10.1038/nature07132 (2008).

S-H Shim, K. Catalli, J. Hustoft, A. Kubo, V.B. Prakapenka, W.A. Caldwell and M. Kunz, **Crystal structure and thermoelastic properties of (Mg0.91Fe0.09)SiO3 postperovskite up to 135 GPa and 2,700 K**, *PNAS*, **105** 7382-7386 (2008).

S. Lundin, K. Catalli, J. Santillan, S-H, Shim, V.B. Prakapenka, M. Kunz and Y. Meng, **Effect of Fe on the equation of state of mantle silicate perovskite over 1 Mbar,** *Physics of the Earth and Planetary Interiors,* **168** 97-102 (2008).

J. Hustoft, K. Catalli, S-H, Shim, A. Kubo, V.B. Prakapenka and M. Kunz, **Equation of state of NaMgF3 postperovskite: Implication for the seismic velocity changes in the D" region**, *Geophysical Research Letters*, **35** L10309 (2008).

S-H. Shim, **The postperovskite transition**, *Applied Physics Letters* **36(10),** 569-599 (2008).

K. Catalli, S-H. Shim, and V.B. Prakapenka, **A crystalline-to-crystalline phase transition in Ca(OH)2 at 8 GPa and room temperature**, *Geophysical Research Letters* **35,** L05312 (2008).

Other

H.Y. Chung, M.B. Weinberger, J.B. Levine, A. Kavner, J.M. Yang, S.H. Tolbert, and R.B. Kaner **Synthesis of ultra-incompressible superhard rhenium diboride at ambient pressure**, *Science* **316** 436-439 (2007).

P.J.M. Monteiro, A.P. Kirchheim, S. Chae, P. Fischer, A.A. MacDowell, E. Schaible, S.M. Clark, and M.A. Marcus, Cement and Concrete Research Using X-rays at the Advanced Light Source in Berkeley, in Proceedings of the 3rd International Symposium "Sustainability in Cement and Concrete, A. Yinobal, Vol 1-2 (Turkish Cement Manufacturers', Istambul, 2007). [Proceedings of the 3rd International Symposium Sustainability in Cement and Concrete, (Istanbul , Turkey, May 21-23 2007].

K. Koskie, N.M. Kamp, R.K. Smith, M. Kunz, J.K. Knight, and A.P. Alivisatos, **Structural distortions in 5-10 nm silver nanoparticles under high pressure** *Physical Review B*, **78** 165410 1 – 165410 10. (2008).

J.C. Crowhurst, A.F. Goncharov, B. Sadigh, J.M. Zaug, D. Aberg, Y.Meng, B.V. Prakapenka, **Synthesis and Characterization of Nitrides of Iridium and Palladium**, *Journal of Materials Research* **23** 1-5 (2008).

C. Infrastructure Development Projects

C.1 Multi-anvil cell assembly project

[PIs: Kurt Leinenweber, Thomas Sharp and James Tyburczy, Arizona State University]

Annual Report and Proposal for Years 3-5 of COMPRES II

Kurt D. Leinenweber[1], James A. Tyburczy[2], Thomas G. Sharp[2]
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[2]School of Earth and Space Exploration, PO Box 1404, Arizona State University, Tempe, AZ 85287-1404

Abstract

The Multi-Anvil Cell Development project of COMPRES has been an outstanding success in developing well characterized, calibrated assemblies that are widely used and distributed globally throughout the multianvil user community. This success involved development of new manufacturing techniques and identification and cultivation of selected manufacturers and machinists who can provide the needed high quality at reasonable cost. These assemblies initially were provided *gratis* to users, but we now propose to move to a model in which users support most of the production costs for standard assemblies and COMPRES funding goes mostly to development of new and experimental assemblies. With these recent developments in fabrication techniques and new materials, we are well positioned to provide major assistance to the development of multianvil cells for use in synchrotron and neutron beamlines, We envision that development of beamline cells will become a significant focus of the COMPRES-supported part of our project. This funding request of $70,000 for year 3 reflects this new system and represents a 30% decrease from our previous COMPRES budget, reflecting current budget realities.

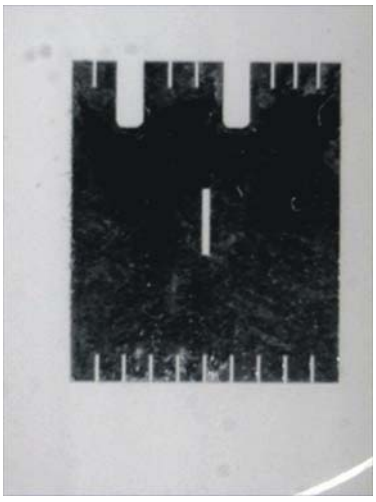

Figure 1. Laser-cut rhenium foil furnace with thermocouple notches, folding contacts, and a slit for x-ray access (center).

<u>Previous Developments</u>

The COMPRES multi-anvil cell development project now involves some 26 large-volume high pressure laboratories around the world (Table 1). The project has so far resulted in the development of six standardized cell assemblies for use in conventional multi-anvil laboratories, and four modified assemblies for use in *in-situ* experiments at x-ray beamlines (these ten cell assemblies are listed in Table 2). The cell assemblies are distributed with detailed instruction manuals and pressure calibration and temperature/power curves. The project has led to the

development and introduction of a significant number of novel materials and techniques into multi-anvil research, including injection-molded octahedra, porous mullite pressure media, forsterite thermal insulation sleeves, laser-cut rhenium furnaces (Figure 1), and new methods of putting x-ray windows into multi-anvil assemblies (Figures 1-3). Many standard materials are also used, such as the lanthanum chromite and zirconia from Japan that have been a mainstay in high pressure research since the 1970's, but we have developed machining techniques to make finished parts available to large numbers of laboratories. The COMPRES lathe that was purchased in the initial stages of the project has allowed the development of automated notching and slitting of ceramic parts for thermocouples and x-ray access (Figure 2). The thermocouple grooves in the octahedral pressure media are molded in (Figure 4). These are all tasks that researchers previously had to do by hand. These developments are documented in two summary publications, one in preparation and one submitted (1, 2). A preliminary report was presented in the COMPRES Newsletter (3). The thermal models that were developed for characterization of the COMPRES assemblies are detailed in reference (4), a publication that references COMPRES support (see Figure 5 for an example of a thermal profile calculated using this model).

Figure 2. $LaCrO_3$ sleeve with thermocouple slots and x-ray window cut on the COMPRES automated lathe. The slit in the rhenium furnace

As part of all this activity, the COMPRES Multi-Anvil Cell Development Project has created a new forum for discussion and comparison of experiments in the multi-anvil community. The new cell assemblies serve as a common basis for comparing techniques in different laboratories. Because they are available in their complete form to any interested laboratory, the COMPRES cell assemblies represent the first time that identical assemblies and materials have been used jointly by so many different laboratories. Thus the laboratories can readily compare the

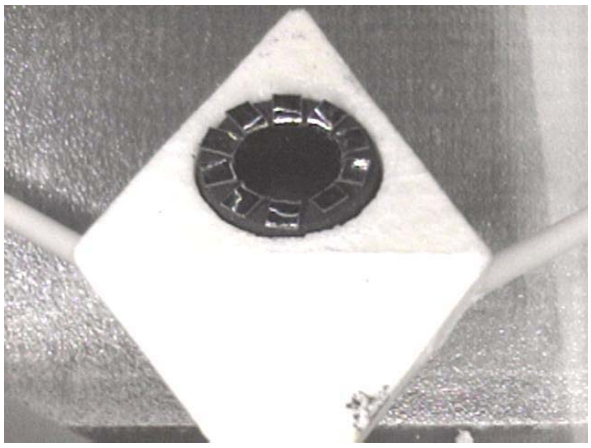

Figure 3. 10/5 in-situ assembly ready to load. The pencil smudge (lower right edge

results obtained with their own high-pressure equipment to those from other laboratories. This project has also aided rapid transfer of multi-anvil technology throughout the community and made possible rapid startups for new laboratories. Community feedback and discussion has led to new ideas and improvements that have been incorporated into the assembly designs. The overall result is a set of assemblies that are easy to learn and use, are well-characterized, have high success rates, and have a broad user base. The assemblies cover a wide range of P-T capabilities (Figure 6) with large volumes.

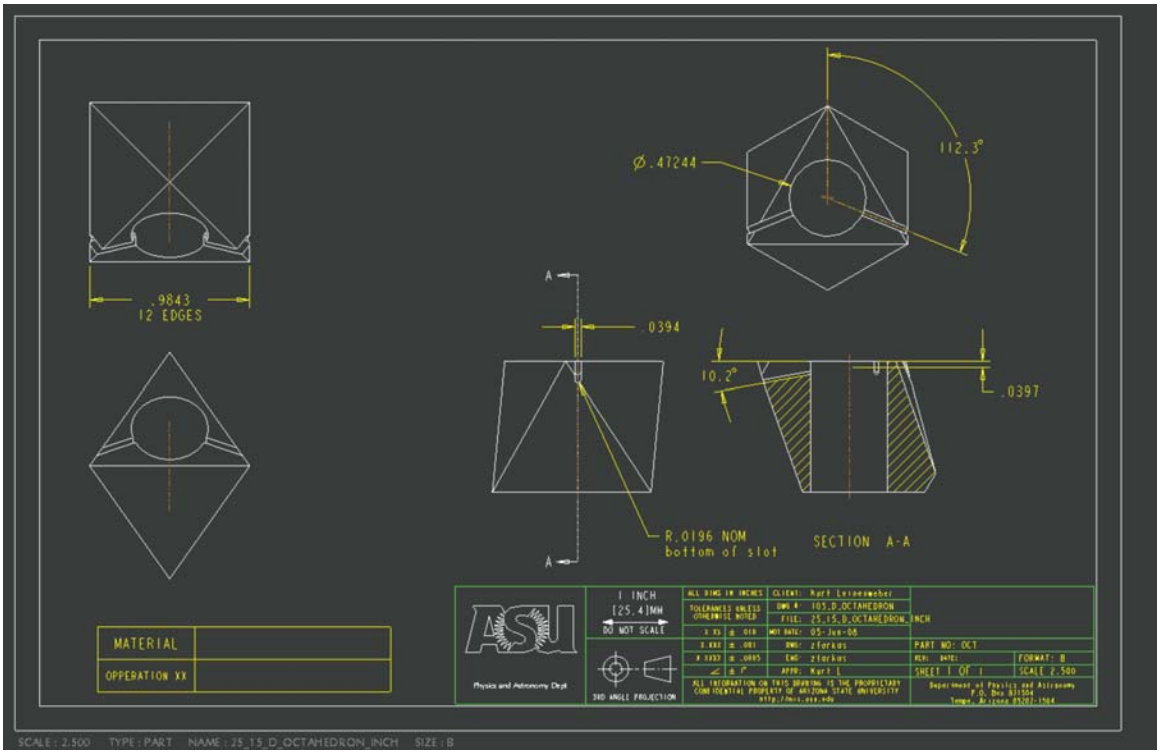

Fig 4. Design drawing for an injection-molded octahedron with sample hole and thermocouple groove.

The building of a community has been promoted by the efforts of the PI's to communicate with many researchers on an individual basis about the techniques and the transfer of the technology, by training visitors at the ASU laboratory (Larissa Dobrzhinetskaya, UC Riverside), by posters and talks at the COMPRES meetings (5-8) and at AGU (9-11), and by input from the COMPRES Facilities Committee and COMPRES Central. The beam line assembly technology has been transferred through contacts with Yanbin Wang at GSECARS, by visits by Kurt Leinenweber to beamline experiments that were using the cells (Righter and Danielson; Jie Li group), and by hosting visitors at the beam line during our own beamline experiments (Jean-Phillippe Perrillat, University of Illinois Urbana-Champaign; E.J. Tronche, University of Amsterdam; Hans Mueller, Potsdam). On March 1-3, 2005, a COMPRES-sponsored Workshop on Multi-Anvil Techniques was organized at APS. The purpose of the

workshop was to demonstrate multi-anvil techniques, the new series of cell assemblies along with other established techniques, and the use of *in-situ* diffraction and radiographic techniques in large-volume experiments. As part of this hands-on workshop three online experiments were performed (12). Several scientific results have also been presented which included detailed developments of the various cells (cf. 13-17).

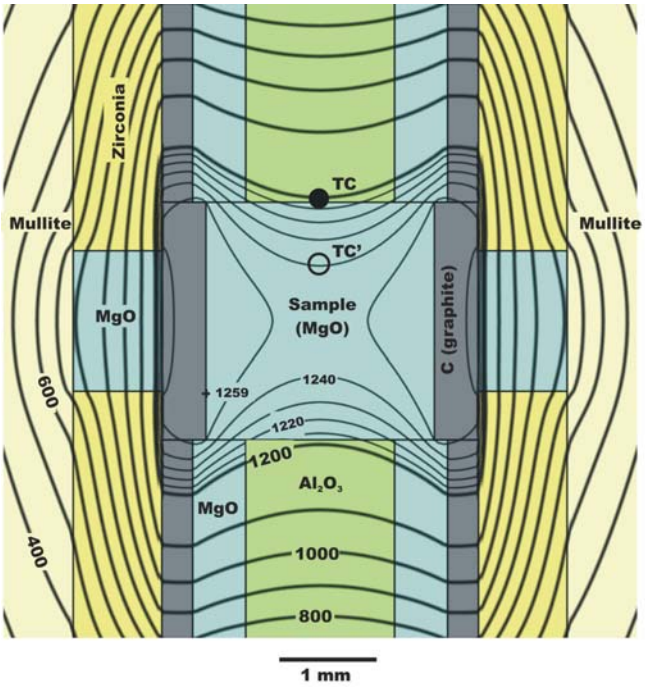

Fig. 5. Thermal calculation for the central part of the 14/8 step-heater assembly with a graphite furnace and MgO windows, combined with a mullite octahedron (10).

Development of multi anvil cells for *in-situ* synchrotron work that resemble the conventional cells (Figures 1-3 show the 10/5 assembly for this purpose) has been pursued in parallel with the cells for conventional multi-anvil laboratories. A primary motivation for this is to make it easier for researchers at conventional laboratories to use synchrotron radiation. The diamond-cell community has a very natural base of synchrotron users, because most diamond cells can be carried to a synchrotron and placed directly on an x-ray stage at the beam line for *in-situ* x-ray experiments. The Large-Volume Press (LVP) facility at the Advanced Photon Source provides an opportunity for the multi-anvil community to have similar access to *in-situ* experiments because the tooling at that press can accept the standard multi-anvil second stage of carbide cubes. To take full advantage of this opportunity, it is necessary to develop easy-to-use pressure cells with the x-ray access needed to allow the collection of diffraction and radiographic images from the sample. The four *in-situ* cells from this project (Table 2) are designed to allow such access. They are based on the familiar designs from the four conventional cells with the

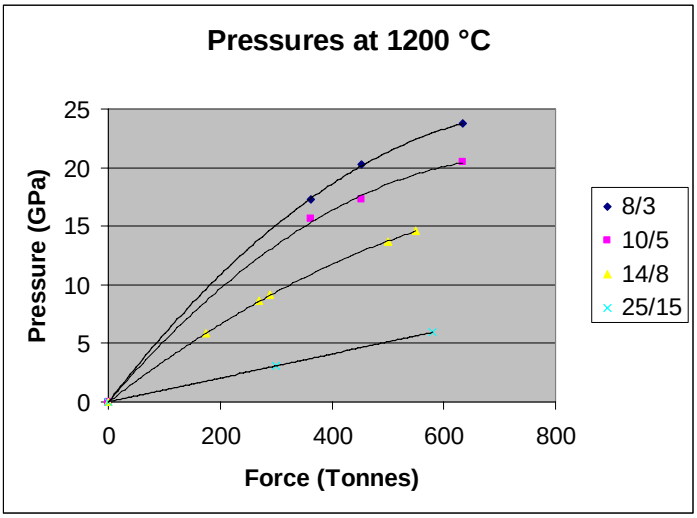

Fig. 6. Summary of the pressure capabilities of several assembly sizes at a temperature of 1200° C.

simple addition of x-ray windows and can be used very easily at the beam line with high success rates similar to those experienced in-house. New beam line users can focus on learning the *in-situ* x-ray techniques rather than worrying about an entirely new style of pressure cells.

The development of conventional cells has focused on 6-8 systems with octahedral pressure media. Some developments, in particular porous mullite pressure media, have been beneficial to the DIA and D-DIA programs for *in-situ* diffraction and deformation experiments using cubic pressure media. The porous mullite ceramic from this project has been heavily developed as a replacement for boron epoxy by the Stony Brook group. Boron epoxy, though it is a highly effective thermal insulator and has low x-ray absorption, has recently been found to introduce H_2O to the sample and assembly, which may cause water weakening in deformation experiments, and simultaneously limits the temperatures that graphite furnaces can reach. Mullite has good thermal insulation capabilities and is reasonably x-ray transparent, but does not introduce H_2O. This has raised temperature capabilities in the DIA by several hundreds of degrees Celsius (18) and allowed more reliable dry or controlled H_2O deformation experiments (19), both major advances in capability.

We have proceeded to make the standardized assemblies for the community upon demand, in quantities up to 200 assemblies per order. We have received a total of 60 orders to date. In the process of fabricating these assemblies, we use 27 different primary outside sources of materials, plus our own machine shop and our undergraduate laboratory assistant. In fiscal year 2007-2008, for example, there were 24 orders that totaled $36,366.

Project Description for years 3-5 of COMPRES II

A. Beamline Support

The COMPRES multi-anvil cell development project has always supported beamline operations. This project has fostered the use of porous mullite ceramic for pressure media in the DIA at BNL and the Kawai-type system at Argonne, including mullite octahedra, mullite cubes and mullite spheres (18, 19). We developed a series of four different 6-8 cell assemblies that are now regularly utilized for in-situ x-ray diffraction experiments at GSECARS, have been used at Daresbury, and have just this year been successfully used at DESY in Germany.

Beyond these developments, there remains significant need for new multianvil capabilities at the beamlines. The Cell Development project has received numerous requests to develop new synchrotron-related cell assemblies and to make major modifications to the existing ones to facilitate their use at beamlines.. We need beam windows in the gaskets and octahedra of the existing assemblies to improve the throughput especially at low energies. There are requests for COMPRES to develop complete D-DIA assemblies (Burnley and others), ultrasonic assemblies for *in-situ* experiments (Manghnani), and completely new designs of 6-8 assemblies using different

components to enhance access to the sample for both diffraction and radiographic studies (Wang). We will pursue all of these requests to the best of our ability as the beamline experiments are scheduled. We do not have a DIA in which to test cubic assemblies, and the frequent testing of assemblies offline is very important to successful beam line experiments. We will seek to collaborate with laboratories that have DIA apparati to test the designs offline as well as at the beam lines.

Our experience thus far in collaborating with beamline scientists, as opposed to those working in conventional laboratories, is that the mode of operation of beamlines does not readily lend itself to or require long-term standardization of the cell assemblies. First of all, the pressure is measured in-situ, so there is no need for the assembly to have a precise pressure calibration. That means that assemblies can be changed much more frequently. In conventional experiments, what is needed is a stable production of well-calibrated pressure and temperature with a low thermal gradient, and once this is achieved, it is best to keep the assembly the same for all subsequent experiments. But at the beamlines, there is also the need for clear x-ray access for both diffraction and radiography, good sample and standard positioning, and optimizing these characteristics is an area of rapid change and improvement in design. Combined with this is the fact that beamlines do not use a large number of assemblies – usually about 10 or at most 20 per group per cycle, with long time intervals between each beam time to reconsider and redesign assemblies. In general for each beam cycle there are two or more individual groups using our assemblies for separate beam times, but they can be using different ones so this still requires a great deal of variety. Finally, beamline scientists often make requests to us on short notice as beamtime approaoches.

These factors – small numbers, complexity of development, frequency of design change because the field is developing and advancing rapidly, and short lead time – make supplying beam-line assemblies more complicated than supplying conventional ones. However, the scientific impact of beam-line experiments is very high, and this more than compensates for these factors.

We are now positioned, with our developments in fabrication techniques and new materials, to provide increasing assistance to the beamlines; we envision that development of beamline cells will become a significant focus of the COMPRES-supported part of our project. The budget items for Materials & Supplies and Services will be used for materials and machining of cell assemblies for beamlines. Part of the Travel budget will be for trips to beamlines to help in the implementation of these assemblies.

Based on the requests for assistance that we have received, we will initially focus on three developments. One will be on complete DIA and 6-8 assemblies for ultrasonics (Burnley and others). We will develop fully functioning ultrasonics assemblies that will be used by the laboratories that are requesting them, as well as any others that are interested. There is a considerable variation in these assemblies depending on the sound velocities of the samples, and we will work with the experimenters to optimize these

variables for each sample. There is also an interest in assemblies for ultrasonics on liquids (Manghnani) which we will work on.

Fig. 7. Mullite spheres and seats made by our project (19)

A second effort will be on deformation assemblies for the D-DIA (Durham, Burnley, others). We already been involved in the development of porous mullite spheres and spherical pyrophyllite seats (Figure 7) which were instrumental in recent success by Durham et al. (19) in measuring the activation volume for creep in olivine to 4.9 GPa. We will extend this to the development of complete D-DIA assemblies that will make these deformation capabilities available to the full range of potential users. A related development is 6-8 assemblies for a new deformation T-Cup (Weidner, personal comm.) which we will also develop.

The third development will be for improved 6-8 assemblies for in-situ x-ray diffraction and radiography studies (Yanbin Wang, Jie Li, others). The assemblies that we have developed to date need improvement to enhance beam throughput (X-ray flux) through the addition of boron epoxy windows in the octahedra and boron nitride windows in the gaskets We will implement and test these improvements. Recently we have published results of in-situ radiography of melting in the Fe-S system with the COMPRES assemblies (20). We will work on assemblies with fuller beam access to the sample for more highly quantitative and complete radiography studies. Some new materials, such as machinable TiB_2/BN composite furnace material from Momentize Performance Materials, combined with our porous mullite pressure media and beam windows, will be utilized for these developments.

We do charge the beamline users for the assemblies that we provide. This helps to recover some of the costs associated with this part of the project. However, the charges are similar to those for the conventional, offline assemblies. They do not take into account the continual development, design changes, and small batch sizes that are

characteristic of beam line assemblies. Also, when designs are extremely new and not well tested, we do not charge for them because the use of the assemblies is part of the development. The beamline aspects of this project will be flexible and responsive to the needs of the beamline community. For this reason, we request COMPRES support for the beamline developments that is in addition to the contribution from the users.

It is advantageous to pursue developments at a location (ASU) that is not affiliated with any particular beamline, so we can assist in parallel developments at all beamlines. We are interested in working with all the beamlines that have capabilities commensurate with our assemblies, including SPring-8 in Japan, HASY in Europe and NSLS and BNL. In addition, as the capabilities at ALS and other beamlines improve, we will work with them. Beamlines are already very busy with users. They will benefit greatly from an interested laboratory that will work on these technical cell developments. Our interests are in advancing state of the art developments that increase capabilities and techniques at large-volume beamlines.

B. Multi-anvil Assembly Production

The development of conventional 6-8 cells for laboratories around the world that are well-calibrated, well-characterized and have high success rates has been the foundation of our work so far.

This part of the project has gone very well, with the development of six major assemblies of differing sizes and capabilities that are supplied to laboratories around the world upon their request. The assemblies have helped supply a common basis around which discussions of high-pressure experiments can be made between laboratories, have provided chances for interlaboratory comparisons and have allowed new laboratories to start up more quickly.

We have made developments to allow a continuous supply of these assemblies to the entire community, without requiring COMPRES support. The assemblies are purchased by the end-users (including ASU) and the purchases offset the costs of all the materials and fabrication costs. These developments have been successful and we have ways, some quite recently developed, to provide a supply of these assemblies no matter how high the demand becomes. Recent developments have even allayed the need for a full-time machinist for production, so the machinist has been removed from our budget. The occasional machining costs for odd items or fill-ins, and for accessories such as brass dummies, specially made diamond files and widgets to help with assembling, are all covered by the purchase prices.

The only items that we have not included in the fabrication price are the labor of an undergraduate student worker who will be involved in inventorying and packaging of materials for shipment, and the time of Kurt Leinenweber which is represented here by a request for 1 month of salary support. For both these individuals, some of the effort will

go to multi-anvil assembly production and distribution, while significant effort will go to the beamline assembly development effort.

C. Technical Developments

Continued technical developments are also desired for our conventional assemblies, which will also provide technical contributions to the beamline assemblies, since the materials and fabrication processes overlap on both types of assemblies.

One significant area of development will be for higher temperature cells, while a related area is to reduce thermal gradients in the sample. Both of these require a cell that has better thermal insulation than current cells, so it is likely that they both can be tackled with the same solution. We have a 14/8 cell design concept that uses a lanthanum chromite box furnace combined with very thin electrical leads and massive zirconia insulation, and we plan to develop this design. When it is finished, it will become a standard COMPRES assembly and will be financed by sales as are the other assemblies.

We will also pursue new production methods. Our experience indicates that the pursuit of new methods requires some investment, because of startup costs for the new methods. Also, these efforts are implicitly experimental in nature, and so are not represented in the material charges for already developed assemblies. Ceramic methods such as extrusion, pressing, and injection-molding will continue to be tested for further developments in new cell materials.

Year 3 Proposed Budget
June 1, 2009 – May 31, 2010
Details of the requested budget for Year #3 and the justification for each budget category are given below in Section E of this report.

Tables

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	Principal 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
California Institute of Technology	Pasadena, CA	Jed Mosenfelder
Case Western Reserve University	Cleveland, OH	James Van Orman, Katherine Crispin
Delaware State University	Dover, DE	Gabriel Gwanmesia
Florida International University	Miami, FL	Jiuhua Chen, Helene Couvy
Helmholtz-Zentrum Potsdam	Hamburg, Germany	Hans J. Mueller
Lawrence Livermore National Laboratories	Livermore, CA	Julien Siebert
Massachusetts Institute of Technology	Cambridge, MA	William B. Durham
NASA Johnson Space Center	Houston, TX	Kevin Righter, Lisa Danielson
National Cheng Kung University	Tainan, Taiwan	Jennifer Kung
Stony Brook University	Stony Brook, NY	Baosheng Li, Matthew Whittaker
Yale University	New Haven, CT	Kazuhiko Otsuka, Justin Hustoft
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
University of California at Riverside	Riverside, CA	Larissa Dobrzhinetskaya
University of Chicago,GSECARS	Argonne, Illinois	Yanbin Wang
University of Hawaii	Honolulu, HI	Murli Manghnani
University of Illinois at Urbana-Champaign	Urbana, IL	Jie Li, Bin Chen
University of Minnesota	Minneapolis, MN	Shenghua Mei, Tony Withers
University of Western Ontario	London, Ontario, Canada	Richard A. Secco

Table 2 – List of the standard and *in-situ* 6/8 assemblies of the COMPRES project.

Assembly name	Peak pressure	Proven temperature	Design
8/3	25 GPa	2319 °C	Rhenium furnace
10/5	20 GPa	2000 °C	Rhenium furnace
14/8 "G2"	13 GPa	1200 °C	Graphite box furnace
14/8 "Bay-Tech"	15 GPa	1400 °C	Graphite/LaCrO3 step furnace
18/12	9 GPa	1500 °C	Graphite box furnace
25/15	5 GPa	1500 °C	Graphite box furnace
8/3 in-situ	25 GPa	2000 °C	Slitted rhenium furnace
10/5 in-situ	20 GPa	2000 °C	Slitted rhenium furnace
14/8 "G2" in-situ	13 GPa	1200 °C	Graphite box furnace, forsterite sleeve
14/8 "Bay-Tech" in-situ	15 GPa	1500 °C	Graphite step furnace, MgO equatorial window, mullite octahedron
18/12	9 GPa	1500 °C	Graphite box furnace

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

[PIs: Wolfgang Sturhahn [1], Jennifer M. Jackson [2], Jay D. Bass [3]]

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2008 Report & 2009 Renewal Request

Report Summary

We report here on the activities to date of Year 2 of a 3-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 first two years with the Executive Committee's expectation of continued funding for the third year of the project. We include here a description of activities to date, planned activities for the coming year, and a budget request for Year 3 of the project.

High-resolution inelastic x-ray scattering (IXS) techniques provide the Earth and planetary science community with 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-P-T 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.

In the first two years of our infrastructure development project, we hired of a full-time postdoctoral researcher 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 beam line (sector 3-ID) to enhance its performance in high-pressure research, we engaged in outreach activities, e.g., a workshop on high-resolution IXS and various presentations at meetings and 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 full-time postdoctoral researcher in December 2007;
2. Organized the workshop "High-resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation", May 31 – June 1, 2008 at Argonne;
3. Generation of user proposals for sectors 3-ID and 30-ID by COMPRES members.

The individual items are described in more detail below.

1. Hiring of Postdoctoral Researcher

The position for the postdoctoral researcher was advertised in EOS and through the COMPRES email system. We received three applications from suitable candidates. The position was then offered to Dr. Hasan Yavas who accepted the offer and started on December 15, 2007. We decided to offer this position to Hasan because of his experience of working with synchrotron radiation in general and with inelastic x-ray scattering techniques in particular. Hasan is located full time at the APS. He co-organized the workshop on high-resolution inelastic x-ray scattering that took place in May/June of 2008.

2. Workshop Organization

We organized a workshop on "High-resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation", on May 31 – June 1, 2008 at the APS, with funding by COMPRES. The 45 participants from the United States, Canada, Germany, France, and Spain included 10 graduate students who learned about the capabilities and the theoretical background of IXS methods and visited sectors 3-ID and 30-ID at the APS where high-resolution IXS is performed. The 16 invited speakers covered introductions to NRS and IXS, applications using Earth materials, as well as theory and simulation of data. The lively and productive discussions after almost every presentation were enjoyed by the participants. During the workshop the following needs could be identified.

- Improve counting rates in experiments by better focusing for momentum-resolved IXS at 3-ID and by increased brilliance and flux from the APS;
- Create new or improved capabilities to enable high-energy x-rays at 3-ID for simultaneous diffraction studies and to increase the energy resolution for access to lower phonon energies;
- Continue support of data evaluation.

The workshop provided an ideal format to collectively address possible solutions to experimental problems and to help building a viable COMPRES user base for this facility. Details on the workshop agenda are still available on the APS web-site at http://www.aps.anl.gov/ixs2008.

3. Generation of New Proposals

In the time period of 2007/2008, 11 independent research groups from 10 COMPRES member institutions submitted 42 proposals to 3-ID and 20 proposals to 30-ID. Of these proposals 20 (= 48 %) and 6 (= 30 %) were granted beam time at 3-ID and 30-ID (see Figure 2). 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 worked well with the PIs to develop effective proposals that were very competitive for beam time. In effect, COMPRES now has it's own expert to help write proposals, consult on technical aspects of experiment design, and to help run experiments.

Planned Activities

In Year 3 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 high-resolution IXS experiments. We plan to organize another tutorial workshop introducing 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. On the instrumental side, we will proceed with the integration and use of the capability of x-ray diffraction with NRS experiments in sector 3-ID. The added diffraction capability will provide us with structural confirmation as well as with an equation-of-state during NRIXS data collection. For IXS experiments in sectors 3-ID and 30-ID, we plan to create an infrastructure in-place supporting high-pressure experiments. This will include optical microscopes and x-ray CCD cameras for in-situ alignment of samples depending on APS capital equipment funding. The successful completion of all these tasks depends on a dedicated postdoctoral researcher like Dr. Hasan Yavas. We expect that proposals for NRS experiments on sector 3-ID and IXS experiments on sector 30-ID will likely result from the workshop, and that Hasan will continue to work with the PIs to develop effective proposals that will be very competitive for beam time. In effect, COMPRES will have it's own expert to help write proposals, consult on technical aspects of experiment design, and to help run experiments. This should be a significant fraction of his workload in Year 3.

Illustrations

Figure 1: The workshop on "High-resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation", on May 31-June 1, 2008 at the APS attracted 45 participants from the United States, Canada, Germany, France and Spain.

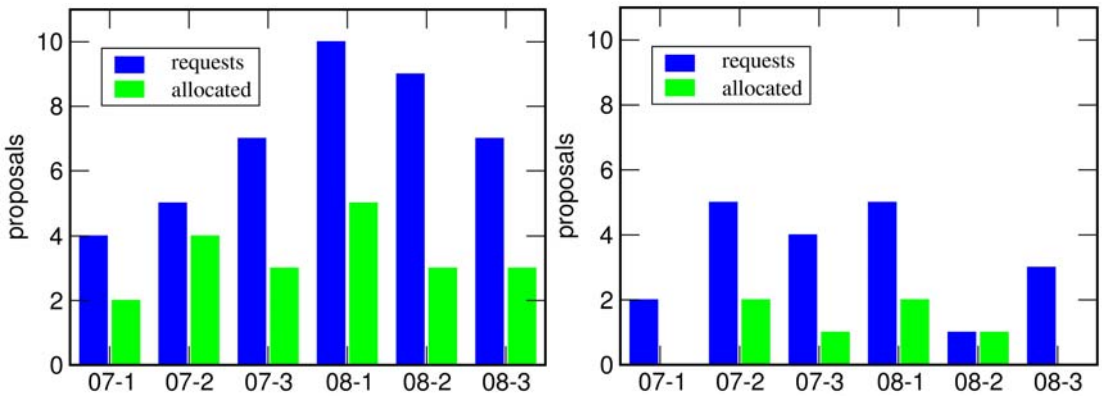

Figure 2: In the time period of 2007/2008, 11 independent research groups from 10 COMPRES member institutions submitted 42 proposals to 3-ID and 20 proposals to 30-ID. Of these proposals 20 (= 48 %) and 6 (= 30 %) were granted beam time at 3-ID and 30-ID, respectively.

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

[PI: Mark Rivers, GSECARS and 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, is working very well. It has now been used by more than 35 users to load over 180 cells.

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.

COMPRES has considered the possibility of duplicating this system at other sites, including perhaps the Advanced Light Source and the NSLS. However, the cost of a complete constructed system is expected to be more than $150,000, and in light of flat funding for COMPRES it makes sense to consider whether there is a cost-effective alternative mechanism to make gas-loading available to the members of the COMPRES community who wish to do experiments at locations other than the 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.

We propose here to have COMPRES fund 50% of a post-doc to reside at the APS. This person would be 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.

The turnaround time for loading cells will be a few days at most. Users who send cells must understand that there is a finite possibility that diamonds will be broken, and not hold GSECARS or COMPRES responsible if a diamond or other component is damaged.

The annual cost to make the APS gas-loading facility available as a mail-in service is less than 25% of the cost of constructing a new system, and a new system might also require similar operating costs to maintain. Thus, we believe the proposal is a good investment for COMPRES.

Year 3 Proposed Budget
June 1, 2009 – May 31, 2010
Details of the requested budget for Year #3 and the justification for each budget category are given below in Section E of this report.

C.4 Workshop Proposals for Year #3 of COMPRES II

a. On-line Brillouin Spectroscopy at GSECARS: basic principles and application for high pressure research

Vitali Prakapenka (GSECARS, Univ. Chicago)
Jay Bass (UIUC)
Stanislav Sinogeikin (HP-CAT, Carnegie Institution of Washington)

November 4, 2008

Introduction

An on-line Brillouin spectroscopy (BS) system was installed in the GSECARS 13BM-D station in 2004. This system was funded by COMPRES as an Infrastructure Development project, the Elasticity Grand Challenge grant from the NSF (to J. Bass), and co-funded by GSECARS. Commissioning and the first scientific experiments were performed during 2005-2007. In beginning of 2008 the system was opened for General User proposals. To promote this unique technique to the high pressure community and to educate potential users we request financial support to cover organization and hosting of a Brillouin Spectroscopy workshop at APS, Argonne National Lab.

Purpose of the Workshop

The main advantage of combining Brillouin spectroscopy with x-ray diffraction is the ability to perform simultaneous measurements of velocities and bulk modulus Ks (by Brillouin spectroscopy), and the volume/density (by XRD) independent of any pressure standard. A Brillouin spectroscopy system, located in the 13BM-D station, provides a new technique for in-situ studies for materials at extreme conditions [Sinogeikin et al, 2006, Prakapenka et al, 2007, Lakshtanov et al, 2007]. With this unique system it is now possible to measure sound velocities and densities of materials simultaneously, resulting in an absolute pressure scale and determinations of important material properties (e.g., equations of state and elastic properties) as a function of pressure and temperature. High resolution x-ray diffraction and Brillouin spectroscopy collected simultaneously from the same sample area and in the same pressure-temperature environment provide information essential for interpreting seismic observations and constraining models of the composition and evolution of the Earth.

The on-line Brillouin spectroscopy system was opened for general users at the beginning of 2008. Although the system is designed to be very user-friendly, successful BS measurements at high pressure using diamond anvil requires training and a thorough understanding of the BS technique. To educate our potential users and to promote this COMPRES-supported project we propose a workshop focusing on the major topics relevant to high pressure research using Brillouin spectroscopy combined with high-resolution x-ray diffraction technique that will include:

- fundamental aspects of Brillouin scattering
- experimental challenges of BS and XRD at high pressures and temperatures

- software for data collection and analysis
- suggestions for future proposals

Business of the workshop will include the plenary lectures, scientific contributions and participation in real experiment with data collection and analysis. It will be organized by Vitali Prakapenka (GSECARS, Univ. Chicago, USA), Jay Bass (UIUC) and Stanislav Sinogeikin (HP-CAT, Carnegie Institution of Washington).

Reasons for Support of the Workshop

The development and installation of the on-line Brillouin spectrometer at 13-BMD station was initially supported by COMPRES as an Infrastructure Development project and by the NSF through the Elasticity Grand Challenge. Since system has became available for the larger COMPRES-community it is vital to further support and promote projects for the high-pressure community and increase the potential user base. We expect a significant impact of the COMPRES-supported workshop on the entire high-pressure community, especially for young scientists and students.

Workshop Details

The Workshop will take place at the Advanced Photon Source, Argonne National Laboratory, Illinois, on 4-6 May, 2009. The workshop will take place as part of the APS User's Meeting. This will allow us to use the organizational structure of the meeting to reduce costs.

An estimated 25 participants will attend. The format of the workshop will include invited talks, contributed presentations and hands-on demonstrations. Ample time will be allotted for formal and informal discussion.
COMPRES mailing lists will be used to disseminate information about the Workshop to all US scientists who might be interested in attending.

Proposed budget and use of requested funds

If this travel request is approved, it is expected that up to 25 US participants will receive the funding necessary to attend the workshop. We will give priority to students and post docs, in terms of support to attend.

Estimated average costs, per person, are as follows:
$450 — Domestic airfare
$100 — Ground transportation
$250 — User-meeting fee
$200 — Room accommodation (3 nights)
$1000 — Total estimated costs

Total budget request:
$25,000

COMPRES approved funding of up to $25,000, or $700 per attendee if less than 35 persons attend. This workshop will be held at the APS in September 2008.

D Budget Request for Year #3

Budget Request for Year #3 [June 1, 2009 to May 31, 2010]. Details may be seen in the NSF 1030 Forms and the associated budget justification pages which are in the appendices to this report.

The COMPRES budget request for $2,100,000 for Year #3 [June 1, 2009 to May 31, 2010] is comprised of three major components (units of $K, which include fringe benefits and indirect costs):

D.1 Community Facilities-operational budgets

$240K for ops	West Coast Synchrotron Facilities [R. Jeanloz and S. Clark]
$288K for ops $95K for equip	X-ray, Diamond-anvil cell facilities at the NSLS [T. Duffy and D. Weidner]
$207K for ops $100K for equip	Infrared, Diamond-anvil facilities at the NSLS [R. Hemley and Z. Liu]
$366K for ops $30K for equip	Multi-anvil Press Facility at the NSLS [D. Weidner and M.Vaughan]
$20K	Beamline user housing
$1121K for ops	Total operational budget for Community Facilities
$225K for equip	See details above

D.2 Infrastructure Development Projects

$72K	Nuclear Resonant Scattering at High P & T:A New Capability for the COMPRES Community [W. Sturhahn, J. Jackson, and J. Bass]
$70K	Multi-anvil Cell Assembly Initiative: New Developments and Production [K. Leinenweber, T. Sharp, and J. Tyburczy]
$37K	Postdoc for Gas-Loading system at GSECARS [M. Rivers]
$52	Workshops (5 to 7 per year)
$8K	Subawards IDC [for new Gas-loading project]
$239K	Total for infrastructure development projects

D.3 Other COMPRES Activities

$128K **Other Community Activities** which includes

$100K	Annual Meeting
$20K	Travel for committees (including that of Advisory Committee, Executive Committee and Standing Committees)
$8K	COMPRES lecture series

$387K **Central Office** which includes: [all items have indirect costs incorporated]

$354K	Salaries and fringe benefits
$13K	Materials and Supplies
$20K	Travel

$515K Total for Other COMPRES Activities

TOTAL BUDGET REQUEST FOR YEAR #2 OF COMPRES II

$1121K	**Operational costs for Community Facilities**
$225K	**Equipment upgrades for facilities**
$239K	**Infrastructure development projects**
$128K	**Other Community activities**
$387K	**Central Office**

$2100K **Total of budget request**

E. Detailed Original Signed Budgets on NSF 1030 forms and Budget Justifications For COMPRES Budget Request for Year #3 [June 1, 2009 to May 31, 2010]

A. Budgets and justifications for Stony Brook University [R. C. Liebermann, PI]

Amount	Purpose	Principal Investigator
$594,959	Central Administrative Budget	R. Liebermann
$382,999	Diamond-anvil –ray facility at the NSLS	T. Duffy and D. Weidner
$396,000	Multi-anvil X-ray facility at the NSLS	D. Weidner and M. Vaughan
$1,373,958	**Total for Stony Brook budget for Year #2**	

B. Budgets and justifications for COMPRES II Subawards for Year #3 [June 1, 2009 to May 31, 2010]

Amount	Institution	Principal Investigator
Current Subawards-extensions from Year #2 to Year #3		
$240,000	University of California, Berkeley	R. Jeanloz and S. Clark
$307,000	Carnegie Institution of Washington	R. Hemley
$72,000	University of Illinois	J. Bass and W. Sturhahn
$70,042	Arizona State University	K. Leinenweber, T. Sharp and J. Tyburczy
$689,042	**Total for existing Subawards for Year #3 [June 1, 2009 to May 31, 2010]**	
New Subaward for Year 3		
$37,000	University of Chicago	M. Rivers
$726,042	**Total of SubAwards for Year #3 [June 1, 2009 to May 31, 2010]**	

$2,100,000 Total COMPRES budget request for Year #3

F. Supplemental Information

Fig. 1. Mark Rivers and new gas-loading system for diamond-anvil cells constructed at the GSECARS beamlines at the Advanced Photon Source with support from COMPRES and GSECARS.

Fig. 2. Attendees at the Workshop to Introduce High-Resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation, held at the Advanced Photon Source, Argonne National Laboratory
May 31 - June 1, 2008

Fig. 3. Attendees at the Workshop on Future Directions in High Pressure Research National Synchrotron Light Source, Brookhaven National Laboratory.
May 21, 2008.

Fig. 4. Attendees at Workshop on Advances in High-Pressure Science Using Synchrotron X-rays held at the National Synchrotron Light Source, Brookhaven National Laboratory, on October 4, 2008.

Fig. 1. Mark Rivers and new gas-loading system for diamond-anvil cells constructed at the GSECARS beamlines at the Advanced Photon Source with support from COMPRES and GSECARS.

Fig. 2. Attendees at the Workshop to Introduce High-Resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation, held at the Advanced Photon Source Argonne National Laboratory May 31 - June 1, 2008. See details Section A.3 and C.2.

Fig. 3. Attendees at the Workshop on Future Directions in High Pressure Research
National Synchrotron Light Source, Brookhaven National Laboratory.
May 21, 2008. See details Section A.3 and B.1.

Fig. 4. Attendees at Workshop on Advances in High-Pressure Science Using Synchrotron X-rays held at the National Synchrotron Light Source, Brookhaven National Laboratory, on October 4, 2008. See details Section A.3 and B.1.