Annual Progress Report for Year #3 and Program Plan and Budget Request for Year #4 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

26 February 2010

2010 Annual Meeting of COMPRES at

Mount Washington Resort in Bretton Woods, New Hampshire

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A COMPRES Year 3: Overview

A.1 Executive Summary

In the first 30 months of COMPRES II [June 2007 to December 2009], 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 55 U. S. institutions which are voting members of COMPRES [the Electorate] and another 37 non-voting institutions overseas which have affiliate membership.

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

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

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

- Using U2A at the NSLS, researchers from UNLV and Caltech have found evidence for small quantities of the mineral wadsleyite forming upon laboratory shock compression of thin layers of magnesium oxide and fused quartz. See Tschauner et al. in Section B.2.

- Experimental work on X17B3 and U2A at the NSLS has confirmed the crystal structure of a new high-pressure phase of boron named c-B28. See Oganov et al. in Sections B.1 and B.2.

- A team led by Sean Shieh from the University of Western Ontario has used the U2A beamline of the NSLS to measure the infrared spectra of polycrystalline samples of Phase D and Phase E synthesized at pressures above 40 GPa. See Shieh et al. in Section B.2.

- A team led by Paul Raterron from Lille, France reported that pressure induces a change in the active dislocation system in dry olivine crystals using X17B2 at the NSLS. See Raterron et al. in Section B.3.

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

- A team led by Rudi Wenk from UC Berkeley has studied texture development in polycrystalline iron during phase transformations and deformation at high P & T using beamline 12.2.2 at the ALS. See Miyagi et al., in Section B.4.

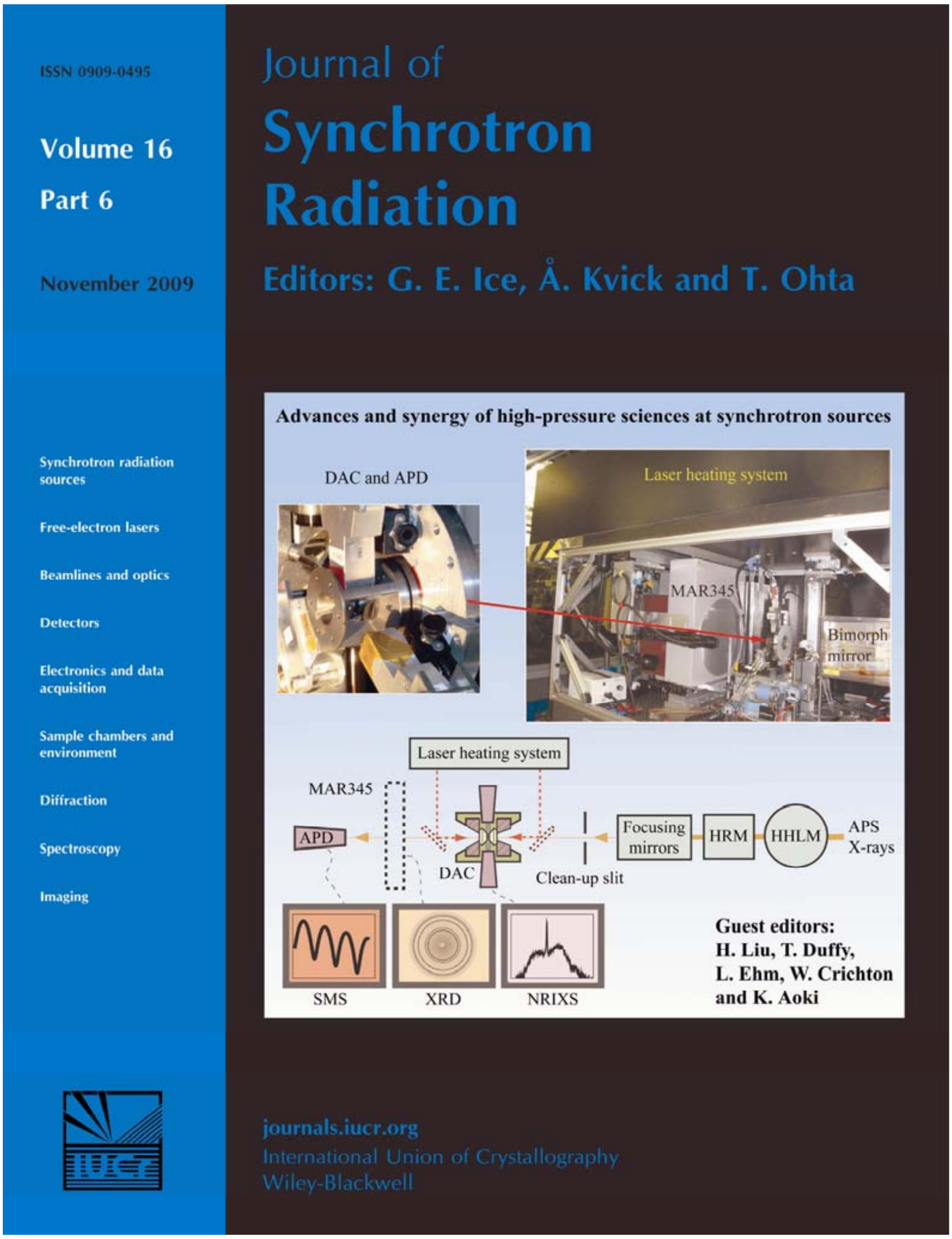
- A team led by David Walker from Columbia has used beamline 12.2.2 to obtain X-ray absorption contrast images of binary chemical reactions. See Walker et al. in Section B.4.

- A team led by Andrew Campbell from the University of Maryland has used special cell assemblies designed by the multi-anvil cell development project at the ASU to study the effects of high pressure on the iron-iron oxide and nickel-nickel oxide oxygen fugacity buffers. See Campbell et al., in Section C.1.

- A team led by Thomas Sharp from the ASU has utilized special cell assemblies designed by the multi-anvil cell development project at the ASU to investigate the effect of small amounts of H_2O on the olivine to ringwoodite phase transformation. See Diedrich et al. in Section C.1.

● A team led by Jennifer Jackson from Caltech has studied the behavior of iron in (Mg,Fe)SiO3 post-perovskite assemblages at Mbar pressures at beamline XOR-3 of the APS with support from the NRIXS development project at UIUC and ANL. See Jackson et al. in Section C.2.

● A team led by Jie Li from the University of Illinois Urbana-Champaign has measured the sound velocities of compressed Fe3C using simultaneous synchrotron X-ray diffraction and nuclear resonant scattering techniques at beamline XOR-3 of the APS with support from the NRIXS development project at UIUC and ANL. See Gao et al. in Section C.2; this paper was featured on the front cover of the Journal of Synchrotron Radiation, November 2009.



A.3 Meetings and Workshops

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

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

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

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

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

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

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

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

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

At one of these workshops last month on Earth and Environmental Sciences, Dr. Lisa Miller (a colleague of Chi-chang Kao, Director of NSLS) gave a splendid presentation on plans for the transition from NSLS to NSLS-II. As part of her presentation, she focussed on the role of COMPRES at the synchrotrons at Brookhaven. Additional details may be found at: http://www.bnl.gov/ls/workshops.asp.

SNAP/COMPRES Meeting at Oak Ridge National Laboratory

April 13-15, 2008

A Joint Meeting of SNAP [Spallation Neutrons at Pressure] and COMPRES was held at the Spallation Neutron Source [SNS] of ORNL from April 13-15. See details of program at: http://www.compres.stonybrook.edu/Meetings/2008-04-13-SNAP/FINAL_ProgramSNAP-COMPRES.doc

Meeting concluded with a guided tour of the new SNAP beamline by Chris Tulk who oversaw the design and construction on behalf of the project team, which also included John Parise, Russell Hemley and Ho-kwang Mao.

Future Directions in High Pressure Research

National Synchrotron Light Source

May 21, 2008.

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

Workshop to Introduce High-Resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation.

Advance Photon Source Argonne National Laboratory

May 31 - June 1, 2008

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

Seventh Annual Meeting of COMPRES

June 25-28, 2008

Cheyenne Mountain Resort, Colorado Springs, Colorado

Program Committee: Carl Agee, Jiuhua Chen, Steven Jacobsen, and James Tyburczy. Lili Gao and Zhu Mao served as student members.

There were 113 registered participants and many accompanying persons to enjoy this splendid site. One of the new features was a set of keynote talks focused on the mantle, geochemical evolution and the core, with speakers for each topic from both within and outside the mineral physics community. Keynote speakers included:

Rajdeep Dasgupta-Rice University	William McDonough-Univ of Maryland
Louise Kellogg-UC Davis	Rebecca Lange-Univ of Michigan
Justin Revenaugh-Univ of Minnesota	Jie Li-Univ of Illinois

The social events of the meeting were underwritten by 9 industrial sponsors: Almax, Blake Industries, D'Anvils, Depths of the Earth, easyLab, MG63, Rockland Research, Scimed and

Technodiamant. In addition, Depths of the Earth provided T-shirts for all attendees [see photo at: http://www.compres.stonybrook.edu/.
Additional details of the Annual Meeting may be found in the October 2008 issue of the COMPRES newsletter and at:
http://www.compres.stonybrook.edu/Newsletter/V7N2/NewsletterV7N2_Revised.pdf

NSLS Workshop: Advances in High-Pressure Science Using Synchrotron X-rays
National Synchrotron Light Source of the Brookhaven National Laboratory
October 4, 2008
This Workshop was held in honor of Drs. Jingzhu Hu and Quanzhong Guo and was organized by by Thomas Duffy (Princeton), Haozhe Liu (Harbin Institute of Technology), Lars Ehm (BNL), Dave Mao (Carnegie Institution of Washington), Zhenxian Liu (Carnegie Institution of Washington), and Jiuhua Chen (Florida International University). It was attended by more than 50 scientists, post-doctoral fellows, and students from the high pressure and synchrotron x-ray research fields.
Financial support was provided by the Consortium for Materials Property Research in Earth Sciences (COMPRES), the Carnegie- DOE Alliance Center (CDAC), and the Harbin Institute of Technology. See additional details at:
http://shp.hit.edu.cn/Meetings/2008NSLS/Home.htm

Long-Range Planning Workshop for High Pressure Earth Sciences
Fiesta Resort Conference Center, Tempe, Arizona
March 2-4, 2009
This workshop was convened by tri-chairs James Tyburczy, Michael Brown and James van Orman on behalf of COMPRES, with support from the School of Earth and Space Exploration [SESE] of the Arizona State University. Robin Reichlin and Sonia Esperanca represented the NSF Division of Earth Sciences. [See photo in Supplemental Information].
Eighty seven scientists from thirty nine institutions gathered at the Fiesta Resort in Tempe to discuss recent scientific successes of the high pressure mineral physics community and articulate directions of our research over the next decade. This two-day workshop featured nine plenary talks and breakout discussion sessions on four themes: 1) The Deeper Reaches of the Planet: Properties of Iron and its Alloys and the Novel Materials of the Deepest Mantle; 2) The Dynamic Ceramic Mantle; 3) Mineral Physics and Society; 4) Enabling Cutting-Edge Science: Tools and the Accomplishments they will drive in the Next Decade of Discovery. Participants of the workshop reviewed etrospective about how our field has impacted other subdisciplines of the earth sciences, including seismology, geodynamics and petrology. They also discussed perspective of high pressure Earth science: what are the next major breakthroughs of our community, and what infrastructure will be necessary to achieve them? While recognizing that incremental progress will occur, what new and different developments could occur? And, what long-standing problems might we solve?
This was the second COMPRES workshop focusing on long range plan for high pressure Earth sciences. The first one "A Vision for High Pressure Earth and Planetary Sciences Research: The Planets from Surface to Center" was held on March 22-23, 2003 in Miami, Florida and led to the 2004 Report on the "Current and Future Research Directions in High-

Pressure Mineral Physics."[the Bass Report]. The product that arises from this meeting will be a new scientific plan for high-pressure Earth sciences, a document that will not only serve as a blueprint for our community as itmoves forward, but will also serve as the input of our community to a new NAS report, commissioned by NSF, on Basic Research Opportunities in the Earth Sciences (BROES). Quentin Williams will serve as Editor-in-Chief of this new report.

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

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

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

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

The meeting also attracted the ten industrial sponsors: Almax, Blake Industries, D'Anvils, Depths of the Earth, easyLab, Foxwoods, Leica Microsystems, MG63, Rockland Research, and

Technodiamant, four of them sent representatives to Bretton Woods.

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

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

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

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

Special Session in Honor of Alex Navrotsky at GSA Annual Meeting

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

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

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

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 2009, there were 53 U. S. institutions which were members of COMPRES and 32 affiliate institutions overseas. In the past year, two U. S. institutions have become members of COMPRES:

Brookhaven National Laboratory: Lars Ehm, Elector; Marcus Hucker, Alternate Elector.
Smithsonian Institution: Elizabeth Cottrell, Elector; Jeffrey Post, Alternate Elector.

These additions brought the membership list to 55 U. S. institutions.

In addition, the following 6 overseas institutions became affiliate members of COMPRES;

Jilin University (China): Xiaoyang Liu, Representative
Peking University (China): Qiong Liu, Representative
Tel Aviv University (Israel): Moshe Pasternak, Representative
University of Calgary (Canada): Sytle Antao, Representative
University of Cambridge (United Kingdom): Michael Carpenter, Representative
University of Edinburgh (United Kingdom): Geoffrey Bromley, Representative

This brings the list of foreign members to 38.

COMPRES US Member Institutions

Institution	Elector	Alternate
Argonne National Laboratory	Wolfgang Sturhahn	Ercan Alp
Arizona State University	Thomas Sharp	James Tyburczy
Auburn University	Jianjun Dong	
Azusa Pacific University	Donald Isaak	
Brookhaven National Laboratory	Lars Ehm	Markus Hücker
California Institute of Technology	Jennifer Jackson	Paul Asimow
Carnegie Institution of Washington	Ronald Cohen	Yingwei Fei
Case Western Reserve University	James Van Orman	Nancy Chabot
Colorado College	Phillip Cervantes	
Columbia University	David Walker	Taro Takahashi
Cornell University	William Bassett	Zhongwu Wang
Delaware State University	Gabriel Gwanmesia	Al Sameen Khan
Florida International University	Jiuhua G. Chen	Surendra Saxena
Harvard University	Sarah Stewart-Mukhopadhyay	Richard O'Connell
Indiana University at South Bend	Henry Scott	Jerry Hinnefeld
Johnson Space Center , NASA	Kevin Righter	John Jones
Lawrence Berkeley National Laboratory	Simon Clark	Corwin Booth
Lawrence Livermore National Laboratory	Daniel Farber	
Los Alamos Natoional Laboratory	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	Liping Huang	Bruce Watson
Smithsonian Institution	Elizabeth Cottrell	Jeffrey Post
Stanford University	Wendy Mao	Jonathan Stebbins
Stony Brook University	Michael Vaughan	John Parise
Texas A&M University	Caleb Holyoke	
Texas Tech University	Yanzhang Ma	Valery Levitas
University of Arizona	Robert Downs	Michael Drake
University of California at Berkeley	Hans-Rudolph Wenk	Raymond Jeanloz

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

COMPRES Foreign Affiliates

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

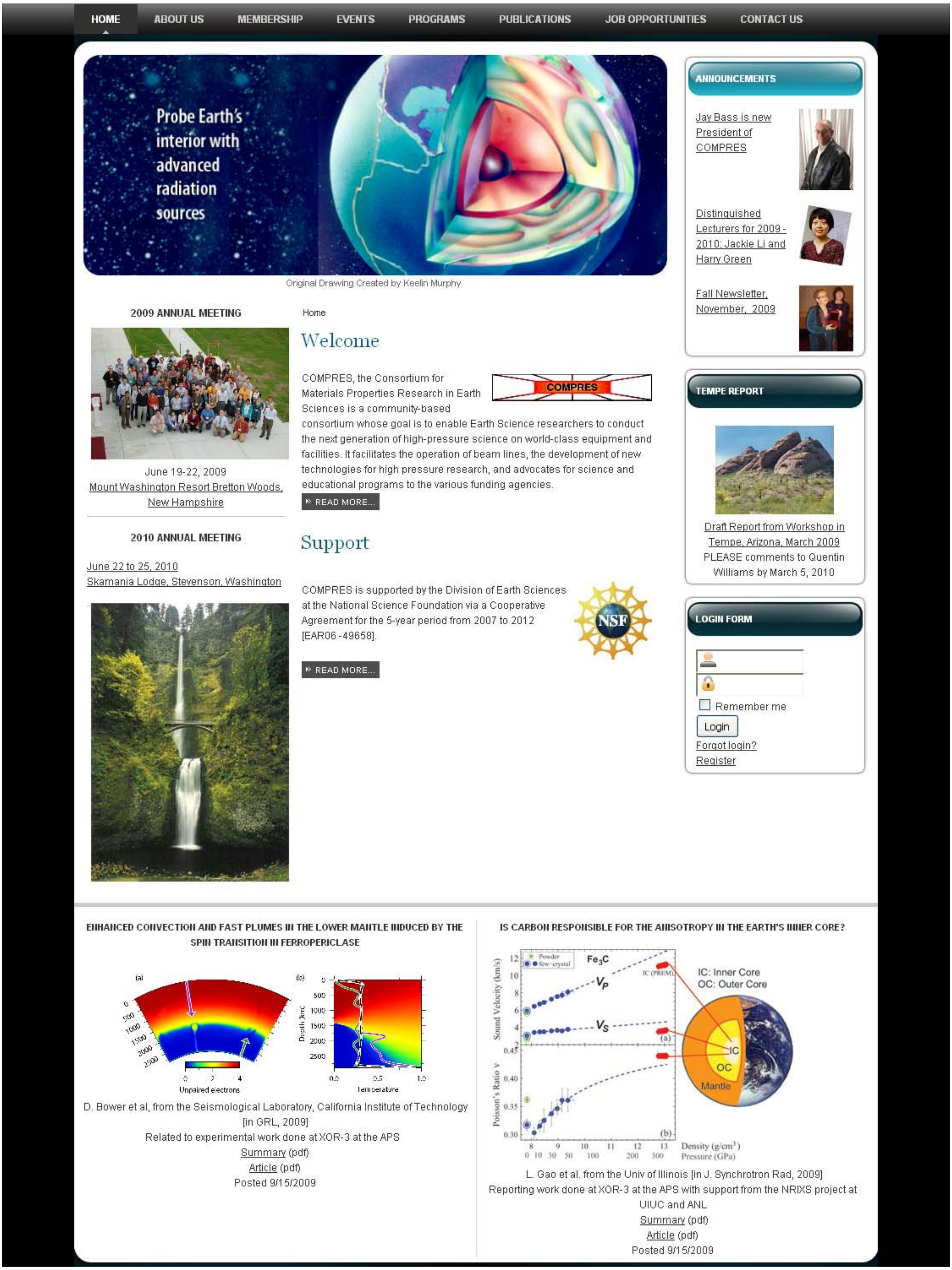
University of Wales at Aberystwyth (United Kingdom)	Takehiko Yagi
University of Western Ontario (Canada)	Martin Wilding
Vrije Universiteit (The Netherlands)	Rick Secco
Yonsei University (Korea)	Wim van Westrenen
Yonsei University (Korea)	Yongjae Lee

A.5 Information Technology and Communications

Website

A more professional appearance of the COMPRES website is \now "live" at www.compres.us. This new website has been designed by a consulting company in Stony Brook, based on advice and guidance of a special subcommittee chaired by Quentin Williams and including Tom Duffy and Nancy Ross. The website now becomes easier for readers to browse and for the webmaster to maintain. The motivation for seeking a new design and format came from comments of the Infrastructure Development Committee and the Executive Committee in December 2008. The COMPRES central office was strongly urged to engage a professional website design firm, and to make the website easier for our staff and volunteers to maintain. Glenn Richard, Michael Vaughan and Ken Baldwin of the Mineral Physics Institute at Stony Brook have offered valuable consultations to the outside company during the development. The new website will be maintained by Emily Vance and Glenn Richard, with oversight by the President of COMPRES. In June 2010, the responsibility for maintaining the website will shift to the University of Illinois at Urbana-Champaign with Steve Hurst as website manager working under the guidance of Jay Bass.

See new website at:
www.compres.us



Science Highlights on the Home Page of COMPRES website

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

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

<u>A general overview of COMPRES</u>

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

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

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

  Minutes of the Executive Committee

  Monthly Messages from COMPRES President

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

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

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

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

Other Electronic Information Technology Services

- **List servers:** The initial list server is now operational that reaches hundreds of the members of the COMPRES community. Additional lists will be established during the coming months that serve the broader high pressure community.
- **People database:** Contact information for people involved in COMPRES. Since 2004, this was made available online through a browser-based form
- **Online Forms for meeting registration:** This offers online registration for meetings and workshops.
- **Videoconferencing:** The Central Office has 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 http://www.compres.us/index.php?option=com_content&task=view&id=49&Itemid=96See COMPRES Home Page for the latest issue for November 2009.

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

A.6 Publications of COMPRES in 2008-2009

[BEAMLINE OR INFRASTRUCTURE PROJECT GIVEN IN CAPS BELOW]

2008

Akhmetov, A. (2008), Strength and elasticity study of MgO, NaCl and Au at mantle pressures *MSc Thesis, University of Western Ontario, London, Ont.* .X17 DAC

Aksoy, R., Selvi, E., Ma, Y. (2008), X-ray diffraction study of molybdenum diselenide to 35.9 GPa *J. Phys. Chem. Solids 69* 2138– 2140 X17 DAC

Aksoy, R. Y. M., E Selvi, Ming C. Chyu, Atila Ertas and Allen White (2008), High pressure x-ray diffraction study of transition metal dichalcogenides,, *Ph.D. Thesis, Texas Tech University, Lubbock, TX* X17 DAC

Antao, S., C Benmore , Baosheng Li, Liping Wang, E Bychkov, J Parise (2008), Network Rigidity in GeSe2 Glass at High Pressure, *Phys. Rev. Lett. (premier) 100(115501)* MAC NSLS

Balogh, L., S Nauyoks, T. Zerda, Cristian Pantea*, S Stelmakh, Bogdan Palosz and T. Ungar (2008), Structure of Diamond-Silicoin Carbide Nanocomposites as a Function of Sintering Temperature at 8 GPa. , *Mater. Sci. Eng. A 487: 180 - 188* MAC NSLS

Bass, J. D., Sergei V. Sinogeikin and Baosheng Li (2008), Elastic Properties of Minerals: A Key For Understanding the Composition and Temperature of Earth's Interior, *Elements (submitted), 4.3.165, 165-170.*MAC NSLS

Burnley, P., D Zhang (2008), Interpreting In-Situ X-ray Diffraction Data from High Pressure Deformation Experiments using Elastic Plastic Self Consistent Models: an Example using Quartz. , *J. Phys.: Condens. Matter*, *20(285201)* MAC NSLS

Chen, B. L., J.; Gao, L.; Leinenweber, K.; Wang, Y.; Sanehira, T. (2008), In Situ Investigation of Melting Behavior in Fe-S System Using Synchrotron X-ray Radiography, *High Pressure Research*, *28, 315-326*.MAC ASU

Chen, J., Yunpeng Yang, Tony Yu, Jianzhong Zhang, Yusheng Zhao and Liping Wang (2008), Strength Measurement of Boron Suboxide B6O at High Pressure and Temperature Using in situ Synchrotron X-ray Diffraction, *High Pressure Res.*, *28(3): 423-430* MAC NSLS

Chen, Z. (2008), Probing spin, charge, and lattice coupling in manganites, *Ph.D. Thesis, New Jersey Institute of Technology, Newark, NJ*.X17 DAC

Dandekar, D., J. Ciezak, M. Somayazulu (2008), Compression and Associated Properties of Boron Carbide, *26th Army Science Conference, Vol GP-05, sponsored by US Department of Army*.U2A DAC

Detrie, T. (2008), Prehnite at the Atomic Scale: Al/Si Ordering, Hydrogen Environment, and High-Pressure Behavior, *MSc Thesis. Virginia Polytechnic Institute and State University, Blacksburg* U2A DAC

Dobson, D. P., Simon A. Hunt, Li Li, Donald J. Weidner (2008), Measurement of Thermal Diffusivity at High Pressures and Temperatures using Synchrotron Radiography, *Miner. Mag*, *72: 653-658* MAC NSLS

Durham, W. B. M., S.; Kohlstedt, D.L.; Wang, L.; Dixon, N.A. (2008), New measurements of activation volume in olivine under anhydrous conditions, *Physics of the Earth and*

Planetary Interiors (in review 2009).MAC ASU

Gao, B. C., J. Wang, E.E. Alp, J. Zhao, M. Lerche, W. Sturhahn, H.P. Scott, F. Huang, Y. Ding, S.V. Sinogeikin, C.C. Lundstrom, J.D. Bass, and J. Li (2008), Pressure-induced magnetic transition and sound velocities of Fe3C: Implications for carbon in the Earth's inner core, *Geophys. Res. Lett., 35, L17306* Nuclear Resonant

Gao, P., T. Tyson, Z. Liu, M. DeLeon, C. Dubourdieu (2008), Optical Evidence of Mixed-Phase Behavior in Manganite Films *Phys. Rev. B: Condens. Matter*, *78, 220404(R)*.U2A DAC

Gleason, A. E., R. Jeanloz, and M. Kunz (2008), Pressure-temperature stability studies of FeOOH using x-ray diffraction *American Mineralogist*, *93, 1882-1885* ALS

Grottoli, A., G., J.F. Adkins, W.R. Panero, D.M. Reaman, K. Moots (2008), Growth Rates, Stable Oxygen Isotopes (δ18O), and Stronium (SR/CA) Composition in Two Species of Pacific Sclerosponges (Acanthocheatetes Wellsi and Astroclera Welleyana) with δ18O Calibration and Application to Paleoceanography, *J. Geophy. Res. Oceans, in press*.U2A DAC

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Higo, Y., T. Inoue, T. Irifune, K. Funakoshi, B. Li (2008), Elastic wave velocities of (Mg0.91Fe0.09)2SiO4 ringwoodite under P-T condition of the mantle transition region, *Phys Earth. Planet Interi. (submitted)*, *66, 167-174*.MAC NSLS

Jacobsen, S. D., Z. Liu, T.B. Ballaran, E.F. Littlefield, L. Ehm, and R.J. Hemley (2008), Effect of water on high-pressure phase transitions in MgSiO3-clinoenstatite: implications for estimating the mantle water content at 270-330 km from the depth of the X-discontinuity, *PEPI, submitted.* .U2A DAC

Jiang, F., Majzlan, J., Speziale, S., He, D., Duffy, T. S. (2008), Single-crystal elasticity of diaspore, AlOOH, to 12 GPa by Brillouin scattering, *Physics of the Earth and Planetary Interiors*, *170* 220-228 X17 DAC

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Karato, S.-I. (2008), Recent progress in the experimental studies on the kinetic properties in minerals, *Phys. Earth Planet. Inter.*, *170: 152-155*.MAC NSLS

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Leinenweber, K. T., J.A.; Sharp, T.G.; Soignard, E.; Diedrich, T.; Petuskey, W.B.; Wang, Y.; Stoyanov, E.; Nite, J.; Mosenfelder, J (2008), Development of a series of cell assemblies

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Li, L., Liping Wang, Michael T. Vaughan (2008), Elastic Softening of Peridotite Due to the Presence of Melt Phases at High Pressure, *Phys. Earth Planet. Interiors*, *170(3-4), 176-180* MAC NSLS
Li, L., Donald J. Weidner (2008), Effect of Phase Transitions on Compressional-Wave Velocites in the Earth's Mantle, *Nature*, *454(984)* MAC NSLS
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Mao, W. L., V.V. Struzhkin, A.Q.R. Baron, S. Tsutsui, C.E. Tommaseo, H.-R. Wenk, M.Y. Hu, P. Chow, W. Sturhahn, J. Shu, R.J. Hemley, D.L. Heinz, and H.-K. Mao (2008), Experimental determination of the elasticity of iron at high pressure, *J. Geophys. Res.*, *113, B09213* Nuclear Resonant
Mao, Z., Jacobsen, S. D., Jiang, F., Smyth, J. R., Holl, C. M., Duffy, T. S. (2008), Elasticity of hydrous wadsleyite to 12 GPa: Implications for Earth's transition zone, *Geophysical Research Letters*, *L21305*.X17 DAC
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Petruska, E. (2008), High-pressure studies of nanocrystalline silver, nanocrystalline silicon carbide, and bulk zirconium pyrophosphate, , *M.S. Thesis, U. Missouri – Kansas City*.X17 DAC

Phatak, N., Kulkarni, S., Drozd, V., Saxena, S., Deng, L., Fei, Y., Hu, J., Luo, W., Ahuja, R. (2008), Synthesis and compressive behavior of Cr2GeC up to 48 GPa, *J. Alloys Compd.*, *463*, 220–225 (2008).X17 DAC

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Weinberger, M., Tolbert, S., Kavner, A. (2008), Osmium metal studied under high pressure and nonhydrostatic stress, *Phys. Rev. Lett. (premier)*, *100, 045506*.X17 DAC

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A.7 Education and Outreach

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

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

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

New outreach initiatives for 2008-2010

<u>Teaching Mineral Physics across the Curriculum</u>

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

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

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

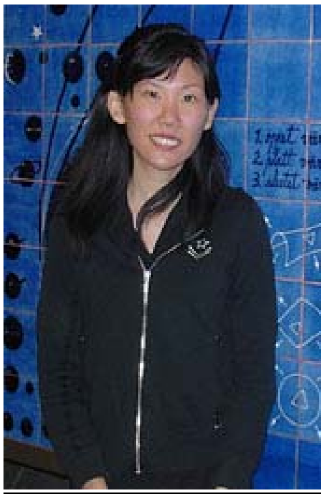
To date, contributions to this module have been received from Alex Navrotsky, Abby Kavner, Pamela Burnley, and Artem Oganov and several other people are working on developing special items on multi-anvil apparatus and use of synchrotron X-radiation facilities for research in mineral physics.

Distinguished Lecturer Program

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

We proposed to select two outstanding scientists and lecturers and offer to send them to U. S. academic institutions to give a COMPRES-sponsored lecture. 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].

The Distinguished Lecturers for COMPRES in 2008-2009 were:



Wendy Mao of Stanford University visited
University of Illinois at Chicago
University of California Davis

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

The Distinguished Lecturers for COMPRES in 2008-2009 are:

Jie (Jackie) Li of the University of Michigan, who will visit:

Univerisit of Western Ontario (Canada)
University of California Davis
University of California Berkeley
Winona State University (Wisconsin)

Harry Green of the University of California Riverside, who will visit:

University of Nevada at Las Vegas
University of Washington
Case Western Reserve University
Northwestern University
Miami University of Ohio
University of Rochester

We plan to continue this program in 2010-2011. By more extensive advertizing in EOS and Earth [the successor to Geotimes], we hoped to attract invitations from more undergraduate liberal arts & sciences colleges and community colleges, which may be less familiar with the field of mineral physics. On the basis of 2 lecturers and 5 lecture visits each @$500 per visit, plus advertising costs and logistics, we have requesed $10,000 for this program in Year #4.

Enhancing Diversity in the Geosciences

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

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

This MS program in Geosciences will be modeled after the existing program for Master of Science in Instrumentation in the Department of Physics & Astronomy at Stony Brook University, and will include both formal courses in Geosciences and Physics & Astronomy and internship research at the beamlines operated by COMPRES at the NSLS of BNL. [Consortium for Materials Properties for Research in Earth Sciences http://www.compres.stonybrook.edu/]. This new OEDG program will also be complimentary to the existing OEDG program led by Gilbert Hanson of the Department of Geosciences at Stony Brook.

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

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

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

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

A.8 Management and Organization

Executive Committee

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

The elected chairs of the Standing Committees on Facilities and Infrastructure Development serve as non-voting advisors to the Executive Committee.
The appointed President attends all meetings of the Executive Committee, as a non-voting member.

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

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

Current members and affiliation (term of service)
Quentin Williams, **Chair [2007-2010]** Member 2004-2010
Carl Agee, **Vice Chair [2008-2010]** Member 2007-2010
James Tyburczy, Member 2008-2011
James van Orman, Member 2009-2012
Donald Weidner, Member 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.

Current members and affiliation (term of service)
Wendy Panero, **Chair [2009-2011]** Member 2006-2012
Andrew Campbell, Member 2008-2011
Thomas Duffy, Member 2007-2010
Wendy Mao, Member 2009-2012
Yanbin Wang, Member 2008-2011

Infrastructure Development Committee

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

Current Members and affiliation (term of service)
Thomas Sharp, **Chair [2008-2010]** Member, 2006-2010
Steven Jacobsen, Member 2008-2011
Abby Kavner, Member 2009-2012
Jie Li (217). Member 2008-2011
Sang-Heon Dan Shim, Member 2004-2010

Advisory Council
Members and affiliation (term of service)
Edward Garnero**,** Arizona State University, Member 2008-2011
Peter Heaney, Pennsylvania State University, Member 2009- 2012
Chi-Chang Kao**,** Brookhaven National Laboratory, member 2003-2011
Louise Kellogg, University of California at Davis, Member 2007-2010
William McDonough, University of Maryland, Member 2007-2010

On 19 June 2009, the Advisory Council met with the Executive Committee just prior to the start of the Eighth Annual COMPRES Meeting in Bretton Woods, New Hampshire. The term one of the members of the Advisory Council ended at Bretton Woods, Wang-ping Chen; we wish to thank him for his service to COMPRES and hope that he will feel welcome to attend future annual meetings of our community.

We were saddened to learn of the death of two former members of the Advisory Council: Malcolm Nicol in May 2009 and Paul Silver in November 2009.

Finally, we would like to welcome the new members of the Advisory Council for three-year terms commencing June 2009:

Peter Heaney from the Pennsylvania State University
Andrew Jephcoat from the University of Oxford (UK)

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.

President of COMPRES

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

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

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

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

New COMPRES Central Office

The new COMPRES central offices will be located in the Geology Department of the University of Illinois Urbana-Champaign (UIUC). The Geology Department at UIUC is part of the School of Earth, Society and Environment (SESE). The Geology Department of UIUC is providing in-kind support of the COMPRES Central Office that is necessary for smooth and efficient COMPRES operations, comparable to the support provided by Stony Brook University for the previous 7 years. UIUC is providing adjoining newly-renovated office space for the President and an Administrative Assistant to form a coherent COMPRES Central Office. Dr. Steven Hurst of SESE will be performing IT support year-round, website maintenance, and assistance in handling IT/computer requirements at the COMPRES Annual Meeting. Scott Morris and Ms Marsha Hatchel will be made available to provide in-house assistance on handling financial and proposal-related aspects of operating COMPRES.

A.9 President's Narrative (by Bob Liebermann)

2009 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.

In mid-February 2009, I spent a week in southern California visiting mineral physics laboratories and meeting students and postdocs. These included:

UCLA—hosted by Abby Kavner.

UC Riverside—hosted by Harry Green. [See photo in Supplemental Information].

Caltech—hosted by Jennifer Jackson and Paul Asimow.

[See photo in Jackson's lab in Supplemental Information].

These visits bring to 31 the COMPRES institutions I have visited during the past 5 ½ years, of the 55 current US members. I have also visited 16 of the 38 foreign affiliates.

In March, I spent five days at Hiroshima University as a guest of Jun-ichi Ando. During a 2 ½ day period, I gave 5 tutorial lectures to 27 graduate students from throughout Japan, as well as a colloquium to the Department of Earth Sciences. [See photo in Supplemental Information].

After the visit to Hiroshima, I spent two days at Ehime University in Matsuyama as a guest of Tetsuo Irifune. While there, I observed the first experiments in BOTCHAN, their 6,000 ton press which will be used to synthesize large specimens of nano-polycrystalline diamonds. I also attended at day-long series of presentations of research activity by the graduate students and postdocs of the Geodynamics Research Center. In an evening event, I offered the congratulations of the COMPRES community to Professor Irifune and his colleagues on the award of a 5-year Global-Center of Excellence grant.

At the end of March, I attended this SMEC 2009: Study of Materials at Extreme Conditions Conference conference in Miami and the Caribbean along with 150 other persons. The conference was organized by Surendra Saxena and his colleagues at the Center for the Study of Materials at Extreme Conditions at the Florida International University. Details of the scientific program may be found at:
http://hipssa.org/smec2009/index.php?ac=abslist
At the invitation of Jiuhua Chen of FIU, I gave an invited talk on "Indoor vs. Outdoor Geophysics."

On April 27 and 28, Quentin Williams and I spent two days in the DC area visiting various federal agencies and research institutions:

a. Division of Earth Sciences of the NSF in Arlington, VA.

We met with Robert Detrick, the new DD for EAR, and David Lambert, Program Director for Instrumentation and Facilities in EAR to discuss the report emanating from the Long-Range Planning Workshop in Tempe, Arizona in early March. We allso met with Robin Reichlin, Russell Kelz, and Lina Patino of EAR and Barbara Ransom of OCE. The Tempe report and other COMPRES items will serve as valuable input for several planned activities/programs, including a strategic plan for EAR, a new BROES [Basic Research Opportunities in Earth Sciences] report by the National Research Council of the NAS, and a new Directorate-wide initiative on "The Dynamic Earth."

b. IRIS Headquarters in central Washington.

We met with David Simpson, President of IRIS to discuss mutually interesting topics of science and funding of science.

c. Basic Energy Sciences Headquarters of the DOE in Germantown, MD.

We met with Nicholas Woodward (Program Director for Geosciences Research), Helen Kerch (Team Lead for Scattering and Instrumentation Sciences), and Pedro Montano (Director of Scientific User Facilities Division). We took the opportunity to thank the DOE for providing the excellent synchrotron and neutron facilities, but also to showcase the science achievements of the COMPRES users, from both the Earth sciences and materials science.

d. Geophysical Laboratory of the Carnegie Institution of Washington in northwest DC.

We met with Bob Hazen and colleagues (Yingwei Fei and Ron Cohen) to learn about their plans for a "Deep Carbon Observatory." Hazen and Russell Hemley are the PIs on a proposal to the Sloan Foundation to develop the concept and plans for a 10-year initiative in this field. See further details at:
http://dco.gl.ciw.edu/

In early May, I attended the High Pressure Synchrotron [HiPreSS] Workshop organized by Malcolm Guthrie and his colleagues at HPSynC [Y. Ding, and M. Lerche]. This workshop was co-sponsored by COMPRES, along with CDAC and the APS, and industrial sponsors Almax, easyLab and Oxford Lasers. Many members of the COMPRES community attended and the following gave talks: Evgeny Gregoryanz, Przemek Dera, Leonid Dubrovinsky, Reinhard Boehler, Thomas Duffy, Viktor Struzhkin, Wolfgang Sturhahn, Charles Lesher, Tetsuo Irifune, Natalia Dubrovinskaia, Wendy Mao, Alexander Goncharov, Stanislav Sinogeikin, and Vitali Prakapenka. Details of the program may be found at:
http://www.hpsync.org/links/HiPreSS/

The Cooperative Institute for Deep Earth Research [CIDER], a NSF-funded program for interdisciplinary research in Earth Sciences, held a strategic planning workshop at the Marconi Center in California from May 17-19., organized by Barbara Romanowicz, Adam Dziewonski, Stan Hart, Louise Kellogg, and Michael Manga. It was attended by 83 scientists from the disciplines of geodynamics, seismology, geochemistry, geomagnetism and mineral physics, as well as Sonia Esperanca and Robin Reichlin, Program Directors in the Division of Earth Sciences at NSF. Speakers from the mineral physics community included Marc Hirschmann, Jackie Li, Dan Frost, Steve Jacobsen, Wendy Panero, Greg Hirth, Dan Shim, and Wendy Mao. I presented at talk on the relationship(s) between COMPRES and CIDER and the opportunities for further collaboration.

Details of the program may be found at:

http://www.deep-earth.org/workshop09.html

I was scheduled to attend the Joint Assembly: The Meeting of the Americas from May 24-27 in Toronto to deliver an invited paper entitled "Indoor vs Outdoor Geophysics" in a special session organized by Hans-Joachim Mueller, but was unable to travel because Air Canada would not accept my alternative travel documents [including copy of passport, original birth certificate, and photo ID (Driver's license-]. A first time for everything. I was particularly disappointed as my principal motivation for attending was to honor the new inductees as Fellows of the AGU from the mineral physics community: Jay Bass, Donald Dingwell, Kei Hirose and Frederic Ryerson.

In July, I visited Harbin Institute of Technology in northern China at the invitation of Professors Haozhe Liu and Luhong Wang and their colleagues. During this visit, I met with administrators, faculty, staff and students of HIT and presented a series of lectures on COMPRES activities and on "Indoor vs. Outdoor Geophysics." In Harbin, I also presented an invited talk at a Workshop on Advanced Crystallography at High Pressure under the auspices of the International Union of Crystallography.

Following a week in Harbin, I visited the Institute of Physics of the Chinese Academy of Sciences at the invitation of Professor Changqing Jin. This visit included a tour of labs in IPCAS, discussions with staff and students, and a two-part seminar on mineral physics and the role of COMPRES.

On September 6-11, I attended the XLVIIth Conference of the European High Pressure Research Group [EHPRG] in Paris, France and presented an invited paper on "Indoor vs Outdoor Geophysics." This conference was organized by A. Polian, M. Gauthier and S. Klotz of the Institut de Minéralogie et Physique du Milieu Condensés. It was held at "Les Cordeliers" , a former convent that now belongs to the Université Pierre et Marie Curie in the Quartier Latin, and included a "field trip" to the Chateau of Versailles and a dinner boat trip on the Seine. Additional details of the program may be found at: http://www-int.impmc.upmc.fr/impmc/47ehprg/

On Friday September 11, I also attended a workshop on a "Partnership for Extreme Conditions Science" organized by the scientific staff from the Institut Laue-Langevin [ILL] and the European Synchrotron Research Facility [ESRF] in Grenoble. The goal of this partnership is to establish support facilities for extreme conditions research at these two European facilities which share the same campus. These developments appear to share some similarities to the Joint Photon Science Institute at the Brookhaven National Laboratory, a new initiative being spearheaded by Chi-chang Kao of BNL and John Parise of Stony Brook University. Additional details on this new PECS initiative may be found at: http://www.ehprg.org/docs/PECS2.doc

Following the EHPRG meeting, I travelled to Potsdam, Germany [near Berlin] to visit the GFZ [GeoforschungsZentrum] German Research Centre for Geosciences of the Helmholtz

Foundation at the invitation of Hans-Joachim Mueller. At the GFZ, I visited labs, including the Brillouin spectroscopy lab of Sergio Speziale, and gave a hybrid seminar on mineral physics and COMPRES.

While in Germany, Mueller drove me to Hamburg for a half-day visit to DESY [Deutsches Elektronen-Synchrotron, where I had a tour of the high-pressure facilities at the

DORIS ring [MAX-80 and MAX-200X], which are operated by staff of the GFZ in Potsdam [See photo in Supplemental Information]. I also met with the Vice Director for Photon Science, Dr. Edgar Weckert to discuss plans for high-pressure beamlines at Petra III, the new synchrotron ring now under development at DESY.

I attended the Annual Meeting of the Geological Society of America in October, primarily to participate in a special session in honor of Alex Navrotsky convened by Gordon Brown, Abby Kavner, Nancy Ross and Glenn Waychunas, and presented another version of my talk on "Indoor vs Outdoor Geophysics."

At the MSA Awards luncheon on October 20, Alex received the 2009 Roebling Medal and Bob Hazen received the 2009 Distinguished Public Service Award. Citations and photos may be seen in the November 2009 issue of the COMPRES newsletter at: http://www.compres.us/files/newsletter/NewsletterV8N2.pdf

Last President's Narrative from Bob

As my term of service to COMPRES came to a close on January 1, 2010, this will be my last President's Narrative to the COMPRES community. The first one was written in February 2004 and said in part:

"On September 1, 2003, I took up my new duties as President of the Consortium for Materials Properties Research in Earth Sciences [COMPRES]. In the first 16 months of its existence, COMPRES made major strides in achieving its objectives. I look forward to working with the Executive Committee and the COMPRES community to build on this initial progress and to continue to develop a shared vision and nurture existing programs and new initiatives over the next few years."

Serving the COMPRES world-wide community has been a great pleasure for me for the past 6+ years and one of the most rewarding experiences of my academic career.

I also very much appreciate and admire the commitment of the many committee members and officers, who have served COMPRES in voluntary, and unpaid, capacities.

Bob Liebermann

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

In preparation for the submission of the Annual Progress Report and Annual Program Plan and Budget to NSF in February, 2010, 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 2009, the two Standing Committees asked the project directors of each of the subawards to submit annual progress reports for Year #3 and program plans and budget requests for Year #4 by November 1, 2009. 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, 2009.

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 2009 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 #4, 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 2010, the Executive Committee met via video and teleconference on four occasions to discuss the reports of the Standing Committees and to formulate recommendations for an Annual Program Plan and Budget for Year #4. Following these meetings, the new President, Jay Bass prepared a budget plan which was discussed, revised, and approved unanimously by the Executive Committee. The budget summary is given in Section D below, with detailed NSF 1030 budget forms and budget justifications given in Section E.

B. Community Facilities

B.1 X-ray Diamond-anvil Facilities at the National Synchrotron Light Source

[PIs: Thomas Duffy, Princeton University, and Donald Weidner, Stony Brook University]

Diamond Anvil Cell X-Ray Diffraction Facility

2009 COMPRES Annual Report for beamlines X17C and X17B3 at the NSLS
November 2008 – November 2009

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) and a sample preparation/spectroscopy laboratory. The X17C beamline is a side station that runs 100% of the time, amounting to a maximum of 81 days for each of the three cycles during the year. The X17B3 beamline operates 33% of the time in dedicated mode with an additional 33% available in shared mode when the X17B2 (multi-anvil) station is running. This nominally provides a maximum of 54 days per cycle. Both X17C and X17B3 beamline are available for energy dispersive (EDXD) and monochromatic (ADXD) experiments.

The 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, and 2009 was no exception.

From January 2008 – October 2009 there are 68 publications in the NSLS publication database for X17C and X17B3. Nine of these are in NSLS-defined premier journals. A total of 7 Ph.D. and 3 M.S. theses in 2008-2009 have been based on work carried out in whole or in part at X17 (Table 1)

Table 1: PhD and MS theses at X17 (2008-2009)

M. Whitaker	Stony Brook University	PhD	2009
D. Liu	Jilin University	PhD	2009
Z. Mao	Princeton University	PhD	2009
Y. Jin	Jilin University	MS	2008
R. Aksoy	Texas Tech University	PhD	2008
Z. Chen	NJIT	PhD	2008
M. Weinberger	UCLA	PhD	2008
M. S. Lucas	Caltech	PhD	2008
L. Petruska	Missouri – Kansas City	MS	2008
A. Akhmetov	U. Western Ontario	MS	2008

Selected Scientific Highlights for 2009

Nanoscale manipulation of the properties of solids at high pressure with relativistic heavy ions

High-pressure and high-temperature phases show unusual physical and chemical properties, but they are often difficult to 'quench' to ambient conditions. In this work, we present a new approach, using bombardment with very high-energy, heavy ions accelerated to relativistic velocities, to stabilize a high-pressure phase. In this case, $Gd_2Zr_2O_7$, pressurized in a diamond-anvil cell up to 40 GPa, was irradiated with 20 GeV xenon or 45 GeV uranium ions, and the (previously unquenchable) cubic high-pressure phase was recovered after release of pressure. Transmission electron microscopy revealed a radiation-induced, nanocrystalline texture. Quantum mechanical calculations confirm that the surface energy at the nanoscale is the cause of the remarkable stabilization of the high-pressure phase. The combined use of high pressure and high-energy ion irradiation provides a new means for manipulating and stabilizing new materials to ambient conditions that otherwise could not be recovered.

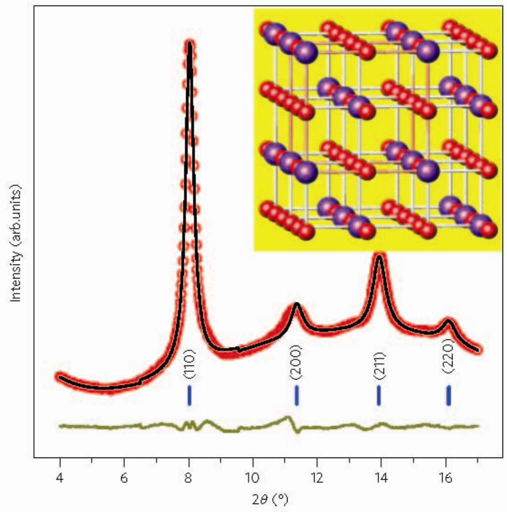


Figure 2 | Synchrotron XRD pattern of the X-phase recovered from 20 GPa after irradiation with 7-GeV uranium ions. (See the corresponding XRD image in Fig. 1e.) Measured diffraction maxima (open circles) can be fully reproduced by the calculated pattern (line) of a cubic $Gd_2Zr_2O_7$ structure ($Im\bar{3}m$). Inset: The crystal structure of the new phase for mixed cation occupancy (large spheres) and fully occupied anions (small spheres).

Publication: M Lang, F Zhang, J Zhang, J Wang, B Schuster, C Trautmann, R Neumann, U Becker, R Ewing, Nanoscale Manipulation of the Properties of Solids at High Pressure with Relativistic Heavy Ions , *Nat. Mater.*, **8**, 793-797 (2009).

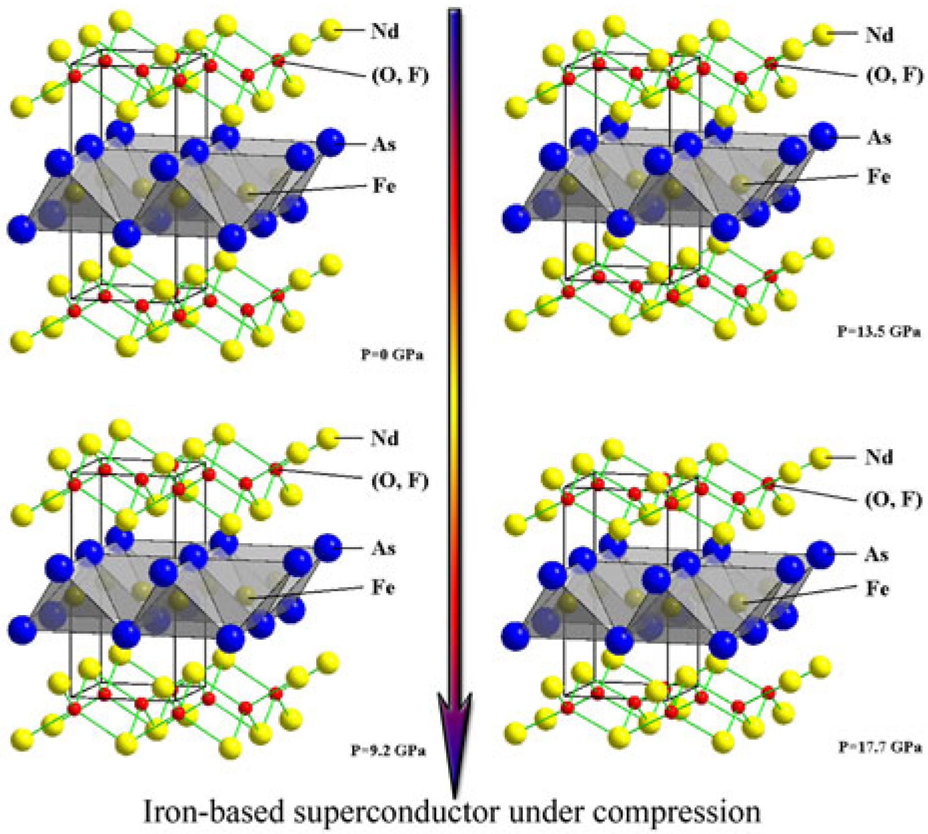
Putting the Pressure on Iron-Based Superconductors

Traditionally, magnetism and superconductivity don't mix. For more than 20 years, the only known superconductors that worked at so-called "high" temperatures (above 30 K, or about -406 degrees Fahrenheit) were almost all based on copper. Materials with strong magnetism, scientists thought, would disrupt the pairing of electrons that is key to achieving the frictionless flow of superconductivity. So when a group of researchers recently found high-temperature superconductivity present in a class of iron-based materials, their discovery shocked and excited the scientific community.

"Many people didn't believe that iron could be an effective superconductor. It went against all prior knowledge," said Haozhe Liu, a professor at the Harbin Institute of Technology, in China. "Now, we've entered the iron age of superconductivity."

Made from conducting layers of iron, arsenic, and various other elements, this new class of materials could lead to applications such as more-efficient power transmission. However, iron-based superconductors are still in the early stages of experimentation and implementation. That why Liu and colleagues from the Chinese Academy of Sciences and the NSLS set out to study the characteristics of a specific iron-and-arsenic-based, neodymium-containing superconductor.

"There is very little information out there right now about this type of superconductor and we want to find out as much as we can about its structure, its behavior, and how it changes under varying conditions," Liu said.



An iron-based superconductor under pressure

The team's results, which are reported in the October 22, 2008, edition of the *Journal of the American Chemical Society*, show that as pressure increases from 0 to 15 GPa, the spacing decreases and Tc increases marginally. But as the pressure increases further, one of the other lattice parameters abruptly increases and the Tc drops.

"After a certain point, there is actually a negative relationship between pressure and Tc," Liu said. "This is a new concept and something that could offer insight on how to design and create other superconducting systems."

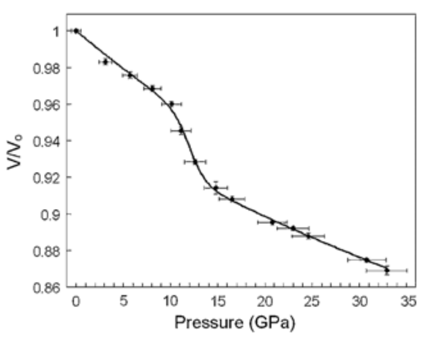
Other authors include Jinggeng Zhao, Luhong Wang, Dawei Dong, and Zhiguo Liu, all from the Harbin Institute of Technology; Genfu Chen, Dan Wu, Jianlin Luo, Nanlin Wang, Yong Yu, and Changqing Jin, from the Chinese Academy of Sciences; and Quanzhong Guo, from the NSLS.

Funding was provided by the National Natural Science Foundation of China, China's Ministry of Science and Technology, and the Excellent Team Program within the Harbin Institute of Technology and the Program for New Century Excellent Talents of China. Use of beamline X17B3 was supported by the Consortium for Materials Properties Research in Earth Sciences (COMPRES), funded by National Science Foundation.

PUBLICATION: J. Zhao, L. Wang, D. Dong, Z. Liu, H. Liu, G. Chen, D. Wu, J. Luo, N. Wang, Y. Yu, C. Jin, and Q. Guo, "Structure Stability and Compressibility of Iron-Based Superconductor Nd(O0.88F0.12)FeAs Under High Pressure," *JACS*, **130 (42)**, 13828-13829 (2008).

Pressure-Induced Invar Behavior in Pd_3Fe

Synchrotron x-ray diffraction (XRD) measurements, nuclear forward scattering (NFS) measurements, and density functional theory (DFT) calculations were performed on $L1_2$-ordered Pd_3Fe. Measurements were performed at 300 K at pressures up to 33 GPa, and at 7 GPa at temperatures up to 650 K. The NFS revealed a collapse of the ^{57}Fe magnetic moment between 8.9 and 12.3 GPa at 300 K, coinciding with a transition in bulk modulus found by XRD. Heating the sample under a pressure of 7 GPa showed negligible thermal expansion from 300 to 523 K, demonstrating Invar behavior. Zero-temperature DFT calculations identified a ferromagnetic ground state and showed several antiferromagnetic states had comparable energies at pressures above 20 GPa.



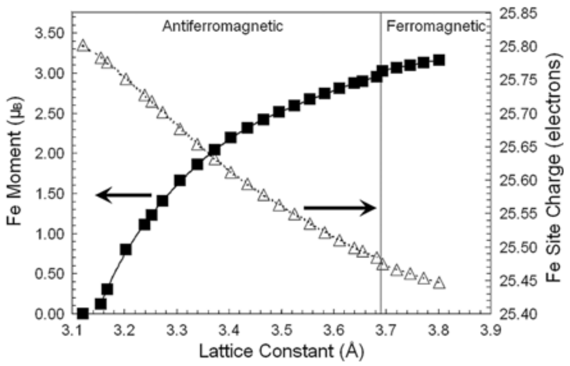


FIG. 1. Volume-pressure data obtained from synchrotron x-ray diffraction measurements (symbols) and the fit of the data to the Weiss-like equation of state [15] (line).

FIG. 4. Magnetic moments at the Fe site (left), and charge at the Fe site (right) versus the lattice constant of Pd3Fe from DFTcalculations. Antiferromagnetic refers to the AFM-I structure(see text). The solid and dashed lines are guides to the eye.

PUBLICATION: M Winterrose, M Lucas, A Yue, I Halevy, L Mauger, J Munoz, J Hu, M Lerche, B Fultz, Pressure-Induced Invar Behavior in Pd3Fe, *Phys. Rev. Lett.*, **102**, 237202 (2009).

Ionic high-pressure form of elemental boron

The results of high-pressure experiments and *ab initio* evolutionary crystal structure predictions have found a new boron phase that we named c-B28. This phase is comprised of icosahedral B12 clusters and B2 pairs in a NaCl-type arrangement, stable between 19 and 89 GPa, and exhibits evidence for charge transfer (for which our best estimate is d<0.48) between the constituent clusters to give (B2)d1(B12)d2. We have recently found that the same high-pressure boron phase may have given rise to the Bragg reflections reported by Wentorf in 1965, although the chemical composition was not analysed and the data (subsequently deleted from the Powder Diffraction File database) seems to not have been used to propose a structure model. We also note that although we used the terms 'partially ionic' and 'ionic' to emphasize the polar nature of the high-pressure boron phase and the influence this polarity has on several physical properties of the elemental phase, the chemical bonding in c-B28 is predominantly covalent.

PUBLICATION: A Oganov, J Chen, C Gatti, Y Ma, Y Ma, C Glass, Z Liu, T Yu, O Kurakevych, V Solozhenko, Ionic High-Pressure Form of Elemental Boron, *Nature*, **457**, 863-868 (2009).

Beamline Overview, 2008-2009

Since June 2007, a multi-institution management team has led X17-DAC. The management team is headed by PIs Thomas Duffy (Princeton University) and Donald Weidner (Stony Brook). 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 as-needed basis.

Beamline Scientists

The last year was a major transition period as two long-serving beamline scientists retired. The new beamline staff members are Sanjit Ghose and Zhiqiang Chen. The transition went remarkably smoothly, and the new staff has instituted a number of changes and improvements to the beamline.

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. Unfortunately for our operation, Sanjit Ghose announced that he accepted a position as staff scientist at the powder diffraction beamline of NSLS-II and will leave X17DAC on January 1, 2010. We are currently conducting a search for his replacement.

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.

Other Key Personnel

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

Beamline operations in 2008-2009

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

In June 2008-Sept2009, X17C had approximately 100 person-visits representing 18 separate universities and institutes while X17B3 had 33 person-visits representing 10 separate universities and institutes. The X17 facility remains oversubscribed and the number of user groups has remained relatively steady for the last few years.

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

X17C

<u>Overview of Major Characteristics</u>

<u>Angle Dispersive Diffraction Experiments</u>

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

Energy Dispersive Diffraction Experiments

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

X17C beamline developments completed in the June 2008-November 2009 period

- The beam line scientists Sanjit K Ghose and Zhiqiang Chen have taken over the beam line operation responsibility from 1st September and 1st November 2008, respectively. Since then, they have been operating and developing the beam lines smoothly without dropping a single day of scheduled beam time.

- A new CCD detector Rayonix SX-165 was installed in place of the old MARCCD which was temporarily borrowed from the NSLS detector pool. The new detector has a larger detection area (165 mm diameter) and faster framing capabilities. This new feature of the MARCCD will facilitate studies on a time scale previously not available in high-pressure and temperature research. New epics control of the MARCCD (Mark River's AreaDetector EPICS control) was installed to control and manage data frame remotely with fully automatic scan protocol. The detector has been in use since June 2009.

- A quick and efficient training procedure with soft and hard documentation was prepared to train new users to learn how to use the beam line with safe and smooth procedure. The same documents are upgraded from time to time with changes and will be soon uploaded to the new website.

- There was a problem of drift of the mono beam observed and analyzed. A heat load diagnosis is made on the double Laue monochromator for 29-30 keV mono beam. With the assistance of Zhong Zhong (NSLS), the upstream slits were closed carefully to reduce the heat load while keeping the beam undisturbed. Now the mono beam is stable and steady.

- Two germanium solid-state detectors, which had been contaminated by Indium fluorescence, were repaired and tested by Canberra. One of these detectors is now in use at X17C for Energy Dispersive X-ray Diffraction (EDXD) experiments.

- Resistive heating setup is reinstalled to heat DACs for both ADXD and EDXD setups. Heating experiments up to 800 degree C could be achieved with special Ar + 4% H gas flow in the cell. The heating set up is done both with the setup used at the beam line as well as setup brought by the users at the beam line.

- The resistive heating set up at the beamline is resumed (previously used) with re-installation of Keithley 2700 digital multimeter and Xantrex XHR 33-33 programmable DC power supply; 33 volts, 33 amp, 1000 watts. The Keithely is connected to the VME system via RS-232 and can be used to measure voltage, temperature, current, etc. from up to 20 inputs. The Xantrex DC power supply is controlled via an external voltage input (VME D/A) to control the output power. An EPICS software feedback loop was set up to control and set the temperature, and could be logged the data at the same time.

X17B3

Overview of Major Characteristics

Angle Dispersive Diffraction and High Energy X-Ray Scattering Experiments

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

Energy Dispersive Diffraction Experiments

White beam E range	20 keV to 100 keV
Focusing optic	K-B mirror
Primary beam size	0.10 mm x 0.080 mm
Focus beam size	0.010 mm x 0.010 mm
Detector	Canberra Ge solid state detector

X17B3 beamline developments completed in the June 2008-November 2009 period

- The operation of the X17B3 beam line has been escalated with regular use of the scheduled beam time both for the focused 30 keV and 80 keV monochromatic beams. This arrangement could accommodate the increase in demand of using ADXD technique with 30 keV at X17C. With the effort of the beam line scientists and maintenance of the facilities, the number of users has been increased during last few cycles.

- An automated X-ray shutter (**XIA** automated X-ray shutter) is installed which operates automatically in sync with the MAR345 image plate operation. This system improved the performance of the beam line significantly as compared to previous operation.

- A multichannel pneumatic valve controller (designed at GSECARS) has been installed to control additional shutters, attenuators, photodiodes and other pneumatically controlled devices. This controller allows us to control sixteen separate pneumatically controlled devices using digitally controlled signals from IPUnidig.

- With Mark River's help a new driver and its epics controls has been installed to drive our digital SONY camera which is used with a Navitar Zoom system to view the beam and samples in the DAC.

- A new Dell workstation is installed along with new MAR software replacing the old computer for the MAR345 image Plate. This improved the performance of the IP as well as data storage management.

- New epics control of the MAR345 IP (Mark River's AreaDetector EPICS control) was installed to control and manage data frame remotely with fully automatic scan protocol. This software allows the users to collect multiple frames (up to 50 frames) preceding with erase cycle after each frame continuously. This helps in collecting data continuously without any intervention.

- New clean up slits were installed to get a sharp Gaussian beam without any extension of the tail of the focused beam. This is achieved with a similar design used at GSECARS with Re and Ta gaskets and inner hole cylinders. The whole slit system is motorized. Further improvement of this system is required for a better and robust clean up slit system which is important for the high-pressure community where use of well defined small gasket hole is essential.

- A preliminary plan for the design of a simple, adequate and fully automated motor controlled high-energy monochromator for X17B3 have been worked out. The motorization of the monochromator would have three 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. Focusing the beam to increase the flux instead of slitting down and use the high flux smaller beam for most DAC users.
    3. The setup time of the monochromator can be drastically reduced, leading to more available user beamtime at X17B2 and X17B3.

  This item will be partly supported by NSLS for which some budget has been requested by Lars Ehm.

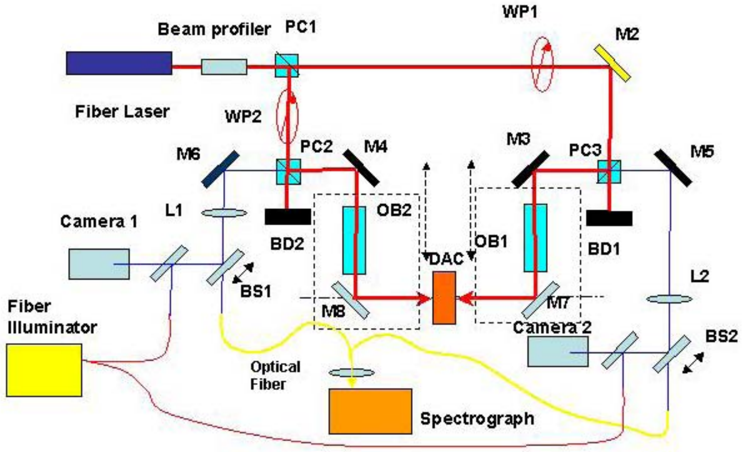


Fig. 1. Schematic for proposed redesign of laser heating system based on Fiber laser

- The new laser heating system is currently being assembled. Due to some issues with the interlock groups at NSLS the scheduled assembly time was delayed. The good news is that these issues have now been fully resolved and the NSLS Interlock Working Group recently approved our interlock design. Here is the list of developments of the laser system achieved so far:
    1. The NSLS interlock group has approved our design and plan for safe operation of the laser.
    2. The old system has been disassembled and the hutch is cleaned up completely to get ready for the new laser system.
    3. The laser bread board with its focusing arrangement is made. (Fig 1 and 2)
    4. New 100 W laser shutter (from Lasermet, UK) is installed along with its logic interface circuit complying with the requirement of the NSLS interlock group. (see Fig 3)
    5. Modification of the optical table and X-ray beam optical components are being made to accommodate the laser heating bread board and shutter system.

  Testing of the system will commence in early 2010, and we expect to have the system assembled at the beamline during the 2nd cycle of 2010.

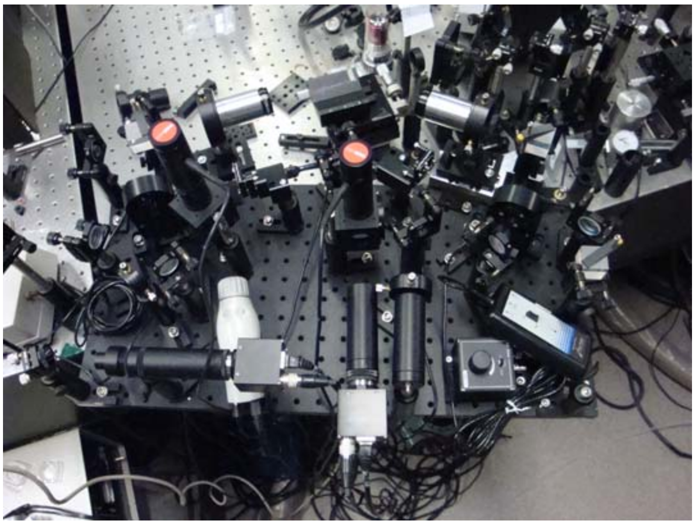


Fig. 2. Laser set up bread board.

Fig. 3. 100 W laser shutter

High-Pressure Laboratory

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

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

<u>Support lab developments completed in the June 2008-November 2009 period</u>

- Last year's supplementary fund was used to procure a set of 3 new diamond cells and related equipment (gaskets, seats, etc) from the Princeton University machine shop. Two of them are in use at the beam line and for experiments at other facilities. The third one has yet to be supplied.

- A new Leica microscope (M165 C) has been set up replacing our old (>15 years) one. This microscope has much improved optics and higher magnification and is a major upgrade for sample loading at very low dimension and has better resolution It includes aperture controls, polarizer & analyzer set up, zoom and camera system. Currently the sample is viewed with an analog camera and soon will be replaced with a digital one with picture capturing and video capabilities.

- Tools for high pressure sample loading such as EDM machine supplies, gaskets (SS & Re), standards and other chemicals are arranged for the users for a hassle- free sample loading experience.

- The lab was used by 50 users from five different beam lines (X17C, X17B3, U2A, X14A, and X27A) affiliated with COMPRES and NSLS, dealing with high pressure and temperature sample loading. The lab safety procedures have been changed as per DOE regulations to maintain a safe and healthy environment.

Outreach Activities

A special issue of *Journal of Synchrotron Radiation* based on the Oct 2008 NSLS workshop on "Advances in High-Pressure Science Using Synchrotron X-rays" was published in November 2009. The special issue includes 12 papers and was edited by H. Liu, T. Duffy, L. Ehm, W. Crichton, and K. Aoki.

A completely redesigned web page for X17-DAC is under construction and should be on-line before the end of 2009.

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

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.

Complete commissioning of the laser heating system, testing and opening for general users, is a major goal of the upcoming year.

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.

For the laser heating system, we will focus the laser beam to about 20-30 micron to heat the sample at specific spots inside the DAC. We also planned to focus the X-ray beam about the similar or less dimension without any figure error from the mirror to get diffraction from the spot of interest. This capability requires a stable, smooth and high resolution Zoom camera system with translational stages for beam diagnosis as well as beam overlapping inside the DAC. We also need to replace our KB mirror system with a new one with better and improved design and stability. The budget for procuring and building these two systems is included in the coming year's budget below.

Working with Z. Zhong (BNL), the Laue monochromator at X17c will be improved to allow for wavelength variation and improved shielding to reduce background.

X17C operates during the full running time of NSLS and two techniques (ADXD and EDXD) must be set up each cycle. Both the techniques have different geometrical pathways and use multi-component assembling units for beam slits and beam detection. The present design and set up follows a tedious procedure and separate set up for each technique which costs not only set up time but also maintenance time.
We would like to improve the design and build adequate set up which could be fixed at the beam lines and a simple switch over to set any of the techniques in a faster and easier way. This would also improve the quality of the experimental procedure and quality of data. We have included an estimated budget for the equipments and components for the same in the next year's budget.

The beam line scientists have initiated and carrying out their own research programs at X17 focusing on high-pressure materials and earth science research as well as facility developments for modern high pressure techniques and data collection. They have plan to increase their activities more involving collaboration from the high pressure communities and other synchrotron facilities.

The X17-DAC facility is one of the most productive COMPRES. 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 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.

X17-DAC Publications (2008-2009)

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Summary of Beamtime Usage for 2009

	Jan-Apr 2009		May-Aug 2009		Sept-Dec 2009	
	X17C	X17B3	X17C	X17B3	X17C	X17B3
# proposals	15	7	17	7	16	7
# days requested	99	58	97	74	100	55
#days beamtime available *	84.73	51.91	60	32.75	66	36
Oversubscription	1.17	1.18	1.62	2.26	1.52	1.53
Funding **						
NSF	9	6	11	4	10	3
DOE	4	1	4	0	2	0
DOD	1	0	2	0	0	0
Foreign	2	1	3	3	4	4

* Available beamtime includes all beam setup, maintenance and development besides beamtime for users.

****** Some proposals are supported by more than one funding.

Total for 2009

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

Summary of beamtime usage for 2008

	Jan-Apr 2008		May-Aug 2008		Sept-Dec 2008	
	X17C	X17B3	X17C	X17B3	X17C	X17B3
# proposals	27	8	22	9	14	5
# days requested	181	76	95	47	69	30
#days beamtime available	85	28	62	20.5	60	19.8
Oversubscription	2.1	2.7	1.5	2.2	1.2	1.5
Funding						
NSF	15	2	8	4	11	5

DOE	8	3	4	3	2	0
DOD	2	0	0	0	0	0
Foreing	4	2	6	2	2	0

Total for 2008

	2008	
	X17C	X17B3
# proposals	63	22
# days requested	345	153
#days beamtime from NSLS	207	68.3
Oversubscription	1.7	2.2
Funding		
NSF	34	11
DOE	14	6
DOD	2	0
Foreign	12	4

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

2009 COMPRES Annual Report for beamline U2A at the NSLS
November 2008-November 2009

Overview

The diamond anvil cell infrared beamline at the National Synchrotron Light Source (NSLS-U2A) 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 diamond high-pressure experiments is one of the unique features of the NSLS for general users. We continue to broaden our user base, and provide convenient access for users from the COMPRES community. In addition, we promote our users' research projects on problems relating to high-pressure geoscience, complemented by studies in materials science, condensed matter physics, chemistry, and biology (many of which are generated by the COMPRES community). The ongoing beamline upgrades provided by the support of COMPRES and CDAC will ensure that this unique facility is supplied/maintained with cutting-edge instrumentation.

I. Selected scientific highlights for 2009

a. Recalibrating the Time Scale of Planet Formation

Wadsleyite is widely believed to be the most abundant mineral in the Earth between 410 and 520 km in depth. Conditions under which wadsleyite forms are known from static high-pressure experiments, but they had never before been recovered from a laboratory-scale shock wave experiment, lasting only a minor fraction of a second. However, wadsleyite has been found in some meteorites consisting of debris that formed upon natural shock events during collisions of proto-planetary bodies in the early solar system. Researchers from **Caltech** and **UNLV**, with the support of scientists from **Carnegie**, have demonstrated a new way to create in the laboratory a mineral that only exists in meteorites and deep below the Earth's crust. The discovery indicates that the formation of planets and certain minerals in the early solar system may have involved collisions between much smaller bodies than previously thought.

In work partly carried out at **NSLS-U2A**, the group reports evidence for small quantities of the mineral wadsleyite forming upon shock compression of thin layers of magnesium oxide and fused quartz.

Based on the size of the wadsleyite grains recovered from the experiment, it can be inferred that the mineral formed in the meteorites from the early solar system could be generated by collisions between bodies one to five meters in diameter, or a thousand times smaller than calculated by earlier models. Therefore high-velocity, destructive collisions among objects in the early solar system may have developed at an early stage of its evolution. Infrared spectroscopy, carried out at **NSLS-U2A**, was used for initial characterization of the shocked sample. Using backscatter electron diffraction techniques, the size of the wadsleyite grains could then be determined to be several micrometers in diameter. Thus, growth rates of the wadsleyite grains during shock were in the range of several meters per second. Usually crystal growth occurs at rates many orders of magnitude slower.

Tschauner, O., P. Asimow, N. Kostandova, T. Ahrens, C. Ma, S. Sinogeikin, Z. Liu, S. Fakra, N. Tamura, Ultrafast Growth of Wadsleyite in Shock-Produced Melts and its Implications for Early Solar System Impact Processes, *Proc Nat. Acad. Sci. USA*, **106**, 13691–13695 (2009).

b. High-Pressure Yields Novel Single-Element 'Compound'

Boron is an element of fascinating chemical complexity. Its complexities arise from frustration: situated between metals and insulators in the periodic table, boron has only three valence electrons, which would favor metallicity, but they are sufficiently localized that insulating states emerge. However, this subtle balance between metallic and insulating states is easily shifted by pressure, temperature and impurities. High-pressure experiments and ab initio evolutionary crystal structure predictions explored the structural stability of boron under pressure and, strikingly, reveal a partially ionic high-pressure boron phase. This new phase is stable between 19 and 89 GPa, can be quenched to ambient conditions, and has a hitherto unknown structure (space group Pnnm, 28 atoms in the unit cell) consisting of icosahedral B12 clusters and B2 pairs in a NaCl-type arrangement. The ionicity affects many properties of the new structure, such as splittings of bands and strong infrared absorption typical of ionic materials. Therefore, infrared spectroscopy is crucial to the characterization of the novel compound. Using intense synchrotron infrared radiation at **NSLS-U2A**, we measured transmission over a very broad wavelength range. The spectrum revealed characteristic features of the predicted structure that arises from different electronic properties of the B2 pairs and B12 clusters and the resultant charge transfer between them.

Oganov, A., J. Chen, C. Gatti, Y. Ma, Y. Ma, C. Glass, Z. Liu, T. Yu, O. Kurakevych, V. Solozhenko, Ionic High-Pressure Form of Elemental Boron, *Nature*, **457**, 863-868 (2009).

c. Anomalous optical and electronic properties of dense sodium

The alkali metals are often presented as textbook examples of simple metals. At low pressures they all take on very simple bcc and fcc crystal structures and display the free-electronlike metallic character predictable for monovalent compounds. However, recent work has shown that the application of pressure results in an unexpected variety of complex phenomena. These include the existence of low-symmetry and even incommensurate phases and significant electronic changes leading to unusual melting behavior, Fermi-surface nesting, phonon instabilities, electron-phonon coupling and superconductivity, and transformations into poor metals or even insulators. Sodium is unique among the alkali metals because of its occupied electronic states; it differs from lithium by the presence of p states, and from the heavier alkalis by the absence of d states under compression. Its Fermi surface remains spherical up to 120 GPa, whereas in all

other alkali metals the Fermi surface is significantly deformed by 7 GPa. It is the only alkali metal not predicted to date to become a superconductor under pressure. It exhibits the largest pressure-induced drop in melting temperature ever reported, dropping from ~1,000 K to nearly room temperature at 120 GPa, and possessing crystal structures in the vicinity of the melting minimum with hundreds of atoms per unit cell. It has been suggested that an observed darkening of the metal at a transition to an incommensurate phase at 125 GPa may signify the onset of semiconducting or insulating behavior suggested in theoretical studies for sodium. To address this, synchrotron infrared reflectivity measurements were performed at **NSLS-U2A**, conventional reflectivity measurements at the Geophysical Laboratory on sodium metal in the low-symmetry phases up to 180 GPa and performed first-principles calculations on the reported crystal structures. Synchrotron infrared spectroscopy on sodium shows a transition from a high reflectivity, nearly free-electron metal to a low reflectivity, poor metal in an orthorhombic phase at 118 GPa. Optical spectra calculated within density functional theory (DFT) agree with the experimental measurements and predict a gap opening in the orthorhombic phase at compression beyond its stability field, a state that would be experimentally attainable by appropriate choice of pressure-temperature path. A transition to an incommensurate phase at 125 GPa results in a partial recovery of good metallic character up to 180 GPa, demonstrating the strong relationship between structure and electronic properties in sodium.
Lazicki, A., A. Goncharov, V. Struzhkin, R. Cohen, Z. Liu, E. Gregoryanz, C. Guillaume, H. Mao, R.J. Hemley, Anomalous Optical and Electronic Properties of Dense Sodium, *Proc. Nat. Acad. Sci. USA*, **106**, 6525-6528, (2009).

d. Novel Pressure-Induced Interactions in Silane-Hydrogen
The strength of the covalent H_2 bond over a range of chemical and thermodynamic environments is of great interest. At extremely high pressure, hydrogen is expected to form a metallic phase and exhibit high temperature superconductivity. However, metallic hydrogen remains elusive as the pressures thought to be required to create it are outside current experimental capabilities. Recent work has suggested that hydrogen dominant materials (*e.g.*, methane, silane, germane, etc.) may undergo insulator to metal transitions at significantly reduced pressures when compared with pure hydrogen. Recent experimental reports have suggested that silane (SiH_4) transforms into a metal around 60 GPa and displays superconductivity at 100 GPa and 17 K. Researchers at the Geophysical Laboratory have revealed a new hydrogen dominant material with indication for molecular hydrogen bond weakening at extremely low pressure when compared with bulk hydrogen. By pressurizing mixtures of SiH_4 and H_2, they discovered the formation of a new compound, $SiH_4(H_2)_2$, that displays abnormally strong intermolecular interaction. Raman and synchrotron infrared spectra (measured at U2A beamline) of the new compound revealed an anticorrelated pressure-frequency dependence of the hydrogen vibrons, indicative of covalent H_2 bond destabilization. Starting at only 7 GPa, this phenomenon is remarkable when compared with solid H_2 where the IR vibron does not soften until pressures well over a megabar. The results of this work point to unusually weak hydrogen covalent bonds, and the possibility of metallization at pressures far below that of pure H_2. The implications for unusual chemical bonding, metallization and superconductivity that arise from the discovery of $SiH_4(H_2)_2$ have been described recently

by N. W. Ashcroft [*Physics*, **2**, 65 (2009)], who points out the importance of this new material to both experimental and theoretical investigations into the nature of hydrogen at high densities.
Strobel, T., M. Somayazulu, R.J. Hemley, Novel Pressure-Induced Interactions in Silane-Hydrogen, *Phys. Rev. Lett.*, **103**, 065701 (2009).

e. Hydrogen Bonds in the Magnesium Silicates, Phase D and Phase E
Hydrogen is a geochemically important element whose abundance is poorly constrained in the Earth's deep crust. The presence of hydrogen even in small quantities can affect phase relations, melting temperature, rheology, and other key properties of the deep Earth. Dense hydrous magnesium silicates (so-called alphabet phases) are a class of hydrous silicates that form under high-pressure-temperature conditions in the MgO–SiO2–H2O. These silicates are potentially important components of the deep Earth water cycle especially in cold slab environments. In particular, phase E is likely to be an important water carrier near the base of the upper mantle and transition zone, while phase D may be the major H_2O-bearing phase at the top of the lower mantle in low-temperature slab environments for peridotite compositions. Using the synchrotron infrared facility at **NSLS-U2A**, we measured the infrared spectra of polycrystalline samples of phases D and E to 42 and 41 GPa, respectively. For both phases, at least three broad OH stretch vibrations were observed at elevated pressures indicating that each phase comprises multiple hydrogen positions that exhibit disorder. No structural phase transition or amorphization was observed for either phase over the measured pressure range. The mode Grüneisen parameters of phases D and E are in the range of −0.12 to 1.14 and −0.17 to 0.83, respectively, with mean values of 0.41 (phase D) and 0.31 (phase E). Using empirical correlations of OH frequency and O· · ·H and O· · ·O bond lengths; the six OH vibrations of phase D at ambient pressure have corresponding O· · ·H and O· · ·O bond distances in the range of 1.519–1.946Å and 2.225–2.817Å, whereas the four OH vibrations of phase E have the corresponding O· · ·H and O· · ·O bond distances in the range of 1.572–2.693Å and 2.557–2.986 Å. These ranges encompass values reported from single-crystal X-ray diffraction measurements. At high pressures, the observable OH stretching vibrations exhibit both positive and negative pressure slopes. Our high-pressure infrared spectra for phase D do not support the occurrence of hydrogen symmetrization as predicted by first-principles calculations.
Shieh, S., T. Duffy, Z. Liu, E. Ohtani, High-Pressure Infrared Spectroscopy on the Hydrous Magnesium Silicates, Phase D and Phase E, Phys. Earth Planet. Interiors, **175**, 106-114, (2009).

II. Beamline Developments

1. **Construction of a new side station at the U2A beamline:** As we pointed out in the previous year's annual report, the U2A beamline has been built as the first dedicated high-pressure IR beamline in the world with many unique features. However, there are important limitations in the present configuration that preclude optimized performance. These limitations, due to the far distance between the U2A beamline end station (spectrometer/microscope) and the synchrotron source spot, are becoming big concern as the IR user community grows. Diagnostic tests have shown that 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 have been running for more than ten years. It's more and more difficult to use the IR microscope because some parts (like motors that control the reflecting mirrors) start malfunctions from time to time.
Recently, we proposed to build a side station that will allow us to perform measurements on high-pressure samples with the highest spatial resolution possible at a synchrotron source while also having the highest broadband IR brightness. An exciting opportunity has arisen to create such 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. Fortunately, we are able to raise sufficient funds to start the side station construction in 2009. A FTIR spectrometer (Bruker Vertex 80v, $150.4 K from COMPRES Year #3 fund $100 K for permanent equipment and the rest from CDAC) has been purchased and will be delivered in early November 2009. In addition, we are fortunate enough to have $60 K contribution from UNLV in order to acquire a Bruker Hyperion 2000 IR microscope. Special thanks to Prof. Malcolm Nicol's kind support and generous contribution from the University of Nevada at Las Vegas; t will be remembered by the COMPRES user community. This new microscope coupled with the FTIR instrument will be ideal for the mapping of natural samples (*e.g.*, solid and fluid inclusions in thin section), heterogeneous charges from high-pressure experiments, as well as laser heated samples *in situ* at very high- pressure in diamond or moissanite anvil cells. Finally, we are also able to purchase a new bolometer detector from IRLabs using the 2009 equipment upgrade monies from NSF via COMPRES. The detector will be delivered in December 2009 and will further improve the far-IR performance at the side station.
Based on current as well as next cycle's beamtime schedule, we plan to install an optical table at the side station before the NSLS winter shutdown. The FTIR spectrometer and the IR microscope are scheduled to be installed by Bruker's engineers in December. Then, we will bring together the FTIR instruments and synchrotron in January 2010. We are confident that the new side station will be accessible for all users in the cycle of Jan-Apr, 2010.

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 the Earth's interior. High-pressure and high-temperature >1000 K extreme conditions are essential for infrared studies of Earth and planetary materials. We are continuing to make progress on the CO_2 laser heating system including purchases and installations of additional accessories such as a controller, a DC power supply, safety shutter, beam expander, and a chiller for the CO_2 laser. However, laser safety is an important issue at BNL, and

we are working very hard with the NSLS interlock group to address the laser safety requirement at BNL. That's the main reason that the laser heating project is behind its current schedule. In addition, the temporary temperature calibration system, as a result of utilizing the dismissed spectrograph and CCD detector from the old Raman system, and a controller for the CCD detector borrowed from the NSLS, are impossible to use because the spectrometer is completely dead. Therefore, an entire new temperature calibration system will be absolutely necessary for the functionality of the CO_2 laser heating system. Again, it's fortunate that we received equipment upgrade funds ($52.4 K) on time to purchase a spectrometer with an OMA-InGaAs detector from Princeton Instruments as well as a standard source for temperature calibration. Another major progress is that the NSLS interlock group was finally approved and will install the laser interlock system soon. The whole system will be moved into a commissioning phase after passing through the laser shutter and interlock inspection.

3. **Laser upgrade for the Raman/IR Microscope system**: The U2A beamline provides access for all users to do not only synchrotron FTIR spectroscopy under extreme conditions but also Raman scattering. The whole system including the microscope, spectrometer, and CCD detector has been upgraded recently using CDAC funds as well as partial COMPRES equipment funds. However, the Ar^+ laser is more than ten years old and running with a refurbished tube. It's necessary to replace it with the solid state lasers. With the available funds from NSF equipment upgrade monies, we will add two DPSS lasers (532 nm and 785 nm) to the micro-Raman system early next year.
4. **Compact cryostat:** The combined high-pressure and low-temperature techniques are very important to address a broad range of problems in planetary sciences. Such capabilities could also attract a lot of users. The existing cryostat at U2A was designed only for Mao-Bell type DACs. It is more than ten years old and the temperature control system doesn't function properly. A new cryostat with a compact design for a standard symmetric DAC has been purchased and will be delivered in December 2009. This cryostat from Cryoindustries will be shared by all DAC facilities at the NSLS.
5. **New sample preparation station:** The number of users at the NSLS DAC facilities is growing and the sample preparation lab at X17C is not sufficient to accommodate this number of people since all three DAC beamlines are running at the same time. In addition, users often need to load samples many times for IR experiments and they have to spend a lot of time moving back and forth between the U2A hutch and the sample preparation lab at X17C. With the available funds, we will purchase a Leica microscope for sample loading and an EDM machine for gasket drilling in the U2A hutch. These tools will be available for users in April 2010 based on the delivery schedule of the EDM machine.

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. Currently, the COMPRES community is the dominant user group in this category. The remaining 25% of beam time is 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 provides the CU group proposed here with the ratings of all proposals for a beam time cycle, so that these ratings may be honored in decisions on requests for the 25% of beam time to be allocated by COMPRES. The remaining 25% goes the Geophysical Laboratory, Carnegie Institution of Washington for development projects and users supported by its grants, including CDAC and EFree.

VIII. U2A Beamline Publications 2008-2009

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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

2009 COMPRES Annual Report for beamline X17B2 at the NSLS
November 2008 – November 2009

Available MAC beamtime. 2008-2009 has been an exciting year at the multianvil facility at the NSLS. The 'B' portion of the superconducting wiggler beam (X17) supports three hutches, X17B1, X17B2, and X17B3. The X17B2 houses the multianvil facility and X17B3 houses a portion of the diamond anvil cell program. Together B2 and B3 are in use 2/3 of the time and can be run simultaneously. Thus the multianvil system is available 2/3 of the time that the NSLS is operating.

The B2 hutch has a white beam and a monochromatic beam that is generated by a single bounce monochromator. Thus it is possible to place two high pressure stations on the floor, each receiving beam. We are still developing the shielding of the mono station so that these two stations can operate simultaneously. We expect this to be finished next week, although we had hoped that it would have been finished earlier. Once completed, we hope to be able to have two groups working two experiments simultaneously on the B2 beam.

Beamtime is allocated on the basis of proposals that are submitted to the NSLS. The allocation committee assigns beamtime totaling 16.7% of the NSLS operations time to the top ranked general user proposals. Often this is allocated to COMPRES type of research projects, but not always. We assign no more than 10% of the time to beamline development purposes, with the rest allocated to the pool of general user proposals. We use the ranking of the review committee, but add a priority to the COMPRES community.

NSLS is now developing X17A. 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 may allow the high pressure portion of the X17B time to increase beyond the current 2/3 allocation. Furthermore, we expect to support some high pressure research on the X17A beamline using either PE or DAC style cells.

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

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

Science Highlights –

Rheology

Here we highlight the rheology program. Many groups are now using this system to define rheological properties of minerals at elevated pressure and temperature. Olivine, pyroxene, garnets have all become subjects of study covering the upper mantle conditions as well as subduction zone P, T conditions.

Rheology of olivine Raterron and his group (Raterron et al., 2009; Raterron et al., 2007; Raterron et al., 2004a; Raterron et al., 2004b; Raterron et al., 2005) have used the deformation system to study the rheology of dry olivine at high pressures (up to 10 GPa) and high temperatures (up to 1800K) for single crystals of both forsterite and San Carlos olivine. Using crystal orientations that promote slip on different slip systems, they concluded that pressure induces a change in the active dislocation system. These results have implications of seismic anisotropy on the flow history of the deep upper mantle. Durham's group (Durham et al., 2009) and Karato's group (Kawazoe et al., 2009b) have pursued the issue of the pressure dependence of creep in olivine polycrystalline samples with implications concerning the strength of the upper mantle to 10 GPa and 2000K. The resulting activation volume has strong implications for the strength of continental roots.

Long (Long, 2008) studied the rheology of olivine at subduction zone conditions. The flow law is generally athermal and strain rate insensitive. Using unconsolidated powders as a model of damage zones, he concluded that such regions may be significantly weakened and become thermally activated at much lower temperatures than sintered samples. This may have implications on the origin of deep earthquakes suggesting that fault zones, once established, may be the site of future earthquakes.

Rheology of wadsleyite Karato's group have begun studies of the flow properties of wadsleyite (Kawazoe et al., 2009a; Nishihara et al., 2008a; Nishihara et al., 2008b). Similar to olivine, steady-state was observed after ~10% strain. They found two flow regimes, a low-temperature regime where the strength is insensitive to temperature, and the high-temperature regime where strength is sensitive to temperature. Only at high temperatures (>1900 K), is there evidence of recovery/recrystallization. Interestingly, samples deformed at high-temperature regime show clear evidence for dynamic recrystallization (grain-size reduction), and most of recrystallized grains have no or little dislocations. They interpret that the low-temperature regime corresponds to the Peierls mechanism, whereas the high-temperature regime corresponds to some mechanisms involving diffusion. However, the exact mechanisms of deformation in high-temperature regime is not well constrained at this time.

Rheology of garnet Li (Li et al., 2006) report a comparative study of the strength of pyrope rich garnet and olivine. This study is possible only with these high pressure systems because of the stability field of pyrope. She concluded that for the magnesium rich end member, pyrope is weaker than olivine (at 1200^{o}C), but the addition of iron weakens the olivine and San Carlos olivine is weaker than a pyrope – almandine garnet that would be in equilibrium with the olivine.

Rheology of polycrystal. Li et al (Li et al., 2004) and Weidner et al (Weidner et al., 2004) demonstrated that a polycrystal often deforms with a large variations of stress among different populations of grains. Those oriented with weak slip relative to the stress field are at a relatively low stress, while strong grains exhibit large stress. Burnley (Burnley and Zhang, 2008) examined this issue with the goal of being able to use this information to constrain slip system and to define the average aggregate stress. Karato (Karato, 2009) has derived a theoretical framework to describe this phenomena.

Rheology of two phase media Li (Li et al., 2007) examined the rheology of two phase mixtures to evaluate the flow properties and to study the partitioning of stress between a strong and a weak phase.

Time resolve studies The dependence of many parameters on time is a critical issue in Earth science research. Sinusoidal variation of the driving field can produce sinusoidal responses of the material. Phase and amplitude analysis enables a wide range of properties to be identified. Dobson's group has adapted this tool to define thermal diffusivity of materials at high pressure. Sinusoidal variations in temperature yield 'heat waves' or diffusion fronts that propagate into the sample. By clever imaging, these heat waves are characterized with thermal diffusivity being derived. Phase transformations (Li Li) are the focus of such studies as the sin wave is a stress wave and the percentage of phases is defined. Stress and strain as such variables defines elastic modulus and Q at seismic frequencies. The ability to obtain a diffraction spectram in 15 seconds gives an enormous boost to this type of study.

New capabilities developed to date for non-hydrostatic pressurizing systems and stress/strain measurements have spawned several collateral spin-offs outside the science of rheologic behavior of rocks. Measurements of seismic attenuation, Q, and dispersion (Li and Weidner, 2007) have been enabled. Since the non-hydrostatic stress is created by a hydraulic system, it can be either increased or decreased with time. This allows a sinusoidal variation in the differential stress. The further use of a corundum rod placed in series with the sample allows one to define a stress proxy from the change in length or strain of the corundum rod. Taking advantage of the fact that an image requires about a millisecond exposure one is able to measure stress and strain of the sample from an image for sinusoidal oscillations of the stress field from 0.1 Hz to 0.001 Hz. Q is determined from the phase lag of the sample strain relative to the corundum strain and effective elastic modulus is defined by the ratio of amplitudes. While the strains are still larger than one would like in such measurements (of the order

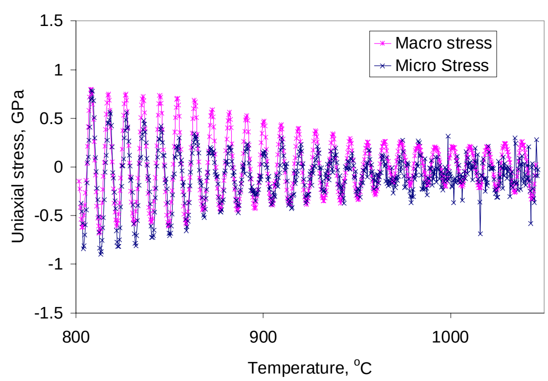

Fig. 1 Sample stress as a function of increasing temperature. One period is 700 seconds. Micro stress is measured from 15 second diffraction spectra of the sample. Macro stress is derived from the length of a corundum rod in the cell in parallel with the sample.

of 10^{-4}), the pressure range is more than an order of magnitude greater than previously available (Jackson and Paterson, 1993), but the results are in good agreement with those of (Jackson et al., 2002) for fine grained olivine. This methodology was used to define the bulk attenuation and dispersion associated with the olivine to ringwoodite phase transition with the implication that two phase regions in the mantle may be softened at seismic frequencies (Li and Weidner, 2007).

From the image analysis system, Dobson's group (University College London) derived a method for measuring thermal diffusivity at high pressure and temperature (Dobson et al., 2008). Placing imagable wires above and below the sample, they defined the characteristic time for a heat wave to diffuse from the cylindrical furnace into the sample. The distance between the wires served as a proxy for temperature as a 50^o amplitude sin wave was applied to the furnace. Frequencies from 1 Hz to 0.01 Hz were used.

The new conical slit system achieves the 10 MPa precision with data collection times of 600 seconds or so. However, the gain in signal to noise actually decreased the amount of time for some measure of differential stress. Fig. 1 illustrates stress data taken during a sinusoidal stress regime (period of 700 seconds) as temperature was increased. The diffraction stress measurements are for 15 second exposures. Also indicated in the figure is the stress defined by the corundum proxy determined from images that were also obtained.

Activities for 2009-10

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 will be installing and commissioning a 1000 ton press with guide block on the white beam. We will be installing and commissioning a new slit system on the monochromatic beam.

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

We are operating two end-stations simultaneously; a white beam and a monochromatic side station. This allows two users to run simultaneously while we have beam, which is now 2/3 of the total NSLS beam days. As X17A is set up, we expect this number to grow. We need a second beamline scientist to carry on this operation.

Our mission in this coming year is 1. to provide user support on both multi-anvil high pressure devices and 2. to construct and install the two items supported by COMPRES on the recent equipment upgrade funding from NSF via COMPRES. Included here is a 1000 ton press with high pressure tooling and a slit system for the monochromatic beam. We have begun the procurement of these items and are targeting December, 2010 for final installation and commissioning. This is an extremely ambitious time line. Our current personnel requests will help to meet this goal.

We are requesting no additional equipment in this budget.

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Beamtime Requests and Usage

In 2009, 27 scientists requested beam time in at least one of the three scheduling periods ("trimesters"). Five were deemed not suitable for beamline X17B2. The requested total for the remaining 22 was 185 days. There were 25 General User days available, to which the NSLS Proposal Review Committee assigned time to 4 users, based on the ratings of their proposals (some more than once). Of the remaining days available, COMPRES assigned 102$^{1}/_{3}$ days. Additional time is found frequently, due to a) Unscheduled Operations or b) people finishing early, starting late or not showing up at all. The last column (Days Used) includes these days. In some cases, that time is less than that assigned. This is usually due to someone else in the same project being allowed to be substituted. The table below details these assignments.

During 2009, there were 49 users from 15 institutions, including 22 PIs. There were 147 separate experiments, lead by 25 users (most proposals required more than one experiment).

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B.4 West Coast Synchrotron Facilities

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

X-ray DAC Facilities at the Advanced Light Source

2009 COMPRES Annual Report for beamline 12.2.2 at the ALS

November 2008-November 2009

NOTE:
This report for 2008-2009 was prepared by R. Jeanloz and S. Clark. Following review of this report by the Facilities Committee and a Site Visit to the ALS in December 2009, the Executive Committee decided to transfer the subcontract for the operation of the high-pressure beamline 12.2.2 at the ALS to the University of California Santa Cruz, with Q. Williams as the PI. Williams and J. Bass will co-chair a new management team which will be formulating the program plan for Year #4 for the COMPRES-funded portion of this facility, starting immediately.

Summary

The laser heating system in the 12.2.2 hutch has been rebuilt on a more solid support structure, and upgraded with 4-color temperature measurement and improved laser beam-shaping optics. We have continued with the validation of our temperature measurement system, and have completed the temperature-pressure calibration of our resistively heated DAC, including development of a set of fluorescence pressure-temperature sensors. The Brillouin system is fully characterized, and in use both for high-pressure and high-temperature measurements on polycrystals. We have continued our support of COMPRES use of the beamline, and seen a growth in beamtime applications.

For next year we propose to complete the validation of our laser-heating imaging/spectroradiometer system, and to implement a more automated temperature measurement system incorporating simultaneous determinations from both the 4-color and spectroradiometer systems. We propose to complete the development and validation of our high-temperature resistively heated DAC (temperatures up to 1000^{o} C), and to upgrade the current MAR345 detector to a CCD based detector to allow us to reduce data collection times. This challenging program of work should be achievable given the level of support we expect from COMPRES, the ALS and UCB Earth and Planetary Sciences.

Activities this year

1. **Complete training of the COMPRES beamline support scientists**
   The three COMPRES support personnel are now fully trained and operating. Their roles are:

Jinyuan Yan	Provide general support and training for Beamline 12.2.2 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 readiness for users.
Selva Vennila Raju	Provide general support and training for Beamline 12.2.2 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 Beamline 12.2.2 users. Provide support and training for cell alignment and loading. Help maintain, calibrate and further develop the laser heating system. Provide support in the high-pressure laboratory including training users in the use of the Brillouin and Raman systems.

   In addition to this Raymond Jeanloz will continue to provide guidance and oversight for the project, Simon Clark will provide day to day management and continue leading the development of the laser heating system at ALS, 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. **Upgrade the laser heating system**
   This year saw a major overhaul of the laser heating and imaging spectroradiometry systems on Beamline 12.2.2.
   a. A new larger optics table with a more robust mounting system was installed. This was necessary to overcome the stability problems we had with the old table, and to provide sufficient space for a rationalized optical layout and the addition of two 4-color systems. This involved a complete strip down and rebuild of the system together with some modification to services in the hutch. The new table is more stable, and matches our needs. The rationalized optical layout (both sides of the temperature measurement system are now symmetrical, which was not possible with the smaller table) is facilitating alignment of the system.
   b. Two 4-color temperature measurement systems were constructed (based on a collaboration with Andy Campbell), and installed on the beamline. We have tested the system, and have robust alignment and data capture in

place. At the moment we are developing the necessary software to allow automated data collection and temperature determination.

c. A laser beam profiler was assembled and commissioned. It has been used to quantify the current laser beam profile at various levels of defocus. A set of pi-shapers have been purchased and tested on the beamline. These were found to give improved control over the laser spot size, allowing us to go to much larger sizes than with the current system.   The shape of the spot was also found to be more like a top hat. A new mounting system incorporating the fiber laser delivery system and the pi-shapers is currently being built, and is due for installation in early December.

Software for temperature determination remains an important issue, which we intend to address during the upcoming year.

3. Continue validation of on-line laser heating system

Validation of the on-line laser heating system has continued in-house with measurements of ambient pressure and high-pressure melting. In addition to Bin Chen, Jinyuan Yan is now fully trained in aligning and operating the laser heating system, and has contributed to the melting curve measurements (Fig. 1).

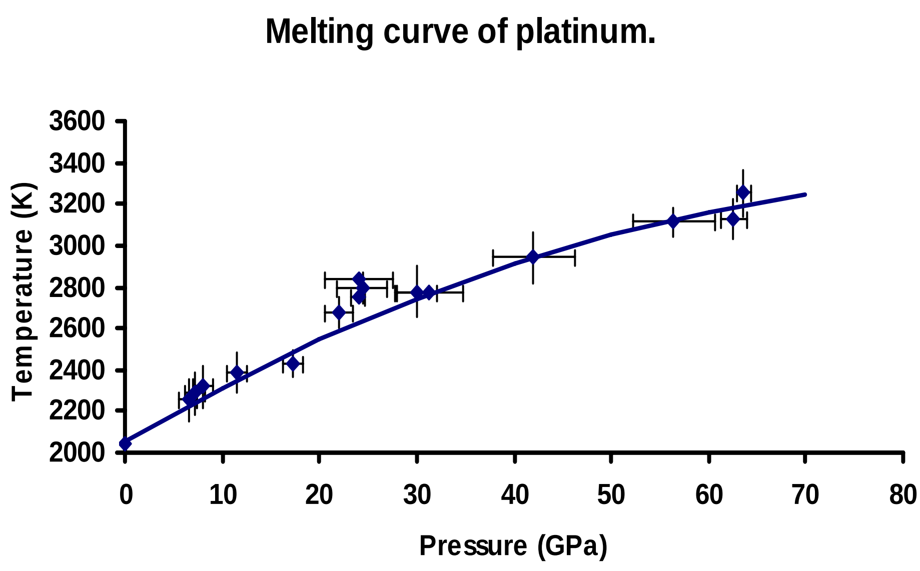


Fig. 1. Melting curve of platinum (S.M. Clark, unpublished measurements). Points below 12GPa are from Lord and Walter (private communication). Points above 12GPa are from our system as determined from plateauing of the power-temperature curve. The line is from Kavner and Jeanloz, J. Appl. Phys., 83, 7553 (1998).

4. Commission resistive heating cell

The development of a resistively heated diamond-anvil cell with a Pt wire heater has been completed by Vennila Raju. It has been tested up to 600^{o} C and 60 GPa, and used for data collection up to 600^{o} C and 25 GPa. Calibration of fluorescence standards as a function of pressure and temperature is completed in this pressure-temperature range, and a method for using these standards to determine both temperature and pressure has been developed. A manuscript describing this work is in preparation. A new power supply that will allow us to operate this cell at higher temperatures has been delivered. We have been working in developing the high temperature resistively heated diamond cell with $MoSi_2$ heater. The power supply and control system have been tested with the $MoSi_2$ heaters. Data have been collected using the resistively heated DAC with a number of groups both on the beamline and with the Brillouin system. These studies include:

d. Alison Pawley, Univ. Manchester. Volume measurement of Lawsonite as a function of pressure and temperature. (bl12.2.2)
e. Jennifer Kung, Diffraction study of a phase transition in (Ca,Sr)SnO3 at high-PT. (bl12.2.2)
f. Sebayachi Sen, UC Davis, Crystallization of a molecular chalcogenide glasses at pressure and temperature. (bl12.2.2)
g. Arianna Gleason, UC Berkeley, Brillouin study of Argon at high pressure and temperature. (Brillouin)

5. Complete development of Brillouin and Raman systems

Raman and Brillouin systems have been commissioned for work with powders at high-pressure, and combined high-pressure and high-temperature. The motivation for developing these capabilities is to offer users independent means of characterizing their samples, both at ambient conditions and at elevated pressures and temperatures. Both can ultimately provide independent validation of temperature-measurement systems. Also, the acoustic-wave velocities documented by Brillouin can help constrain equations of state determined on the x-ray beamline, and can ultimately provide independent determinations of melting in the diamond-anvil cell. Because of these intended applications, we have focused on developing polycrystal capability.

Data have been collected on a number of materials, and publications are either in review (2) or preparation. We have validated our system with joint studies with Tom Duffy in Princeton and Sergio Speziale in Potsdam, and demonstrated that our data – both single crystal and powder – are equivalent to those collected using the other systems. The following projects are complete or in progress using this system:

h. Kristie Koski (UCB Chemistry). Studies of organic solvents, including ethylcyclohexane, under pressure.

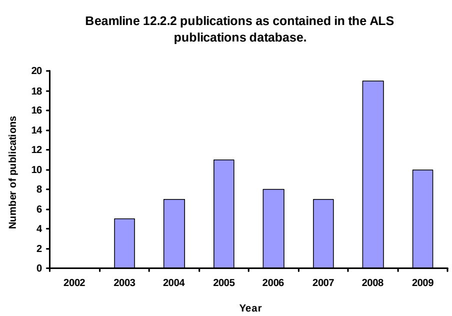
i. Arrianna Gleason (UCB EPS). Studies of powders, including NaCl and MgO and studies of noble gases including Ar and Ne under pressure and at combined P and T.

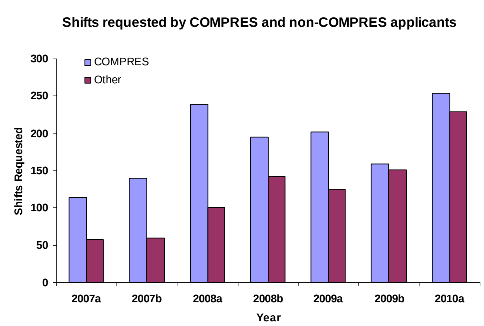
j. Haulke Marquardt (GFZ, Potsdam). Studies of ferro-periclase under pressure coupled with radial diffraction studies on beamline 12.2.2.

A paper is in press describing our powder Brillouin measurements, both at ambient and high pressures (A. Gleason, et al., Geophys. Res. Lett. (2009)). Finally, we are adding remote viewing and alignment systems to allow users to operate the system while it is inside a laser enclosure. This adds greatly to laser safety, and reduces the necessary user training by effectively lowering the laser risk to users from Class 3 to Class 1.

6. Support a program of outstanding scientific research.

We have continued to support a program of outstanding scientific research, both on the beamline and in the high-pressure laboratory (see figure below). Demand for the beamline has increased, although much of the growth has been in proposals from non-COMPRES users. This growth in the number of shifts requested by non-COMPRES users has reduced the percentage of time allocated to COMPRES users from about 70% to about 50%. Nevertheless, demand from COMPRES users remains strong, with about 42% of the time in the next allocation period identified for laser heating experiments.





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 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

Continue to provide high quality user support

We propose to continue providing support for COMPRES users of Beamline 12.2.2. This year Jinyuan Yan, Simon Clark and Jason Knight have taken on the majority of this work. Now that the Brillouin system is fully validated, we propose to focus Bin Chen on supporting users of bl 12.2.2, along side Jinyuan Yan. Since Jinyuan Yan is now fully trained in aligning and using the laser heating system, we would expect him to work side by side with Bin Chen in supporting users for high-temperature measurements. This will have the advantage of freeing up Simon Clark and Jason Knight to concentrate more on completing the developments and validation work outlined below.

Improved infrastructure

It has become clear to us that we have fallen behind in the provision of basic infrastructure for high-pressure research. In particular our current facilities for gasket preparation and pressure transmitting fluid loading need upgrading.

Our current equipment for drilling holes (a drill press and a spark eroder) are difficult to train visitors to operate effectively, and even the in house staff can only achieve about a 60% success rate. Upgrading to a laser cutting system similar to that at GSECARS will enable us to reliably cut accurate holes, and this will lead to more reliable loadings. At the moment, virtually all of our failed experiments are due to gasket failures. We feel that provision of a laser drill will eliminate most of these failures and lead to a largely improved productivity. We have quotes for a turn-key system of around $110 K, and believe that we could build a suitable system for around $60 K for parts plus ALS labor.

Currently we typically load silicone oil, methanol-ethanol or argon as our pressure transmitting fluid. The argon is loaded cryogenically and has a 50:50 success rate. Both methanol-ethanol and silicone oil have cause problems with interpretation of measurements due to non-hydrostaticity. A reliable system for loading noble gases is a prerequisite at any state of the art high-pressure facility, and the system at GSECARS has been proven to work effectively. The plans and parts list have been made available to us. We believe that we can build a copy of the GSECARS system for about $90 K for parts and ALS labor.

Provision of these systems will greatly improve our users' effectiveness and productivity.

Complete validation of laser heating system and complete development of an automated temperature measurement system

Now that we have upgraded the laser heating optical table, installed the 4 color systems, and upgraded the laser-beam delivery and diagnostic systems with addition of pi-shapers and beam profiler, we are in a position to complete the commissioning and validation of the full laser-heating system. This is already in progress. We have a Ph.D. student, Zack Geballe (working with Raymond Jeanloz) who is characterizing the spectroradiometry system. We also have an experienced researcher, Robin Benedetti, (funded by Raymond Jeanloz) who is working with us to develop software for automated temperature measurement and to participate in the validation of our laser-heating system. This provides valuable additional personnel to help us complete the validation process this year. The in house team together with this additional UCB resource plan to work together to validate the system by a series of melting curve measurements using combined 4-color and spectroradiometry to measure temperature. A range of melting criteria, including diffraction, will be documented. In parallel with this development, we are constructing a set of software to enable the rapid collection and temperature determination from both 4-color and spectroradiometry systems. This activity is on going, and expected to be completed this year.

Complete testing and validation of our high temperature resistively heated diamond anvil cell

All of the components for the high-temperature diamond-anvil cell, including power supplies but not the inert-gas enclosure, have now been delivered. We aim to design and build the inert-gas enclosure this year, and start commissioning the cell early next year. We hope to complete testing to 1000^{o} C and 40 GPa by summer 2010. The cell will then be available for users on both the x-ray beamline and the Brillouin/Raman systems.

Upgrade of beamline, optics and and x-ray detectors.

The beamline and its K-B optics were designed by Howard Padmore and his group. Howard is the ALS Division Deputy for Experimental Systems (ESG) at ALS and his team includes experts in many areas of synchrotron science and instrumentation. He has indicated that greater input can now be expected from his team in two areas. In optics, we will be investigating improvements to beamline performance resulting from a funded upgrade to the storage ring that will increase the brightness by a factor of 10. This increase is on top of a factor of 2 improvement that has been achieved from operation in topoff mode at twice the previous average current, and a factor of 2 increase from reduction in vertical bream size. The benefits in flux in a high-pressure experiment will only be realized if we upgrade the beamline optics, and this will be analyzed in the next year. In addition, the imaging spectroradiometry and 4-color systems will be analyzed with an aim of improving performance and ease of use.

For the second contribution, a thrust area at the ALS is in improving the performance of detectors. Padmore together with Peter Denes (head of ALS engineering and acting division director for LBNL Engineering) have been developing fast silicon detectors for x-ray experiments under a strategic LDRD (internal LBNL funding totaling around $1 M over the last 3 years). This work has just been approved for new ARRA funding of $2M, and a new 3 year R&D program at $1.7 M/year has been funded. This potentially could have significant impact for high-pressure research at ALS. One product of this work has been fast (200 frames/second), ultra-low noise column parallel CCDs that can be used for either optical or x-ray detection. One version of this detector is being used for direct detection, and has around 200 eV energy resolution; it has potential applications in diffraction-free x-ray fluorescence, energy resolved Laue and speckle diffraction. We are currently working with the ESG group to develop these advances for high-pressure research. In the meantime, Padmore is making available a new Bruker P200 CCD-fiber -phosphor detector for work at 12.2.2 as required. The value of this new detector is approximately $260 K. In addition, the ESG group has a small (80 x 36 mm) Dectris pixel detector, and this will be tested at 12.2.2 in order to assess its performance for experiments where rapid framing is needed

Establish off line facility for developing spectroradiography.

We have interested Howard Padmore and his team in our temperature measurement problem. He will assess the level of effort required to fully model the present system, the likely benefits of such a study, and the availability of a specialist to take on this task. This would be part of on-going efforts to document the design and expected performance of this system.

One issue that we face is that it is difficult to characterize let alone develop our temperature measurement systems in the x-ray hutch, due to the constant demand of beamline users and maintenance personnel. We therefore propose to build a development system in the high-pressure lab to allow us to test and fully characterize new optical configurations or optical elements prior to deployment onto the beamline. If we went for a full system with lasers (2 x 50 W), one spectrometer and one 4-color system, we estimate that it would cost about $80 K.

Summary of publications

So far this year, ten publications are reported in the ALS database. A list of publications for Year 2 of COMPRES II is contained in the appendix.

Other highlights

The LBNL guest house has opened. This provides affordable housing close to the ALS. One of the first groups to stay there were the Winkler group (Pictured here) while they were working on Beamline 12.2.2.

Appendix : List of ALS high-pressure publications for 2008-2009

COMPRES

Miyagi, L., M. Kunz, J. Knight, J. Masiatka, M. Voltolini, and H.R. Wenk, "In-situ Phase Transformation and Deformation of Iron at High Pressure and Temperature," *Journal of Applied Physics* **104**(10), 103510 (2008).

Gleason, A.E., R. Jeanloz, and M. Kunz, "Pressure-temperature stability studies of FeOOH using x-ray diffraction," *American Mineralogist* **93**, 1882-1885 (2008).

Miyagi, L., M. Kunz, J. Nasiatka, M. Voltolini, J. Knight, and H.-R. Wenk, "In-situ study of texture development in polycrystalline iron during phase transformations and deformation at high pressure and temperature.," *Journal of Applied Physics* **104**, 103510 (2008).

Walter, M.J., 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**, 622-626 (2008).

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

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

Grant, C.D., J.C. Crowhurst, T. Arsenlis, E.M. Bringa, Y.M. Wang, J.A. Hawreliak, P.J. Pauzauskie, and S.M. Clark, "X-ray diffraction of electrodeposited nanocrystalline Ni under high pressure," *Journal of Applied Physics* **105**, 084311 (2009).

Juarez-Arellano, E.A., B. Winkler, A. Friedrich, L. Bayarjarga, V. Milman, J. Yan, and S.M. Clark, "Stability field of the high-(P,T) Re2C phase and properties of an analogous osmium carbide phase ," *Journal of Alloys and Compounds* **481**, 577-581 (2009).

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

Walker, D., O.T. Lord, M.J. Walter, and S.M. Clark, "X-ray Absorption Contrast Images of Binary Chemical Reactions," *Chemical Geology* **260**, 211-220 (2009).

Weinberger, M.B., J.B. Levine, H.Y. Chung, R.W. Cumberland, H.I. Rasool, J.M. Yang, R.B. Kaner, and S.H. Tolbert, "Incompressibility and Hardness of Solid Solution

Transition Metal Diborides: Os1-xRuxB2," *Chemistry of Materials* **21**(9), 1915-1921 (2009).

Winkler, B., E.A. Juarez-Arellano, A. Friedrich, L. Bayarjargal, J. Yan, and S.M. Clark, "Reaction of titanium with carbon in a laser heated diamond anvil cell and reevaluation of a proposed pressure-induced structural phase transition of TiC," *Journal of Alloys and Compounds* **478**, 392-397 (2009).

Other

Zhuravlev, K.K., W.M. Hlaing Oo, M.D. McCluskey, J. Huso, J.L. Morrison, and L. Bergman, "X-ray diffraction of MgxZn1-xO and ZnO nanocrystals under high pressure," *Journal of Applied Physics* **106**(1), 013511 (2009).

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

C. Infrastructure Development Projects

C. Infrastructure Development Projects

C.1 Multi-anvil cell assembly project

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

Multi-anvil Cell Assembly Project at ASU
2009 COMPRES Annual Report
November 2008-November 2009

Prior accomplishments of the project

The COMPRES Cell Assembly Development Project (COMP-CAD) began in September of 2002. The objective of the project is to create a broad collaboration in the multi-anvil community in order to develop, fabricate and use multi-anvil cell assemblies. In the beginning, the project was fully COMPRES funded and the cell assemblies and parts were distributed for free, and the results of testing and the impressions of the users were acquired in return.

As the project progressed and the first cell assemblies were tested and calibrated and could be used routinely, the COMPRES Infrastructure Development Committee requested that some of the costs be covered by providing the established assemblies to the multi-anvil community at or near cost. We started doing this in 2005. A formula was developed for pricing the assemblies: summing the idealized minimum costs incurred during the fabrication of each piece of the assembly to get a base price, and then applying a safety margin for non-ideality in the process. We initially set what we consider to be a modest margin of 20% (most companies use 50- 100% or more) and began sending out quotations in response to inquiries. The interested users would place purchase orders and we would set about procuring, organizing, and packing the materials.

This system works very well – the margin has remained at 20%, the costs have been recovered appropriately, and the challenge of supplying a large number of assemblies and parts has driven us to make many improvements in the fabrication and processing of the cell assembly parts. Since 2005, we have had 93 orders from 26 institutions world-wide, involving some 2000 cell assemblies composed of some 40,000 parts. In May 2008-May 2009, the most recent full year of the project, we had \$48065 in revenues from cell assemblies. This provides an “engine” for keeping the cell assemblies in constant production and ensuring their ready availability to the community. A list of the participating researchers and laboratories is given in Table 1.

The project has resulted in a series of “standard” cell assemblies used for multi-anvil laboratory work. Care is taken to maintain the same materials for the assemblies once they are calibrated and standardized. Materials are procured in large batches for longer-term consistency, densities and x-ray patterns of all the materials are checked, and the shipments include a packing slip with batch dates for all the parts in order to track any problems that occur with the assemblies during use. The COMPRES standard assemblies are listed in Table 2.

In addition to the standard assemblies, we create under the auspices of this project novel beam line assemblies for use in *in-situ* x-ray diffraction studies. These are not subject to the constraints of consistency because pressure is measured *in-situ*, are made in smaller numbers because beam times are of short duration with longer times in between, and are subject to more frequent modifications in order to optimize their use for a variety of *in-situ* studies. The current lineup of *in-situ* assemblies is also listed in Table 2.

<u>Providing standard multi-anvil cells</u>

A significant portion of the materials costs are supplied and maintained by providing cell assemblies to the multi-anvil community at or near cost. This allows a flow of materials to be developed and maintained, which makes the materials less expensive, and provides a consistent methodology for high-pressure experiments. The interlaboratory consistency and sharing of experiences working with the same set of materials is to the overall benefit of the high-pressure community.

The orders for cell assemblies are overseen by K. Leinenweber, while the assembling and packing of materials is usually done by undergraduate student workers, and since summer 2009 by the technical support person, Jacob Nite. The employment of a dedicated technical support person for this aspect of the project has greatly improved the flow of orders and materials, and kept us up-to-date on orders so that an order for materials that are already in stock can take an average of only about a week to ship. We find it expedient to put the orders together when the customers express the intention of ordering, rather than when a purchase order is actually received, as would be required by a typical company. This allows the materials to ship immediately upon receipt of a purchase order.

The stocks for the standard assemblies are now maintained ahead of the orders, because the assemblies are static (in order to preserve the calibrations) and it is virtually certain that the parts will be used. Large orders of as many as 1000 pieces per batch are made, which saves some money per piece, and also makes the operation smoother because we need to order less often. The majority of the ordering, and communication with suppliers, is done by K. Leinenweber.

We have also made some parts that are not part of the standard assemblies "to order" for other laboratories. These are provided at cost for the materials and machining, and are done partly as a COMPRES-supported community service, and partly to gather experience in the fabrication of parts that we might incorporate into future designs. Various specialized sample capsules for UNM and NASA Johnson Space Center are recent examples of this activity.

Other more innovative and experimental assemblies are provided at less than cost, because they are part of the COMPRES development project and can thus be justifiably subsidized for materials, but we recover part of the cost of the development this way. New beam line assemblies that are being tested and used by UIUC, NASA Johnson Space Center, and others are examples of this.

Calibration and Testing Program

As the project has developed and grown, the amount of experimental work necessary to calibrate and test both the new and the standard assemblies has risen and has reached a rate of 50 runs per year on the multi-anvil. The bulk of testing is, as expected, done on new designs and on newly developed materials and parts. The assemblies are thoroughly vetted before being listed as standard items. When other laboratories are interested in testing them and reporting back their results, as always we will provide the trial cells free of charge. But naturally much or most of the testing of a new design will be carried out in the ASU laboratory where the results of the testing can feed quickly back into the design process.

Testing is also done for new developments in materials for our cells. Furnaces with TiB_2+BN composites replacing graphite in the diamond kinetic stability region, for example, have been successfully tested in recent months, have been used at the beam lines in a 14/8 "equatorial" assembly (Leinenweber et al., 2006; Chen et al., 2009) and will be used for December 2009 beam times in a new 10/5 assembly that we have just finished testing.

Even for the established "standard" assemblies, it is often required for the cells to be tested to ensure uniformity, reproducibility and reliability. If a user experiences problems with an assembly, new testing immediately is undetaken to determine the causes and whether the assembly is still performing according to expectations. We keep careful track of the batch information for all the parts of each order, and this also allows problems to be tracked. Cells are tested by performing multi-anvil runs with complete records of the power consumption to compare to previous records, and usually with a calibrant inside to verify the pressure generation. With the significant numbers of assemblies that are being sent out, it is important to have a control for the performance of the assemblies at the point of manufacture (ASU). We have performed several runs to test standard assemblies this year based on issues reported to us, have shared the results with those labs using the assemblies, have successfully addressed many of the issues, and are working on others. In addition, we need to extend the calibrated range of the standard assemblies – for instance, this year we have calibrated the 10/5 assembly at 2000 °C and 12 GPa using the coesite-stishovite transition, which enhances the calibration information because it previously went up to only 1500 °C.

The last but very important type of testing is bringing assemblies to the beam time, either to obtain detailed calibration curves for the standard offline assemblies (Diedrich et al., 2009; Stoyanov et al., 2009) or to use the in-situ assemblies for scientific studies. The in-situ assemblies are first carefully tested offline, as described above, and even sample centering can be tested in this way by post-run sectioning, plus the x-ray throughput can be calculated as a function of wavelength using x-ray absorption calculations. So, in theory, there is little left to surprise at the beam line. However, for the very new designs, it has been found to be expedient for KL to join some of the beam line experiments of other groups if invited. This has been done in the case of the NASA/JSC group of Kevin Righter (Danielson et al., 2007) and Jie Li's group at UIUC (Chen et al., 2008).

<u>Need for the technician position</u>

Early in the project, the pressure calibration and high-pressure testing of cells, as well as the supply of the cell materials to the community, were done by K. Leinenweber and by undergraduate workers as the needs arose. However, as the project has moved forward and the number of working assemblies and new designs has grown, the testing requirements have risen, and have now reached what we consider to be a steady state of 50 runs per year, which is a significant experimental load. The volume of orders for cell assemblies and new designs have also have become quite significant. This has raised an issue relating to the success of this project: if we can meet the community demand, and supply cell assemblies and materials in a reliable way that creates confidence within the user base and allows experimental programs to proceed unimpeded by supply problems, then the project is serving its purpose.

In order to approach this issue, an undergraduate worker who was especially effective and who graduated with a B.S in Chemistry (Jacob Nite) was hired as a technician starting in summer 2009 full-time, specifically for the COMPRES project. What we found was that the backlog of cell assembly orders and needs for experimental testing significantly cleared up within a few months of the hiring of the technician. We were then able to keep up quite steadily with the demand, and many important test runs that had been waiting to be done, were done. The technician has done 25 COMPRES-related testing experiments, a rate of about 1 per week, since his full-time appointment, and taken care of many COMPRES-related orders – our orders are now able to be filled very quickly compared to before, which should increase the confidence of the user base in the project.

For this project to reach its full potential as a community service, we therefore request that this work continue to be done by a full-time technician. The salary is modest and thus this is a cost-effective use of COMPRES funds to facilitate this project.

<u>Cost reduction for multi-anvil cells</u>

One very important function of the centralized project is to look for ways to reduce costs on assemblies while keeping the quality (and therefore the pressure and temperature capabilities and calibrations) the same. The prices are based on actual manufacturing costs versus yield for each part, which we keep track of carefully each time a batch of parts is fabricated. Thus by finding less expensive ways to manufacture the parts, we can reduce the price of the whole. This is also sometimes possible by ordering in larger quantities at a lower cost per piece.

For parts such as the frequently used zirconia pieces, extrusion was attempted as a very inexpensive alternative, but so far, unfortunately, our testing has concluded that the extruded zirconia does not have desirable deformation properties for high-pressure research such as that of the zirconia available from Mino Yogyo in Japan. The cost of this material per block is quite high ($600 or more for a larger block 120x120x 25 mm). Combined with machining the parts, and considering cost savings on other parts, this had become one of the main costs of many of the assemblies. Therefore, we searched for less expensive ways to process the zirconia and also to increase the yield per block to offset the high cost of the material. In June, 2008, we found a more efficient way to make complex zirconia pieces (pieces having thermocouple slots, steps, off-center holes, or other complex features) by cutting the block into slabs of the right thickness and milling the parts from a single slab as close together as possible. This has worked well for medium-sized parts.

This type of milling is still not the ideal solution for all the parts, especially very small ones. The milling tool is typically 2.4 mm in diameter in order to have sufficient surface speeds for machining the ceramic, and the material in the path of the tool is wasted. Also, the overall machining costs can be fairly high. In April, 2009 we found a better alternative for small, simple cylindrical plugs or sleeves: the ultrasonic coring of cylindrical parts directly from the block. The coring tools are very thin, so much less material is wasted. As an example, for the small zirconia end-plug for the 10/5 assembly, by machining, we obtained 188 parts per smaller zirconia block and experienced costs of $4.42 per piece in 2008. With the new procedure – the use of dimensionally accurate ultrasonic coring tools combined with slicing on a diamond wafering saw - the yield per block is increased to 2000 pieces, and the total price per piece is now $0.83 per piece, a savings of $3.59 per 10/5 assembly.

The ultrasonic coring method is now used to make 2 of the 3 zirconia parts for the 14/8 “G2” assembly, for a savings of several dollars per assembly. The third piece has thermocouple slots and is made by milling.

We will continue to search for ways to reduce the cost per assembly. For a given design using a particular set of materials, at some point the costs stabilize and it becomes very difficult to make them any lower, but currently there is still room for some additional savings on most of the standard assemblies that we produce, and new techniques for the new assemblies will continue to be sought.

New Developments

New developments will use the materials and supplies budgets from COMPRES (see budget explanation). This allows innovative techniques and materials to be tried. One recent new development is larger cells (18/12 and 25/15) which now have completed designs (Stoyanov et al., 2009) and which have begun to be provided to the community. An important issue with the larger cells again becomes price; costs for some of the pieces increase in proportion to the sizes of the components. This is particularly true for the 25/15 which has a 12 mm hole in the octahedron that is occupied by a zirconia sleeve. Only 64 pieces can be obtained from a large block of zirconia, at a cost of $17.19 per sleeve. A new idea is to use low-fired pyrophyllite for low pressures. It may be recalled by some that low-fired pyrophyllite was used as thermal insulation for diamond syntheses. This material was used historically but has been to some extent "forgotten" by the multi-anvil community because it was replaced by zirconia at pressures higher than 7 GPa, where it transforms to silica plus alumina and loses its thermal insulation capabilities. We can obtain fired pyrophyllite sleeves for this assembly for $7.25 apiece. This type of insulation needs to be tested and compared to zirconia; if it is satisfactory, it will lead to cost-savings for these large assemblies which are used for phase equilibrium studies and synthesis at pressures up to 7 GPa.

New developments are being undertaken for assemblies to measure electrical conductivity (based on the Bayreuth design and piggybacking on a pre-existing COMPRES cell that is the Bayreuth 14/8 cell), a project that is entering the testing stage. There is a demand for ultrasonics assemblies and we are basing these on the pre-existing 10/5 and 8/3 assemblies. These are in the design stages and will be tested in the spring of 2010. There is also an interest in deformation assemblies; we are providing some parts for deformation assemblies for the D-DIA (Durham et al., 2008), and are interested in providing full assemblies for deformation experiments.

The other major thrust of current development is in beam line assemblies. There is a new improvement in the "windowed" assemblies with laser-cut rhenium heaters that have x-ray windows. The windows have been partly closing under experimental conditions for unknown reasons, resulting in reduced sample access. At a recent beam time (July 2009) at GSECARS, it was observed through radiography and diffraction that because one of the windows was cut along the seam of the furnace, in the very early stages of compression the furnace would wrap and the one window along the seam would close, while the other remained open. This observation resulted in a re-design with both windows cut away from the seam, and a second seam added for symmetry (Figure 1). This will be tested at the beam line in December (KL beam time), and we are very optimistic that the sample x-ray access problem will be solved. The great advantage of these assemblies is that they can easily reach very high temperatures (in excess of 2200 °C) and still allow x-ray diffraction to be performed (Danielson et al., 2007). These are also easily modified for ultrasonic experiments.

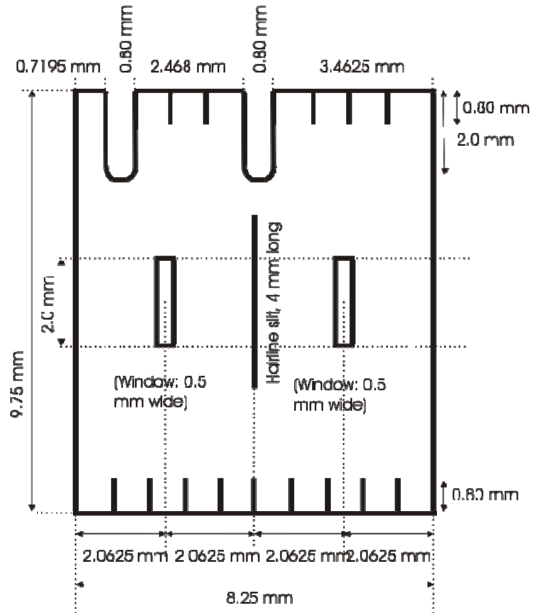


Figure 1. Improved laser-cut rhenium furnace for in-situ x-ray diffraction, Sept. 2009. Thermocouple grooves are along the top, slits for folding furnace are along top and bottom, and x-ray windows are in the center. The foil is rolled up along the vertical axis for use as a tube-shaped furnace.

For studies that require full radiographic access, not just diffraction access, we are developing a series of "equatorial" assemblies – assemblies with full equatorial windows in the thermal insulation sleeves that are normally zirconia or lanthanum chromite, which are far too absorbing to be useful. To avoid heat loss through the windows, the octahedron is made of mullite. The windows themselves are made of MgO, because mullite breaks down at high pressures and temperatures near the furnace. We developed a 14/8 windowed assembly based on the Bayreuth step-heater assembly, first using a graphite furnace (Mosenfelder et al., 2005) and more recently with a TiB_2 + BN furnace (Chen et al., 2009) which can stably reach significantly higher temperatures than a graphite furnace, though probably not as high as the rhenium heaters described above. For the next beam time, we are making prototypes of a new 10/5 equatorial assembly at the request of Jie Li's group at UIUC, who would like to have full radiographic access at higher pressure than before. The new 10/5 assembly uses mullite octahedra, MgO windows and a straight TiB2 + BN heater. It has been tested successfully in our lab and we are also sectioning it to check the centering of the sample, which is most important for beam line use, and is adjusted by changing the lengths of the pieces inside. It will be used at the beam line immediately after KL's experiments (Jie Li's beam time) and KL will join the beam line team for the experiments.

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* multi-anvil 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 step heater	15 GPa	1400 °C	Graphite/$LaCrO_3$ step furnace
18/12	9 GPa	1500 °C	Graphite box furnace
25/15	5 GPa	1500 °C	Graphite box furnace
8/3 window assembly in-situ	25 GPa	2200 °C	$LaCrO_3$ sleeve and rhenium furnace with windows
10/5 window assembly in-situ	20 GPa	2200 °C	$LaCrO_3$ sleeve and rhenium furnace with windows
10/5 equatorial assembly	20 GPa	1700 °C	TiB_2+BN straight furnace, MgO equatorial window, mullite octahedron.
14/8 "G2" in-situ	13 GPa	1200 °C	Graphite box furnace, forsterite sleeve
14/8 equatorial assembly in-situ	15 GPa	1500 °C	TiB_2+BN step furnace, MgO equatorial window, mullite octahedron

References and publications associated with the Multi-anvil Cell Development Project

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

Chen, B.; Li, J.; Gao, L.; Leinenweber, K.; Wang, Y.; Sanehira, T. (2008). In Situ Investigation of Melting Behavior in Fe-S System Using Synchrotron X-ray Radiography. High Pressure Research 28, 315-326.

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

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Hernlund J, Leinenweber K, Locke D, Tyburczy, JA (2005) A numerical model for steady-state temperature distributions in solid-medium high-pressure cell assemblies. American Mineralogist 91, 295-305.

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Leinenweber, K.; Tyburczy, J.A.; Sharp, T.G.; Soignard, E.; Diedrich, T.; Petuskey, W.B.; Wang, Y.; Stoyanov, E.; Nite, J.; Mosenfelder, J (in preparation). Development of a series of cell assemblies for reproducible multi-anvil experiments (the COMPRES assemblies).

Mosenfelder, J., Leinenweber, K., and Wang, Y. (2005) A new multi-anvil assembly for beamline experiments up to 15 GPa: application to in situ measurement of the pyroxene-ilmenite transition in $ZnSiO_3$. EOS Trans. AGU, 86(52), Fall Meet. Suppl., Abstract MR23C-85.

Stoyanov, E.; Haussermann, U.; Leinenweber, K. (2009) Large-volume multianvil cells designed for chemical synthesis at high pressures. In press, High Pressure Research.

Tronche, E.J.; van Westrenen, W.; van Kan, M.; de Vries, J.; Li, J.; Chen, B.; Gao, L.; Wang, Y.; Sanehira, T.; Leinenweber, K. (2008). Equation of State of Ilmenite at lunar pressures and temperatures. EMPG (Experimental Mineralogy Petrology and Geochemistry) XII, Sept. 2008.

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

[PIs: Wolfgang Sturhahn and Ercan Alp, Argonne National Laboratory; Jennifer Jackson, California Institute of Technology; and Jay Bass, University of Illinois at Urbana-Champaign*]

- **As of 1 January 2010 when he assumed his position as President of COMPRES, Jay Bass is no longer a Co-PI on this project.**

Inelastic X-ray Scattering Project at the APS
2009 COMPRES Annual Report
November 2008-November 2009

Report Summary

We report here on the activities to date of Year 3 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 full term with the possibility of continued funding beyond this time period. We include here a description of activities to date, planned activities for the coming year, and a budget request for an extension of the project.

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

During 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&IXS 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 (Dr Hasan Yavas) 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;
4. Created high-pressure capabilities at for IXS at 3-ID.

The latter two items are described in more detail below. On the instrumental side, we proceeded with the integration and use of the capability of x-ray diffraction with NRS experiments in sector 3-ID. Hasan's effort has now provided more accurate NRIXS data by effective use of the added diffraction capability with structural confirmation as well as pressure calibration.

Generation of Proposals

In the time period of 200782009, 11 independent research groups from 10 COMPRES member institutions submitted 59 proposals to 3-ID and 22 proposals to 30-ID. Of these proposals 28 (= 47 %) and 7 (= 32 %) were granted beam time at 3-ID and 30-ID, respectively (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 many of the PIs to develop effective proposals that were very competitive for beam time. Table 1 shows details on proposals allocated for beam time in 2009.

High-pressure IXS at 3-ID

In the last year, we have explored the possibility of reducing the size of the x-ray beam at the momentum-resolved IXS station in sector 3-ID. Hasan's contributions were crucial in this effort. We were able to demonstrate a 20□20 micron^2 spot size (prior 150□150 micron^2) and obtain the highest spectral flux density of any IXS beam line in the world. This success will enable high-pressure studies using momentum-resolved IXS at 3-ID. Even though not immediately apparent to some COMPRES users, the effort of Hasan is important for our future growth potential, e.g., by increasing the total amount of beam time available.

Publications

In the time period of this proposal, the following publications in refereed journals had partial support by COMPRES. Reference 8 was featured on the front cover of the printed version of the journal (see Fig. 2). Several papers are in preparation or in the review process.

- Gao, B. Chen, J. Wang, E.E. Alp, J. Zhao, M. Lerche, W. Sturhahn, H.P. Scott, F. Huang, Y. Ding, S.V. Sinogeikin, C.C. Lundstrom, J.D. Bass, and J. Li Geophys. Res. Lett. 35, L17306 (2008), doi:10.1029/2008GL034817L Pressure-induced magnetic transition and sound velocities of Fe_3C: Implications for carbon in the Earth's inner core

- W.L. Mao, V.V. Struzhkin, A.Q.R. Baron, S. Tsutsui, C.E. Tommaseo, H.-R. Wenk, M.Y. Hu, P. Chow, W. Sturhahn, J. Shu, R.J. Hemley, D.L. Heinz, and H.-K. Mao
  J. Geophys. Res. 113, B09213 (2008), doi:10.1029/2007JB005229
  Experimental determination of the elasticity of iron at high pressure

- J.-F. Lin, A.G. Gavriliuk, W. Sturhahn, S.D. Jacobsen, J. Zhao, M. Lerche, and M. Hu
  American Mineralogist 94, 594-599 (2009), doi:10.2138/am.2009.3108
  Synchrotron Mössbauer spectroscopic study of ferropericlase at high pressures and temperatures

- S.-H. Shim, A. Bengston, D. Morgan, W. Sturhahn, K. Catalli, J. Zhao, M. Lerche, and V. Prakapenka
  Proc. Nat. Acad. Science 106, 5508-5512 (2009), doi:10.1073/pnas.0808549106
  Electronic and magnetic structures of the postperovskite-type Fe_2O_3 and implications for planetary magnetic records and deep interiors

- J.M. Jackson, W. Sturhahn, O. Tschauner, M. Lerche, and Y. Fei
  Geophys. Res. Lett. 36, L10301 (2009), doi:10.1029/2009GL037815
  Behavior of iron in (Mg,Fe)SiO_3 post-perovskite assemblages at Mbar pressures

- J.M. Jackson, E.A. Hamecher, and W. Sturhahn
  Eur. J. Mineral. 21, 551-560 (2009), doi:10.1127/0935-1221/2009/0021-1932
  Nuclear resonant X-ray spectroscopy of (Mg,Fe)SiO_3 orthoenstatites

- D.J. Bower, M. Gurnis, J.M. Jackson, and W. Sturhahn
  Geophys. Res. Lett. 36, L10306 (2009), doi:10.1029/2009GL037706
  Enhanced convection and fast plumes in the lower mantle induced by the spin transition in ferropericlase

- L. Gao, B. Chen, M. Lerche, E.E. Alp, W. Sturhahn, J. Zhao, H. Yavas, and J. Li
  J. Synchrotron Rad. 16, 714-722 (2009), doi:10.1107/S0909049509033731
  Sound velocities of compressed Fe_3C from simultaneous synchrotron X-ray diffraction and nuclear resonant scattering measurements

- K. Catalli, S.-H. Shim, V. Prakapenka, J. Zhao, W. Sturhahn, P. Chow, Y. Xiao, H. Liu, H. Cynn, and W.J. Evans
  Earth Planet. Sci. Lett. (2009), doi:10.1016/j.epsl.2009.10.029
  Spin state of ferric iron in $MgSiO_3$ perovskite and its effect on elastic properties

Planned Activities

In the extension of our infrastructure development project, we will continue the outreach effort to the COMPRES community by assisting interested groups in design, preparation, execution, and evaluation of 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 sector 30-ID, we plan to create an infrastructure in-place supporting high-pressure experiments. For the new opportunity of IXS experiments in sector 3-ID, we plan to invest $100k into an instrument upgrade to enable high-pressure experiments. This will include optical microscopes and micro-positioning stages for convenient in-situ alignment of samples. The successful completion of all these tasks depends on a dedicated postdoctoral researcher like Dr. Hasan Yavas. We expect 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. Together with the upgrade of IXS at 3-ID for high-pressure studies and COMPRES user support during and preceding experiments, this should be a significant fraction of his workload.

Illustrations

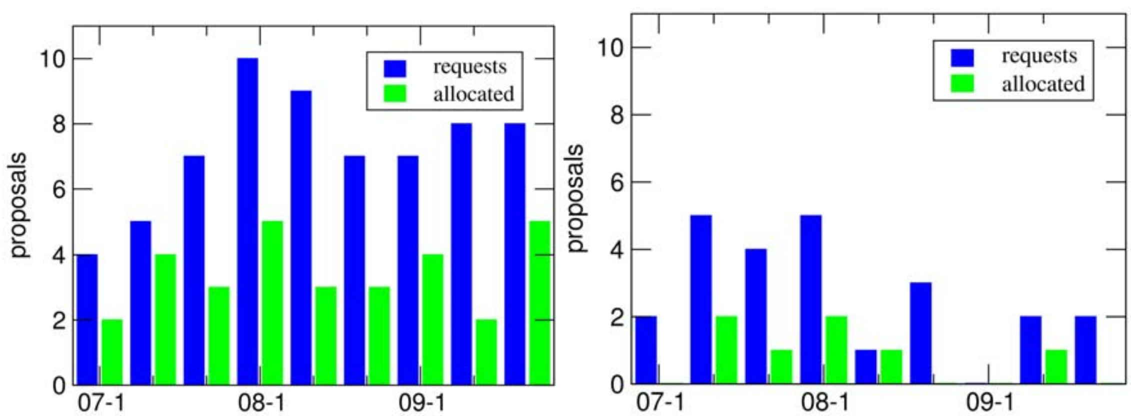

Figure 1: In the time period of 2007-2009 11 independent research groups from 10 COMPRES member institutions submitted 59 proposals to 3-ID and 22 proposals to 30-ID. Of these proposals, 28 (=47%) and 7 (=32%) were granted beam time at 3-ID and 30-ID, respectively.

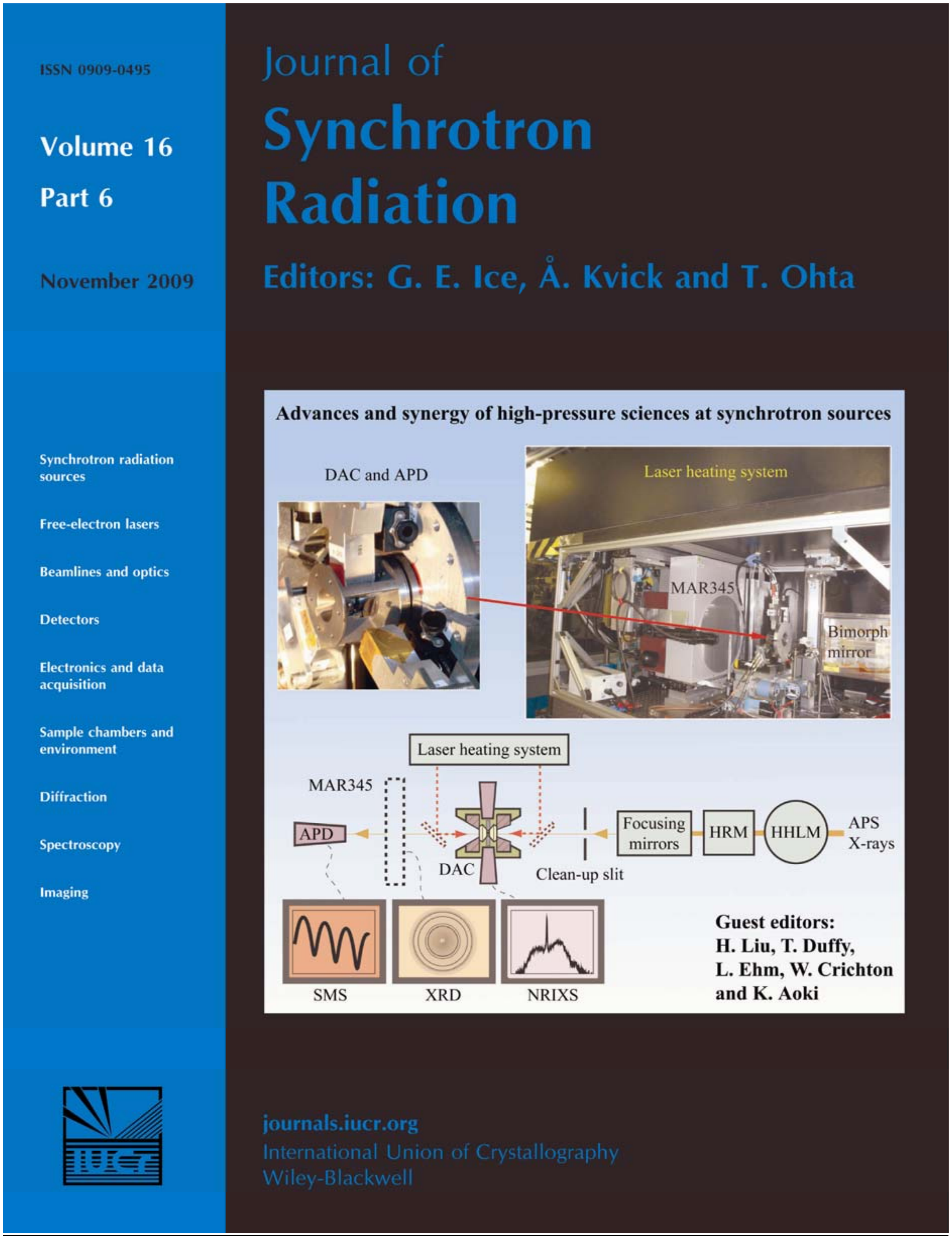

Figure 2: The cover of the November 2009 issue of the Journal of Synchrotron Radiation features the achievements of the present COMPRES ID projects

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

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

2009 Annual Report for gas-loading system at GSECARS
November 2008-November 2009

Progress Report

The COMPRES 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 50 users to load many hundreds of cells. The system works extremely well, with the only significant problems being some failures of the commercial compressor. We have in-house technical support (Guy Macha) to repair such problems, and the mean time to repair has typically been 1 day.

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

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

This COMPRES project is intended to fund 50% of a post-doc to reside at the APS. This person will 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.

We have interviewed 3 prospective candidates for this position since receiving this funding from COMPRES. Unfortunately these candidates have all either accepted positions elsewhere or were not found qualified for the position. None of the funds received to date have been expended. We have several new candidates in mind, and will be arranging interviews in the near future.

This new infrastructure project was funded in Year #2 at $37K. To date [Feb 2010], a suitable candidate for the postdoc has not been found. We propose to continue this ID project in Year #3, but will not allocated any new funds unless a postdoc is hired prior to June 1, 2010.

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

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

New Infrastructure Development Project

We propose to establish a facility for comprehensive characterization of melt/liquid properties, allowing users to study structure (by x-ray diffraction), density (by absorption measurements), elasticity (by ultrasonic interferometry), and viscosity (by radiographic imaging) at high pressure and temperature. This proposal is based on the extensive development at GSECARS and HPCAT in the past two years. A new Paris-Edinburgh (PE) press with pressure control system has been constructed and tested to 10 GPa and 2000 K. HPCAT has developed x-ray instrumentation at 16-BM-B equipped with a large Huber circle for accurate two-theta control using a solid-state detector, allowing angular scans to a maximum two theta of 37°. The PE system has been successfully operated in this station, with a very large coverage in Q ($=2\pi\sin\theta/\lambda$). Preliminary experiments, based on multiple-angle energy-dispersive diffraction, showed that intensities with Q up to 20 $Å^{-1}$ are usable; with further optimization in beamline optics, a greater Q range up to 35 $Å^{-1}$ is expected. Ultrasonic measurements on melts are planned in the end of Oct, 2009, using the Tektronix acoustic interferometer available at GSECARS. With these developments well underway, we seek modest fund from COMPRES to complete the system and to promote the facility to the COMPRES community. Our goal is to develop a portable system, which can be used at 16-BM-B and 16-BM-D at HPCAT and 13-BM-D at GSECARS. These three stations are complimentary: 16-BM-B is a white beam station, ideal for structural studies; both 13-BM-D and 16-BM-D have monochromatic capability, best suited for absorption-based density measurements. Ultrasonic and radiographic measurements can be carried out at all stations. 16-BM-B will offer up to 50% of the total available beam time to this technique, and time available at 13-BM-D and 16-BM-D may be up to 15%. We plan to complete the system in two years and hold a hands-on workshop at the end of the second year. With significant investment already devoted from GSECARS and HPCAT, we believe this project is extremely cost-effective for the COMPRES community.

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

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

New Infrastructure Development Project

Mössbauer Spectroscopy (MS) is a well-established method to study minerals at ambient and extreme conditions of temperature, pressure, and magnetic field. The laboratory of Ercan Alp and Wolfgang Sturhahn is located at the Advanced Photon Source building in a dedicated, appropriate room at Argonne National Laboratory.

Alp and Sturhahn propose to expand and enhance the existing off-line Mössbauer spectroscopy laboratory at the Advanced Photon Source to accommodate high-pressure experiments. Currently, experiments involving Fe, Sn, Eu and Sb can be conducted at the laboratory. More recently, in collaboration with Jie Li, a "point" 57Co radioactive sealed source was purchased to test the feasibility of Mössbauer measurements inside a diamond-anvil cell.

Mössbauer spectroscopy can be used for the following purposes:

1. Determination of abundance of different mineral phases by analysis of the spectra, based on models derived from previous measurements and crystal structures;

2. Behaviors of materials under pressure as a function of temperature and external magnetic field for better characterization of mineral phases that may have overlapping spectral lines;

3. Identification of crystalline and amorphous or glassy phases.

Our laboratory has been receiving requests from the high-pressure community who first come into contact with us through the beamline related activities. We realize that many of sample characterization needs can be addressed at the Mossbauer laboratory, without the need for waiting synchrotron beamtime. In order to facilitate some of their requests, we recently (2008) obtained a 10mCi ^{57}Co radioactive source in the form of "point" geometry. We have demonstrated that it is possible to obtain Mossbauer spectra from small samples inside the DAC. However, for isotopically un-enriched samples or for very small samples with dilute iron concentration data acquisition times can exceed a month, tying up the existing spectrometer. So to facilitate data acquisition for earth science users, we propose to purchase a dedicated new spectrometer, a new radioactive source, special set-up for DAC mounting, and a few perforated diamonds. The last item is needed to minimize the absorption of 14.4 keV gamma-rays (A 2 mm thick diamond anvil reduces the transmitted intensity by one half).

C.6 Workshop Proposals for Year #4 of COMPRES II

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

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

COMPRES Summer School in High Pressure Research

Stony Brook University - Brookhaven National Laboratory

Earth Materials at high pressure and temperature
One week in August 2010
at Brookhaven National Laboratory

Organizer:
Lars Ehm
lars.ehm@stonybrook.edu
National Synchrotron Light Source
Brookhaven National Laboratory
&
Mineral Physics Institute
Stony Brook University
1

<u>Scope and goals of the summer school</u>

Recent developments in synchrotron radiation based techniques for the *in-situ* investigation of atomic structure and properties of earth materials at high pressure and temperature have lead to a deeper understanding of the structure, composition and properties of Planet interiors. Many of the groundbreaking technique developments have been initiated by members of the Mineral Physics community. COMPRES has been a major facilitator in the advancement of synchrotron based techniques. Alone at the National Synchrotron Light Source (NSLS) four dedicated high-pressure endstations are currently supported by COMPRES. These facilities provide a wide range of high-pressure techniques for the user community, including X-ray diffraction in diamond anvil cells and large volume presses, imaging, ultrasonic interferometry, and infrared spectroscopy capabilities.

Currently, substantial upgrades are planed for existing 3rd generation synchrotron sources,such as the Advanced Photon Source (APS) in the USA and the European SynchrotronRadiation Facility (ESRF) in France. Furthermore, next generation synchrotron sourceswith enhanced beam characteristics, such as NSLS-II and PETRA-III, are already underdesign or in construction. These new or upgraded sources will provide enhancedexperimental capabilities for the Mineral Physics community and will lead to a surge of new discoveries.

The next generation of scientists will play a crucial role in exploding these new experimental capabilities in their research program. Therefore, it should be paramount to train the current generation of undergraduate, graduate students and postdoctoral scholars in the use of synchrotron based techniques for their research, in order to grow the user community for the future and currently operating synchrotron radiation sources. Furthermore, workshops and summer schools are an important part of professional developments of young researchers and a great networking opportunity.

The goal of the school is to attract participants from research groups that don't already have a well established synchrotron based Mineral Physics program. Therefore, the summer school program will cover a broad range of experimental high-pressure techniques available at the COMPRES supported beamlines at the NSLS, instead of an in-depth introduction of one particular experimental method. The lectures and hand-on experiments will lay a foundation for the participant, which will enable them to perform experiments at synchrotron beamlines and evaluate the collected data.

Agenda

The summer school will be organized as a five day event with lectures in the morning and hands-on experiments at the COMPRES supported beamlines at NSLS during the afternoon. The emphasis of the school is to transfer the fundamental knowledge on how to conduct a high pressure experiment at a synchrotron radiation source and evaluate the collected data.

The following topics will be covered during the school:

- Preparation and handling of diamond anvil cells
- Preparation and handling of large volume presses
- Data analysis of high pressure diffraction data
- Stress-Strain measurements
- Single crystal diffraction at high pressure
- Measurement of properties such as sound velocities, resistance etc.
- Heating in diamond anvil cells and large volume presses

Participants and Lectures

The school will be restricted to a maximum number of 20 participant due focus on handson experience. Besides the established high pressure groups in the United States, effort will be made to reach out to groups in the Earth and Planetary science community that currently don't belong to the frequent users of the high pressure instruments at synchrotron sources. Preference will be given to undergraduate, graduate student and post -doctoral scholars.

Lectures in the morning by experts in the field of high pressure research followed byhands-on activities at the NSLS beamlines, including those supported by COMPRES at X17B2,, X17B3, X17C, and U2A.

Instructors at the Beamlines

The hands-on part of the workshop will be lead by the beamline staff at participating beamline. It is expected that the lecturers will participate as instructors during the hands on experiments as well.

D Budget Request for Year #3 of COMPRES II [June 1, 2010 to May 31, 2011]

All numbers in $K

D.1 Community Facilities-operational budgets

$219	for ops	West Coast Synchrotron Facilities [Q. Williams and J. Bass]
$292	for ops	X-ray Diamond-anvil cell facilities at the NSLS [T. Duffy and D. Weidner]
$54	for equip	[Ops funds includes $42K to Princeton and $250K to Stony Brook]
$203	for ops	Infrared Diamond-anvil facilities at the NSLS [R. Hemley and Z. Liu]
$50	for equip	
$377	for ops	Multi-anvil X-ray Facility at the NSLS [D. Weidner and M.Vaughan]
$70		Beamline user housing
$44		Subawards IDC
$1135	for ops	Total operational budget for Community Facilities
$104	for equip	See details above

D.2 Infrastructure Development Projects

$73	Nuclear Resonant Scattering at High P & T:A New Capability for the COMPRES Community [W. Sturhahn, J. Jackson, and J. Bass]
$90	Multi-anvil Cell Assembly Initiative: New Developments and Production [K. Leinenweber, T. Sharp, and J. Tyburczy]
$0	Postdoc for Gas-Loading system at GSECARS [M. Rivers]
$37	Portable Paris-Edinburgh Cell for APS [G. Shen and Y. Wang]
$42	Mössbauer Spectroscopy at the APS [E. Alp]
$100	Workshops (5 to 7 per year)
$0	Subawards IDC
$342	Total for Infrastructure Development projects

D.3 Other COMPRES Activities

$345		**Other Community Activities** which includes
	$150	Annual Meeting
	$40	Travel for committees
	$10	COMPRES lecture series
	$65	Contingencies [early hires, salary adjustments]
$474		**Central Office** which includes: [all items have indirect costs incorporated]
	$410	Salaries and fringe benefits
	$40	Materials and Supplies
	$24	Travel
$919		Total for Other COMPRES Activities

TOTAL BUDGET REQUEST FOR YEAR #4 OF COMPRES II

$1135	**Operational costs for Community Facilities**
$104	**Equipment upgrades for facilities**
$342	**Infrastructure Development Projects**
$345	**Other Community activities**
$474	**Central Office**
$2400K	**Total of budget request**

E. Detailed Original Signed Budgets on NSF 1030 forms and Budget Justifications
For COMPRES Budget Request for Year #4 [June 1, 2010 to May 31, 2011]

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F. Supplemental Information

Figure 1. Attendees at On-line Brilouin Spectroscopy Workshop at GSECARS of the APS, Sept 23-25, 2009. Conveners: V. Prakapenka, Stanislav Sinogeikin and Jay Bass.

Figure 2. Visit by Bob Liebermann to diamond-anvil cell laboratory of Jennifer Jackson at Caltech, February 2009.

Figure 3. Junfeng Zhang [China University of Geosciences in Wuhan] in laboratory of Larissa Dobrezhenitskaya and Harry Green at UC Riverside, during visit by Bob Liebermann in February 2009.

Figure 4. Marc Hirschmann from University of Minnesota lecturing on "Deep Earth Volatiles" at Long-Range Planning Workshop in Tempe, Arizona, in March 2009.

Figure 5. Graduate students from throughout Japan at Hiroshima University for series of tutorial lectures on mineral physics by Bob Liebermann in March 2009.

Figure 6. Dave Mogk from Montana State University demonstrating the new module on "Teaching Mineral Physics across the Curriculum" to Joseph Smyth, Thomas Sharp and James Tyburczy at 2009 Annual Meeting of COMPRES in Bretton Woods, New Hampshire.

Figure 7. Lara O'Dwyer [UC Davis] presenting her poster at 2009 Annual Meeting of COMPRES in Bretton Woods, New Hampshire.

Figure 8. Hans-Joachim Mueller showing Bob Liebermann to the DIA-type guideblock in the MAX-200X at the DESY Synchrotron in Hamburg, Germany in September 2009.

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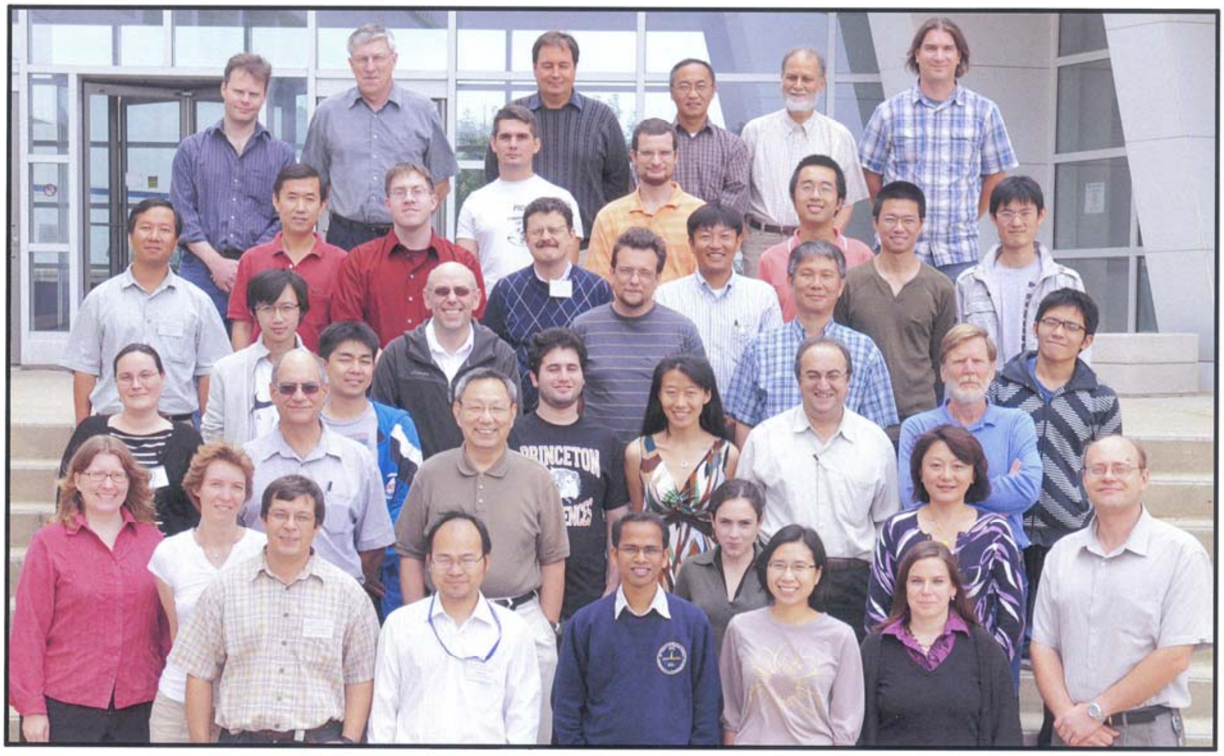

On-line Brillouin Spectroscopy at GSECARS: Basic Principles and Application for High Pressure Research
GSECARS, Advanced Photon Source
September 23-25, 2009

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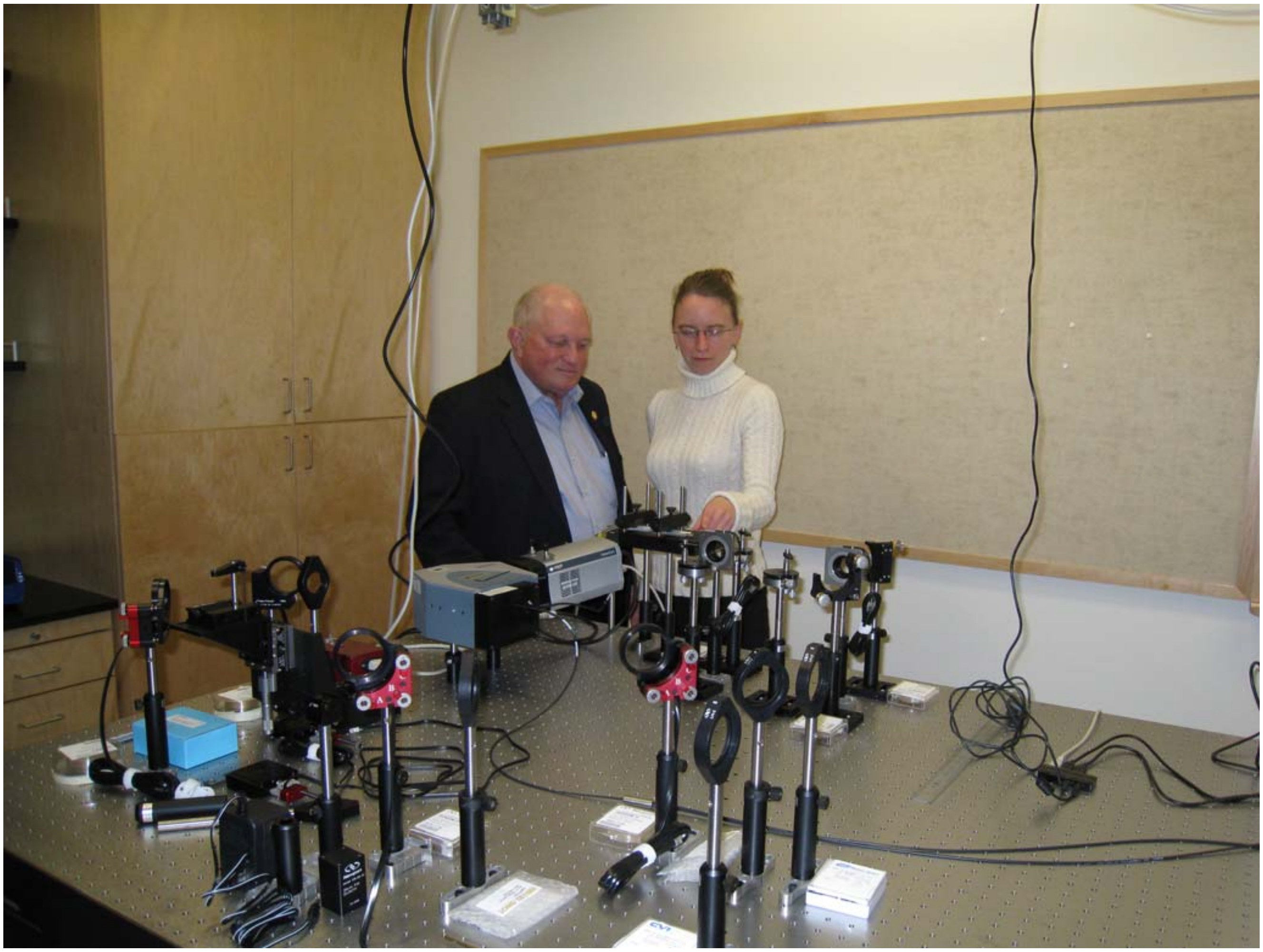

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