Year 1 Annual Progress Report of the Consortium for Materials Properties Research in Earth Sciences (COMPRES) for

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

1 March 2008



2007 Annual Meeting of COMPRES at Lake Morey Resort in Vermont.

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Section

A COMPRES Year 1: Overview

A.1 Executive Summary

In 2007, 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 51 U. S. institutions which are voting members of COMPRES [the Electorate] and another 31 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 for funding of COMPRES as follows:

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

In this section of the Annual Report for Year #4, we present an overview of the activities of COMPRES. Subsequent sections include detailed reports from each of the Community Facilities operations and Infrastructure Development projects supported by COMPRES. The final section presents the budget plan for Year #2 [June 1, 2008 to May 31, 2009]; detailed budgets and justifications are given in the appendices to this report.

A.2 Research Accomplishments

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

- A new gas-loading system for diamond-anvil cells has been constructed and commissioned with COMPRES support at the GSECARS facilities at the APS by Mark Rivers and his team. The system is now "open for business" and several investigators have already taken advantage of it. See Section C.3.
- A team from Jie Li's laboratory at the University of Illinois at Urbana-Champaign has conducted experiments at beamline X17C of the NSLS on the thermal expansion of iron-rich alloys, with implications for the behavior of the Earth's core. See Chen et al. in Section B.1.
- The research team of Rod Ewing at the University of Michigan has performed experiments at beamline X17C of the NSLS which show dramatically different behaviors between isostructural pyrochlore materials at high pressures. See Zhang et al. in Section B.1.
- A Brillouin spectroscopy system developed by Jay Bass and his team at the University of Illinois at Urbana-Champaign has been installed and commissioned on the 13 BM beamline at the GSECARS sectors of the APS. Initial experiments include work on the post-stishovite phase transition in hydrous alumina-bearing SiO₂ by D. Lakshtanov and colleagues. See Section C.3.
- The team of Larissa Dobrzhinetskaya and Harry Green at UC Riverside has examined the occurrence of water in microdiamons from subduction zones using the infrared facilities at the beamline U2A of the NSLS. See Section B.2.
- The theoretically predicted high to low spin transition of Fe in magnesiowustite has been confirmed and the associated volume change measured as a function of pressure and composition in experiments performed at beamline 12.2.2 of the ALS by the team of Raymond Jeanloz at UC Berkeley. See Speziale et al.. in Section B.4.
- Single crystal studies by a team led by Paul Raterron of the Universite Lille in France demonstrate a pressure induced change in slip systems in olivine undergoing deformation in the D-DIA apparatus at high pressure and temperature. See Section B.3.
- A fully functional monochromatic side-station running simultaneously with the main energy-dispersive station at the X17B2 beamline at the NSLS has been installed and commissioned in 2007 by a team led by Jiuhua Chen (now of Florida International University). The side-station at beamline X17B2 of the NSLS not

only doubles the beamtime for high pressure experiments but also broadens the experimental capacity for different measurements.

• A customized cell consisting of a mullite sphere and pyrophyllite cradles for D-DIA apparatus was fabricated in multi-anvil cell development program at the Arizona State University by Kurt Leinenweber and colleagues for deformation experiments at the X17B2 beamline of the NSLS. See Section C.3 and photo in Supplementary Documents for this report.

A.3 Meetings and Workshops

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

Workshop on Current Status and Prospects for Establishing Precise and Accurate **Pressure Scales at High Temperatures**

January 26-28, 2007 Geophysical Laboratory of the Carnegie Institution of Washington. **Organizing committee:** Alexander Goncharov, Geophysical Laboratory Kurt Leinenweber, Arizona State University Tom Duffy, *Princeton University* Russell Hemley, Geophysical Laboratory Yingwei Fei, Geophysical Laboratory

Workshop on Calorimetry-on-a-Chip

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

Fourth Biennial Conference of CeSMEC

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

7th High Pressure Mineral Physics Seminar (HPMPS-7)

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

Sendai) May 8 to 12, 2007.

Gordon Conference on Earth's Interior

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

Sixth Annual Meeting of COMPRES

June 17-20, 2007

Lake Morey Resort, Vermont

Program Committee: Michael Brown, Jennifer Jackson, Boris Kiefer, Sara Gaudio, Lara O'Dwyer

There were 102 registered participants and many accompanying persons to enjoy this splendid site. One of the new features was a set of keynote talks focused on the mantle, geochemical evolution and the core, with speakers for each topic from both within and outside the mineral physics community. The social events of the meeting were underwritten by 9 industrial sponsors: Almax, Blake Industries, Bruker AXS, D'Anvils, Depths of the Earth, Foxwood Instruments, Rigaku MSCHKL, Rockland Research and Technodiamant. Additional details of the Annual Meeting may be found in the July issue of the COMPRES newsletter and at:

http://www.compres.stonybrook.edu/Meetings/2007 Annual Meeting/index.htm

The Second VLab Workshop

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

International Workshop on Synchrotron High-pressure Mineral Physics and Materials Science

December 6-7, 2007 Advanced Photon Source, Argonne National Laboratory, Chicago Organizers: Tetsuo Irifune-GRC, Ehime University (Japan) and Yanbin Wang-GSECARS, University of Chicago.



Attendees at 2007 Annual Meeting of COMPRES at Lake Morey Resort in Fairlee, Vermont on June 17-20, 2007

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 2007, there were 50 U. S. institutions which were members of COMPRES and 27 affiliate institutions overseas. In the past year, one U. S. institution has become a member of COMPRES:

University of Michigan

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

Universite Paul Sabatier in Toulouse, France

Okayama University in Misasa, Japan.

Université Blaise Pascal in Clermont-Ferrand, France.

Harbin Institute of Technology in China.

This brings us to a total of 51 U. S. institutional members and 31 affiliated members of COMPRES. They are listed in the following table.

COMPRES US MEMBER INSTITUTIONS

Institution

Argonne National Laboratory Arizona State University Auburn University Azusa Pacific University California Institute of Technology Carnegie Institution of Washington Case Western Reserve University Colorado College Columbia University

Cornell University

Delaware State University

Florida International University Georgia State University Indiana University at South Bend Johnson Space Center, NASA Lawrence Berkeley National Laboratory Lawrence Livermore National Laboratory Los Alamos Natoional Laboratory Louisiana State University

Massachusetts Institute of Technology

New Mexico State University Northern Illinois University Northwestern University **Ohio State University** Princeton University Rensselaer Polytechnic Institute Stony Brook University Texas Tech University University of Arizona

University of California at Berkeley

Elector

Wolfgang Sturhahn Thomas Sharp Jianjun Dong **Donald Isaak** Paul Asimow **Ronald Cohen** James Van Orman Nancy Chabot Phillip Cervantes David Walker

William Bassett

Gabriel Gwanmesia Surendra Saxena Pamela Burnley Henry Scott Kevin Righter Simon Clark **Daniel Farber** Yusheng Zhao Bijaya Karki San-Heon (Dan) Shim Kanani Lee Mark Frank Steven Jacobsen Wendy Panero **Thomas Duffy** Anurag Sharma Michael Vaughan Yanzhang Ma Robert Downs Hans-Rudolph Wenk

Alternate

Marcos Grimsditch James Tyburczy

Jennifer Jackson Yingwei Fei

Taro Takahashi Donald

Bilderback

Al Sameen Khan

Jerry Hinnefeld John Jones **Corwin Booth**

Gary Chesnut

Robert van der Hilst Boris Kiefer Jonathan Berg **Craig Bina** Michael Barton **Guust Nolet** John Schroeder John Parise Valery Levitas Michael Drake **Raymond Jeanloz**

University of California at Davis	Charles Lesher	<u>Alexandra</u> <u>Navrotsky</u>
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	<u>Sofia Akber-</u> <u>Knutson</u>	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	<u>Murli Manghnani</u>	Li Chung Ming
University of Illinois at Urbana-Champaign	Jay Bass	Jie Li
University of Louisville	George Lager	
University of Maryland at College Park	Andrew Campbell	John Tossell
University of Michigan	Rebecca Lange	Youxue Zhang
University of Minnesota	<u>Renata</u> <u>Wentzcovitch</u>	David Kohlstedt
University of Missouri - Kansas City	Michael Kruger	Ray Coveney
University of Nevada at Las Vegas	Oliver Tschauner	Malcolm Nicol
University of New Mexico	Carl Agee	David Draper
University of Washington	Michael Brown	
University of Vermont	Tracy Rushmer	
University of Wyoming	David Anderson	
Virginia Polytechnic Institute and State University	Nancy Ross	Ross Angel
Yale University	Shun-ichiro Karato	David Bercovici

COMPRES FOREIGN AFFILLIATES

Australian National University Canberra (Australia)	<u>]</u>
Bayreuth Universitat (Germany)]
Chinese Academy of Science (China)	<u>(</u>
Ecole Normale Supérieure de Lyon (France)]
Ehime University (Japan)	2
Eidgenossische Techniche Hochschule Zurich (Switzerland)	4
GeoForschungsZentrum Potsdam (Germany)]
Harbin Institute of Technology (China)]
Institut de Physique du Globe Paris (France)	<u>(</u>
Institute of Experimental Mineralogy, Chernogolovka (Russia)	2

Hugh O'Neill David Rubie Changqing Jin Jan Matas Tetsuo Irifune Artem Oganov Frank Schilling Haozhe Liu Guillaume Fiquet Yuriy Litvin Johann Wolfgang Goethe Universitat Max-Planck Institute for Solid State Research, Stuttgart (Germany) National Cheng Kung University (Taiwan) Novosibirsk State University (Russia) Okayama University (Japan) Royal Institution of Great Britian, The (United Kingdom) Ruhr-Universitat Bochum (Germany) Seoul National University (Korea) Tohoku University, Sendai (Japan) Universitat Frankfurt AM Main (Germany) Universite Blaise Pascal (France) Universite de Poitiers (France) Universite des Science et Technologies de Lille (France) Universite Paul Sabatier (France) University College London (United Kingdom) University of Manchester (United Kingdom) University of Tokyo (Japan) University of Wales at Aberystwyth (United Kingdom) University of Western Ontario (Canada) Vrije Universiteit (The Netherlands) Yonsei University (Korea)

Jennifer Kung Elena Boldyreva Eiji Ito Paul McMillian Sumit Chakraborty Haemyeong Jung Eiji Ohtani **Bjorn Winkler Denis Andrault** Jacques Rabier Paul Raterron Jannick Ingrin David Dobson Alison Pawley Takehiko Yagi Martin Wilding Rick Secco

Bjorn Winkler

Paul Balog

<u>Wim van</u> <u>Westrenen</u> Yongjae Lee

A.5 Information Technology and Communications

Web Site

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

<u>http://www.compres.stonybrook.edu</u> server and are being maintained by Glenn Richard, Emily Vance, and Michael Vaughan. At present, the COMPRES site provides the following information:

A general overview of COMPRES

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

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

Annual Reports for NSF from Years #105 of COMPRES I [2002 to 2007]

COMPRES Booth Powerpoint presentation at December 2007 AGU

Minutes of the Executive Committee

Monthly Messages from COMPRES President

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

• The quarterly COMPRES Newsletters

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

[link at: http://www.compres.stonybrook.edu:8080/COMPRESImageLibrary/index.html]

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

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 and may be found on the COMPRES web site at <u>www.compres.us/Newsletter/</u>. See COMPRES Home Page for the latest issue for February 2008.

In addition to a column in the quarterly COMPRES newsletter, the President of COMPRES [Robert Liebermann] has sent a Monthly Message to the COMPRES community using the listserv distribution, beginning in October 2003 [see link at: http://www.compres.stonybrook.edu/Publications/Monthly%20Messages%20from%20C OMPRES%20President/Index.html]. The purpose of these monthly messages from the President is to keep the COMPRES community informed of recent developments as well as activities of the Executive and Standing Committees. These Monthly Messages are also sent to the Program Directors of the Division of Earth Sciences at the NSF.

COMPRES Exhibition Booth at Fall 2007 AGU Meeting

At the Fall 2007 Meeting of the American Geophysical Union in San Francisco in December 2007, COMPRES had a special booth in the Exhibition Area. This exhibition booth was jointly sponsored by GSECARS and COMPRES, and attracted lots of visitors.

Jiuhua Chen and Ann Lattimore created the materials for the booth based on input provided by the Community Facilities and Infrastructure Development projects. Glenn Richard and Michael Vaughan helped in staffing the booth, in cooperation with Nancy Lazarz and Mark Rivers of GSECARS.

A Powerpoint presentation created for the COMPRES Booth by Glenn Richard can be found on the COMPRES website.

A.6 Publications of COMPRES in 2006-2007

2006

- Aksoy, R. Y. M., E Selvi, Ming C. Chyu, Atila Ertas and Allen White (2006). Equation of state measurement of molybdenum disulfide. <u>J. Phys. Chem. Solids</u> 67: 1914-1917. X17 DAC
- Atkinson, T., K. Chynoweth, P. Cervantes, (2006). Electronic Band Gap of SrSe at High Pressure,. <u>Solid State Commun.</u> 139(215). U2A DAC
- Bud'ko, S. L. T. A. W., R. A. Ribeiro, P. C. Canfield, Y. Lee, T. Vogt and A. H. Lacerda (2006). Effect of pressure and chemical substitutions on the charge-density-wave in LaAgSb2. <u>Phys Rev, B</u> 73(184111). X17 DAC
- Campbell, A. J., L. Danielson, K. Righter, Y. Wang and G. Davidson (2006). Oxygen fugacity at high pressure: equations of state of metal-oxide pairs. <u>Lunar and</u> <u>Planetary Science XXXVII</u>. MAC ASU
- Carpenter, M. A. P. S., B. Li, R C. Liebermann, J.W. Walsh, J Schreuer, and T W. Darling (2006). Structural evolution, strain and elasticity of perovskitesat high pressures and temperatures. <u>Journal of Mineralogical and Petrological Sciences</u> **101**: 95-109. MAC NSLS
- Chen, J., L. Li, T. Yu, H. Long, D. Weidner, L. Wang and M. Vaughan (2006). Do Reuss and Voigt bounds really bound in high pressure rheology experiments? <u>Journal of Physics: Condensed Matter, special issue: Rheology and Elasticity studies at Ultra-High Pressures and Temperatures</u> 18 (25): S1049-S1059. MAC NSLS
- Cunningham, N. C. W. Q., and Y. K. Vohra (2006). Observation of complete regular trivalent rare earth sequence in heavy lanthanide metal holmium under high pressure. <u>High Pressure Research</u>, In Press **26**(**43**). X17 DAC
- Dobrzhinetskaya, L. F., Z. Liu, P. Cartigny, J. Zhang, D. Tchkhetia, R. J. Hemley and H. W. Green II (2006). Synchrotron infrared and Raman spectroscopy of microdiamonds from Erzgebirge, Germany. <u>Earth Planet Sci. Lett.</u>, submitted 248: 325-334. U2A DAC (X17 DAC)
- Gatta, G. D. Y. L. (2006). On the elastic behaviour of zeolite mordenite: a synchrotron powder diffraction study. <u>Phys Chem Minerals</u> **32**: 726-732. X17 DAC
- Gilbert, B., H. Zhang, B. Chen, M. Kunz, F. Huang and J. F. Banfield (2006). The Compressibility of Zinc Sulfide Nanoparticles, . Phys. Rev. B. ALS
- Gleason, A. E., S. Parry, M. Kunz, W. A. Caldwell, A. R. Pawley and S. M. Clark (2006). Pressure Temperature Stability Studies of Talc and 10-Å Phase using xray diffraction. <u>Am. Min. (in press)</u>. ALS
- Goncharov, A. F. a. R. J. H. (2006). Probing hydrogen-rich molecular systems at high pressures and temperatures, <u>Chem. Soc. Rev.</u> U2A DAC
- Gwanmesia, G. D., J. Zhang, K. Darling, J. Kung, B. Li, L. Wang, D. Neuville and R. C. Liebermann (2006). Elasticity of polycrystalline pyrope (Mg3Al2Si3O12) to 9
 GPa and 1000 oC. <u>Physics of the Earth and Planetary Interiors</u> 155: 179-190. MAC NSLS
- He, D. W. and T. S. Duffy (2006). Static strength of tungsten to 69 GPa. <u>Physical Review</u> <u>B, in press</u>. X17 DAC

- He, D. T. S. D. (2006). X-ray Diffraction Study of the Static Strength of tungsten to 69 GPa.). <u>Phys. Rev. B.</u> 73(13416). X17 DAC
- Hernlund, J., K. Leinenweber, D. Locke and J. A. Tyburczy (2006). A numerical model for steady-state temperature distributions in solid-medium high-pressure cell assemblies. <u>American Mineralogist</u> 91: 295-305. MAC ASU
- Higo, Y. T. I., B. Li, T. Irifune, and R C Liebermann (2006). The effect of iron on the elastic properties of ringwoodite at high pressure. <u>Phys. Earth Planet. Inter.</u> 159: 276-285. MAC NSLS
- Hu, J., H. Mao, J. Shu, Q. Guo and L. H (2006). Diamond Anvil Cell Radial X-ray Diffraction Program at the National Synchrotron Light Source. <u>J. Phys.: Condens.</u> <u>Matter.</u> 18: (S1091-S1096). X17 DAC
- Hu, J. H. M., J Shu, Q Guo, H Liu (2006). Diamond Anvil Cell Radial X-ray Diffraction Program at the National Synchrotron Light Source. <u>J. Phys.: Condens. Matter.</u> 18(S1091-S1096). X17 DAC
- Iezzi, G., Z. Liu and G. D. Ventura (2006). Synchrotron infrared spectroscopy of synthetic Na(NaMg)Mg5Si8O22(OH)2 up to 30 GPa: Insight on a new amphibole high pressure polymorph. <u>American Mineralogist</u> 91 (2-3): 479-482. U2A DAC (X17 DAC)
- Jiang, F., S. Speziale and T. S. Duffy (2006). Single-crystal elasticity of brucite, Mg(OH)2, to 15 GPa by Brillouin scattering. <u>American Mineralogist, in press.</u> X17 DAC
- Jiang, F., S. Speziale, and T. S. Duffy (2006). Single-crystal elasticity of brucite, Mg(OH)2, to 15 GPa by Brillouin scattering. <u>American Mineralogist</u> 91: 1893-1900. X17 DAC
- Klug, D., J. Tse, Z. Liu and R. Hemley (2006). Infrared Absorption and first-Principles Study of Hydrogen-Bond Symmetrization in Methane Filled Ice. J. Chem. Phys., submitted. U2A DAC
- Klug, D. D., J. Tse, Z. Liu, R. Hemley, (2006). Hydrogen-bond Dynamics and Fermi Resonance in High-pressure Methane Filled Ice,). J. Chem. Phys. 125(154509). U2A DAC
- Kung, J., B. Li and R. Liebermann (2006). Ultrasonic Observations of Elasticity Changes across Phase Transformations in MgSiO3 Pyroxenes. <u>Journal of Physics and Chemistry of Solids</u> 67: 2051-2055. MAC NSLS
- Lee, K. K. M., O. Tschauner and P. D. Asimow (2006). Phase Assemblage and stability of pyroxenite at Lower-Mantle conditions. ALS
- Lee, Y. J. H., J. Parise and T. Vogt (2006). Pressure-induced hydration in zeolite tetranatrolite. <u>American Mineralogist</u> **91**: 247-251. X17 DAC
- Leinenweber, K., J. Mosenfelder, T. Diedrich, E. Soignard, T. Sharp, J. Tyburczy and Y. Wang (2006). High-pressure cells for in-situ multi-anvil experiments. <u>High</u> <u>Pressure Research.</u> MAC ASU
- Levitas, V. Y. Z. M., and J Hashemi, M Holtz and N Guven (2006). Strain-induced disorder, phase transformations and TRIP in hexagonal boron nitride under compression and shear in a rotational diamond anvil cell: in-situ X-ray diffraction study and modeling. J. Chem. Phys., 25(044507): 1-14. X17 DAC
- Li, B. (2006). Elasticity of Ringwoodite at high P and T. Geophys. Res. Lett. In press. MAC NSLS

- Li, L., D. Weidner, P. Raterron, J. Chen, M. Vaughan, S. Mei and W. Durham (2006). Deformation of olivine at mantle pressure using the D-DIA. <u>European Journal of</u> <u>Mineralogy</u> 18(1): 7-19. MAC NSLS
- Li, B. K. W., and J. Kung (2006). Elasticity of MgO to 11 GPa with an independent absolute pressure scale: Implications for pressure calibration. <u>J. Geophys. Res.</u> 111(B11206). MAC NSLS
- Li, L. L., H., Weidner, D.J. and Raterron, P. (2006). Plastic flow of pyrope at mantle pressure and temperature. <u>American Mineralogist</u> **91**: 517-525. MAC NSLS
- Lin, J. F., A. G. Gavriliuk, V. Struzhkin, S. D. Jacobsen, W. Sturhahn, M. Y. Hu, P. Chow and C. S. Yoo (2006). Pressure-induced electronic spin transition of iron in magnesiowustite-(Mg,Fe)O. <u>Phys. Rev. B</u> 73(113107). Nuclear Resonant
- Liu, H., H.-R. Wenk, and T. S. Duffy (2006). Rheology and elasticity studies at ultrahigh pressures, preface to special issue. <u>Journal of Physics: Condensed Matter</u>, **18**(25), June 28, 2006. X17 DAC
- Liu, W. a. B. L. (2006). Thermoelasticity of olivine to 8 GPa 1073K. <u>Phys. Earth. Planet.</u> <u>Inter.</u> **157**: 188-195. MAC NSLS
- Lufaso, M. W. R. B. M., Y. Lee, T. Vogt and H. Loye (2006). Pressure induced octahedral tilting distortion in Ba2YTaO6. <u>Chem. Commun</u> 168: 168-170. X17 DAC
- Lufaso, M. W. G., S Mugavero, Y Lee, T Vogt, H zur Loye (2006). Compression mechanisms of symmetric and Jahn-Teller distorted octahedra in double perovskites: A2CuWO6 (A ¹/₄ Sr, Ba), Sr2CoMoO6, and La2LiRuO6. J. Solid State Chem.. **179**: 3571-3576. X17 DAC
- Ma, Y., E. Selvi, V. Levitas and H. J (2006). Effect of Shear Strain on the ?-? Phase Transition of Iron: a New Approach in the Rotational Diamond Anvil Cell. . <u>J.</u> <u>Phys.: Condens. Matter.</u> **18:** (1075). 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.

In order to advance the practice of using digital tools to work with real Earth systems data, COMPRES is promoting the use of geographic information systems (GIS) and other data analysis tools in educational settings. At Stony Brook University, Glenn Richard has served as one of the instructors for an undergraduate field methods course in which students collect and map their own field data. During the spring, 2006 semester, he is co-teaching a group of undergraduate students who are studying Long Island's Carmans River using geospatial tools and chemical testing equipment in order to investigate anthropogenic effects on the river.

COMPRES collaborates with the Department of Geosciences and the Department of Technology and Society at Stony Brook to offer students of the Brentwood School District an Honors Earth Science program modeled after Stony Brook's introductory environmental geology undergraduate course. During the summers, about 15 students from Brentwood engage in a four week residential program, emphasizing scientific methodology, research techniques and data collection in the field. During the following academic year, students work in teams to conduct research projects.

COMPRES, the Department of Geosciences, the Department of Technology and Society, and the Center for Environmental Molecular Science at Stony Brook collaborate to offer an honors Earth science course to students at Sayville High School, equivalent to Stony Brook's undergraduate introduction to physical geology. During the first year of the program, which runs over a two year cycle, lecture and laboratory components of the undergraduate course are incorporated into the honors course at Sayville. During the second year students complete a major research project that is carried out over the duration of the academic year.

Educational networks need to leverage their resources by working with teachers in order to reach large numbers of students. CEN 514: Long Island Geology is a professional development-level course designed for teachers, offered each fall, that explores processes that have governed the geological development of Long Island and other parts of New York State. Topics include mantle processes and their relation to plate tectonics, the tectonic history of New York State, local seismicity, the origin of local rocks, and a brief overview of current research in mineral physics and its relation to processes that have played a role in the geologic history of New York.

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 initiative for 2008-2009

COMPRES is requesting \$6,000 in funds to support a lecture series. This would be based on the successful models of other organizations, such as the Mineralogical Society of America.

We propose 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 would be provided by COMPRES, and local subsistence expenses would be provided by the host institutions [to be chosen on the basis of applications in response to ads in EOS and on the COMPRES website]. On the basis of 2 lecturers and 4 lecture visits each @\$500 per visit, plus advertising costs and logistics, we estimate \$6,000 for the first year of this new initiative.

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 nonvoting member.

A statement of the Polices and Procedures for the COMPRES Executive Committee can be found at: <u>http://www.compres.stonybrook.edu/People/Committees/ExComm%20Pol%20&%20Pro</u>

c-revised%2010%20June%202004.doc

Current members and affiliation (term of service)

Quentin Williams, **Chair** University of California at Santa Cruz (2007-2010) Carl Agee, University of New Mexico (2007-2010) Jay Bass, University of Illinois at Urbana-Champaign (2006-2009) Michael Brown, **Vice Chair** University of Washington (2005-2008) Donald Weidner, Stony Brook University (2007-2010)

Facilities Committee

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

A statement of the Polices and Procedures for the COMPRES Facilities Committee can be found at: <u>http://www.compres.stonybrook.edu/People/Committees/4%20June%202004%20Pol%2</u> <u>0and%20Proc--Fac%20Comm.doc</u>

Current members and affiliation (term of service)

Thomas Duffy, **Chair**, Princeton University (2007-2010) Charles Lesher, University of California at Davis (2006-2009) William Durham, Massachusetts Institute of Technology (2005-2008)

Wendy Panero, Ohio State University (2006-2009) Mark Rivers, University of Chicago (2005-2008)

Infrastructure Development Committee

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

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

ucture%20Development%20Comm--

Policies%20and%20Procedures%204%20June%202004.doc

Current Members and affiliation (term of service)

Nancy Ross Chair, Virginia Polytechnic Institute and State University (2006-2009) Pamela Burnley, University of Nevada at Las Vegas (2005-2008) Russell Hemley, Carnegie Institution of Washington (2005-2008) Thomas Sharp, Arizona State University (2006-2009) Sang-Heon Dan Shim, Massachusetts Institute of Technology (2007-2010)

Advisory Council

Members and affiliation (term of service) Bruce Buffett, University of Chicago (2002-2007) Wang-ping Chen, University of Illinois at Urbana-Champaign [2006-2009] Chi-Chang Kao, Brookhaven National Laboratory [2003-2008] Louise Kellogg, University of California at Davis [2007-2010] Guy Masters, University of California at San Diego [2003-2008] William McDonough, University of Maryland [2007-2010] Malcolm Nicol, University of Nevada at Las Vegas [2006-2009] Richard O'Connell, Harvard University (2002-2007)

On 19 June 2007, the Advisory Committee met with the Executive Committee just prior to the start of the Sixth Annual COMPRES Meeting in Lake Morey, Vermont. The terms of two of the founding members of the Advisory Council ended at Lake Morey: Bruce Buffett and Rick O'Connell. We especially wish to thank them for their service during the formative years of COMPRES and hope that they will feel welcome to attend future annual meetings of our community.

Finally, we would like to welcome two new members of the Advisory Council for three-year terms commencing June 2007:

Louise Kellogg from UC Davis

and

William McDonough from the University of Maryland.

Relationship to National Facilities

- GSECARS: COMPRES will review the high pressure facilities and assure highest service to the user community.
- NSLS: COMPRES funds Multi-anvil and Diamond-anvil facilities at NSLS. COMPRES will review the high pressure facilities and assure highest service to the user community.
- ALS: COMPRES funds Diamond-anvil facilities at ALS. COMPRES will review the high pressure facilities and assure highest service to the user community.
- ORNL: The COMPRES community has succeeded in obtaining DOE funding to build a high pressure facility at the Spallation Neutron Source that is now under construction. COMPRES will work to build the user community and assure access to this facility.

Operation of the COMPRES Central Office

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

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

The administrative operation of COMPRES is also supported by the following personnel who are employees of the Mineral Physics Institute of Stony Brook University: Jiuhua Chen, Research Associate Professor. COMPRES role: Editor of Newsletter 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.

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

Special Committee on Incorporation of COMPRES

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

The committee concluded that there were no compelling reasons for COMPRES to incorporate at this time, but that COMPRES should reevaluate the incorporation issue periodically, especially if one or

more of the following changes occur:

(1) There is an increase in its scientific advising or lobbying activities in Washington DC.

(2) COMPRES is funded by multiple agencies. At present, all of COMPRES funding comes from the NSF EAR division.

(3) The COMPRES constituency requests that the organization not be tied to a home institution.

A.9 President's Narrative

2007 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.

On November 30, The Program Directors from the Division of Earth Sciences led a Site Visit from Instrumentation and Facilities Panel to the NSLS at Brookhaven, as part of the review of the proposal from COMPRES for renewed funding in the period 2007-2012. Nineteen members of our community represented COMPRES at the Site Visit. The oral presentations included introductory remarks by Bob Liebermann, a talk on the partnership of COMPRES and the NSLS by Chi-chang Kao [Director of NSLS and a member of the Advisory Committee of COMPRES], an overview of the program plans for COMPRES by Harry Green, and talks by representatives of the major users of COMPRES facilities [David Walker], leaders of infrastructure development projects [both current and future, Kurt Leinenweber and Ho-kwang Mao. The Panel and the Program Directors of EAR will also have tours of the beamlines at the NSLS operated with support from COMPRES led by Russell Hemley, Jiuhua Chen and Don Weidner, as well as a "virtual tour" of the high-pressure facilities at the ALS led by Simon Clark.

Congratulations to Hans-Rudolf [Rudi] Wenk and his colleagues for organizing the very successful "MSA Workshop on Neutron Scattering in the Earth Sciences," which was held in Emeryville, California from Dec 7-9, 2006. Details of this Workshop can be found at: <u>http://www.minsocam.org/MSA/RIM/Rim63.html</u>. COMPRES provided travel support for graduate student attendees to this Workshop

On January 26-28, 2007, I attended a COMPRES sponsored a "Workshop on the Current Status and Prospects for Establishing Precise and Accurate Pressure Scales at High Temperatures." This Workshop was convened by Alex Goncharov, Kurt Leinenweber, Tom Duffy, Rus Hemley, and Yingwei Fei and included more than 50 attendees from around the world.

From March 21 to April 1, I was in France for two events:

Visiting the laboratories at the Institut de Minéralogie et de Physique des Milieux Condensés in their new location at Boucicaut in southwest Paris on March 22-23. I gave a seminar on « Indoor Seismology » and discussed research projects with Guillaume Fiquet, James (Jimi) Badro, François Guyot, Frederic Decremps, Stefan Klotz and Michel Gauthier.

Attend the First EuroMinSci Conference in La Colle-sur-Loup near Nice in the south of France from March 26-29. This conference was convened by Bjorn Winkler of Universität Frankfurt and brought together faculty, staff and students from many countries in Europe who are engaged in the new European Mineral Sciences initiative, a 4-year collaborative research program supported by the

European Collaborative Research Scheme [EUROCORES] of the European Science Foundation [ESF]. I gave the opening keynote talk on "Outdoor vs Indoor Geophysics." Other keynoters included H-k. (Dave) Mao of the Carnegie Institution of Washington.

On April 19, I was at Delaware State University in Dover to help honor Gabriel Gwanmesia, who was recognized for his research and educational achievements by an Innnovative Technologies Breakfast sponsored by the Central Delaware Economic Development Council and the Delaware Economic Development Office, and Delaware State University.

On April 25, the Executive Committee of COMPRES visited NSF Headquarters to meet with Program Directors of the Division of Earth Sciences and the Department of Energy to discuss the current status of funding and future strategic initiatives for COMPRES.

On 8-13 May 2007, the High Pressure Mineral Physics Seminar-7 was held in Matsushima, Japan. Eiji Ohtani of Tohoku University in Sendai and his colleagues organized and executed a very successful meeting, both on a scientific and social level. Michael Brown of the University of Washington and Yanbin Wang of the University of Chicago served as the US conveners and Denis Andrault of Université Blaise Pascal in Clermont-Ferrand and David Rubie of the Bayerisches Geoinstitüt served as the European conveners.

As you may recall, this Seminar was the 7th in a series which dates back to 1976, when it was supported by the US-Japan cooperative program of the NSF International Program office. Although it is a continuation of that tradition, it has taken on a new flavor in the past two occurrences, the 2002 Seminar in Verbania, Italy, and the 2007 Seminar in Matsushima, Japan. It is now truly international, with strong contingents from Europe, Japan and the U. S., as well as attendees from Taiwan, China, and Canada.

The 2007 meeting was attended by more than 140 people, including 31 from European countries and 91 from the host country Japan. The U. S. was represented by 23 scientists from academic institutions and national laboratories. Although there were no graduate students in the U. S. contingent, there were 10 young faculty/staff persons, many of whom had never been to Japan. Of these young scientists, 4 were women. COMPRES received \$35,000 in special fund from the Office of International Science Exchanges and the Divison of Earth Sciences at NSF to provide partial travel support fot the US contingent.

The attendees have expressed a strong desire to have the next Seminar in 2012 in the U. S., and we in COMPRES have issued an "Olympic-style" invitation to all. We are already working to identify conveners for this Seminar and searching for an attractive venue.

Following the HPMPS-7 meeting in Japan, I visited Taiwan for a week at the invitation of Jennifer Kung, now an Assistant Professor of Earth Sciences at the National Cheng Kung University in Tainan. In addition to visiting NCKU, I gave a seminar at the National Research Synchrotron Science Center in Hsinchu at the invitation of Qong Cai, and participated in a Mineral Physics Special Session of the Taiwan Geosciences Assembly in Taoyuan convened by Professor Kung.

On June 10-12, I was an observer at a DOE Workshop on Basic Research Needs for Materials under Extreme Conditions at the invitation of Russell Hemley, one of the workshop co-conveners. I participated in the sessions on Thermomechanical Extremes co-chaired by Malcolm Nicol; Michael Brown was one of the members for this sub-panel.

The Gordon Reseach Conference on "Interior of the Earth" was held at Mount Holyoke College in Massachusetts from June 10-15, 2007, with Goran Ekstrom as Chair and Bruce Buffett as Vice Chair. More than 121 people attended, of whom 20 were from the mineral physics community. Of the 22 keynote lectures, 26% were presented by mineral physicists.

The Virtual Laboratory for Earth and Planetary Materials Studies [VLab] held its 2nd Workshop at the University of Minnesota on August 6-10, 2007 convened by Renata Wentzcovitch, PI of the VLab Project. In conjunction with this workshop, the members of the the Elasticity Grand Challenge of the COMPRES Initiative held a two-day meeting. Details of the program may be found on the website at: http://www.vlab.msi.umn.edu/events/secondworkshop.shtml.

On September 12-16, I attended a Seminar on Density, Temperature and Elastic Constants of Earth's Mantle at the Castle of Linderhof in the Bavarian Alps south of Munich. This seminar was convened by Hans-Peter Bunge, John Brodholt and Brian Kennett and sponsored by the Wilhelm and Else Heraeua Foundation. Invited lectures were presented by representatives of the seismology, mineral physics and geodynamics communities. Representing mineral physics were Tetsuo Irifune, Artem Oganov, Lars Stixrude, Bob Liebermann and Guy Masters masquerading as a closet mineral physicist.

The joint AIRAPT and EHPRG conference was held in Catania, Italy from September 17-21. I attended as a representative of COMPRES and also delivered a paper on "Ultrasonic measurements of the elasticity of materials at elevated pressures and remperatures: Implications for determination and calibration of pressure.

At this conference, two members of the COMPRES community were honored by receiving major awards:

Takehiko Yagi of the University of Tokyo was awarded the Bridgman Medal of AIRAPT, thus joining a distinguished group of mineral physicists who have won this award since its inception in 1977: Francis Birch in 1983, Ho-kwang Mao in 1989, William Bassett in 1997 and Sergei Stishov in 2005.

Agnes Dewaele from the Commissariat à l'Energie Atomique in France was awarded the Outstanding Young Scientist Award of the European High Pressure Research Group [EHPRG]. Previous awardees from our COMPRES community include Alex Goncharov in 1991, Stefan Klotz in 1995, and Artem Oganov in 2004.

On November 30, 2007, Jay Bass and I attended the first meeting of the Board of Governors for HPSynC, a new research initiative at the APS and learned of progress and plans in the first year of operation.

On December 5-6, I attended an International Workshop on Synchrotron High-Pressure Mineral Physics and Materials Science at the APS of the Argonne National Laboratory. This workshop was convened by Tetsuo Irifune of Ehime University and Yanbin Wang of the University of Chicago and was attended by more than 50 persons from throughout the world of mineral physics.

Elsevier Publications recently announced a list of the Top 50 Most Cited Authors in PEPI for the period 2004-2007. Papers from the field of mineral and rock physics comprise more than half of this list. Our congratulations to all of the authors, and especially to those from our COMPRES community.

The 2007 Fall meeting of the AGU in San Francisco was most certainly the highlight of December for the COMPRES community.

a. Special Sessions on mineral and rock physics

There were many special sessions organized by mineral physicists, including Union sessions as well as those in Mineral and Rock Physics. Our compliments and thanks to Heather Watson of the Lawrence Livermore National Laboratory for serving on the AGU Program Committee.

b. AGU Awards for Mineral Physicists

(1). Ho-kwang (Dave) Mao was honored by receiving the 2007 Lehmann Medal in recognition of outstanding contributions to understanding of the structure, composition, and dynamics of the Earth's mantle and core.

(2). Eiji Ohtani from Tohoku University and Hugh O'Neill from the Australian National University were selected to receive the Bowen Award from the Section on Volcanology, Petrology and Geochemistry and delivered special lectures.

(3) The Outstanding Student Award in Mineral and Rock Physics was presented to Yasuhiro Kuwayama of the Tokyo Institute of Technology. Kuwayama-san joins a long list of previous awardees from 1990 to 2007 which can be seen on the AGU website http://www.agu.org/inside/mineral.html.

c. Exhibition Booth

Once again, COMPRES and GSECARS co-sponsored an exhibition booth at the Fall AGU Meeting. Our thanks to Glenn Richard and Michael Vaughan for

staffing the booth for COMPRES, along with Mark Rivers and his colleagues from GSECARS.

Among the newly elected Fellows of the AGU for 2008 are 4 members of the mineral physics community: Patricia Dove from Virginia Polytechnic Institute and State University Greg Hirth from Brown University Tetsuo from Ehime University in Matsuyama, Japan Renata Wentzcovitch from the University of Minnesota

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.

New faculty appointments in mineral physics in the U. S. and overseas. We take great pleasure in noting the following new faculty appointments in mineral physics:

Carmen Sanchez-Valle as Professor at the ETH in Zürich, Switzerland.

Denis Andrault at the Universite Blaise Pascal [France]

Haozhe Liu as Professor at the Harbin Institute of Technology in China.

Wendy Mao as an Assistant Professor at Stanford University.

Burkhardt Militzer at the University of California at Berkeley.

Razvan Caracas at the École Normale Supérieure Lyon [France].

Takao Okuchi at Okayama University [Japan]

Daniele Antonangeli and

Anne-Line Auzende—both at the Institut de Minéralogie et de Physique des Milieux Condensés in Paris.

A number of mineral physics faculty have recently announced their transition to a new academic institution, including:

Pamela Burnley from Georgia State University to the University of Nevada at Las Vegas in June 2007.

Tracy Rushmer from the University of Vermont to Macquarie University in Australia in July 2007.

Jiuhua Chen from Stony Brook University to Florida International University in September 2007.

Lars Stixrude from the University of Michigan to University College London in 2008. Carolina Lithgow-Bertelloni will also join the faculty of UCL.

Kanani Lee from New Mexico State University to Yale University in June 2008.

2008 Annual Meeting of COMPRES at Cheyenne Mountain Resort, Colorado Springs Planning is proceeding for the 2008 Annual Meeting from June 25-28.

Keynote Speakers include:
Rajdeep Dasgupta-Rice University Louise Kellogg-UC Davis Rebecca Lange-Univ of Michigan Jie Li-Univ of Illinois

William McDonough-Univ of Maryland Sean Raymond-Univ of Colorado Justin Revenaugh-Univ of Minnesota

A.10 Annual Program Plan and Budget Request

In preparation for the submission of the Annual Progress Report and Annual Program Plan and Budget to NSF in February, 2008, 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 2007, the two Standing Committees asked the project directors of each of the subawards to submit annual progress reports for Year #1 and budget requests for Year #2 by November 1, 2008. The Infrastructure Development Committee also issued a call to the COMPRES community for proposed new initiatives for technological projects that would contribute to the COMPRES mission, with a deadline of November 1, 2007.

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 2007 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 #2, 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 2008, the Executive Committee met via video and teleconference on three occasions to discuss the reports of the Standing Committees and to formulate recommendations for an Annual Program Plan and Budget for Year #1. Following these meetings, the President prepared a budget plan which was discussed, revised, and approved unanimously by the Executive Committee.

B Community Facilities

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

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

Prepared by:

Tom Duffy (Princeton), Don Weidner (Stony Brook), Lars Ehm (Brookhaven-Stony Brook), Alex Goncharov (Carnegie Institution of Washington), Jiuhua Chen (Florida International), Mark Rivers (Chicago), Chi-chang Kao (Brookhaven), Jingzhu Hu (Stony Brook), Quanzhong Guo (Stony Brook)

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 (X-17C and X-17B3) together with a sample preparation laboratory. The X-17C beamline is a side station that runs 100% of the time, amounting to about 81 days for each of the three cycles during the year. Dr. Jingzhu Hu has been the beamline scientist at X-17C since 1990. Both X-17C and X-17B3 beamline are available for energy dispersive (EDXD) and monochromatic (ADXD) experiments. Beginning September 1, 2007, the fraction of beamtime allocated to X-17B2 and X-17B3 was increased to 33%. The X-17B3 beamline thus now runs 33% of the time in dedicated mode with an additional 33% available in parasitic mode when the X-17B2 (multi-anvil) station is running. This is a total of 54 days per cycle. Dr. Quanzhong Guo has been beamline scientist at NSLS since 1999.

The DAC-XR facility is one of the longest-running high-pressure beamlines in the world, and has been a workhorse for diamond anvil cell research for more than two decades. The X17-DAC beamline is one of the most productive beamlines at the NSLS. Over the last 8 years, the beamline has recorded 149 publications, including 31 in premier journals.

2007 was a transition year for the facility: a new management team is now in place and a new Stony Brook-NSLS staff member is on-board. Significant improvements have been made in the areas of beamline controls, motorization, and detectors. We are planning to accelerate these improvements in 2008 while also planning for new capabilities in high-pressure research at NSLS-II. In 2008, we will develop a new laser heating system, and upgrade and improve our beam delivery system (monochromator, slits, and mirrors) and propose to make a major upgrade in our detector capabilities. Our current beamline scientists are planning to retire in 2008, and replacing them also will be a major task in the next year.

Selected Scientific Highlights for 2007

Structure and compression mechanism of liquid Gallium at high pressure

Recent development of high-energy monochromatic diffraction at the X-17B3 makes it possible to study pair distribution functions (PDF) of disordered and amorphous materials

at high pressures. X-ray total scattering experiments of the high-pressure and temperature behavior of liquid gallium have been carried out using a hydrothermal diamond anvil cell and 80 keV x-rays. The analysis of the PDF indicates that the 1st and 2nd nearest neighbor distances are insensitive to pressure whereas the 3rd and 4th nearest neighbor distances are decreasing with pressure. A model for liquid Gallium comprised of locally ordered units can be derived form the PDF and the compression mechanism. These experiments require high x-ray energy to cover large Q-range, and X-17B3 is currently the only dedicated high-pressure beamline in the nation where such experiments can be performed.

This project received the "Best Poster" Award at 2007 NSLS User's Meeting

T. Yu, L. Ehm, J. Chen, Q. Guo, J. Parise, Structural changes in liquid gallium at high pressure and temperature, in preparation

Thermal Expansion of Iron-Rich Alloys and Implications for the Earth's Core

The Earth's core makes up nearly one-third of the planet's mass. Its composition, properties, and dynamics are fundamental issues in the study of the Earth's interior. A critical test for any candidate core composition model is that it must be able to reproduce the physical properties of the core. On the basis of observing seismic rays penetrating the deep interior of the Earth and the orbital dynamics of the Earth as a planet in the solar system, models have been constructed to describe the physical state, density profile, and velocity profiles of the Earth's interior. One of the most widely used models is the Preliminary Reference Earth Model (PREM). To perform the test of consistency between a composition model and the PREM model, we must know the thermal state of the core and the equation-of-state (EOS) of various Fe-rich allovs at the pressure and temperature conditions of the core. A survey of literature revealed a significant lack of thermal expansion data on Fe-rich alloys under static high pressure. In this study, we have determined thermal expansion of Fe₃S, Fe, and Fe–Si alloys using in-situ synchrotron techniques. We have determined the unit-cell parameters and thermal expansivity of the iron-sulfur compound Fe₃S by using synchrotron x-ray diffraction techniques and externally heated diamond-anvil cells at pressures up to 42.5 GPa and temperatures up to 900 K. Our data at 42.5 GPa and 900 K suggest that 2.1 atom % sulfur produces 1% density deficit in iron.

B Chen, L Gao, K Funakoshi, J Li, Thermal Expansion of Iron-Rich Alloys and Implications for the Earth's Core, *Proc Natl Acad Sci USA*, 104: 9162-9167 (2007)

Synthesis of Ultra-Incompressible Superhard Rhenium Diboride at Ambient Pressure

The quest to create superhard materials rarely strays from the use of high-pressure synthetic methods, which typically require gigapascals of applied pressure. We report that rhenium diboride (ReB₂), synthesized in bulk quantities via arc-melting under ambient pressure, rivals materials produced with high-pressure methods. Microindentation measurements on ReB₂ indicated an average hardness of 48 gigapascals under an applied load of 0.49 newton, and scratch marks left on a diamond surface confirmed its superhard nature. Its incompressibility along the *c* axis was equal in magnitude to the linear incompressibility of diamond. In situ high-pressure x-ray diffraction measurements yielded a bulk modulus of 360 gigapascals, and radial diffraction indicated that ReB₂ is able to support a remarkably high differential stress. This combination of properties suggests that this material may find applications in cutting when the formation of carbides prevents the use of traditional materials such as diamond.

H Chung, M Weinberger, J Levine, A Kavner, J Yang, S Tolbert, R Kaner. Synthesis of Ultra-Incompressible Superhard Rhenium Diboride at Ambient Pressure. *Science*. 316: 436 (2007)

Structural Distortions and Phase Transformations in Sm₂Zr₂O₇ Pyrochlore at High Pressures

The structural characteristics of Sm₂Zr₂O₇, an ordered pyrochlore, were studied by angledispersive X-ray diffraction (XRD) and Raman scattering methods with increasing pressure. A structural distortion was observed at low pressures; but the distortion disappeared at pressures above 13.5 GPa. Above 18 GPa, the pyrochlore structure is unstable and a pressure-induced phase transition occurred. The high-pressure phase is a distorted fluorite structure in which the cations and anion vacancies are disordered. The disordered structure is accompanied by the formation of partially amorphous domains. With the release of pressure, the high-pressure phase partially transforms to the amorphous state.

F Zhang, J Lian, U Becker, L Wang, J Hu, S Saxena, R Ewing, Structural Distortions and Phase Transformations in Sm₂Zr₂O₇ Pyrochlore at High Pressures, *Chem. Phys. Lett.*, **441**: 216-220 (2007)

Beamline Developments 2006-2007

Management and Manpower

New Management Team

Since September, 2005, the operations of NSLS X-17C and X-17B3 diamond cell beamlines were managed by the University of Chicago (Mark Rivers PI). In June 2007, a new multi-institution management team was established to lead the X17 DAC effort. The management team is jointly led by PIs Thomas Duffy (Princeton) and Donald Weidner (Stony Brook). The other members of the management team are: Mark Rivers (Chicago), Alex Goncharov (Carnegie), Jiuhua Chen (FIU), and Chi-chang Kao (Director, NSLS). The management plan that was submitted to and approved by COMPRES is attached in the Appendix.

The management team met at NSLS in October, 2007 to define goals and strategies for the DAC program at X17. One outcome of the workshop was that a set of workgroups were established to lead the effort at beamline upgrades in the following areas: laser heating (Alex Goncharov, leader), beam stability (Lars Ehm, leader), and detectors (Jiuhua Chen, leader).

Joint Stony Brook - NSLS staff member in high-pressure research

Lars Ehm was jointly appointed as Research Assistant Professor at the Mineral Physics Institute at Stony Brook University and the National Synchrotron Light Source at Brookhaven National Laboratory in September 2007. He will provide scientific and technical support to the high-pressure program at X17. Due to his area of expertise in crystallography at extreme conditions and diamond anvil cell research, Lars will contribute to the improvement of existing and the development of new experimental capabilities at X17B3 and X17C. Furthermore, Lars will play a central role in the construction and operation of the new facility-operated beamline X17A (see below). The joint nature of the appointment allows Lars to function as an additional liaison between the COMPRES beamline and the NSLS. The research program of Dr. Ehm in the year 2008 will focus on two areas: determination of structure-property relationships in carbonates and determination of the atomic structure of partially and non-crystalline materials as a function of pressure and temperature using high-energy total X-ray scattering.

Beamline operations in 2006-2007

The X-17 beamlines are NSLS Facility Beamlines with a Contributing User agreement with COMPRES. The NSLS is responsible for the operation of the beamline (optics, safety systems, etc.) while COMPRES is responsible for operation of the experimental stations. 50% of the beamtime is given to general users (GU) and 50% of the available beamtime (CU) is assigned to COMPRES. All proposals are first submitted through the proposal system at NSLS to compete for GU time. CU time may be assigned to proposals without a sufficiently high rating to obtain GU time, to increase the number of days for a successful GU proposal, or for use by beamline staff.

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

Funding for the X17-DAC effort is provided 100% by COMPRES. A DOD DURIP proposal was submitted in 2007 to obtain additional funding for equipment but this request was declined.

Beamline improvements completed in 2007

A number of upgrades and improvements to beamline capabilities have been made over the last year.

<u>X17C</u>

Computer systems, software, and electronics

New beamline control computers were purchased and upgraded operating systems were installed on the beamline. A variety of new software was installed or upgraded and we now have Linux installed at the beamline for the first time. For beamline control, an

obsolete CAMAC system was removed and replaced with modern VME modules. The EPICS control system has been upgraded to the latest version from CARS. P. Dera (GSECARS) installed his new software for single-crystal diffraction. It is expected that this software will eventually supplant the current outdated software that is used for energy-dispersive single-crystal diffraction. An updated version of the program with new features for energy dispersive and angle dispersive single-crystal diffraction is expected in February 2008.

Kirkpatrick-Baez mirrors

Focusing the KB mirrors at the X17 beamline has been time-consuming and difficult due to lack of key motorization and visualization components. This problem was partially addressed in 2007 by the installation of a Sony Firewire CCD camera camera for imaging the focal spot and by motorizing the in-hutch microscope. This equipment is shared between X17C and X17B3.

Detectors

The NSLS has made a 135-mm CCD detector (MarCCD) available for X17C users starting from February, 2007. This detector is available for X17C users except when needed by NSLS as a back-up. For the few occasions in which the MarCCD was unavailable, users have access to the (off-line) Fuji image plate system at NSLS. Although not optimum, this availability of the MarCCD for the vast majority of users is a big improvement. However, the lack of dedicated, on-line detectors for diffraction experiments remains a major limitation of the facility.

The two Ge detectors for EDXD experiments are undergoing repairs at this time to remove stray fluorescence lines that often contaminate users' spectra.

Other

The set-up for energy dispersive experiments was streamlined by adding motors to both the front (so-called "tip") and back (Huber) slits thereby allowing for remote scanning which speeds the alignment process. A new Watec video camera was installed in the station for sample alignment. We have also added a Keithley 2700 digital multimeter and Xantrex XHR 33-33 programmable DC power supply, both of which are connected to the VME system.

<u>X17B3</u>

Laser Heating

Motor control of YAG laser focusing lenses was set up, allowing remote focusing of the laser heating system. A longer focal distance lens was also installed in the system to

make alignment easier. An overheating problem of the CCD detector used for spectrometric temperature measurements has been solved.

Sample Stage

A new zoom microscope system was set up for rapid and improved sample imaging in the diamond cell.

Detectors

A major drawback to X17B3 was that the available detector was limited to an off-line IP which made data collection inefficient and slow. In 2007, an on-line image plate detector (Mar345) became available for X17B3 courtesy of a loan from the NSLS. This detector has been used successfully by several groups.

X-ray system

A new beamline slit system in combination with the KB mirror system has resulted in reduction of the focused beam size to 30 μ m from 50 μ m previously. In collaboration with K. Evans-Lutterodt of NSLS, a kinoform lens was successfully tested at X17B3 with x-ray energy of 30 keV and vertical focused beam of better than 8 μ m was achieved. The flux through the B3 monochromator was increased by a factor of two by optimizing the crystal thickness in the Laue monochromoter system.

Diamond Cells

A symmetric diamond cell and a pair of anvils were obtained for use by the beamline staff in testing the laser heating system and conducting experiments.

Planned Activities for January - April, 2008

Two key beamline developments are necessary to enhance the X17 DAC facility for COMPRES users. The first is to improve the size and cleanliness of the focused beam using the KB mirror system. The second is to rebuild the laser heating system using a new fiber laser and improved optical design and layout. For the first issue, we have already installed and tested the motor controls and optical imaging capabilities necessary for rapid testing of the KB mirrors. A diagnostic visit by the mirror's designer, Peter Eng, is being planned for early 2008. Our goal is to make improvements to the KB mirrors to achieve stable focused beam of 15 x 15 μ m at 35 keV and 25 x 25 μ m at 80 keV. Based on the results of Dr. Eng's visit, we will carry out repairs and upgrades. Funds have been budgeted to cover costs of replacement materials and to build a permanent inert-gas enclosure to house the mirrors.

For the laser heating system, the goal is to improve the performances and reliability of the system. Ultimately, we are planning to enable *in situ* measurements of thermal equations of state, phase transitions (including melting), high-temperature rheology, and chemical

reactivity. This will require new laser heating source, improved optics and controls. The estimated cost is \$96,000 and is contained within our current equipment budget.



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

The major tasks for 2008 include:

Purchasing of a fiber laser (the order has been placed; the delivery is in January 2008).
Working out safety issues related to the new laser (interlocks, control box, etc) and setting up the laser.

3. Working out an improved optical layout (Fig. 1). Currently the improvements planned include: improved the overall stability of the optical and x-ray systems; polarization laser power controls; beam profiler which provides uniform illumination of a controlled diameter laser spot at the sample; motorized x-ray transparent steering mirrors; rugged and optically uniform optical collection path with high throughput.

4. Construction, setting up, and testing the system.

Other tasks to be completed by the end of this budget year:

--Further testing of Kinoform lens concept in collaboration with Kenneth Evans-Luterodt of BNL

-- Test and improve beamline slit system up to 80 keV energy

-- Build improved clean-up slits to eliminate gasket lines in laser heating.

-- Improve the Laue Monochromator for X17C to make it quick and easy to change energy from current fixed 30 keV value. This is being planned in collaboration with Zhong Zhong of BNL.

-- Improve beamline shielding when in-hutch X17C monochromator is set up.

-- A new Ar laser for the ruby spectrometer system will be purchased

Planned Activities for COMPRES II – Year 2 (May 2008 – April 2009)

Staffing

The current beamline scientists, Jingzhu Hu and Quanzhong Guo will retire on September 30, 2008. We will advertise for two beamline scientists, and we expect to have one of these two in place by mid-summer 2008 to allow for several months overlap with Drs. Hu and Guo. The other beamline scientist will be hired in Fall 2008.

Beamline Components

We anticipate that construction, testing, and commissioning of the laser heating redesign will continue through the first part of the new budget year. No funds are being requested for laser heating equipment as we anticipate being able to purchase all necessary components from existing funds.

The lack of an area detector owned by and dedicated to the X17-DAC facility is a major problem area that we propose to address in year 2. Currently, the area detectors from the NSLS detector pool are used at the X17-DAC beamlines. These detectors, a marccd detector at X17C and the mar345 image plate detector at X17B3, can be requested by NSLS facility beamlines at any time, and therefore may not be available for experiments at the X17-DAC beamlines. Furthermore, to take full advantage of the capabilities of the new laser heating system at X17B3 a fast area detector is necessary. The readout time on the mar345 image plate detector of 2.5 minutes limits the detection of fast phenomena and studies of reaction and transition kinetics. The currently most cost effective detector system on the market is the SX-165 marccd detector. The active area of the detector is 165 mm (2048×2048 pixels) and it is sufficiently large for powder and single-crystal diffraction experiments in a diamond anvil cell. The readout time of 2.5 seconds is fast enough for experiments on kinetics of phase transitions and reactions. Previous generations of the 165 marccd detector system are currently in use at many dedicated high-pressure beamlines (e.g. GSECARS, HPCAT) and are very efficient and reliable. A new feature of the SX-165 marccd is the capability to partially read out the detector in milliseconds. This will facilitate studies on a time scale previously not available in high-pressure and temperature research. We request funds from COMPRES for the purchase of a SX-165 marccd detector.

Outreach

While the X17-DAC facility has a steady and accomplished group of users, we recognize that beamline improvements must be coupled with outreach efforts to be successful. Concurrently, we need to organize and lead the community in planning for the NSLS-II facility. In January, 2008, two planning workshops for NSLS II that are of interest for the high-pressure community will be held. One workshop will address the needs of the material science community, whereas the other has geoscience/environmental science as a focus. Lars Ehm (geo/enviro) and John Parise (materials) are involved in this activity as we continue to make the science case for a major role for high-pressure research in NSLS-II. We are also planning to hold a workshop on "Future of High-Pressure Research" at the annual NSLS meeting in May, 2008. This workshop is being organized by L. Ehm, J. Chen, B. Li and Z. Liu and will highlight some of the research opportunities available at the current NSLS facility as well as future opportunities at NSLS-II.

Future Developments at the NSLS

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



Development of X17A

Fig. 2. X17 beamline layout and proposed location of the new X17A station (courtesy of Z. Zhong, NSLS).

In the latest 5-year plan for NSLS, it is proposed to develop a new side station, X17A, to enhance utilization of the superconducting wiggler beamline of X17. While mainly serving the materials science community, the addition of X17A will increase the share of beamtime available to the X17 end-stations, X17B2 and X17B3 and thus directly impact the amount of beamtime available for high-pressure activities. The project is viewed as a high-priority and is expected to commence in FY 2007-8.

NSLS-II

NSLS-II is a proposed new storage ring at Brookhaven that promises to deliver x-rays with 10^4 times the brightness of the current NSLS. Design and engineering of the new light source is in progress and operations are expected to commence in 2015 (and the current NSLS will be decommissioned shortly thereafter). Design goals for the project include achieving spatial resolution of 1 nm and energy resolution of 0.1 meV. Current plans involve the development of 6 insertion device beamlines as part of the construction project, with additional insertion device beamlines pursued via separate Major Items of Equipment (MIE) DOE-BES funding. There will also be a number of beamlines (~20) that will be transitioned and upgraded from current NSLS beamlines. The project can accommodate up to 58 beamlines in total. A superconducting wiggler beamline for high pressure/high energy diffraction is proposed as an MIE insertion device beamline (Fig. 3). The possibility of including a 6-T superconducting wiggler at NSLS-II is being currently evaluated. High-pressure activities will also likely be incorporated into the project beamlines which tentatively include powder diffraction, nanoprobe, and IXS beamlines. The NSLS-II will also include infrared beamlines and thus high-pressure infrared capabilities can be maintained and improved.

This project is considered a near-term priority for the US Department of Energy's office of Science. In 2007, the project achieved "Critical Decision One" designation in the five-step DOE approval process.



Fig. 3. Brightness versus energy for various proposed NSLS-II insertion devices. SCW – superconducting wiggler

High-Pressure Research at NSLS-II

The NSLS and NSLS-II management recognizes high-pressure research as an emerging field across scientific disciplines. In July 2007 Brookhaven National Laboratory held a user workshop to discuss science opportunities and possible beamline designs at NSLS-II. The high-pressure community was well represented at this meeting and attended many of the technique-focused breakout sessions and science-based discussion groups. It was striking that high-pressure research played a significant role in the scientific cases and designs of the first suite of six beamlines build as part of the facility construction project. The goal of NSLS-II is to be able to accommodate high-pressure equipment (e.g. diamond anvil cells or Paris-Edinburgh cells) on almost any beamline. However, the high-pressure community determined during the meeting of the high-pressure discussion group at the NSLS-II workshop, that the additional high-pressure capabilities at these beamlines are no alternative to dedicated high-pressure beamlines at NSLS-II. The high-pressure community defined as a goal for the high-pressure research at NSLS-II a minimum of three dedicated high-pressure beamlines:

One beamline for single-crystal and powder diffraction in diamond anvil cells with *in situ* laser-heating and cryogenic capabilities.

One beamline for experiments in a large volume press.

One beamline for infrared spectroscopy in diamond anvil cells with *in situ* laser-heating and cryogenic capabilities.

A report outlining the needs of the high-pressure community for NSLS-II in detail was prepared by Don Weidner.

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Appendix I

Management Plan for X17 Diamond Cell Facility

June 6, 2007

We plan to institute a new multi-institution management plan where participants from each institution will bring unique capabilities that together will provide an excellent team for development and maintenance of this facility. The management team will be led by Thomas Duffy and Donald Weidner and who will jointly lead the project as PIs. The other members of the management team are: Mark Rivers, Alex Goncharov, Jiuhua Chen, and Chi-chang Kao.

Thomas Duffy, Princeton University. Duffy is a diamond anvil cell specialist and has been a user of the NSLS since 1993. He has experience in a wide variety of synchrotron based high-pressure experiments, and formerly served as beamline scientist at the GSCECARS facility of the Advanced Photon Source. Duffy will coordinate the scientific agenda for the new DAC-XR program, co-supervise beamline postdoc fellows, serve as interface to the user community as well as seek for external funding for facility development and related scientific research.

Donald Weidner, SUNY Stony Brook. Weidner has experience in synchrotronbased multi-anvil and diamond cell experiments. He also has extensive knowledge of beamline development at NSLS. As PI, Weidner will provide overall guidance and supervise beamline personnel for the DAC-XR facility. Weidner will also serve as a liaison between the diamond cell and multi-anvil programs at X17C. In this way, we will achieve synergy and coordination between the high-pressure groups that could not be achieved otherwise. Weidner provides on-site leadership that is essential for proper management and oversight as well as rapid response to both technical problems and scientific opportunities as they develop. Weidner will also direct scientific research direction that takes unique advantages at the facility (e.g. high energy melt/glass x-ray scattering) and seek external funding and supports (e.g. personnel support from SBU and the NSLS) to the facility.

Mark Rivers, GSECARS, U. of Chicago. Mark Rivers is manager of the GSECARS sector at the Advanced Photon Source which is one of the most productive and successful beamlines at the APS. He is also part of the team that has also remotely managed X-26 of the NSLS for many years. Rivers brings the technical resources of GSECARS to help strengthen the NSLS program. This has already been done informally over the years in critical areas such as focusing optics, detectors, and software. GSECARS has expertise in these areas and also in mechanical design. The participation of GSECARS also enables development of common tools across beamlines which makes it easier for users to carry out experiments at multiple beamlines. Rivers will thus supply technical expertise to the management team.

Alex Goncharov, Geophysical Laboratory, Carnegie Institution of Washington. Goncharov has extensive experience in optical systems for high-pressure research. He will be intimately involved in the design, testing, construction, and operation of the new laser-heating system at X17B3. He also will serve as a liaison between the x-ray and infrared facilities at NSLS.

Jiuhua Chen, Florida International University. Chen, the previous PI of the DAC program at X17, has experience in synchrotron-based multi-anvil and diamond cell experiments. He also has extensive knowledge of beamline development at NSLS. Chen will direct scientific research direction that takes unique advantages at the facility (e.g. high energy melt/glass x-ray scattering).

Chi-chang Kao is the director of the NSLS. It is essential to involve the NSLS in the strategic planning for the beamline and the transition to NSLS-II. Chi-chang will serve to link and develop the high-pressure activities at X17-DAC within the broader community of materials scientists and crystallographers at Brookhaven. Chi-chang will also serve as a liaison with NSLS staff for new beamline and facility developments at X17-DAC including beamline optics (monochromators, focusing optics, detectors) and large-scale infrastructure development (X17A, NSLS-II).

Hiring Plans There is currently a research faculty search that is jointly supported by the NSLS and the Mineral Physics Institute of Stony Brook. In addition, with the departure of Chen from the MPI, we anticipate a second position at the research faculty status who will have an intellectual investment in this DAC program. We anticipate that one of the successful candidates will assume the PI role in this project. However, we feel that it is premature to commit to the time frame over which this role develops.

We also anticipate that the current beamline scientists will be replaced over a time frame of the next twelve months. We will aggressively seek to recruit the best candidates for this position.

The new management structure together with new scientific and beamline staff will provide this facility with the energetic, committed team to make this a world-class facility.

Responsibilities The management team is responsible to maintain a strategic plan that provides the vision for the next three years. This strategic plan will be continually evaluated and altered as new input becomes available. The goals of the strategic plan should include the following: 1. Provide a vital community facility for mineral physics, 2. Define a significant focus for the NSLS program that enables it to become unique in the world in diamond cell research, 3. Look forward to the NSLS II in such a manner that COMPRES will have significant access to this new facility. The management team is also responsible to supplement the COMPRES funding with additional resources for operating and growing the beamline. The management team is responsible to keep in touch with the user community through workshops. The PIs are charged with overseeing the development of the strategic plan, supervising local support personnel, and coordinating with the management team.

Funding host. Stony Brook University will be the host institution for COMPRES funding associated with this project. In this way, resources for scientific and beamline staff and scientific equipment can be managed under a single entity.

B.2 Infrared Diamond-anvil Facilities at the National Synchrotron Light Source

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

Overview

U2A beamline is an integrated and dedicated facility for measurement of far- to nearinfrared spectra of materials from ambient to ultrahigh pressures at variable temperatures by coupling synchrotron infrared microspectroscopic techniques with diamond-anvil cell methods. During phase I of COMPRES (2002-2007), we built a broad user base, provided convenient access for users from the COMPRES community, and promoted user research projects on problems in high-pressure geoscience, complemented by studies in materials science, condensed matter physics, chemistry, and biology (many of these studies by the COMPRES community).

Selected Scientific highlights

Synchrotron infrared reflectivity of iron at high pressure – The physical properties of iron (Fe) at high-pressure place important constraints on the state and evolution of terrestrial planetary cores. Many techniques for measuring the physical properties of Fe at high pressures and temperatures rely on spectroradiometry for temperature measurement. Knowledge of the spectral emissivity of iron at high pressures is of immense significance for accurate temperature determination in laser-heated diamond anvil cells and dynamic shock wave experiments. It is commonly assumed that most materials are greybodies simply because emissivity data at high pressures do not exist. It is clear from measurements of the emissivity of Fe at 1 bar that iron is not a greybody, and almost no data exists for the optical properties of iron at high pressure. A group from the University of Chicago (C. Seagle and D. Heinz) measured the infrared reflectivity of iron at pressures up to 50 GPa and room temperature at U2A beamline using the Fourier Transform Infrared Reflectivity technique in order to evaluate the greybody assumption often applied in spectroradiometry. The emissivity and other optical properties were derived with a Kramers-Kronig analysis. All the optical properties depend on pressure and undergo a discontinuous change in both slope and magnitude at the body centered cubic (bcc) to hexagonal close packed (hcp) phase transition in iron. The errors associated with the greybody assumption can be as high as 25% for bcc Fe assuming there is no temperature dependence of the emissivity, hcp Fe is nearly a perfect greybody at room temperature. The addition of high temperature data to this knowledge base will allow more accurate temperature determinations using spectroradiometry. The analysis of the high temperature data will also provide the pressure and temperature dependence of the conductivity, which is important for geodynamo simulations, and provide a fundamental understanding of the effect of pressure and temperature on the optical properties of Fe. More beam time has been scheduled for these high pressure and temperature experiments in November [C. Seagle at. al., AGU Fall Meeting, 2007].

High-pressure infrared studies of talc and lawsonite – The high-pressure stability of hydrated metamorphic phases and their importance in transporting water into Earth's deep interior is well appreciated. Yet, the manner in which hydrogen is retained within

these phases is a topic of considerable uncertainty. In particular, the role of hydrogen bonding (and its pressure dependence) in stabilizing these metamorphic phases at high pressure remains unclear. Among metamorphic phases stable to high pressures, talc, Mg,Si,O, (OH), and lawsonite, CaAlSi,O, (OH), HO, represent two different means of sequestering hydrogen. Talc is a chemically simple layer silicate, with the hydroxyl unit oriented nearly perpendicular to the layers and weak hydrogen bonding. In contrast, lawsonite contains both hydroxyl units and water molecules; it has both weak and intermediate strength hydrogen bonding. The effect of pressure on the vibrational spectrum of lawsonite has been examined by both mid-infrared spectroscopy and by Raman spectroscopy to ~20 GPa (Daniel et al. 2000; Scott and Williams 1999), but the far-infrared spectrum of lawsonite under pressure has not been reported. The vibrations in this long wavelength range are associated with translations of the water molecule and are critical for calculating the thermochemical properties of the material. In contrast, Raman spectra of talc have been collected to only 3.5 GPa (Holtz et al. 1993), and its infrared spectrum under pressure has not been reported. We present high-pressure infrared spectra of talc and lawsonite at room temperature. For lawsonite, our data span the far infrared region from 150 to 550 cm-1 and extend to 25 GPa. The spectroscopic data were combined with previously published high-pressure mid-infrared and Raman data to constrain the Grüneisen parameter and vibrational density of states under pressure. In the case of talc, the high-pressure infrared data span both the mid and far-infrared from 150 to 3800 cm-1, covering lattice, silicate, and hydroxyl stretching vibrations to 30 GPa. Both phases show remarkable metastability well beyond their nominal maximum thermodynamic stability at simultaneous high-pressure and high-temperature conditions [H. Scott at. al, Am. Mineral. 92: 1814-1820 (2007)].

Water in microdiamonds from subduction zones: evidence from synchrotronassisted infrared spectroscopy – All natural diamonds are formed in the Earth's deep interior -- upper mantle, mantle transition zone, and perhaps below the 660-km seismic discontinuity. Due to the chemical inertness of diamond, it is a near-perfect container stable over geologically relevant times for fluid and solid inclusions trapped during its growth. The chemistry and structure of inclusions are used to reconstruct mantle mineralogy, and conditions and compositions of diamond-forming media. Though most natural diamonds of gem and industrial quality originate from kimberlites and other ultramafic magmas, unusual small diamonds (1-300 micron in size) have been discovered within some orogenic belts of Kazakhstan, China, Norway, Germany and Greece. All of them were formed as a result of Paleozoic and Mesozoic continental collisions and subduction of continental lithologies, followed by exhumation from minimum depths of ~150-250 km. Because these microdiamonds are hosted by metasedimentary rocks of continental affinity, their formation is unexpected according to mainstream geological thinking; they are thus currently the focus of study to understand subduction zone processes and rock exhumation. A group led by L. Dobrzhinetskaya from Univ. California Riverside carried out synchrotron infrared microspectroscopy studies of samples from the Late Paleozoic crystalline massif of Erzgebirge at U2A beamline. These studies showed that the Erzgebirge diamonds contain nitrogen impurities. molecular H₂O, OH- and CO₃ radicals. The presence of both nitrogen C- and A defects classifies the studied diamonds as Type Ib-IaA, which is similar to other diamonds from

metamorphic terranes such as the Kokchetav massif, Kazakhstan and the island of Fjortoft in the Western Gneiss region of Norway. Presence of H_2O and $CO_3^{2^-}$ strongly supports a concept of diamond crystallization from C-O-H fluids [L. Dobrzhinetskaya at. al., Earth Planet Sci. Lett., **248**: 325-334 (2006); Proc Nat. Acad. Sci. **104**: 9128-9132 (2007)].

Ongoing and Future Beamline Upgrade Plans

- 1. New IR/Raman Microscope system (also supported by CDAC): This setup will include an independent and user-friendly Raman microscope system and the capacity of far-IR reflection with higher spatial resolution and will be available for general users after the NSLS winter shutdown. An Olympus microscope (model BXFM) has been purchased (\$12.4 K) with CDAC funds. Optical components including notch filters, Newport XYZ stage, mirrors, and optical mounts (~\$15 K) will be delivered in November.
- 2. CO₂ laser heating system: Numerous users require high pressure and high temperature >1000 K extreme conditions are essential for infrared studies of Earth and planetary materials. Considering the intrinsic phonon absorption $\sim 10 \ \mu m$ in a large number of hydrate silicates and to overcome 1000 K temperature barrier due to the external resistance heating, an off-line but on-site CO_2 laser heating has the highest priority on the list of beamline's upgrade in order to accommodate users need on infrared studies of hydrous minerals at high pressure and high temperature. As first step, we decided to purchase a CO_2 laser with outstanding power stability (<3%) from Coherent (\$20 K). Additional accessories including chiller and optical table (~\$9 K) will be purchased as well. All the equipment will be delivered in this year and NSLS will provide a space to locate this laser system. We request additional funds in the next year's permanent equipment budget in total amount of \$65 K (see below) to develop an in situ temperature calibration system with FTIR spectroscopy. This will enable us to cover the gap of high temperature calibration in DACs between the resistance and laser heating techniques. In addition, high pressure and high temperature (up to several thousand K) are generated in DACs, while the sample serves as an IR source for emission measurements. Specifically, these in situ high P-T IR techniques are critically important for understanding the behavior of hydrogen in hydrous minerals.

Proposed budget for next year

With the significant amount of beam time available to general users and contributing users as well as plans for beamline upgrades needed by our user community, we request \$225 K for operating, maintaining, and upgrading the IR beamline for the year beginning June 1, 2008 and ending May 31, 2009. The budget and budget justification are given in the Detailed Budget section below.

The fraction of beam time on the IR beamline available to the community next year

Under the new NSLS Contributing User Proposal, U2A became a facility beamline from January 1, 2006. Thus 50% of the beam time allocated to U2A will be available to General Users. This reflects a 100% increase of available beam time to general users. Currently, the COMPRES community is the dominant user group in this category. The remaining 25% of beam time will be allocated by COMPRES with at least half of this time being dedicated to support research by members of the COMPRES community through proposals vetted by the NSLS General User program; the NSLS User Administration will provide the CU group proposed here with the ratings of all proposals for a beam time to be allocated by COMPRES. The remaining 25% will go to Geophysical Laboratory, Carnegie Institution for development projects and users supported by its grants such as CDAC.

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

[Donald Weidner and Michael Vaughan, Stony Brook University]

Recent Developments in 2007:

Parasitic beamtime The 2006-2007 year has been an exciting year at the multianvil facility at the NSLS. We are continuing to expand the user time available by increasing access to multi-anvil experiments in time periods that were previously unavailable. The first phase is to time-share with the B3 diamond anvil cell hutch. When the new hutches were designed, the beam was split so that one part fed the B2 hutch and the other went through the hutch to the B3 station. By placing a shutter between hutches, we are able to run experiments in the B2 hutch while they can enter the B3 hutch. The multi-anvil facility has access to 25% of the total time as an unencumbered allocation. Now it has parasitic access to the B3 time – another 25%. During B3 time we are more restricted as to when we can enter our hutch, and we are sometimes shut out as they need access to the entire beam line. Still we are finding that we can very effectively use this parasitic time. In fact, we have begun to schedule users in this time with an additional allowance to make up for the added difficulties scheduling when we can enter the hutch.

Beam allocation to high pressure The Scientific Advisory Committee recommended this year that the beam time to high pressure be increased to 2/3 of the total time from $\frac{1}{2}$ of the total time.

In-hutch monochromatic side station We are now near completion of a second high pressure station within the high pressure hutch. A single bounce monochromator will remove a thin slice of beam from the white beam and deliver it behind the main press to a second press equipped with a T-cup high pressure device. We have received all of the hardware for this installation. Now we are finishing lead shielding around the mono station. We have begun to work with the new DTcup cell which will be used in the side station. The completion of this system will enable another doubling of the total high pressure time.

Beam time allocation We are continuing our process of beam time allocation. Now all experiments must be submitted to NSLS review panel using the NSLS review process for general users. NSLS then assigns up to 50% of the standard mode beam time on the basis of their review (this does not count parasitic time). We reserve 10% for beamline development. We assign the remaining time following the rating of the NSLS review, but upgrading proposal that are consistent with a COMPRES agenda.

Summary of X17B2 Beam Usage

In 2007, the Multianvil Cell program hosted 45 users at X17B2. They were from 17 Institutions. 125 separate experimental runs were performed, with an total time of 139 days. There were 122 days of scheduled operations time allocated to X17B2 and X17B3, so not only were there apparently zero days of wasted time, there were 17 days unscheduled time made available to the users by the Light Source.



Installation of Monochromatic Side Station in X17B2 Hutch

Science Highlights - activities of 2007

- **Deformation experimental technique breakthrough and scientific research:** The Rotational Drickamer Apparatus, developed by Shun Karato of Yale has been deployed on our beamline. Karato brings his research team and high pressure apparatus to the hutch. We have been successful measuring strain and stress with this device. This machine is capable of very large strains because of the rotational mechanism, and very high pressures (in excess of 20 GPa) because of the Drickamer style pressure generation.
- The D-DIA has become a routine experimental system for rheology experiments. This new apparatus has typical cubic-anvil geometry with independent control of top and bottom rams. Therefore under high pressure and temperature, the top and bottom ram can advance or retreat independently to deform the sample. In conjunction with synchrotron x-ray, the sample stress and strain can be measured by x-ray diffraction and radiograph imaging. Multiple x-ray diffractions along different direction relative to the principal stress axis yield an accurate measurement of stress in the sample to 100 MPa, and correlation of strain-mark images on the radiograph provides a precise strain measurement to $10^{-4} 10^{-3}$.
- High pressure Rheology of olivine: Olivine continues to be a central theme for D-DIA experiments. Single crystal studies by Raterron demonstrate a pressure induced change in slip systems. Several groups are converging on the activation

volume for power law creep. While initially divergent, it is clear that the results are beginning to converge. Papers are being submitted by these groups.

• *Q* Measurements are now being made that are sensitive to the Q and dispersion of elastic properties. While publicized only a year ago, we have had three beam time projects by groups outside of the Stony Brook program come an pursue these types of experiments.

Activities for 2007-8

We plan to fully implement the monochromatic side station during the upcoming year. We will work to use monochromatic measurements for differential stress. We hope to run two simultaneous experiments by the end of the coming year, at which time we can accept proposals for both systems – thereby doubling the available time. We will continue to serve users with the DDIA for deformation/controlled stress measurements. We will continue ultrasonic measurements in the DDIA. We hope to return to the T-cup to refine the high pressure limits of our system. We have obtained 28 GPa with cBN anvils. We have not had time to push this limit. We will also work on additional megabar strategies.

Major Support Personnel	Source of Funding
Liping Wang beam line scientist	COMPRES
Carey Koleda machinist	COMPRES
Michael T. Vaughan NSLS coordinator	MPI at SBU
Donald J. Weidner, scientist spokesperson	Geosciences at SBU
Ken Baldwin, software support	MPI at SBU
William Huebsch, electronics expert	Geosciences at SBU

MPI: Mineral Physics Institute of Stony Brook University Geosciences: Department of Geosciences of Stony Brook University

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B.4 West Coast Synchrotron Facilities

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

Summary

Beamline 12.2.2 is working well for axial and radial diffraction, high-pressure, high-temperature studies using laser heated diamond anvil cells.

This year we have been implementing the recommendations of the Williams report [February 2007] with a focus on improving the performance of our laser heating system. Our operations and development program has been badly effected by both of our COMPRES user support staff leaving to take up permanent positions. To minimize the immediate impact on beamline users Jason Knight, our new ALS associate beamline scientist on beamline 12.2.2, is spending almost all of his time providing user support. This has led to a slow down in our facility development: the new resistively heated cells have not been commissioned and the end station 1 upgrade is on hold. The laser heating system is working really well at the moment. We have installed and commissioned two new fiber lasers, which has increased our total laser heating power from 50W to 200W allowing us to increase our laser spot size for the same achievable temperature. We have also developed improved alignment tools and procedures that both reduce the time needed for alignment and improve the reliability of our temperature measurement system. Reliable temperatures are now measured simultaneously from both sides of the diamond cell. Nevertheless, we are determined to continue to develop the system until it is demonstrated to be the best laser heating system in the world.

Our highest priority at the moment is to get new COMPRES user support personnel in post and fully trained. We also plan to upgrade the temperature-measurement and control capability of our laser heating system during a Spring shutdown of the ALS. This upgrade will include installation of an improved laser optics table mount system that will greatly reduce vibration. We will also install improved optics, including pellicle beam splitters, remotely controlled spectrometer slits and a beam stabilization feed back system. In addition we plan to add a four color temperature measurement system to operate in parallel with our existing spectroradiometery system to give us an on-line probe of spatial variations of temperature. In parallel with these developments we plan to move the diamond cell preparation and loading facility into a new laboratory and use the current high-pressure laboratory to install our old YLF laser and interface it with our Brillouin and Raman systems. This will enable us to validate the temperatures that we obtain from our on-line system and allow us to gain the necessary experience to allow us to implement these techniques on the beamline.

Summary of beamtime allocation process

Beamtime on beamlines 1.4, 11.3 and 12.2.2 is made available to COMPRES users as part of the COMPRES-ALS Approved Program. This guarantees a minimum of 20% of the beamtime on beamlines 1.4 and 11.3 to COMPRES users, and a proportion of the time on 12.2.2. The proportion of the time on beamline 12.2.2 depends on the amount of monies contributed by the approved program partners (COMPRES, UCB, LLNL) in any

particular year. The current COMPRES approved program has been active for almost three years. It ends in June 2008. A renewal request has been submitted in December 2007.

Currently, the agreement with the ALS is that potential COMPRES users should apply under the general user program in place at the ALS for COMPRES beamtime. The reason for doing this is that it establishes the COMPRES community's credibility with respect to the ALS, not only helping us justify COMPRES' Approved program status but also giving us an opportunity to request special funding allocations for new equipment and other expenditures. All applications deemed eligible for COMPRES beamtime, as decided by the Calipso program manager, will be allocated COMPRES time on one of these beamlines if they pass the normal peer review process that all ALS applications are subject to. Successful proposals at the ALS are active for four cycles (two years). In the last round of applications demand for COMPRES beamtime exceeded available beamtime by almost a factor of three.

Summary of the major accomplishments for the past year

This year has been overshadowed by our two COMPRES user support scientists leaving. This has led us to focus our resources on user support with less emphasis on facility developments. Within this context, we have been doing what we can to implement the recommendations of the William's review. This sets the first priority as the laser heating system on beamline 12.2.2 with implementation of the single crystal system as a secondary objective to be pursued once the laser heating system is world leading. Given the lack of people resources and the guidance of the review recommendations we decided to put the resistive heating and single crystal developments on hold while we recruited new staff and to focus what resources we have on user support and laser heating. This has worked adequately well, with laser heating user visits generally reporting successful experiments. Much of this success is due to the two new fiber lasers. These come with built in HeNe alignment lasers that are coaxial with the infrared laser beam. This allows almost complete alignment of the system as a class 1 system with no need for safety goggles, and has reduced the time we need for atotal realignment of the laser heating system from one or two days to two or three hours. We have also added additional translation stages and motors. We can now get much more precise alignment resulting in improved imaging and reduced aberrations in the spectroradiagraphic system.

Summary of proposed activities for next year

For next year we have five main goals:

- 1. Appoint new COMPRES user support scientists. Advertisements have been placed in national and international journals and job search sites. So far we have had thirty eight applicants. First waves of interviews have been completed and we hope to have the first person in post early next year.
- 2. Reorganize high-pressure laboratory.

The current high-pressure laboratory is extremely heavily used, often with three or four user groups sharing the space. It is not really possible to perform spectroscopy with this number of people using the lab. We propose to move the diamond cell preparation and loading to a new workspace in the new user support building. This will not be ready for two years. In the interim we propose a move to a temporary work area close to beamline 12.2.2. This will allow us to fully utilize the current laboratory in our drive to validate the temperatures that we get from our spectroradiometric measurements. To achieve this we intend to install our old YLF laser in that laboratory and interface it with the Raman and Brillouin systems. We will then use Brillouin and Raman for ancillary temperature measurement. If this is successful then we can use that to check the temperatures from our spectroradiometery with near ambient pressure measurements from melting point standards in our diamond cells. Potentially this could lead to future online systems that will greatly improve the absolute accuracy and reliability of our temperature measurement. We have all of the hardware necessary for this development except for spectrometers. Capital equipment money was included in our budget from COMPRES last year to allow us to buy a fiber laser. The William's report allowed us to make the case for new lasers with the ALS management and they helped pay for the new lasers. We therefore have capital equipment money for new spectrometers for the off-line system.

3. Upgrade laser heating system.

The current laser heating set up is working well and COMPRES users are reporting satisfaction with it. Nevertheless we believe that we can significantly improve the reliability and absolute accuracy of this system, and decrease the time for optics alignment by a number of small upgrades:

- a. Install vibration damped support system for the laser optics table to improve stability.
- b. Install improved objective lens mount system to aid in alignment.
- c. Install pellicle beam splitters to reduce the number of ghost images.
- d. Install new spectrometers with motorized slits to allow change from imaging to dispersion mode with out entering the hutch.
- e. Improve temperature stability by installing a two loop temperature feed back system using both the laser power and light emitted from the sample to control the temperature on both sides.

We also aim to install a four-color imaging system to give an alternative and complimentary measurement of temperature distributions simultaneously with our current system.

4. Continue validation of on-line laser heating system.

We plan to continue the validation of the temperature measurement with determinations of the melting curves of Fe and Pt.

5. Support a program of outstanding scientific research.

We will continue to provide the current high level of support for COMPRES users of the beamline. Demand for the COMPRES time has risen to the current level of over demand which, we believe, will increase the quality of the research done. Also, the improvements in the reliability of the laser heating system should result in greater productivity.

If resources allow we will also endeavor to:

Commission resistive heating cell.

We have a new resistively heated diamond cell which should be capable of reaching temperatures in excess of 1000° C. We need to change the objective lens of the online ruby fluorescence system to allow us to measure pressure with the cell at temperature in it's heating shroud using SrBO₄ as the internal standard. We also need to check the accuracy of the temperature measurement. Once this is done and the system validated with a measurement of the thermal equation of state of MgO we will make this cell available for our general users.

Staff issues

We aim to have our new staff in post at the beginning of 2008. It will take some months before they are trained in the beamline operation and contributing fully to our program. We really need to make significant progress with improving and validating our laser heating system this year. We propose to use the available monies on visiting staff to provide address targeted issues in improving our laser-heating and temperature-determination systems.

Requested capital equipment

The determination of accurate and reliable temperatures of samples held in our diamond cells during laser heating is the biggest challenge facing our community at the moment. Our strategy is to provide a range of complementary temperature measurement systems to provide cross checks to aid in determining if the temperatures that we determine are reasonable. At present we have two dispersing spectrometers that image a line across the laser hot spot and are used to determine temperatures across that line. An alternative approach is to split the image of the hot spot into a number of beams that are then filtered by notch filters and imaged onto a CCD camera. From the point to point intensity of these images it is possible to build up a temperature profile of the whole laser heated spot. We can easily add such a system to operate in parallel with our current spectrometers. All we require is a suitable CCD detector and some optics. We estimate the cost will be about \$10,000 which we have included in our capial equipment request.

At the ALS we provide a complete high-pressure service. Diamond cells, gasketing materials and necessary gases are provided so that totally inexperienced geo-scientists may perform high-pressure experiments. Also, in order for our facilities to be at the highest level of usability and readiness it is important that our beamline scientists engage themselves in high-pressure research using our facilities. A certain level of consumable support is required to sustain these two activities. At the ALS \$10,000 is a normal yearly level of support for consumables on a superbend beamline. We therefore request this amount in our budget for next year.

Summary of COMPRES beamtime proposals

For the February to June 2007 scheduling period there was one COMPRES proposal for beamline 11.3 and for the July 2007 to December 2007 there was none. There was one other high-pressure proposal for beamline 11.3 during the July to December allocation period. On beamline 12.2.2 there were 13 proposals from COMPRES users asking for a total of 136 shifts of beamtime during the February to June allocation period and 16 proposals totaling 144 shifts of beamtime during the July to December allocation period. We were able to accommodate all of these proposals.

Summary of publications for 2006-2007

Publications from COMPRES users are beginning to appear in print. Most COMPRES user groups report successful use of their beamtime, with multiple publications in preparation. All publications arising from data collected on beamlines 12.2.2, 11.3 and 1.4 listed below.

COMPRES

S. Speziale, I. Lonardelli, L. Miyagi, J. Pehl, C. Tommaseo, and H-R. Wenk. **Deformation experiments in the diamond-anvil cell: Texture in Copper to 25 GPa**, *J. Phys. Condensed Matter.* 18, S1007-S1020, doi:10.1088/0953-8984/18/25/S08, (2006)

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

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

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

S.M. Clark, B. Colas, M. Kunz, S. Speziale and P.J.M. Monteiro, Effect of pressure on the crystal structure of ettringite, *Cem. Conc. Res.* **38** 19-26 (2007).
S. Speziale, V.E. Lee, S.M. Clark, J.F. Lin, M.P. Pasternak and R. Jeanloz, Effects of Fe spin transition on the elasticity of (Mg, Fe)O magnesiowustites and implications for the seismological properties of the Earth's lower mantle J. Geophys. Res., 112, B10212, doi:10.1029/2006JB004730.

J.C. Crowhurst, A.F. Goncharov, B. Sadigh, J.M. Zaug, D.Aberg, Y. Meng, B. Vitali-Prakapenka, **Synthesis and Characterization of Nitrides of Iridium and Palladium.** *Journal of Materials Research* In Press (2007).

A.E.Gleason, S. Parry, M. Kunz, W.A. Caldwell, A.R. Pawley and S.M. Clark, **Pressure Temperature Stability Studies of Talc and 10-Å Phase using x-ray diffraction**, *Am. Min.* In Press. (2007).

J. Yan, P. D. Adams, R. J. Angel, N. L. Ross, M. Rivers, J. B. Parise and S. M. Clark, **The Development of an Automated Data Analysis System for powder diffraction data collected using an area detector,** Submitted to J. Appl. Cryst. (2007).

S. Speziale, R. Jeanloz, S.M. Clark, S. Meenakshi, V. Vijayakumar, A.K. Verma, R.S. Rao and B.K. Godwal, **Axial ratio anomalies and Electronic Topological Transitions in Cd_{0.80}Hg_{0.20} at High Pressures, Physics of the Earths Interior, In Press (2007).**

Other

H.Y. Chung, M.B. Weinberger, J.B. Levine, A. Kavner, J.M. Yang, S.H. Tolbert, and R.B. Kaner **Synthesis of ultra-incompressible superhard rhenium diboride at ambient pressure**, *Science* 316 (5823): 436-439 (2007)

D.V.S. Muthu, B. Chen, B.A. Cook, and M.B. Kruger, **Effects of sample preparation** on the mechanical properties of AlMgB₁₄, High Pressure Research, In Press (2007).

C. Infrastructure Development Projects

C.1 Multi-anvil cell assembly project

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

In this year of COMPRES we have worked on the system for letting our users order the COMPRES multi-anvil cell assembles. It works in the following way: the users that want to do their own research with our cells simply request a quote, then we send one, which also indicates a commitment on our part to provide the assemblies. If the users then send a purchase order, we set about preparing the assemblies, packaging them and sending them. We have done this only for assemblies that have been extensively tested and proven, while the assemblies that are untested are provided free of charge as part of the development part of the project.

The COMPRES price structure includes 20% overhead on materials, but does not include the time of any of the PI's or of the COMPRES machinist. The PI's time is paid for by Arizona State University, while the machinist is paid for by COMPRES.

In the period since May 1, 2006, we have filled 26 orders totaling \$50,683.85. The level of interest has been significant, and in fact some inquiries had to be put on hold until the future because we had not yet geared up to the level necessary to accommodate them, and so the potential is even greater than this. It does seem that there is a strong need for this type of assistance in our community, and our feeling is that the demand is going to continue to increase in the near term. Table 1 is a current list of regular users of the standard assemblies.

In the process of going through these orders, we were also able to improve the production methods significantly, which makes it feasible to meet the existing and expected demand for these assemblies. Much of the improvements simply consisted of outsourcing some of the work to help us meet the demand. We found a company that can cut our ceramic blocks into square rods for us, so that our ceramic is now ready for us to machine without us having to cut it first, which took many hours per block on our saw. We also procured a "rod puller," which is an automated clawlike device that can grab the ceramic and advance it in the lathe, so that we don't have to intervene manually during the machining of a ceramic rod. We will now only have to intervene when a new rod needs to be loaded into the lathe, or when tools wear out and need replacement. The rod-puller is on-site but has not been set up and programmed yet – when it is it will save significant operator time. In fact, at that point we will probably be as efficient as we can be with specialty ceramics like LaCrO₃, and ZrO₂, which are absolutely necessary for multi-anvil research, but can only be purchased in small blocks and so are inherently somewhat inefficient.

The project also makes available small accessories for multi-anvil work, such as pellet dies, furnace-rolling dies and pins, assembly stands (dummies) and alignment plates for putting carbide nests together (nesting plates).

Finally, detailed instructions for the assemblies, including all the known calibration data, thermal gradient calculations, and other information are available for free download on the web. Our computer program for doing thermal gradient calculations is also available for free download, and is in use in several laboratories for helping with cell assembly design.

The supplying of these assemblies is combined with consultation on the performance and capabilities of the assemblies, discussions back and forth between the users and the project directors, and planning for further developments. The experiences the users have with the assemblies are used for further design improvements, or when the assemblies already work very well, they are used for more detailed characterization of pressure, temperature, and capabilities of the assemblies. Several beam times have occurred in this period, including the August 2006 ASU beam time at GSECARS where assemblies and CsCl pressure standard were characterized, a March, 2007 NASA beam time at GSECARS where improvements in the pressure-temperature capabilities of the 8/3 assembly were proven on-line and an upcoming beam time in November 2007 with Jie Li using the 10/5 *in-situ* assembly. Kurt Leinenweber attended all these beam times as part of the cell assembly effort.

We have been working with several companies to try to make zirconia parts that are equivalent to our machined ones, and can be used in their place. We are making progress on it, but this has proven to be one of the more difficult goals, and we have not succeeded yet though we are getting closer. Extruded tubing is being attempted at Du-co Ceramics, and though there are still problems with cutting and grinding the material without chipping it, that process is nearly working and the company is still engaged with us trying to fix the problems. That will take care of the zirconia "middle sleeves" such as those used in the Bayreuth-style 14/8 assembly. Prototype pieces of the material have already been tested and it is a good replacement for the machined pieces. And, for the first time, we have also succeeded in getting an injection-molding company to try developing a porous zirconia for molding. That project is currently in progress at the company, where different firing conditions are being tested to achieve the desired porosity of 30%. This will allow complex shapes to be made, and our intention is to use it for parts with thermocouple grooves and for molding compound parts that will replace two of the current parts in the 14/8 box furnace assembly. Another effort to use pressed zirconia has been discontinued because that material caused carbide failure and blowouts, exemplifying how tricky the development of suitable zirconia has been.

We have also, as planned in the original proposal, developed new designs for larger assemblies, the 18/12 and 25/15 assemblies. The purpose of this is to develop the lower-pressure, higher-volume end of the assembly series. These new designs will be presented at the Fall 2007 AGU meeting (see references). These are still prototype designs and have not been developed for larger-scale production yet, but are currently available in small quantities for testing purposes free of charge.

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Leinenweber, K. Development of a CsCl pressure standard and a series of multi-anvil cells for in-situ high-pressure experiments, with examples of some recent results. Abstract for International Workshop on Synchrotron High-Pressure Mineral Physics and Materials Science. 6-7 December 2007, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois USA

Table 1. Users

Institution:	Primary users:
Arizona State University	Kurt Leinenweber, Thomas Sharp, Ulrich
	Haussermann, James Tyburczy
Australian National University	Robert Rapp
California Institute of Technology	Jed Mosenfelder, Jennifer Jackson
Lawrence Livermore National Laboratories	Julien Siebert
NASA Johnson Space Center	Kevin Righter, Lisa Danielson
National Cheng Kung University, Taiwan	Jennifer Kung
State University of New York at Stony	Liping Wang, Baosheng Li, Jiuhua Chen
Brook	
University of Arizona	Mike Drake, Kenneth Domanik
University of California at Davis	Charles Lesher, Alisha Clark
University of Chicago, GSECARS	Yanbin Wang
University of Delaware	Gabriel Gwanmesia
University of Hawaii	Murli Manghnani, Roni Greenberg
University of Illinois at Urbana-Champaign	Jie Li, Bin Chen
University of Minnesota	Tony Withers
University of Reykjavik, Iceland	Siggurdur Jacobsson
University of Western Ontario	Rick Secco

C. 2 High-resolution Inelastic X-ray Scattering at High P & T:

[Wolfgang Sturhahn¹, Jennifer M. Jackson², Jay D. Bass³]

1: Argonne National Laboratory, Argonne, IL 60439

- 2: California Institute of Technology, Pasadena, CA 91125
- 3: Geology Department, University of Illinois, Urbana, IL 6180

Report Summary

We report here on the activities to date of Year 1 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 last year to COMPRES, and it was funded for the first year with the Executive Committee's expectation of continued funding for the next year of the project. We include here a description of activities to date, planned activities for the coming year, and a budget request for Year 2 of the project.

High-resolution inelastic x-ray scattering (IXS) techniques provide the Earth and planetary science community with opportunities for new and exciting results on the properties of materials at high pressure and temperature conditions. Our infrastructure development project is aimed at outreach to the COMPRES community on the capabilities and use of these techniques and at creating state-of-the-art IXS techniques for characterizing the properties of materials under the high-P-T conditions of planetary interiors. We are pursuing the development of two related techniques: Nuclear Resonant Scattering (NRS), which provides information on electronic, vibrational, and elastic properties, such as the density of states and sound velocities, and momentum-resolved IXS which directly gives the dispersion relation of low-energy collective excitations to provide directional information on vibrational and elastic properties, such as the elastic tensor and sound velocities. Both methods are in many ways ideally or even uniquely suited for addressing a number of important geophysical questions.

In the first year of our infrastructure development project, we focused on the hiring of a full-time postdoctoral researcher to support the goals laid out in the original proposal text. We initiated high pressure experiments at the new IXS beam line (sector 30-ID) of the Advanced Photon Source and improved the experimental capabilities of the NRS beam line (sector 3-ID) to enhance its performance in high-pressure research. Both beam lines are now accessible to the COMPRES community. Outreach activities, e.g., an upcoming workshop on high-resolution IXS and various presentations at meetings and conferences, have broadly disseminated information on applications of NRS and IXS to understand Earth materials. In particular, we accomplished the following tasks:

- 1. Identified candidates and hired of a full-time postdoctoral researcher in November 2007;
- 2. Started to organize the workshop "High-resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation", March 2008 at Argonne;
- 3. Generation of new proposals for sectors 3-ID and 30-ID by COMPRES members.

- 4. Installation of a new focusing mirror at 3-ID for increased x-ray intensity;
- 5. Installation of image plate device for NRS with x-ray diffraction at 3-ID.

The individual items are described in more detail below.

1. Hiring of Postdoctoral Researcher

The position for the postdoctoral researcher was advertised in EOS and through the COMPRES email system. We received three applications from suitable candidates. The position was then offered to Dr. Hasan Yavas who accepted the offer and will start on November 15, 2007. We decided to offer this position to Hasan because of his experience of working with synchrotron radiation in general and with inelastic x-ray scattering techniques in particular. Hasan is located full time at the APS. He would also be coorganizing the workshop on high-resolution inelastic x-ray scattering that is planned for March 2008.

2. Workshop Organization

We are planning to organize a workshop on "High-resolution Inelastic X-ray Scattering on Earth Materials using Synchrotron Radiation", to take place in May, 2008 at the APS pending on the support requested from COMPRES separately. Participants would learn about the capabilities and the theoretical background of IXS methods, visit sectors 3-ID and 30-ID at the APS where high-resolution IXS is performed. The goals are formulated as follows:

- provide a basic introduction of high-resolution IXS to the Earth science community;
- define the state-of-the-art of high-resolution IXS especially at high pressure;
- > discuss the applications to important geophysical problems;
- develop productive collaborations;
- > address common experimental issues confronting users.

This workshop would provide an ideal format to collectively address possible solutions to experimental problems and will help to build a viable COMPRES user base for this facility. Details on the workshop agenda could soon be available on the APS web-site.

3. Generation of New Proposals

In the time period starting May 2007, we were able to catalyze eight new beam time proposals for NRS studies at sector 3-ID and six new beam time proposals for IXS studies at sector 30-ID from COMPRES member institutions. Proposals from COMPRES member institutions were among the first-ever high-resolution

experiments allocated beam time at the new sector 30-ID beam line (see Fig. 1). Many proposals over the last year have produced novel results, e.g., to be presented in "Effect of alloying elements on the magnetic transitions in iron-rich alloys" by J. Li et al. (UIUC), "The Electronic Structure of Iron in (Mg,Fe)SiO₃ Perovskite and Post-Perovskite Under Megabar Pressures" by J.M. Jackson et al. (Caltech), "Synthesis and Crystal Structure of Ferric-Rich MgSiO₃-Perovskite" by K. Catalli et al. (MIT), "Pressure-Induced Phase Transitions In Gadolinium Iron Borate" by S.A. Kharlamova et al. (APS), "Magnetic transition and sound velocities of Fe₃C at high pressure" by L. Gao et al. (UIUC), Abstracts for Fall 2007 AGU meeting, San Francisco. Several papers based primarily on data obtained at 3-ID or 30-ID are in preparation.

With improvements of the x-ray intensity, e.g., by the mentioned mirror upgrade project, we are addressing the present oversubscription of sector 3-ID. Also the total amount of NRS beam time in sector 3-ID was increased by 20 % with the beginning of operations at the new IXS beam line 30-ID.

4. Installation of New Focusing Mirrors

Experiments with small samples require a small x-ray beam. In particular, high-pressure studies with sample sizes of 50 μ m or less benefit tremendously by focusing of the x rays. At sector 3 Kirckpatrick-Baez mirrors are implemented for this task. The spatial acceptance of the system is determined by mirror size, incident angle of the x rays, and energy of the x rays. At 14.4 keV the vertical and horizontal acceptance of about 300 μ m and 700 μ m, respectively, have been upgraded to about 400 μ m and 1.6 mm by installation of new mirrors of 20 cm and 60 cm length (see Fig. 2). The longer horizontally focusing mirror has a piezo-electric bending mechanism build into the mirror itself for optimal shape adjustment and captures most of the x-ray beam at 14.4 keV. The x-ray flux on the sample doubled, and this increase in flux directly translates to enhanced capabilities, either by reduction of data collection times (crucial for experiments at very high temperatures) or by increased statistical accuracy.

5. Installation of Image Plate Device

An image plate device has been installed at the sector 3-ID NRS beam line (see Fig. 3). This addition of an x-ray diffraction capability can provide us with structural confirmation as well as with an equation-of-state during NRIXS data collection. The possibility to perform NRS (for sound velocities and elastic parameters) and x-ray diffraction (for density, elastic parameters, and structure confirmation) simultaneously under high pressure and temperature conditions will be groundbreaking.

Planned Activities

In Year 2 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 will organize a second tutorial workshop introducing high-resolution IXS and its applications for studying planetary interiors. 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. This will include optical microscopes and x-ray CCD cameras for in-situ alignment of samples depending on APS capital equipment funding. The successful completion of all these tasks depends on a dedicated postdoctoral researcher like Dr. Hasan Yavas who we will hire in November 2007. We expect that proposals for NRS experiments on sector 3-ID and IXS experiments on sector 30-ID will likely result from the workshop, and that Hasan will work with the PIs to develop effective proposals that will be very competitive for beam time. In effect, COMPRES will have it's own expert to help write proposals, consult on technical aspects of experiment design, and to help run experiments. This should be a significant fraction of his workload in Year 2.

Illustrations





C. 3 Ongoing Infrastructure Development Projects from COMPRES I

In addition to the two Infrastructure Development projects for which funding was renewed in Year #1 of COMPRES II [see reports in Sect. C.1 and C.2], there was progress on Infrastructure Development projects which had received no-cost extensions to complete their goals beyond the end of the first 5 years of COMPRES I. We report that progress briefly in this section of the report.

Gas-loading system for diamond-anvil cells

[Mark Rivers, University of Chicago]

In January 2008, commissioning of a new gas-loading system for diamond-anvil cells was completed at GSECARS at the APS. The team successfully loaded a diamond cell with Heat 23,000 PSI (about 1580 bar) and was able to accurately close the cell by watching the pressure increase with the on-line ruby fluorescence system. The system is currently able to load symmetic cells. Additional clamping mechanisms for other cell designs will be built soon. The system is now "open for business" and several investigators have already taken advantage of it.

Congratulations are due to Mark Rivers and his team of Clayton Pullins, Fred Sopron, Ellen La Rue, Guy Macha, Mike Jagger, Vitali Prakapenka, and others for their work in building this system. Support was provided by NSF-EAR via COMPRES and GSECARS.

A feature article on this new system will appear in the February 2008 issue of the COMPRES Newsletter.





CO₂ laser-heating system for diamond anvil cells.

[T. Duffy, Princeton University; V. Prakapenka and D. Heinz, University of Chicago; G. Shen, Carnegie Institution of Washington]

A newly-designed CO_2 laser-heating system for diamond anvil cells was installed on the 13ID-D station of GSECARS in early 2007. Commissioning of the system and initial experiments by local users ensued, with the system to be available for general users in mid-2008.



<u>Monochromatic side-station for angle-dispersive X-ray diffraction at X17B2</u> [J. Chen, Stony Brook University]

A fully functional monochromtatic side-station running simultaneously with the main energy-dispersive station at the X17B2 beamline at the NSLS has been installed and commissioned in 2007., thereby enabling studies of deformation and melt properties.





The side-station at X17B2 not only doubles the beamtime for high pressure experiments but also broadens the experimental capacity for different measurements. For the first time, Couvy *et al* are able to characterize the stress field of a shear deformation configuration using the side station.

Helene Couvy performing rheological experiment on MnGeO₄.

Brillouin spectroscopy in conjunction with synchrotron X-radation [J. Bass, University of Illinois at Urbana-Champaign; V. Prakapenka, University of Chicago]

A Brillouin spectroscopy system developed by Jay Bass and his team at the University of Illinois at Urbana-Champaign has been installed and commissioned on the 13 BM beamline at the GSECARS sectors of the APS.

Initial experiments include work on the post-stishovite phase transition in hydrous alumina-bearing SiO_2 by D. Lakshtanov and colleagues. <u>Proceedings of the National Academy of Science</u>, <u>104</u>, 13588-13590, 2007.

Fig. caption. Acoustic velocities (solid symbols) and squares of the Raman frequencies (open symbols) across the rutile-CaCl₂ phase transition in K324 stishovite. Solid line – linear fit to square of the Raman frequencies; dashed line indicates P_{tr} derived from the Raman



<u>Johnson noise thermometry</u> [Yanbin Wang, University of Chicago, and Ivan C. Getting, University of Colorado]

Realistic signals have been observed with the Johnson Noise Thermometer in a multianvil high pressure cell in the GSECARS hutch at APS with the synchrotron running. Complex electrical issues involving the heater power supply, ground loops, shielding, and cable geometry have been successfully addressed. First high temperature data were recorded up to 800 K.



Figure: Numerically correlated output recorded in the Johnson noise thermometry (blue squares) plotted against the product of sensor resistance and absolute temperature. Data were recorded in a large DIA cell at low pressure, 180 kN (~20 ton) load, ~ 100 MPa. Red line is the result from ambient bench test, by varying probe resistor only. Further investigation is needed to understand the deviation from the linear trend for the high temperature data above 450 K.

Calorimetry-on-a-Chip[

[A. Navrotsky and C. Lesher, UC Davis and F. Hellman, UCBerkeley]

Silicon micromachined calorimeters ("calorimeter on a chip") are used to measure heat capacities and phase transition enthalpies for thin film, single crystal, and powder samples (5 – 500 micrograms), compatible with samples made at high pressure.. The calorimetric entropy of the olivine - spinel transition in Fe₂SiO₄ (-16 \pm 5 J/mol·k) is in good agreement with that calculated from phase equilibrium data (-14 \pm 3 J/mol·K).



Comparison of the specific heat of the spinel phase of Fe_2SiO_4 as measured by calorimetry on a chip for a 108 microgram sample to that of olivine (measured by adiabatic calorimetry on about 10 g of sample). Entropy is shown in the inset.

D-DIA 30 Apparatus for Multi-Anvil Deformation Experiments to 30 GPa [Y. Wang and M. Rivers, University of Chicago; C. Lesher, UC Davis]

The DDIA-30 design work is in its final stage; most major components have been completed, detailing and peripheral component design work are being finished (see figure below). Parallel to the DDIA-30 designing effort, a DIA-26 module has been build, which is modified from the C3MA apparatus in Chip Lesher's lab at UC Davis and will enable us to conduct tests (starting in May 2007) using the 6/8 configuration, with 10 and 14 mm second-stage sintered diamond anvils for ultrahigh pressure generation.



Figure: The DDIA-30 module. Linear dimensions of the guide blocks are about 480 mm, and the entire module weighs about 300 kg.

Multi-anvil cell assembly project

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

Durham, Kohlstedt, Mei "Rheology of Earth's Interior", funded by BES

Kurt Leinenweber's infrastructural project in support of the COMPRES community has made a critical contribution to the progress of our high-pressure deformation research. In our D-DIA experiments on olivine at high pressure and high temperature we have had a persistent problem with conventional pressure media. They either have sufficient water content to water weaken the sample material, a phenomenon we wish to avoid, or they lack the mechanical competence to retain pressure at high loads, thereby preventing us from reaching high pressures. We recognized that a hybrid medium that combined the dry chemistry of the one with the mechanical competence of the other had the potential to solve our problems, and Leinenweber saw that such a configuration could be fabricated quickly and at reasonable cost. He proceeded to do so, under the auspices of the COMPRES infrastructure project, and our research was able to move forward. Within less than one year we went from concept, to execution, to carrying out successful experiments, to writing and submitting a paper presenting results on activation volume for creep in olivine (Durham et al., submitted). See next page for a couple of photos.

W. B. Durham, S. Mei, D. L. Kohlstedt, L. Wang, N. A. Dixon, New measurements of activation volume in olivine under anhydrous conditions, *Phys. Earth Planet*. *Interiors*, submitted.





Shown above is the new hybrid D-DIA cell. (a) Cube parts. A 6-mm diameter mullite sphere is cradled and lightly cemented between two pieces of unfired pyrophyllite to form a solid cube of 6-mm edge length. The pyrophyllite has excellent pressure-sealing properties but its water content is undesirably high for the experiments; the mullite is bone dry, but too friable to hold a pressure seal. (b) Appearance of cell following testing in the D-DIA. Gasketing "fins" (some are broken off) of pyrophyllite have been extruded at the edges the cubic cell, now approximately 5 mm in edge length. A spot of mullite is visible on the front face, but no mullite has extruded into the gaskets. The top of the deformation column is visible at the center of the top face.

D Budget Request for Year #2

<u>Budget Request for Year #2</u> [June 1, 2008 to May 31, 2009]. Details may be seen in the NSF 1030 Forms and the associated budget justification pages which are in the appendices to this report.

The COMPRES budget request for \$2,100,000 for <u>Year #2</u> [June 1, 2008 to May 31, 2009] is comprised of three major components (units of \$K, which include fringe benefits and indirect costs):

D.1 Community Facilities-operational budgets

\$240K for ops \$10K for equip	West Coast Synchrotron Facilities [R. Jeanloz and S. Clark]	
\$280K for ops \$200K for equip	X-ray, Diamond-anvil cell facilities at the NSLS [T. Duffy and D. Weidner]	
\$180K for ops \$45K for equip	Infrared, Diamond-anvil facilities at the NSLS [R. Hemley and Z. Liu]	
\$315K for ops \$60K for equip	Multi-anvil Press Facility at the NSLS [D. Weidner and M.Vaughan]	
\$20K	Beamline user housing	
\$1035K for ops	Total operational budget for Community Facilities	
\$315K for equip	5K for equip See details above	

D.2 Infrastructure Development Projects

\$35K	Nuclear Resonant Scattering at High P & T:A New Capability for the COMPRES Community [W. Sturhahn, J. Jackson, and J. Bass]		
\$100K	Multi-anvil Cell Assembly Initiative: New Developments and Production [K. Leinenweber, T. Sharp, and J. Tyburczy]		
\$91	Workshops (5 to 7 per year)		
\$226K	Total for infrastructure development projects		
D.3 Other	COMPRES Activities		
\$130K	Other Community Activities which includes		
\$90K	Annual Meeting		
\$30K	Travel for committees (including that of Advisory Committee,		
Executive Committee and Standing Committees)			
\$10K	COMPRES lecture series		
\$394K Central Office which includes: [all items have indirect costs incorporated]			
\$346]	X Salaries and fringe benefits		
\$15K	Materials and Supplies		
\$20K	Travel		
\$13K	Consultant services for website design		

\$524K Total for Other COMPRES Activities

TOTAL BUDGET REQUEST FOR YEAR #2 OF COMPRES II

\$1035K	Operational costs for Community Facilities
\$315K	Equipment upgrades for facilities
\$226K	Infrastructure development projects
\$130K	Other Community activities
\$394K	Central Office

\$2100K Total of budget request

* Note: Budget Impact Statement attached requesting restoration of \$100,000 increment authorized in the Cooperative Agreement of April 2007, thereby bringing the total funding requested for Year #2 to \$2200K.

E. Detailed Original Signed Budgets on NSF 1030 forms and Budget Justifications For COMPRES Budget Request for Year #2 [June 1, 2008 to May 31, 2009]

\$1,490,000	Total for Stony Brook budget for Year #	ŧ2
\$374,803	Multi-anvil X-ray facility at the NSLS	D. Weidner and M. Vaughan
\$479,999	Diamond-anvil –ray facility at the NSLS	T. Duffy and D. Weidner
\$635,198	Central Administrative Budget	R. Liebermann
A. Budgets a <u>Amount</u>	and justifications for Stony Brook Univers Purpose	sity [R. C. Liebermann, PI] Principal Investigator

B. Buddgets and justifications for COMPRES II Subawards for Year #2 [June 1, 2008 to May 31, 2009]

\$610,000	Total for existing Subawards for Year #2 [June 1, 2008 to May 31, 2009]			
		and J. Tyburczy		
\$100,000	Arizona State University	K. Leinenweber, T. Sharp		
\$35,000	University of Illinois	J. Bass and W. Sturhahn		
\$225,000	Carnegie Institution of Washington	R. Hemley		
\$250,000	University of California, Berkeley	R. Jeanloz and S. Clark		
Current Subawards-extensions from Year #1 to Year #2				
<u>Amount</u>	Institution	Principal Investigator		

No new Subawards for Year #2

\$610,000 Total of SubAwards for Year #2 [June 1, 2008 to May 31, 2009]

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

* Note: Budget Impact Statement attached requesting restoration of \$100,000 increment authorized in the Cooperative Agreement of April 2007, thereby bringing the total funding requested for Year #2 to \$2200K.

Detailed NSF 1030 Budget Forms and Budget Justifications deleted in this website version as they contain confidential salary information.

F. Supplemental Information

Fig. 1. Jennifer Jackson and June Wicks from Caltech preparing for experiment at the new inelastic X-ray scattering beamline at ID-30 of the Advanced Photon Source.

Fig. 2. Customized cell of a mullite sphere and pyrophyllite cradles for D-DIA apparatus fabricated in multi-anvil cell development program at the Arizona State University by Kurt Leinenweber and colleagues for deformation experiments at the X17B2 beamline of the National Synchrotron Light Source.

Fig. 3. The DDIA-30 module for new multi-anvil deformations experiments to 30 GPa, being developed by Yanbin Wang and Mark Rivers at the University of Chicago and Charles Lesher at UC Davis as an Infrastructure Development project of COMPRES. D-DIA 30 Apparatus for Multi-Anvil Deformation Experiments to 30 GPa

Fig. 4. 2007 Annual Meeting of COMPRES at Lake Morey Resort in Fairlee, Vermont.



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