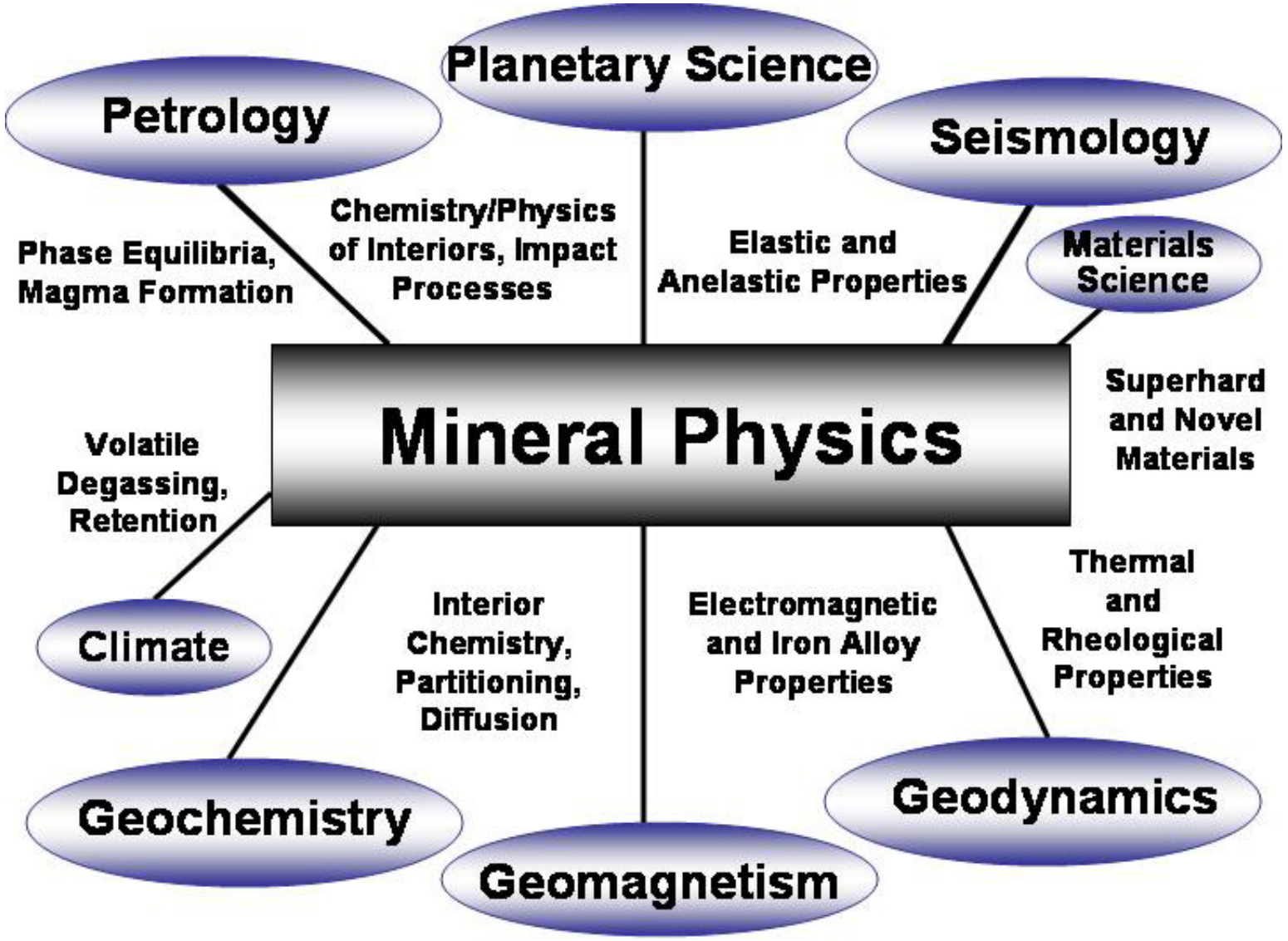
# Year 4 Annual Progress Report of

# Consortium for Materials Sciences Research in Earth Sciences

# COMPRES

February 2006


Planetary Science
Petrology
Seismology
Chemistry/Physics of Interiors, Impact Processes
Phase Equilibria, Magma Formation
Elastic and Anelastic Properties
Materials Science
Mineral Physics
Superhard and Novel Materials
Volatile Degassing, Retention
Climate
Interior Chemistry, Partitioning, Diffusion
Electromagnetic and Iron Alloy Properties
Thermal and Rheological Properties
Geochemistry
Geomagnetism
Geodynamics

# *A COMPRES Year 4: Overview*

## A.1 Executive Summary

In 2005, 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. There are now 45 U. S. institutions which are voting members of COMPRES [the Electorate] and another 20 non-voting institutions overseas which have affiliate membership.

COMPRES has sponsored and/or organized many workshops and scientific meetings in 2005. These include the COMPRES Fourth Annual Meeting at the Mohonk Mountain House in New Paltz, NY in June and a High Pressure Summit Meeting on Long Island in September. Other workshops: (1) "Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation," at the Advanced Photon Source in February; (2) "Multi-Anvil Techniques" at the Advanced Photon Source in March; (3) "High-Pressure Melts," in Albuquerque, NM in July; and (4) "Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science," at the National Synchrotron Light Source in November.

In March 2005, a new poster was created for COMPRES based on the report on "Current and Future Directions of Research in High-Pressure Mineral Physics", otherwise known as the "Bass Report". A copy may be downloaded from the Publications page of the COMPRES website. Full-size, glossy copies at 24" x 36" of this poster were available at the 2005 Annual Meeting and may be requested from Ann.Lattimore@stonybrook.edu. See also Fig. 1 of this report.

In October 2005, a feature article entitled "The Future of High-Pressure Mineral Physics" appeared in EOS in the 4 October 2005 issue [Vol. 86, No 40, pp. 365, COMPRES Home Page at http://www.compres.stonybrook.edu/Publications/RCL%20EOS%20MS/Published_article.pdf

Fig 1. of this article showing the linkages between mineral physics and other Earth science fields appears as the frontispiece to this Annual Report.

In this section of the Annual Report for Year #4, we present an overview of the activities of COMPRES. Subsequent sections include detailed reports from each of the

Community Facilities operations and Infrastructure Development projects supported by COMPRES. The final section presents the budget plan for Year #5 [May 1, 2006 to April 30, 2007]; 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 Brillouin spectrometer has been developed by Jay Bass and his team at the University of Illinois at Urbana-Champaign and installed on sector 13-BM-D at the Advanced Photon Source in collaboration with the staff of GSECARS. See details in the November 2005 issue of the COMPRES newsletter.

A Virtual Laboratory for Earth and Planetary Materials 9VLab) has been established at the University of Minnesota under the leadership of Renata Wentzcovitch with four-year funding from the Information Technology Research Program of the NSF. See details in March 2005 issue of the COMPRES newsletter and in Sec. C.3 below. A team led by Malcolm Nicol and Przemek Dera was awarded a Major Research Instrumentation grant by the NSF for "Development of Six New Approaches for Micro-focus Single-Crystal X-ray Diffraction for Materials Structure Research at Synchrotrons". This proposal was an outgrowth of a COMPRES-sponsored workshop organized by Dera and Charles Prewitt at the APS in November 2004.

Synchrotron-based infrared spectroscopy facilities at the U2A beamline of the National Synchrotron Light Source have been used by Steve Jacobsen and colleagues to study the high-pressure behavior of near-IR absorption bands in single-crystal samples of hydrous wadsleyite and laser-heated hydrous ringwoodite in a diamond-anvil cell. See details in Sect. B.2.

The National Synchrotron Light Source at Brookhaven National Laboratory has approved four Contributing User Agreements with COMPRES to operate high-pressure facilities at the superconducting wiggler X-ray beamline (X17) and the ultraviolet beamline (U2A), with teams from the Carnegie Institution of Washington, Stony Brook University and the University of Chicago.

Deformation of rocks and minerals: New experimental technologies for rheological experiments at high pressures and temperatures; see details in Sec. B.3.

A new high pressure deformation apparatus D-DIA has been married to the synchrotron x-ray source at the multi-anvil beamline at the NSLS. The D-DIA can generate pressures of 8 GPa in an apparatus of cubic-anvil geometry.

A rotational Drickamer-type apparatus [RDA] for high-pressure, temperature, large strain rheological experiments has been developed by Shun Karato and his team at Yale University and installed on the multi-anvil beamline at the NSLS.

## A.3 Meetings and Workshops

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

**Workshop on Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation**
February 11-13, 2005
Organizers: Wolfgang Sturhahn, Jay Bass and Michael Lerche
Advanced Photon Source of the Argonne National Laboratory
This workshop brought together more than 30 people, including experts in these techniques and new potential users from the COMPRES community. See additional details in the March 2005 issue of the COMPRES newsletter and on the COMPRES website at: http://www.nrs2005.aps.anl.gov.

**Workshop on Multi-Anvil Techniques**
March 1-3, 2005
Organizers: Kurt Leinenweber, Charles Lesher and Yanbin Wang
GSECARS Beamlines at the Advanced Photon Source of the Argonne National Laboratory
See report in the July 2005 issue of the COMPRES newsletter and other details at:
http://cars9.uchicago.edu/gsecars/LVP/LVP_workshop_05/Main_index.htm

**Third Biennial Conference of CeSMEC**
April 21-23, 2005
Organizers: Surendra Saxena, Hexiong Yang and colleagues
Hotel Deauville, Miami Beach
More than 160 scientists from 20 countries attended, with a heavy emphasis on non-U. S. participants. The principle themes of the conference were high-pressure physics, solid state physics, and materials science. Additional details may be found at the meeting website: http://www.cesmec.fiu.edu/SMEC2005/. COMPRES was one of the sponsors and more than 29 members of the COMPRES community attended.

**Gordon Research Conference on Earth's Interior**
June 12-16, 2005
Organizers: Lars Stixrude
Mt Holyoke College, South Hadley, MA
This biennial included many fine invited talks: those from mineral physics were by Paul Asimow, Guillaume Fiquet, Daniel Frost, Kei Hirose and Jie Li.

**Fourth Annual Meeting of COMPRES**
June 16-19, 2005
Mohonk Mountain House, New Paltz, NY
Program Committee: Thomas Duffy, Harry Green and Abby Kavner
There were 109 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 11 industrial sponsors: Almax, Blake Industries, D'Anvils, Delaware Diamond Knives, Diacell, HKL, MAR-USA, Rigaku MSC, Rockland Research, Scimed, 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/2005-06-16-19/Index.html

**Workshop on Calorimetry-on-a-Chip**
June 17, 2005

Organizers: Alexandra Navrotsky and Frances Hellman
Mohonk Mountain House, New Paltz, NY
A mini-workshop was convened within the Annual Meeting to present and discuss the new infrastructure development initiative on application of nanotechnology to the study of ultra-small quantities of sample in calorimetry apparatus.

**Workshop on VLab**
July 20-23, 2005
Organizer: Renata Wentzcovitch
Minnesota Supercomputing Institute, University of Minnesota.
See report and other details at:
http://www.vlab.msi.umn.edu/events/workshops.shtml

**Workshop on High Pressure Melts**
July 20-22, 2005
Organizer: Carl Agee
Los Poblanos Conference Center, Albuquerque, New Mexico
The participants of this Workshop are preparing a Grand Challenge collaborative research proposal to submit to the NSF Earth Sciences Division, perhaps in the CSEDI program.

**3rd Workshop on Earth's Mantle Composition, Structure, and Phase Transitions**
August 30-September 3, 2005
Organizers: Guillaume Fiquet, Jay Bass, Kei Hirose, and James Badro
Saint Malo, France
This COMPRES-sponsored Workshop was attended by more than 35 people, including many young scientists from Europe and a large contingent from Fei's lab at the Carnegie Institution of Washington. The scientific program was excellent, the site superb, the excursions well-planned and interesting, and the weather remarkable for this time of year

in Brittany. See details of the program and associated activities at:
http://deep.earth.free.fr/

**Workshop on Neutrons at High Pressure**
September 13, 2005

Organizer: Yusheng Zhao
Los Alamos National Laboratory
This half-day workshop was held during the LANSCE Users Meeting at the Los Alamos National Laboratory. Keynote speakers included Yusheng Zhao of LANL on the conceptual design for a LAPTRON facility at LANSCE and Christopher Tulk of Oak Ridge National Laboratory on the design and progress of the SNAP project at the SNS, followed by discussion of the needs of users and tour of the high-pressure facilities at the Lujan Center.

**Elasticity Grand Challenge Workshop**
September 16-18, 2005
Organizer: Jay Bass
Stony Brook University
This working group meeting was attended by G. Gwanmesia of Delaware State University, L. Stixrude of the University of Michigan, R. Wentzcovitch of the University of Minnesota, and B. Li, L. Li, M. Vaughan, D. Weidner and Liping Wang of Stony Brook University. This is one of the four Grand Challenge initiatives submitted to the NSF contemporaneous with the COMPRES core proposal in August 2001; three of these were funded by EAR and have been an important scientific compliment to the COMPRES programs to support beamline operations at national facilities and nurture infrastructure development projects.

**High Presssure Summit Meeting**
September 24-25, 2005
Organizer: Robert Liebermann
Ronkonkoma, Long Island, NY
This meeting was held at the suggestion of David Lambert of the NSF-EAR and Nicholas Woodward of DOE-BES. Attendees include representatives COMPRES [H. Green, N. Ross, R. Liebermann], GSECARS [M. Rivers, S. Sutton], NSLS High Pressure Teams [D. Weidner, R. Hemley, M. Rivers, H-k. Mao], HP-CAT [H-k. Mao], SNAP [C. Tulk, J. Parise, R. Hemley, H-k Mao] ALS-High P Partners [S. Clark, J. Zaug, H. Green], CDAC [R. Hemley], LANSCE [Y. Zhao], and CHESS [D. Bilderback]. The attendees prepared a report which they presented en masse to the program managers of the NSF and DOE in Washington on November 29, 2005.
Special Topical Session on High Pressure Mineral Physics
October 17-19, 2005
Organizers: William Bassett, Russell Hemley and Anne Hofmeister
GSA Annual Meeting, Salt Lake City, Utah
This session was co-sponsored by the Mineralogical Society of America, Geophysical Laboratory of the Carnegie Institution of Washington and COMPRES. It celebrated Ho-kwang Mao's receipt of the 2005 Roebling Medal and covered a broad spectrum of

research in mineral physics. Areas that Dr. Mao pioneered were highlighted along with their importance to all geology.

**Workshop on Rheology and Elasticity Studies at Ultra High Pressures and Temperatures**
October 21-23, 2005
Organizers: Haozhe Liu, Hans-Rudi Wenk, and Thomas Duffy
This COMPRES-sponsored
**Workshop on Evaluation of Synchrotron Mossbauër Data**
October 29-30, 2005
Organizers: Wolfgang Sturhahn, Michael Lerche and Jay Bass
Advanced Photon Source of the Argonne National Laboratory
This workshop was designed to teach new users of the nuclear resonant inelastic scattering beamline at the APS to reduce their Mossbauër data.See details at: http://www.aps.anl.gov/News/Conferences/2005/Mossbauer_Data_Workshop/.

**Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science**
November 3-5, 2005
Organizers: Russell Hemley and Zhenxian Liu
National Synchrotron Light Source of the Brookhaven National Laboratory
More than 50 people attended this two-day formal workshop, of whom 47% were under 38 years of age and 23% were women. Following the workshop, the organizers arranged for students/postdocs were able to conduct real experiments at the U2A beamline supported by COMPRES. See details at:
http://www.nsls.bnl.gov/newsroom/events/workshops/ir./ and also a more complete report in the November 2005 issue of the COMPRES newsletter

**Workshop on New Directions in High-Pressure Science: Probing Extreme Conditions with Ultrashort X-ray Sources**
December 3, 2005

Organizers: by Simon Clark, Yogendra Gupta, Jerry Hastings, Russell Hemley and Raymond Jeanloz
Advanced Light Source of the Lawrence Berkeley National Laboratory
This COMPRES-sponsored workshop was attended by more than 81 people from the extended COMPRES community. Invited talks focused on (1) New ultra short pulse X-ray sources; (2) Overview of shock-wave techniques; (3) Status of shock-wave measurements and (4) Scientific challenges.

## 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 2005, there were 41 U. S. institutions which were members of COMPRES and 16 affiliate institutions overseas. In the past year, four new U. S. institutions have become members of COMPRES:

1 Lawrence Berkeley National Laboratory
2 Los Alamos National Laboratory
3 Ohio State University
4 University of Missouri at Kansas City

In addition, four overseas institutions became affiliate members of COMPRES:

1 Australian National University (Australia)
2 Ehime University (Japan)
3 National Cheng Kung University (Taiwan)
4 Vrije University (The Netherlands)

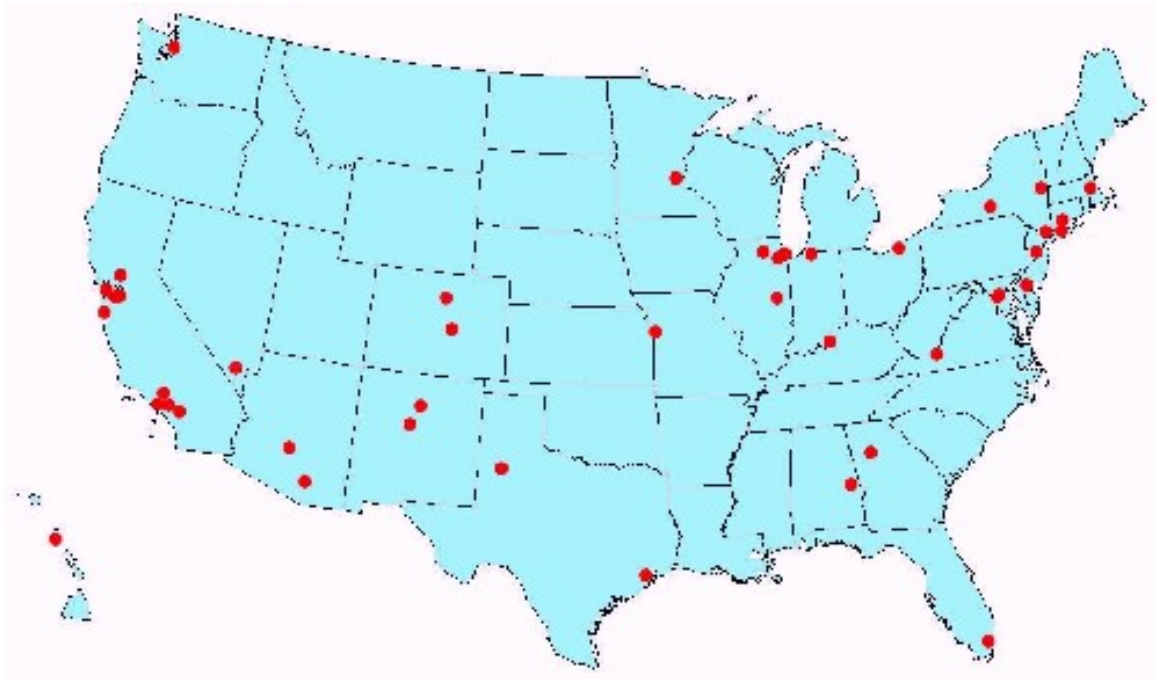
This brings us to a total of 45 U. S. institutional members and 20 affiliated members of COMPRES. They are listed in the following table and indicated on the maps.

**COMPRES Member Institutions**

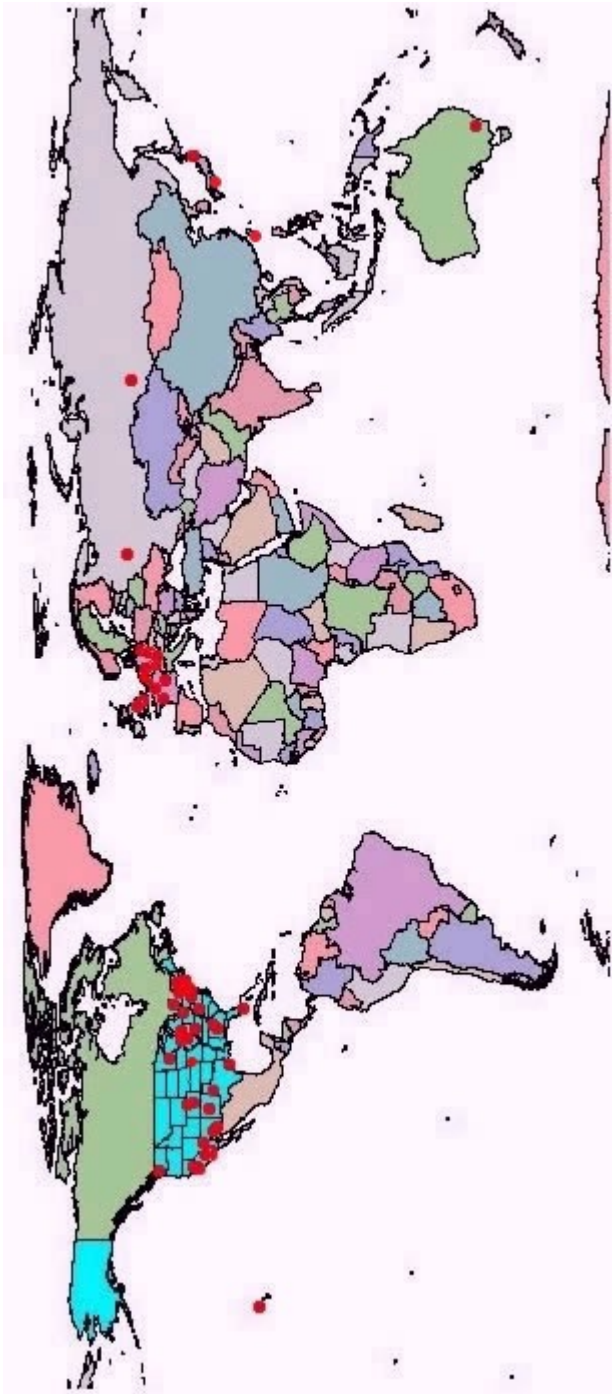
| Institution | Elector | Alternate |
|---|---|---|
| Argonne National Laboratory | Wolfgang Sturhahn | Marcos Grimsditch |
| Arizona State University | Thomas Sharp | James Tyburczy |
| Auburn University | Jianjun Dong | |
| Australian National University Canberra (Australia) | Hugh O'Neill | |
| Azusa Pacific University | Donald Isaak | |
| Bayreuth Universitat (Germany) | David Rubie | |
| California Institute of Technology | Paul Asimow | Thomas Ahrens |
| Carnegie Institution of Washington | Ronald Cohen | Yingwei Fei |
| Case Western Reserve University | James Van Orman | Nancy Chabot |
| Colorado College | Phillip Cervantes | |

| | | |
|---|---|---|
| Columbia University | David Walker | Taro Takahashi |
| Cornell University | Chang-Sheng Zha | William Bassett |
| Delaware State University | Gabriel Gwanmesia | Al Sameen Khan |
| Ecole Normale Supérieure de Lyon (France) | Jan Matas | |
| Ehime University (Japan) | Tetsuo Irifune | |
| Eidgenossische Techniche Hochschule Zurich (Switzerland) | Artem Oganov | |
| Florida International University | Surendra Saxena | Hexiong Yang |
| GeoForschungsZentrum Potsdam (Germany) | Frank Schilling | |
| Georgia State University | Pamela Burnley | |
| Indiana University at South Bend | Henry Scott | Jerry Hinnefeld |
| Institut de Physique du Globe Paris (France) | Guillaume Fiquet | |
| Institute of Experimental Mineralogy, Chernogolovka (Russia) | Yuriy Litvin | |
| Johnson Space Center , NASA | Kevin Righter | John Jones |
| Lawrence Berkeley National Laboratory | Simon Clark | Corwin Booth |
| Lawrence Livermore National Laboratory | Daniel Farber | William Durham |
| Los Alamos Natoional Laboratory | Yusheng Zhao | Gary Chesnut |
| Massachusetts Institute of Technology | San-Heon (Dan) Shim | Robert van der Hilst |
| Max-Planck Institute for Solid State Research, Stuttgart (Germany) | Paul Balog | |
| National Cheng Kung University (Taiwan) | Jennifer Kung | |
| Northern Illinois University | Mark Frank | Jonathan Berg |
| Novosibirsk State University (Russia) | Elena Boldyreva | |
| Ohio State University | Wendy Panero | Michael Barton |
| Princeton University | Thomas Duffy | Guust Nolet |
| Rensselaer Polytechnic Institute | Anurag Sharma | John Schroeder |
| Royal Institution of Great Britian, The (United Kingdom) | Paul McMillian | |
| Ruhr-Universitat Bochum (Germany) | Sumit Chakraborty | |
| Stony Brook University | Michael Vaughan | John Parise |
| Texas Tech University | Yanzhang Ma | Valery Levitas |
| Tohoku University, Sendai (Japan) | Eiji Ohtani | |
| Universite de Poitiers (France) | Jacques Rabier | |
| Universite des Science et Technologies de Lille (France) | Paul Raterron | |
| University College London (United Kingdom) | David Dobson | |

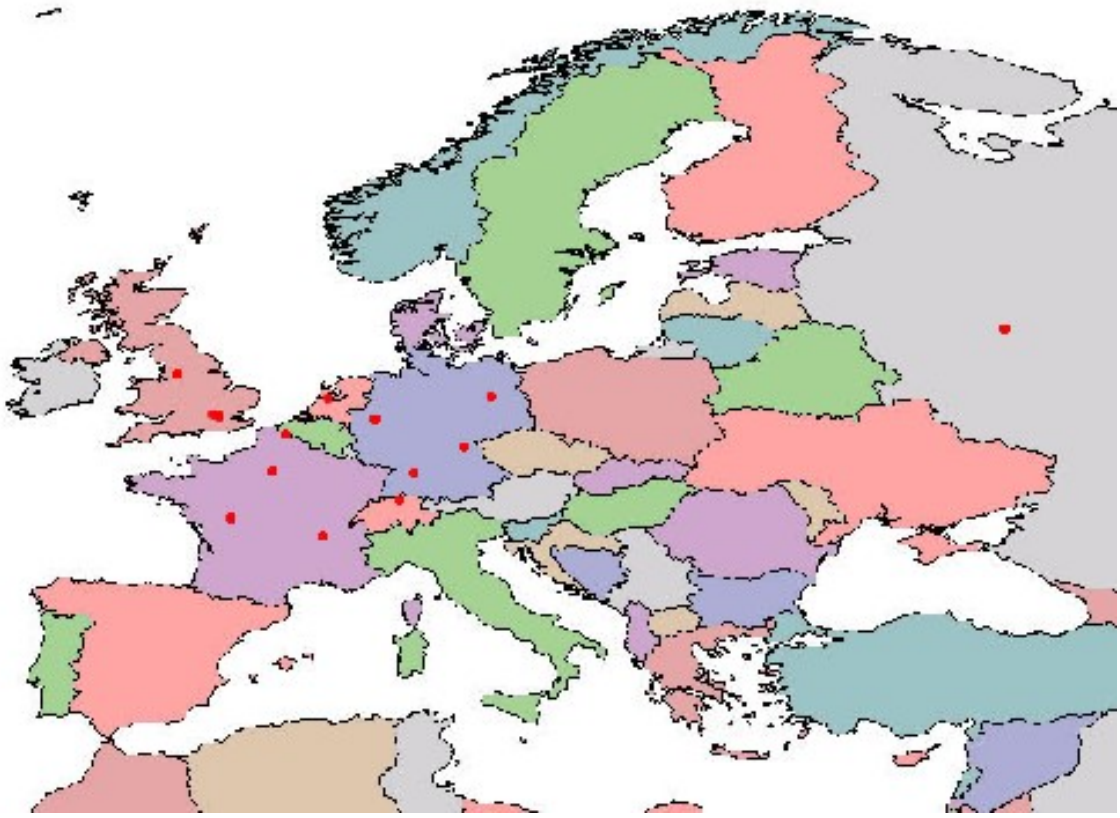
| | | |
|---|---|---|
| University of Arizona | Robert Downs | Michael Drake |
| University of California at Berkeley | Hans-Rudolph Wenk | Raymond Jeanloz |
| University of California at Davis | Charles Lesher | Alexandra Navrotsky |
| University of California at Los Angeles | Abby Kavner | Donald Isaak |
| University of California at Riverside | Harry Green | Stephen Park |
| University of California at Santa Cruz | Quentin Williams | Elise Knittle |
| University of Chicago | Dion Heinz | Mark Rivers |
| University of Colorado at Boulder | Joseph Smyth | Hartmut Spetzler |
| University of Illinois at Urbana-Champaign | Jay Bass | Jie Li |
| University of Hawaii at Manoa | Murli Manghnani | Li Chung Ming |
| University of Louisville | George Lager | |
| University of Manchester (United Kingdom) | Alison Pawley | |
| University of Maryland at College Park | Andrew Campbell | John Tossell |
| University of Minnesota | Renata Wentzcovitch | David Kohlstedt |
| University of Missouri - Kansas City | Michael Kruger | Ray Coveney |
| University of Nevada at Las Vegas | Oliver Tschauner | Malcolm Nicol |
| University of New Mexico | Carl Agee | David Draper |
| University of Washington | Ann Chopelas | Michael Brown |
| University of Western Ontario (Canada) | Rick Secco | |
| University of Wyoming | Jeffrey Yarger | David Anderson |
| Virginia Polytechnic Institute and State University | Nancy Ross | Ross Angel |
| Vrije Universiteit (The Netherlands) | Wim van Westrenen | |
| Yale University | Shun-ichiro Karato | David Bercovici |



Locations of COMPRES Institutional Members in the United States.



Locations of COMPRES Institutional Members Throughout the World.



Locations of COMPRES Institutional Members in Europe.

## A.5 Information Technology and Communications

### Web Site

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

(a) EOS Article "The Future of High-Pressure Mineral Physics" by Liebermann on behalf of COMPRES—4 October 2005
(b) Annual Reports to NSF for Years #1-3.
(c) ©COMPRES Booth Powerpoint presentation at December 2005 AGU
(d) Minutes of the Executive Committee
(e) Monthly Messages from COMPRES President
(f) Current and Future Research Directions in High-Pressure Mineral Physics
(g) The Bass Report [August 2004]
(h) 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. In 2004, this was made available online through a browser-based form

*Online Forms for meeting registration:* This offers online registration for meetings and workshops

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*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.

The 2005 issues have featured reports on the Virtual Laboratory for Earth and Planetary Materials (VLab at the University of Minnesota), COMPRES-sponsored Workshops, the 2005 COMPRES Annual Meeting, Beamline interns, recent PhDs in mineral physics, membership updates, and the Brillouin spectroscopy infrastructure development project (led by the University of Illinois at Urbana-Champaign for installation at the Advanced Photon Source).

These newsletters are edited by Jiuhua Chen and may be found on the COMPRES web site at www.compres.us/Newsletter/

In addition to a column in the quarterly COMPRES newsletter, the President of COMPRES [Robert Liebermann] has sent a Monthly Message to the COMPRES

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

*COMPRES Exhibition Booth at Fall 2005 AGU Meeting:*

At the Fall 2005 Meeting of the American Geophysical Union in San Francisco in December 2005, 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 Lazarx and Mark Rivers of GSECARS.

A Powerpoint presentation created for the COMPRES Booth by Jiuhua Chen can be found at www.compres.us/Meetings/2005-12-12-AGU-Powerpoint/COMPRESbooth05.ppt

## A.6 Publications of COMPRES

### Papers


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Amulele, G., M. Manghnani, B. Li, D.J. Errandonea, M. Somayazulu, Y. Meng, High pressure ultraonic and X-ray studies on SiC composite, J. Applied Physics, 2003 (accepted).

Angel RJ, Bismayer U, Marshall WG (2004) Local and long range order in ferroelastic lead phosphate at high pressure. Acta Crystallographica B-Structural Science 60:1-9.

Antao, S.M., Wang, L, Li, B., Chen, J., Benmore, C.J., Parise, J.B.: Acoustic anomalies accompanying structural changes in GeSe2 glass with pressure. In Preparation. (2005)

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Chen, B., D. Penwell, J.H. Nguyen, and M.B. Kruger, High Pressure X-ray Diffraction Study of Fe2B, Solid State Comm., in press, 2003. –X17C

Chen, J., D. J. Weidner, and M. T. Vaughan, Strength of Mg0.9Fe0.1SiO3 Perovskite at High Pressure and Temperature, Nature, 419, 824-826 (2002).

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Chen, J.H., T. Inoue, H. Yurimoto, and D.J. Weidner, Effect of water on olivine-wadsleyite phase boundary in the (Mg, Fe)(2)SiO4 system, Geophysical Research Letters, 29 (18), -, 2002b.

Chen, J; L. Li, D.J. Weidner and M. Vaughan, Deformation Experiments using Synchrotron X-rays: In situ stress and strain measurements at high pressure and temperature, Physics of The Earth and Planetary Interiors 143-144, 347-356, 2004.

Chen, J; Schmidt, N; Chen, JH; et al: "Yield Strength enhancement of MgO by nanocrystals", Journal of Materials Science, 40 (21): 5763-5766 Nov 2005

Chen, Jiuhua, Donald J. Weidner, Liping Wang, Michael T. Vaughan, and Christopher E. Young: "Density measurements of molten materials at high pressure using synchrotron x-ray radiography: Melting volume of FeS in "Advances in High Pressure Technology for Geophysical Applications" Elsevier, 185-194 (2005)

Chen, Jiuhua; Haozhe Liu, C. David Martin, John B. Parise, Donald J. Weidner: "Crystal chemistry of NaMgF3 perovskite at high pressure and temperature", American Mineralogist, 90 (10): 1534-1539 Oct 2005

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Couvy, Hélène (2005) Experimental deformation of forsterite, wadsleyite and ringwoodite: Implications for the seismic anisotropy of the Earth's mantle, Bayerisches Geoinstitut, Universität Bayreuth (Germany) and Laboratoire de Structure et Propriétés de l'Etat Solide, Université des Sciences et Technologies de Lille (France)

## 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.

During the fall, 2005 semester, Glenn Richard assisted Donald Weidner in the development of inquiry-based computer lab activities for GEO 305: Global Concerns. These activities engaged the students in the analysis of data to investigate issues such as energy sources and the effects of seismic events on human society. During the spring, 2005 he is developing similar activities for GEO 304: Energy, Mineral Resources, and the Environment that focus on geothermal energy.

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. In the fall of 2005, GEO 514 was taught by Glenn Richard, Steven Englebright, a University Adjunct who is a New York State Assemblyman, and Mirza Beg of the Center for Environmental Molecular Science. Each participant in CEN 514 is required to perform a research project or develop a lesson plan that is designed to familiarize secondary school students with Earth science as an investigative process.

In 2004 and 2005, Glenn Richard served as Founding Director of the Flax Pond Summer Institute, in which high school students and community members collected field data and created maps to investigate changes that are occurring in the distribution of biological communities in the Flax Pond salt marsh. He co-mentored Samantha Baer from Ward Melville High School as she conducted an investigation in Flax Pond for which she has been recognized as an Intel semi-finalist.
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

**Future Plans**

During the summer of 2006, Glenn Richard plans to co-mentor an REU student with Bill Holt. The student will develop strain rate models for the western United States. The output of the model will be represented in the form of raster maps of the western United States and numerical geospatial data that students can use in a GIS or other mapping tool to study the model.

## A.8 Management and Organization

### Executive Committee

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

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

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

A statement of the Polices and Procedures for the COMPRES Executive Committee can be found at:
http://www.compres.stonybrook.edu/People/Committees/ExComm%20Pol%20&%20Proc-revised%2010%20June%202004.doc

Current members and affiliation (term of service)

Harry Green, Chair, University of California at Riverside (2004-2007)
Jay Bass, University of Illinois (2003-2006)
Michael Brown, University of Washingtonb (2005-2008)
Donald Weidner, Stony Brook University )2004-2007)
Quentin Williams, University of California at Santa Cruz (2004-2007);
Vice Chair (2005-2007)

Previous members and affiliation (periods of service)

Thomas Duffy, Princeton University (2002-2003)
Russell Hemley, Carnegie Institution of Washington (2002-2004)
Shun-ichiro Karato, Yale University (2002-2005)
Donald Weidner, Chair, Stony Brook University (2002-2004)

### Facilities Committee

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

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

**Current members and affiliation (term of service)**

Mark Rivers, Chair (2003-2005), University of Chicago. Member (2002-2005).
Thomas Duffy, Princeton University (2003-2006)
William Durham, Lawrence Livermore National Laboratory (2005-2008)
Abby Kavner, University of California at Los Angeles (2004-2007)
Charles Prewitt, University of Arizona (2003-2006)

**Previous members affiliation (periods of service)**

Michael Brown, University of Washington (2002-2003)
Yingwei Fei, Carnegie Institution of Washington (2002-2005)
Harry Green, University of California at Riverside (2002-2004)
Quentin Williams (Chair), University of California at Santa Cruz (2002-2003)

**Infrastructure Development Committee**

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

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

**Members and affiliation (term of service)**

Nancy Ross, Chair (2004-2006), Virginia Polytechnic Institute and State University, Member (2003-2006).
Pamela Burnley, Georgia State University (2002-2005)
Russell Hemley, Carnegie Institution of Washington (2005-2008)
Kevin Righter, NASA Astromaterials Laboratory (2003-2006)
Sang-heon (Dan) Shim, Massachusetts Institute of Technology (2005-2008)

**Previous members affiliation (periods of service)**

David Walker, Columbia University (2002–2003)
Raymond Jeanloz, University of California at Berkeley (2002–2003)
James Tyburczy, Chair, Arizona State University (2002-2004)
Yanbin Wang, University of Chicago (2002-2005)

**Advisory Committee**

**Members and affiliation (term of service to be determined)**

Bruce Buffett, University of Chicago
Chi-chang Kao, Brookhaven National Laboratory
Guy Masters, University of California at San Diego
Richard O'Connell, Harvard University
Paul Silver, Carnegie Institution of Washington

On 17 June 2005, the Advisory Committee met with the Executive Committee during the Fourth Annual COMPRES Meeting in New Paltz, New York.

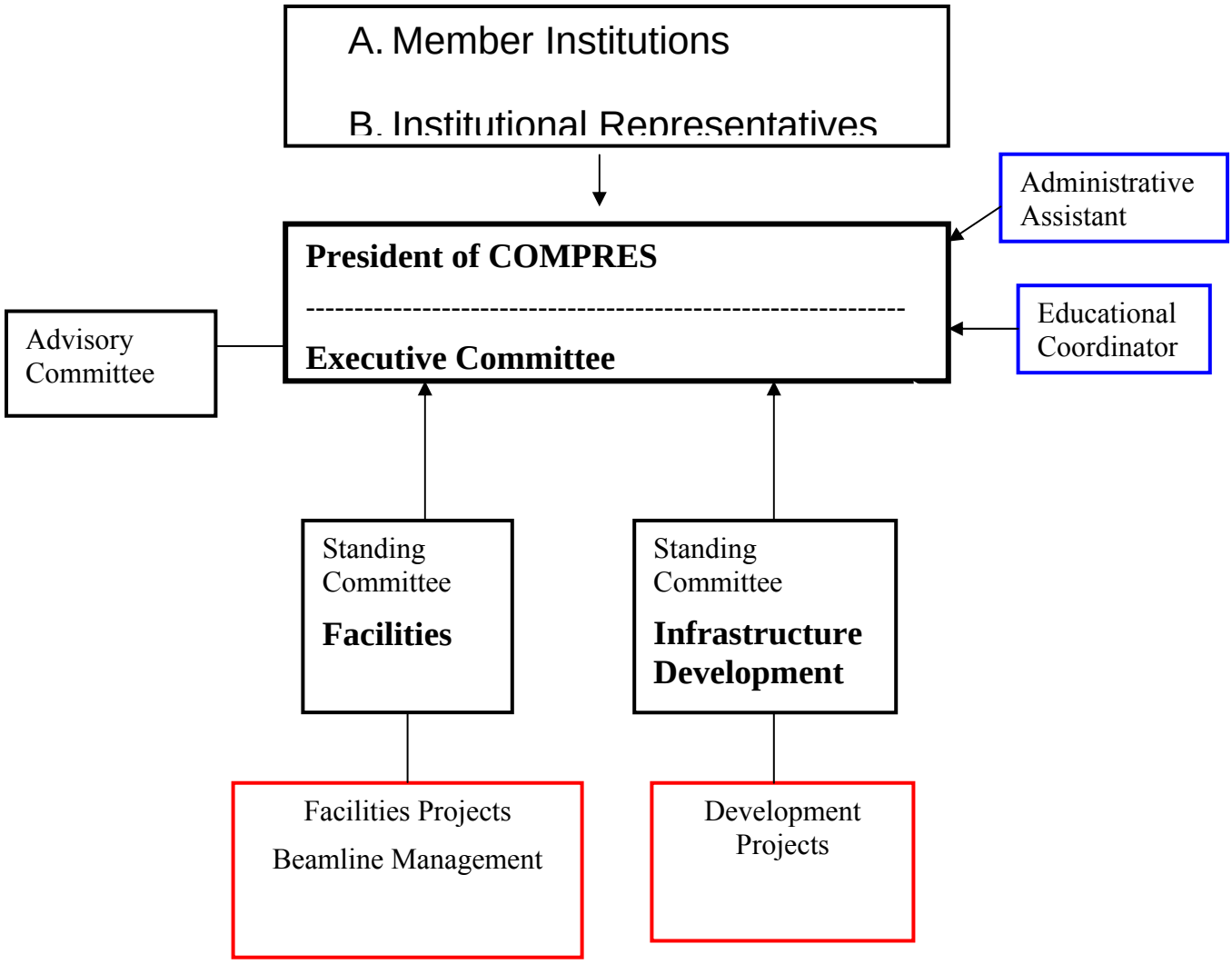
**Relationship to National Facilities**

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, along 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 1, 2003) and Ann Lattimore, Administrative Assistant, both of whom are supported by the COMPRES Collaborative Agreement with the NSF.

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. Lattimore to provide administrative support to COMPRES activities.

In addition to the MPI staff contributions, we have profited from the advice and logistical support of three staff members of the Department of Geosciences at Stony Brook: Owen Evans, Director of Laboratories; Claire Ondrovic, Assistant to the Chair; and Benedict Vitale, Electronics Engineer.

## A.9 President's Narrative

The major activity of the Executive Committee in January 2005 was the preparation of the Year #3 Annual Report of COMPRES to the NSF, and the Annual Program Plan and Budget request for Year #4 [May 1, 2005 to April 30, 2006]. In preparation for this submission, the Executive Committee developed a process that involved the COMPRES community and the two elected Standing Committees for Community Facilities and Infrastructure Development Projects. This revised Annual Program Plan and Budget was submitted to the NSF on February 3, 2005. The report, plan and budget for Year #4 [May 1, 2005 to April 30, 2006] was approved by David Lambert of NSF-EAR and the budget increment for Year #4 of $2.1 million authorized. The full Year #3 Annual Report can be viewed on the COMPRES website along with photos which accompanied these reports at the new url: www.compres.us.

In January 2005, the American Geophysical Union announced the election of 43 new Fellows. On behalf of the mineral and rock physics and chemistry communities, COMPRES can point with pride to the members of its extended community who will be honored this year, including the new AGU Fellows: Bruce Buffett, University of Chicago; Reid Cooper, Brown University; Geoffrey David Price, University College London; David Yuen, University of Minnesota; and Vladimir Zharkov, Institute of Physics of the Earth, Moscow.

The Science Advisory Committee (SAC) of the National Synchrotron Light Source at the Brookhaven National Laboratory reviewed all of the beamline operations of the NSLS. On January 31 and February 1, 2005, the subpanel responsible for reviewing the activities at the high-pressure beamlines met. These high-pressure beamlines include the Diamond-Anvil Cell facilities at X17B3 and X17C and U2A and the Multi-Anvil Facilities at X17B2, which are operated by members of the COMPRES community.

For the DAC facilities, H-k. Mao and R. Hemley of the Carnegie Institution of Washington made presentations of the current status and future needs. D. Weidner made a presentation for the Multi-Anvil facilities. R. Liebermann represented COMPRES and its Executive Committee. M. Rivers represented the University of Chicago, which will assume responsibility for the management of the X-ray DAC facilities on May 1, 2005.

Renata Wentzcovitch (University of Minnesota) and her investigator team were awarded a grant for $2.8M for a four-year program to establish a Virtual Laboratory for Earth Materials [VLab] from the Information Technology Research for National Priorities Program of the NSF. Co-PIs are: Yousef Saad, Ilja Siepman, Donald Truhlar, D. Yuen, all at University of Minnesota. P. Allen [Stony Brook University], G. Erlebacher [Florida State University], B. Karki [Louisiana State University], M. Marlon Pierce [Indiana University], F. Spera [University of California at Santa Barbara].

In consultation with the Executive Committee, we prepared a one-page PowerPoint slide for David Lambert at NSF-EAR to use in presentations within the NSF. A copy may also be downloaded from the Publications page of the COMPRES website.

In collaboration with Ellen Kappel of GeoProse, we designed a poster based on the report on "Current and Future Directions of Research in High-Pressure Mineral Physics", the so-called Bass Report. A copy is attached to this report and may also be downloaded from the Publications page of the COMPRES website. Full-size copies at 24" x 36" of this poster may be obtained by writing to Ann.Lattimore@stonybrook.edu.

Since November 2002, COMPRES has been publishing quarterly Newsletters to inform the COMPRES and broader communities of the current activities of COMPRES as an organization and high-pressure mineral physics as a scientific discipline. These have been edited by Jiuhua Chen, Associate Director of the Mineral Physics Institute of Stony Brook University. The Executive Committee of COMPRES has concluded after the first two years of these quarterly newsletters that they are an important and effective means of communication and have decided to continue publishing the Newsletter, but at a reduced frequency of every three months. It is our intention to publish new issues of the COMPRES Newsletter each February, June and October. See the Publications link on the COMPRES website to download copies.

I attended the European Geosciences Union General Assembly in Vienna, Austria from April 24-29. Special features included a Union symposium on "Neutrons at the Frontier of Earth Sciences and Environment" convened by H. Schober, J. Parise and H. Kagi. I gave a paper in the symposium on "High-pressure and high-temperature mineral physics: Contributions towards the understanding of planetary interiors" convened by D. Frost. At the EGU, special awards were given to two members of the COMPRES community: David Dobson received the Outstanding Scientist Award from the European Mineralogical Union; David Kohlstedt received the Louis Neel Medal and delivered a lecture entitled: "Mantle Flow, Melt Migration, and Seismic Anisotropy: Aligned Against the Flow."

On May 10, the Facilities Committee [M. Rivers-Chair, Y. Fei, A. Kavner, C. Prewitt] paid a Site Visit to the high-pressure beamlines at the National Synchrotron Light Source of the Brookhaven National Laboratory. The purpose of this visit was to learn the current status of the diamond-anvil and multi-anvil facilities operated for COMPRES by the Carnegie Institution of Washington [H. Mao and R. Hemley] and

Stony Brook University [D. Weidner and M. Vaughan], respectively, and to discuss future plans for enhancing these facilities to serve the COMPRES community.

In May, the U. S. National Academy of Sciences announced the election of 72 new members, including three from the mineral and rock physics community: Marcia McNutt from the Monterey Bay Aquarium, Barbara Romanowicz from the University of California at Berkeley, and Paul Tapponier [Foreign Associate] from the Institut de Physique du Globe in Paris.

On May 17, H. Green, M, Rivers and I visited the Advanced Light Source at the Lawrence Berkeley National Laboratory to see the new facilities for high-pressure mineral physics operated for COMPRES by the University of California [R. Jeanloz]. We were hosted by Simon Clark and his team of associates including Martin Kunz, Sander Caldwell and Arianna Gleason [COMPRES Beamline Intern]. As part of a western trip in mid-May, I also visited the Lawrence Livermore National Laboratory [hosted by William Durham, Daniel Farber, Jeffrey Roberts, and Brian Bonner] to see their high-pressure facilities. On the way home, I stopped for a day to visit Ivan Getting at the University of Colorado to get an update on the Johnson noise thermometry project that he is conducting part of the COMPRES infrastructure development program.

The 15th Goldschmidt Conference was held in Moscow, Idaho from May 20-25,with many special symposia of interest to the COMPRES mineral physics community, including "Geochemical, Rheological, and Geophysical Aspects of Deep Mantle Phase Changes" [convened by J. Bass and I. Daniel] and "Mantle Heterogeneity, Past and Present" [convened by F. Albarede and P. Tackley]. Additional details of the meeting may be found at: http://www.the-conference.com/2005/gold2005/index.php.

At the Goldschmidt Conference, Alexandra Navrotsky received the 2005 Harold Urey Medal of the European Association of Geochemistry.

In early June, the Royal Academy of Sciences awarded the Gregori Aminoff Prize for 2005 to Ho-kwang (Dave) Mao of the Carnegie Institution of Washington. Several mineral physicists from the U. S. participated in a symposium in Dave's honor in Stockholm.

In June, Guy Masters, one of the members of the COMPRES Advisory Committee, was elected Fellow of the Royal Society of London.

At the AIRAPT Meeting in Karlsruhe, Germany in early July, Sergei Stishov received the Bridgman Medal for his pioneering research into the properties of materials at high pressures and temperatures.

While in New Mexico to attend the High Pressure Melts Workshop in July, I took the opportunity to visit Santa Fe to see one of the potential sites for the 2006 Annual Meeting and to visit the Lujan Center of LANSCE at the Los Alamos National Laboratory and see the high-pressure facilities being developed there by Yusheng Zhao,

Jianzhong Zhang and their colleagues. This is part of a program to visit mineral physics laboratories in the U. S. and overseas on behalf of COMPRES.

While in France in September 2005 to attend the "3rd Workshop on Earth's Mantle Composition, Structure, and Phase Transitions" in Saint Malo, I also be visited the high-pressure beamline facilities at the European Synchrotron Radiation Facility [ESRF] in Grenoble and gave a seminar entitled: "Sound Velocities in Minerals under Mantle Conditions." My host was Wilson Crichton, Beamline Scientist on ID27. It was a special pleasure to see the wide range of high-pressure experiments being conducted on many different beamlines; see details at: http://www.esrf.fr/.

On September 6, the International Balzan Foundation announced that its 2005 Balzan Prize in Mineral Physics is to be awarded to Russell J. Hemley and Ho-kwang (David) Mao of the Carnegie Institution of Washington. This prize carries a cash award of one million Swiss francs, half of which must be allocated to research projects involving young researchers. Drs. Hemley and Mao were honored in a special ceremony in Bern, Switzerland in November 2005.

Frances Hellman, Professor at the University of California at Berkeley, has be selected to be the 2005 recipient of the Keithley Award of the American Phyical Society for her work in nanocalorimetry. Professor Hellman is collaborating with Alexandra Navrotsky of the University of California at Davis on a COMPRES infrastructure development project on "Calorimetry-on-a-Chip."

John Hall, a physicist at the National Institute of Standards and Technology [NIST] and the University of Colorado was one of the 2005 winners of the Nobel Prize in Physics. Dr. Hall has been collaborating with Ivan Getting on the Johnson noise thermometry project sponsored by COMPRES under the Infrastructure Development Program

.

George Rossman of the California Institute of Technology has been awarded the 2005 Friedrich Becke Medal of the Austrian Mineralogical Socieity for his "outstanding contributions in the fields of mineralogy, petrology and geochemistry."

On 14 October 2005, I attended the CARS Board of Governors meeting at the Advanced Photon Source as the new representative of GeoSoilEnvironCARS. A report on the review of the GSECARS operations was one of the features of the meeting, in which the close collaborative relationship between COMPRES and GSECARS was highlighted.

On 20-21 October, I visited the Department of Geology and Geophysics at the University of Minnesota and gave a seminar entitled: "Sound Velocities in Minerals under Mantle Conditions." My host was David Kohlstedt, and I had the opportunity to visit the experimental laboratories of Kohlstedt and Mark Zimmerman [rock deformation], Marc Hirschmann [experimental petrology], and Subir Banerjee [rock

magnetism], as well as discuss mutual interests with Rama Murthy, Justin Revenaugh, Emi Ito and Donna Whitney.

The Facilities Committee of COMPRES paid a site visit to the GSECARS sectors at the APS on Oct 23-24, 2005. Charles Prewitt organized and chaired the visit, inasmuch as Mark Rivers is one of the two Project Managers/PIs of GSECARS; William Durham, Thomas Duffy and Abby Kavner all attended. Green and Liebermann attended as observers. The visit included talks by Rivers, Yanbin Wang, Vitali Prakapenka, and Steve Sutton, as well as a tour of the Sector 13 beamlines [both bending magnet and insertion device stations]. This visit also included a presentation by Guoyin Shen, now Project Manager of HPCAT and a visit to the Sector 3 beamline [hosted by Wolfgang Sturhahn] at which COMPRES is partially funding a postdoc to provide access to the nuclear resonant inelastic X-ray scattering facilities.

I attended a meeting of the Science & Technology Steering Committee of the Brookhaven Science Associates on November 2-3 at the Brookhaven National Laboratory. The principal agenda item was the announcement that the NSLS-II project had been awarded Critical Decision-0 by the Department of Energy; now that CD-0 has been achieved, the principal challenge for the NSLS management is to perform the critical development research will lead to CD-0 late next year.

The major event of December 2005 for COMPRES was the Fall AGU Meeting in San Francisco. Highlights included:

Many special sessions convened by colleagues in mineral and rock physics, and organized by Steve Jacobsen as the representative for Mineral and Rock Physics on the Program Committee. There were 242 abstracts [2% of the meeting total] submitted under the MRP designation, of which 72 were first-authored by students. This creasted 7 different special sessions with 80 oral presentations. There were additional papers from our field submitted under the Tectonophysics and Volcanology-Geochemistry-Petrology sections. Our congratulations and thanks to Steve for such a splendid job on behalf of our community.

Exhibition booth jointly sponsored by GSECARS and COMPRES, which attracted lots of visitors, and which featured copies of the new COMPRES poster based on the "Bass Report," reprints of the October 2005 EOS article on "The Future of High Pressure Mineral Physics," and COMPRES pocket calendars for 2006. Our thanks to Jiuhua Chen for creating the PowerPoint presentation, to Ann Lattimore for overseeing preparations, and to Glenn Richard and Michael Vaughan for staffing the booth, as well as to Nancy Lazarz and Mark Rivers of GSECARS for their collaboration.

We all took special pride in the award of honors and medals to our colleagues in Mineral and Rock Physics and related fields, including:

Paul Asimow—James Macelwane Medal
Thomas Jordan—Inge Lehmann Medal

Sean Solomon—Harry Hess Medal

New AGU Fellows [honored in New Orleans in May]: Bruce Buffett, Reid Cooper, David Price, David Yuen, and Vladimir Zharkov.

The Mineral and Rock Physics Focus Group hosted a wine and cheese reception on Dec. 5, sponsored jointly by Almax Industries, Digital Technology, Technodiamant and Oxford Instruments. During the reception, the 2005 Outstanding Student Award in Mineral and Rock Physics was presented to Jennifer Jackson of the University of Illinois at Urbana-Champaign.

The Physical Properties of Earth Materials group once again organized a fantastic dinner celebration at the Aziza, a Moroccan restaurant on Geary Blvd. Our congratulations to Brian Bonner and Bill Durham for discovering such a wonderful venue for this special evening.

COMPRES convened a Town Hall Meeting on Thursday, Dec 8 to discuss plans and strategies for submitting a proposal to the NSF in August 2006 for renewal of the Cooperative Agreement for COMPRES for the period May 2007 to April 2012.

**5th Annual Meeting of COMPRES**

Dates:
Arrival: Tuesday, June 20 in afternoon or evening
Departure: Friday, June 23 after lunch

Site:
Snowbird Alpine Village, Snowbird, Utah [http://www.snowbird.com/meetings]

Details of the program and registration/logistics will follow early in the 2006 new year. In the meantime, please send your suggestions for program content and format to me [Robert.Liebermann@stonybrook.edu].

This site was specifically chosen to allow those persons who will be attending the Gordon Research Conference on Research at High Pressure at the University of New England in Main [June 25-30] to attend the COMPRES meeting.

## 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, 2006, 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 2005, the two Standing Committees asked the project directors of each of the subawards to submit annual progress reports for Year #4 and budget requests for Year #5 by November 1, 2005. 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, 2005.

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 2005 AGU Meeting in San Francisco. Each of the Standing Committees gave oral reports on their deliberations to the Executive Committee at the Fall AGU Meeting, and then submitted their written report, with evaluations of progress and recommendations for funding in Year #5, to the Executive Committee. In the case of the Infrastructure Committee, this report included recommendations for initial funding of new projects and community workshops.

In January 2006, 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 #5. 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

[M. Rivers, J. Hu, and Q. Guo, University of Chicago]

### Overview of Year 4 for NSLS X-17C and X-17B3

The operations of NSLS X-17C and X-17B3 diamond cell beamlines was transferred from Carnegie Institution of Washington (Dave Mao PI) to University of Chicago (Mark Rivers PI). This transfer was planned for May 1, 2005 but did not actually occur until September 1, 2005. From May through August Drs. Jingzhu Hu and Quanzhong Guo remained employees of Carnegie, and became University of Chicago employees on Sept. 1. The COMPRES sub-award for year 4 to Chicago is still being finalized, because we are trying to generate a single award to cover the $CO_2$ laser heating, gas-loading, and Johnson noise infrastructure projects, as well as the X-17 diamond-anvil operations.

A new agreement with the NSLS for these beamlines has been finalized. This agreement converts the beamlines to "Facility Beamlines" with a "Contributing User" agreement with COMPRES. The main differences from the previous PRT arrangement are:

- The amount of general user time has increased from 25% to 50%.
- The amount of COMPRES time is 50% of the available beamtime on each beamline.
- The NSLS assumes responsibility for the operation of the "beamline" (optics, safety system, etc.), while
- COMPRES is responsible for the operation of the experimental stations.

The X-17C beamline can run 100% of the time, since it is a side-station. The X-17B3 beamline only runs 25% of the time in dedicated mode, with an additional 25% available in parasitic mode when the X-17B2 (multi-anvil) station is running.

The X-17C beamline has been productive during the year, with nearly all of the beamtime being used for experiments from a large number of institutions. The publication rate remains quite high. X-17B3 has had a number of technical problems, with both the laser heating system and the Laue monochromator. These problems are being addressed, and we plan to have the station running reliably for the first run in 2006.

The X-17C and X-17B3 beamlines continue to be funded at a very minimal level. Having a single person responsible for a beamline that runs 100% of the time (X-17C) or 50% of the time (X-17B2), is not sustainable in the long run, and is fewer than any other COMPRES beamline except U2-IR at the NSLS.

**X17C COMPRES 2005 Annual Report**
[Prepared by J. Hu and M. Rivers]

**Major accomplishments in 2005**

1 Developed Laue diffraction for single crystal and tested Dr. Dera's software 2). Started to run monochromatic beam at 23, 25 and 30 keV energies. Improved lead shielding box. That reduced the background.

2 Plans for 2006 : 1). Continue single crystal program development 2). Improve mirrors focus capability 3). Improve beam alignment system for easier convert between EDXD and ADXD

3 2005 Jan – April: General user beam time is 25%, May-August: General user beam time is 50%, Sept- Nov: General user beam time is 50%

4 2006 General use beam time will be 50%

5 Beam time allocation procedure: 1) Users submit proposals to NSLS GU program. 2) Committee review proposals 3) Allocate beam time that NSLS approved 4) Allocated some rejected proposals if users still request time. 5) Accept temporary beam time requesting from COMPRES if beam time is available. (Some users missed submitting dead line time).

**X17B3 COMPRES 2005 Annual Report**
[Prepared by Q. Guo and M. Rivers]

**Major accomplishments in 2005:**

1 Setup YAG laser heating optical system.
2 Optimized 4-Laue monochromator system

**2006**
***List of things to do:*** 1). Continue Monochromator development 2). Update YAG laser heating system. 3). Improve beam alignment system.
**2005**
General user beam time through NSLS was 25%; COMPRES beam time is 50% CIW time was 25%
**2006**
General user beam time will be 50%.
COMPRES beam time will be 50%

**Beam time procedures:**
1) Users submit proposals to NSLS GU program. 2) Committee review proposals 3) Allocate beam time that NSLS approved 4) Allocated some rejected proposals if users still requested time 5) Accept rapid access beam time requests from COMPRES users if beam time available. (Some users missed submitting time).

**X17B3 and X17C Publications in 2005**

1 Duffy, T. S., Synchrotron facilities and the study of deep planetary interiors,

*Reports of Progress in Physics*, ***68***, 1811-1859, 2005. (X17C).
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## B.2 Infrared Diamond-anvil Facilities at the National Synchrotron Light Source

[R. Hemley and Z. Liu, Carnegie Institution of Washington]

Summary of the Workshop on Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science

Sponsored by COMPRES and the NSLS, the workshop on Synchrotron Infrared Spectroscopy for High Pressure Geoscience and Planetary Science was held at the NSLS, Brookhaven National Laboratory on Nov. 3-5, 2005. Thanks to the members of the COMPRES Executive Committee for suggesting, promoting, and supporting the IR workshop. It was a great success in terms of the excellence of the lectures, broad attendance that included many new potential users and student participation, extensive program, hands-on experiences for new users. More than 50 attendees took part in (the maximum allowed by the budget and lecture room).

The workshop consisted of five sessions designed to accommodate the broad range of attendees from experts to new users. The Friday morning session was directed toward attendees new to modern IR spectroscopy techniques in the field but it was also very useful review of fundamentals and new developments for experienced users. Q. Williams (Univ. Calif. Santa Cruz) gave a thorough overview on IR spectroscopy (and FT techniques in general) and its applications in the Earth sciences. G. Rossman (California Institute of Technology) gave a talk on hydrous components in the nominally anhydrous minerals, which was crucially important for many users who are interested in the calibration of the water content in minerals. A. Hofmeister (Washington University in St. Louis) discussed about high pressure far-IR spectroscopy of mantle candidate minerals that are worth pursuing with the synchrotron technique. Finally, J. Tse (University of Saskatchewan, Canada) described theoretical methods for vibrational spectroscopy and many other applications.

The Friday afternoon session was started by L. Carr (NSLS, Brookhaven National Laboratory). He gave a very comprehensive talk on Fourier transform spectroscopy techniques using the synchrotron infrared source as well as an overview on the IR programs at the NSLS. There were seven speakers discussed different topics related the works they have done at the U2A beamline. These talks include simple molecular systems under high pressure (A. Goncharov, Geophysical Laboratory); Infrared absorption and first-principles studies of ice-VIII and high-pressure clathrate hydrate structural changes (D. Klug, Canadian Research Council); Infrared and visible spectroscopy in diamond anvil cells: reflectivity measurements and data analysis (V. Struzhkin, Geophysical Laboratory); High-pressure synchrotron-FTIR studies of hydroxyl in Mg2SiO4 and MgSiO3 polymorphs in Earth's mantle (S. Jacobsen, Geophysical Laboratory); Using infrared spectroscopy to characterize volatile-bearing Earth materials (H. Scott, Indiana University South Bend); Correlation between crystallographic and spectroscopic measurements at high pressure (G. Lager, University of Louisville); Host-guest interactions in Zeolites under pressure: combined synchrotron XRD and IR measurements (Y. Lee, Brookhaven National Lab). These talks not only

addressed a broad range of problems in Earth and planetary sciences but also reflected new techniques developed at the U2A beamline in past years.
The Saturday morning session first focused on imaging techniques combined with synchrotron sources. L. Miller (NSLS, Brookhaven National Laboratory) gave an extensive overview of chemical imaging at high spatial resolution using a synchrotron infrared microscope. L. Wang (SUNY) and L. Dobrzhinetskaya (Univ. Calif. Riverside) discussed about experimental constraints on the incorporation mechanism of water in mantle olivine and fluid inclusions in microdiamonds: from direct observations with transmission electron microscope to IR synchrotron radiation studies, respectively. In addition, M. Koch-Müller (GeoForschungsZentrum Potsdam, Germany) and S. Clark (Advance Light Source) also gave talks featuring high-pressure IR studies at other synchrotron sources.

The facility tour and hands-on session on Saturday afternoon attracted more than 30 people. At the IR beamline, new users received detailed information on the beamline facility and its capabilities as well as first hand experience on how to perform high pressure IR experiments from the beginning to the end.

The last session for student/post-doc experiments at U2A beamline started right after the workshop. Two students and one post-doc submitted their research proposals and a one day beamtime were allocated per proposal. This new session offered not only a great opportunity to learn how to use the synchrotron IR facility but also a chance to collect valuable data for their research projects. The experiments went very well and the IR data they obtained are very interesting and will be publishable in scientific journals.

Finally, an open discussion brought a lot of attention on the future beamline developments. R. Hemley and Z. Liu described the current status of the IR facility and its feasibility and abilities for general users as well as proposed beamline upgrades in the near future, such as combined laser heating and synchrotron IR spectroscopy for high pressure and high temperature experiments, new side station, imaging at ambient and high pressure, etc. The feedback from attendees has overall been very positive. It seems urgent to set up a CO2 laser heating system at the NSLS site as the first step. This will greatly benefit all users who are interested in doing high P-T experiments at the NSLS. Currently, only one laser heating system is available for general users at X17B3 beamline but it is old and outdated. It is also not suitable to high P-T experiments for most hydrous minerals.

**Scientific highlights**

High-pressure synchrotron-IR studies of hydrated transition zone and lower-mantle minerals in the laser-heated diamond cell – Synchrotron-based infrared spectroscopy capabilities at the U2A beamline have been used to study the high-pressure behavior of near-IR absorption bands in single-crystal samples of hydrous wadsleyite and laser-heated hydrous ringwoodite in a diamond-anvil cell. The sample of pure-Mg hydrous wadsleyite contained roughly 1 wt% water and was studied to 20 GPa. In agreement with previous results on Fe-bearing samples [Cynn and Hofmeister 1994, JGR

99, 17717], the band group at lower wavenumber (3200-3400 cm-1) displays a negative shift upon compression whereas the group at higher wavenumber (3580-3700 cm-1) displays a slightly positive shift, or no shift at all. These results confirm that there are at least two very different hydrogen bonding geometries in wadsleyite. A single-crystal of Fo90 hydrous ringwoodite also containing ~1wt% water was transformed to a silicate perovskite plus magnesiowüstite assemblage at 35 GPa and various temperatures between 1200 and 1800 oC. Laser heating and phase analysis were carried with in-situ X-ray diffraction on the 13-ID-D beamline at GSECARS, Advanced Photon Source. The use of synchrotron-IR techniques facilitated study of the recovered sample at 35 GPa at various points of the sample where heating was carried out at different temperatures. In addition to spectra corresponding to unconverted ringwoodite, magnesiowüstite, and possibly phase D and quench glass, we observe two new sharp bands at 3060 and 3160 cm-1, which may correspond to the elusive O-H stretching of structurally bound hydroxyl in silicate perovskite not normally observed in recovered samples at room pressure. (S. Jacobsen at. al., AGU meeting, 2005)

Effects of water on the behavior of MgSiO3-clinoenstatite at high pressure – Just 1000 ppm of $H_2O$ stored in the major minerals of Earth's upper mantle would represent more than one ocean-mass equivalent of liquid water. The incorporation of water as hydroxyl into clinoenstatite (MgSiO3) was investigated using synchrotron-based IR spectroscopy on the U2A beamline U2A at NSLS, and the effects of water on the low-density clinoenstatite (LCEN) to high-density (HCEN) phase transformation were studied using high-pressure Raman spectroscopy. Single-crystal samples of low-clinoenstatite with varying water contents were synthesized in a multianvil press at 16-18 GPa and around 1100 oC. IR-absorption bands in the region of O-H stretching at 3675, 3600, and 3550 cm-1 were monitored to 17 GPa. The bands shift to lower wavenumber upon compression, but between 6 and 8 GPa a change in the pressure dependence of the band at 3675 cm-1 was observed, accompanied by broadening and disappearance of the 3600 cm-1 band. Changes in the FTIR spectra are attributed to the low- to high-clinoenstatite phase transformation, and indicate that there are differences in the hydrogen bonding environment between the two structures. Raman spectroscopy was used to monitor the transformation pressure (PT) of hydrated and anhydrous crystals loaded together in the same diamond cell. On compression, PT is reduced from 8.1 GPa for the dry sample to about 5.7 GPa for the most hydrous sample containing about 1000 ppm H2O. Upon decompression, all samples back-transformed to low-clinoestatite at around 4.5 GPa. The results indicate that hydration narrows the transformation hysteresis and that water reduces the transformation pressure by about 1 GPa per 1000 ppm H2O, if PT is taken to be the mid-point of the hysteresis. If hydroxyl defects affect the orthoenstatite to high-clinoestatite transformation similarly in the mantle, a shift in PT of 1 GPa would uplift any corresponding seismic discontinuity by about 30 km. Thus, relatively small amounts of water may have seismically detectable effects on the behavior and properties of the upper mantle. (E. Littlefield et. al., AGU meeting, 2005)

High-pressure vibrational study of dense hydrous magnesium silicate 10Å Phase – Dense hydrous magnesium silicates (DHMS) could be important hosts for H2O in the Earth's mantle and subduction zones, and their dehydration may be responsible for deep

focus earthquakes. Among these phases, the so-called 10Å phase (Mg3Si4O10(OH)2.nH2O) is characterized by a phlogopite-like structure which accommodates molecular water in the interlayer. However, the amount of interlayer water, its precise structural position and response upon compression remain uncertain. To better understand the high pressure behavior of hydroxyl groups and interlayer water in 10Å phase, we have conducted in situ synchrotron IR and Raman spectroscopic measurements up to 20 GPa at 300 K. The high brightness and spatial resolution of the synchrotron IR radiation available at the U2A beamline at NSLS, high-quality mid-IR spectra with high signal/noise ratio have been collected in the diamond-anvil cell. The 10Å phase samples were synthesized at 6.5 GPa and 650 ºC in a Kawai-type multianvil press using talc and excess water as starting materials. At ambient conditions, the IR spectrum shows a strong band at 3675 cm-1 and two less intense and broader bands at 3258 and 3589 cm-1. With increasing pressure up to 5.5 GPa, the band at 3675 cm-1 displays a linear negative frequency shift. Near 6.2 GPa a new band emerges at 3680 cm-1 and its intensity progressively increases with pressure up to 15.5 GPa, indicating major changes in the hydrogen bonding. All pressure-induced changes in the IR spectra are fully reversible upon decompression and occur without any noticeable hysteresis. On the basis of combined high pressure IR and Raman results, it is possible to reevaluate the assignment of the OH–vibrational bands of the 10Å phase and constrain the response to compression of SiO4 tetrahedra, MgO6 octahedra, hydroxyl units and molecular water. (C. Sanchez-Valle et. al., AGU meeting, 2005)

**Future Beamline Upgrade Plans (not included in present budget)**

New IR/Raman Microscope system (also supported by CDAC): This setup with higher spatial resolution will be available to general users early next year. A dedicated resistively heated diamond anvil cell (EHDAC, or hydrothermal cell) cell was added to the current complement of diamond cells and already served for users from the COMPRES community. This high pressure and high temperature device will be solely used at U2A, and will routinely cover the P-T range of up to 40 GPa and 1000 K. In addition, large volume cells (e.g., for far-IR spectroscopy and imaging) will be added. The first will use moissanite anvils and then large diamonds synthesized by CVD (anvils made of both materials were tested this past year). It will be initially attached to the Bruker IFS 66v/S spectrometer. If the requested funds mentioned below are awarded, this system will be permanently attached to the new FTIR spectrometer for high P-T studies. This cell has been ordered from Foxwood Instruments and was delivered in April 2005.

New side station and CO2 laser heating system at U2A beamline: Measurements at the side station will be conducted for infrared imaging experiments. We also expect an increase in the S/N compared with the current in-hutch system because of the reduced distance between the storage ring and the end station. We can adapt the custom-built high P-T IR microscope to the FTIR spectrometer and dedicate the system to studies of Earth and planetary materials. As a first step, funds are needed to purchase an FTIR spectrometer (~$100 K). Combined with the new IR microscope discussed above, users will be able to carry out imaging studies of samples under pressure as well as ambient conditions (e.g., whole rock samples). Further developments would focus on laser heating

and IR emission techniques, requiring the purchase of a CO2 laser (~$50 K). In these experiments, high pressure and high temperature (up to several thousand K) are generated in a DAC, 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.

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

Under the new NSLS Contributing User Proposal, U2A will become 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, and in the past year nearly all of the General Users were from COMPRES. The remaining 25% of beam time will be allocated by COMPRES with at least half of this time being dedicated to support research by members of the COMPRES community through proposals vetted by the NSLS General User program; the NSLS User Administration will provide the CU group proposed here with the ratings of all proposals for a beam time cycle, so that these ratings may be honored in decisions on requests for the 25% of beam time to be allocated by COMPRES. The remaining 25% will go to Geophysical Laboratory, Carnegie Institution for development projects and users supported by its grants such as CDAC.

**2004 U2A Publications**


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Lu, J., G. Rozgonyi, A. Schönecker, A. Gutjahr, and Z. Liu, "Impact of oxygen on carbon precipitation in polycrystalline ribbon silicon", J. Appl. Phys., 97, 033509, 2005.
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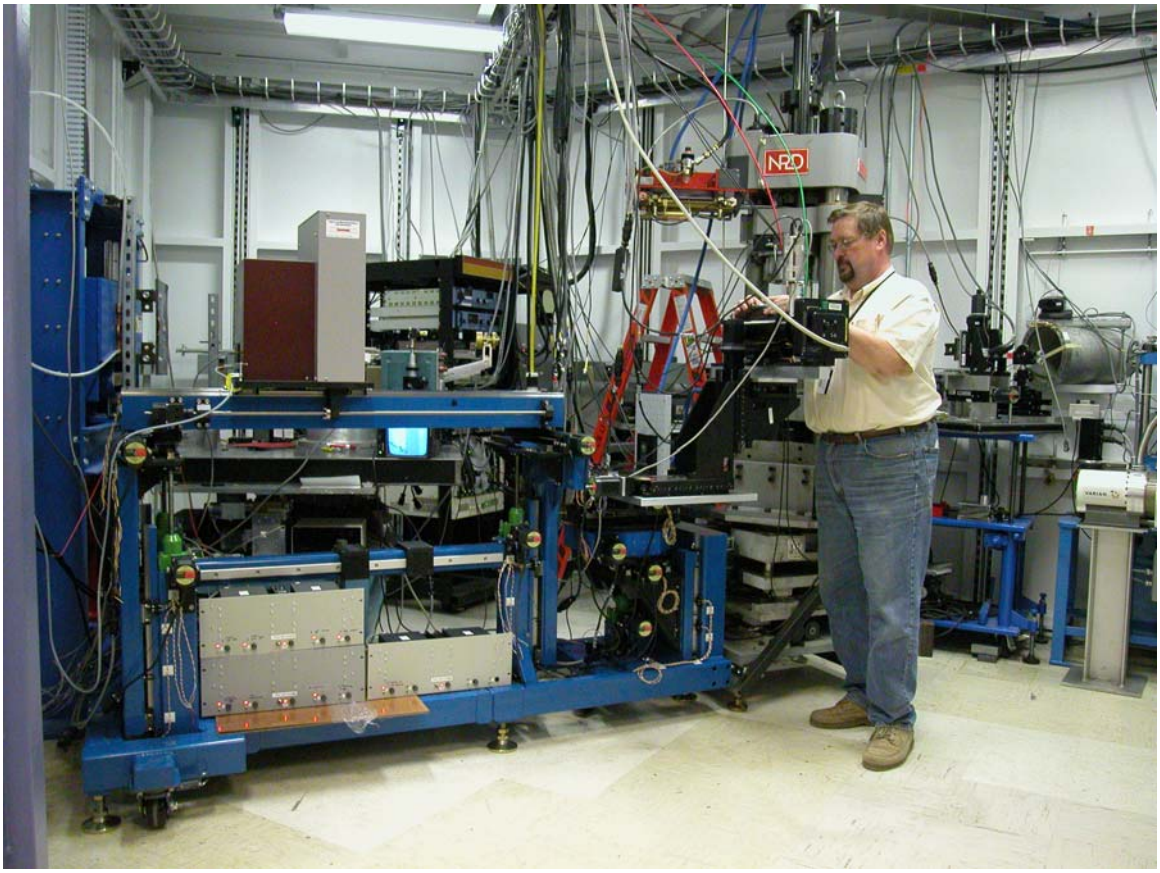
## B.3 Multi-anvil Cell Facilities at the National Synchrotron Light Source

[D. Weidner and M. Vaughan, Stony Brook University]

*Parasitic beamtime*: The 2005 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.

In-hutch monochromatic side station: We have now begun development of a second phase designed to increase the available beam time in the multi-anvil hutch. We are building a monochromatic in-hutch-side-station. 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 been funded by the Air Force ($182,000) and Stony Brook ($50,000) for a significant portion of the equipment that is required. We have acquired the main detector, a MAR345 imaging plate system. Just this past month, we have installed the monochromatic side station for shakedown and for the first experiments. We are using the DIA press and guidblock at the current time. In the future, this press will be moved back to the white beam position, as a new system in installed on the monochromatic line. We can report that the initial installation has been successful and within the week, we hope for new data.
We are looking at presses to place on the side station. Our concept is to obtain a light weight press for this purpose. The main beam (white) and the monochromatic beam will be able to operate simultaneously. This has the possibility of doubling the number of experiments that we can do. Further, it will open a new class of experiments – namely, monochromatic, that will be run on a continuous basis.

Beam time allocation: We are continuing our process of beam time allocation. Now proposals for all experiments must be submitted to General Users Program and evaluated via the NSLS review process for general users. NSLS then assigns up to 25% of the standard mode beam time on the basis of their review (this number will become 50% with the newly negotiated MOU's). We reserve 10% for beamline development. We assign the remaining time using the rating from the NSLS review, but weighting those proposals which are consistent with a COMPRES-earth sciences agenda and the special considerations for the parasitic time.



**Installation of Monochromatic Side Station in X17B2 Hutch**

**Science Highlights – activities of 2005**

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. We have been working with Ringwood Superabrasives in Australia to develop sintered diamond anvils that are both x-ray transparent and enable

higher pressure runs. To date this system is working to about 8 GPa, while our goal is to double this in the D-DIA.

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. Mei et al and Li et al are finding a low activation volume for olivine (0-5 cc/mol), while Karato finds evidence for a larger value (15 cc/mol). The story here is still unfolding, but we now have the facilities to address this important issue.

Polycrystalline stress field: Multi-phase aggregates have been the focus of recent studies, capitalizing on the D-DIA. Different stresses in different samples indicate the organization of the grains in order to support the stress.

Melt property study at high pressure: A technique has been developed to measure the melt density at high pressures using x-ray radiograph and absorption simulation. Studies include: EOS of liquid FeS; viscosity of silicates, FeS and metal alloy; melting curve and elasticity of NaCl. Measurements have also been carried out on tin and promise to be quite interesting.

Activities for 2006

We plan to fully implement the monochromatic side station during the upcoming year. We have the possibility of using a Paris-Edinburgh cell as the pressure device and may try to use Karato's RDA device. 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 D-DIA for deformation/controlled stress measurements. We will continue ultrasonic measurements in the D-DIA. 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.

Our main agenda will be to serve the proposals that we receive.

**Beamline Usage - Calendar Year 20052004 Summary**

For the 2004 2005 calendar year we received 2024 General User beam time requests from 2022 individuals totaling 166161 days. NSLS awarded beam time to 57 of these users totaling 12.531 days. There were 59.5 47.5 Operations days assigned to X17B2, and 55 53.5 assigned to X17B3, of which we were able to use 5052.5., giving a total of 100 days available in the X17B2 hutch. Subtracting the 31 12.5 days assigned by the NSLS, 78.587.5 were left as PRT time. COMPRES assigned 8169.5 of these days to 1715 of the proposals which had not been allocated beamtime by the NSLS Proposal Review Committee., and 6.59 days were used for beamline development and other maintenance projects.

**Major Support Personnel**

| | |
|---|---|
| Liping Wang beam line scientist | COMPRES funds |
| Carey Koleda machinist | COMPRES funds |
| Michael T. Vaughan NSLS coordinator | MPI |
| Jiuhua Chen scientist/advisor to users | MPI |
| Donald J. Weidner, scientist spokesperson | SUNY |
| Ken Baldwin, software support | MPI |
| William Huebsch, electronics expert | SUNY |

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## B.4 West Coast Synchrotron Facilities

[R. Jeanloz and S. Clark, University of California, Berkeley]

### Summary

This year has seen the completion of the commissioning period on beamline 12.2.2. Both end stations 1 and 2 are now up and running. We have managed to fit a number of COMPRES users into the commissioning phase and publications are starting to appear. We expect productivity from the beamline to increase as our experience of using it grows. We will continue to improve the reliability and efficiency of the beamline as we deliver the science program with our COMPRES users during the next year.

Beamline 11.3 is working routinely for ambient temperature high-pressure measurements. No improvements are planned for this beamline during the next year since we will be totally focusing our efforts on beamline 12.2.2.
Up take of beamtime on the infrared beamline 1.4 has been disappointing. The infrared workshop at NSLS gave us the opportunity to advertise this facility to the general COMPRES community may of who are based in California. We now have a new high-temperature diamond cell suitable for use on this beamline which we hope will further increase interest.

We are still developing resistively heat diamond cells in collaboration with Lawrence Livermore National Laboratory and hope to be able to make these routinely available during 2006. The high-pressure laboratory is being upgraded with the addition of Raman and Brillouin systems. Plans for upgrading end station 1 of beamline 12.2.2 for single crystal measurements are being developed and will be shared with the general COMPRES community at the next COMPRES Annual Meeting.

### 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. In the January to June 2006 allocation period COMPRES was due 73 shifts on beamline 12.2.2. This amount will increase or decrease depending

on the level of funding from COMPRES. The current COMPRES approved program will be active for three years, at which time it will be reviewed by the ALS Science Advisory Council. Depending on the strength of the COMPRES program at the ALS at that time the percentage of beamtime available for COMPRES users on these beamlines may be increased, decreased or the whole approved program may be terminated.

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. 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).

**Summary of the major accomplishments for the past year**

Diamond anvil cells (DAC): The heatable diamond anvil cell developed and tested last year was successfully used for HT-HP studies on talk, goethite, garnet and zircon. Shortcomings of the present design were identified and a modified version of the heater as a MoSi2 ribbon rather than a wound Pt-Rh wire is in production.

Beamline 12.2.2: After completing commissioning of end-station 1 (ES-1), this station has been successfully used for experiments by approved program groups. About 20 % of the experiments on ES-1 were P-T experiments making use of the externally heated diamond anvil cell, developed in-house. The energy / flux characteristics and the ease of wavelength selection across the full spectrum make ES-1 also a very useful beamline to perform radial diffraction experiments. First publications stemming from these experiments are in preparation or in review process.

During the May shut-down, the K-B mirrors were installed on end-station 2 (ES-2). Commissioning and testing of this system started in July 2005. Commissioning included the following tests:

- Setting mirror bend for optimal focusing in the metrology lab.
- Aligning mirror position in the hutch on a virtual source defined by a set of off-set slits.
- Optimizing focus spot using mirror tilt.
- Measuring the optimized focus spot using blade scans and using an imaging system: 10 x 13 μm2. Full width at 1 % intensity is ~ 40 μm.
- Measuring the energy dependence of the focus spot: ~ 1 μm/10keV; i.e. negligible.
- Measuring peak shape using imaging system: Almost pure Gaussian (low tails), no flat top => needs more work to understand.
- Measuring net intensity loss at K-B mirrors. Iout/Iin = 50%.
- Measuring the dependence of FWHM on position along beam. ~ 2μm/cm => too small: needs more work to fully understand.

- Comparison of peak shape between off-set slits and opposed slits. No difference in peak shape: However FWHM seems to half when changing from opposed-slits to off-set-slit configuration. Encouraging!

The X-ray system has been interfaced with the laser-heating system. First hot patterns have been collected on garnet and Pt. In addition, the microfocused beam on ES-2 is now also very popular with users not depending on laser-heating and is being widely used for experiments. These commissioning experiments help iron out the remaining glitches and problems of the K-B mirror assembly.

Together with Brent Grochoslki (UCB) a rotatable and heatable DAC holder has been designed in order to enable viscosity measurements using the rolling sphere techniques. For this, X-ray shadowgraphs of the DAC were taken in rapid sequence in order to determine the acceleration and final velocity of a sphere in a liquid within the DAC. The imaging technique made use of both the multiplayer monochromator as well as the Si(111) monochromator. In the latter case, a 'dithering' function to spread out the beam over the area of the DAC sample chamber was applied. The imaging technique was also used by COMPRES members Dave walker and Michael Walter. They made use of X-ray shadowgraphs to determine elemental diffusion by measuring changing absorption in adjacent oxides and metals

.

An in-situ ruby fluorescence system has been assembled and pre-installed on ES-2 of 12.2.2. Its final installation and alignment is imminent. A replacement for the present off-line pressure measurement system, which had various safety concerns, was evaluated and purchased. Its final installation is imminent.

*Beamline 11.3.1:* In 2005, a total of 141 shifts of COMPRES experiments were scheduled/performed. They were used for combined high-pressure – high-temperature experiments. It turns out that the software limitations of the commercial data-collection software for the 11.3.1 single-crystal set-up are the limiting factor for an immediate success of this project. Work to resolve these issues are in progress in collaboration with VPI, Oxford diffraction and the crystallography lab at UCB.

*Beamline 1.4:* A new high-temperature infrared cell has been obtained from Diacell products Ltd. This is being commissioind and will be used during December COMPRES time on the beamline.

**Summary of proposed activities for next year**

For next year we have three main priorities:

1 Making sure, the allocated COMPRES and GU experiments can be completed successfully and yield publishable data.
2 Getting ES-2 with the KB mirrors and in situ laser heating in a safe, easy to use user-facility. This will mean some additional tweaking and commissioning, especially of the K-B mirrors. Although these mirrors already proved to give a

nicely focused X-ray spot, there remain some questions as to spot shape (further reduction of tails in return for a flat top) and general stability to be resolved. We are confident, that by the middle of FY 06/07, 12.2.2 / ES-2 will routinely produce high quality in-situ laser heated powder diffraction data.

3 Upgrading ES-1. We propose to upgrade ES-1 with a monochromatic single crystal diffractometer. This is pursued in context with the NSF-MRI initiative by Dera, Downs, Nicol, Denton, Rivers and Kunz. The aim is to establish 12.2.2 ES-1 as one of the synchrotron based high-pressure single-crystal stations within the US. This upgrade, if approved, could be completed by mid 2006, with commissioning ended by end of 2006. The monochromatic single crystal technique shall be complemented by a monochromator-scanning technique for polychromatic single crystal diffraction. This will enable to extract structural information of immobile samples at extreme conditions of pressure and temperature.

Furthermore, the promising X-ray imaging technique will be perfected during next year. This will be mainly done with Dave Walker (Columbia) and Brent Gricholsky (UCB). We also hope to continue the program on axial X-ray diffraction in collaboration with Rudy Wenk (UCB). On a more ambitious note, we hope to interface also this technique with laser heating. Last but not least, we hope to start the high-pressure EXAFS program in FY 2006/2007.

**Summary of COMPRES beamtime proposals**

For the Jan-Jun 2006 scheduling period there were eight beamtime proposals for beamline 12.2.2, 1 for beamline 11.3 and none for beamline 1.4. One group applied for time on 11.3 and no applications from COMPRES users for time on 1.4 were received. A summary of beamtime application for the January 2006 to June 2006 beamtime allocation period are contained in appendix 7 [not included in this public version of the report].

**Summary of publications**

Development of COMPRES activities on the West Coast are in an early stage. Our flagship beamline 12.2.2 is in commissioning this year and becomes available for general use January 2006. Nevertheless, we have tried to fit in as much science around the commissioning work as possible which has resulted in the papers listed below.

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## B. 5 Neutron Studies

[N. Ross and H. Sitepu, Virginia Institute of Technology and State University]

### Introduction

The goals of the neutron initiative of COMPRES are to:

1. Identify and broaden the neutron scattering community of Earth Scientists in the U.S.
2. To stimulate and promote the use of neutron scattering, with emphasis on high-pressure research, in the Earth Sciences.
3. To carry out educational activities which support the above goals.
4. Identify the needs of the community, including future requirements for instrumentation and sources, and to represent these needs to the neutron facilities (and funding agencies).

### Summary of Activities in Year 4

Husin Sitepu was employed as a Postdoc on the COMPRES Neutron Grant on

3/1/05. He has been responsible for outreach to the COMPRES community with the following activities:

- Updating and modifying COMPRES Neutron website (*http://www.crystal.vt.edu/compres*) to include deadlines for proposal submission, power points from recent neutron workshops and conference proceedings, and educational material *(e.g. "Recent Examples of High P-T Neutron Applications in the Earth Sciences"; "High Pressure Neutron Diffraction").*
- Providing updates of neutrons at high pressure to the community in "Neutron Corner", a new feature of the COMPRES Newsletter *(http://www.compres.stonybrook.edu/ Newsletter/V4N2/ Newsletterv4n2.pdf)*
- Investigating number of days available for high-pressure research at neutron facilities in
- U.S. and abroad (data that may be used in COMPRES renewal proposal).
- Exploring new opportunities for high-pressure neutron diffraction in U.S. He has contacted Dr Anna Llobet-Megias, HIPD (High-Intensity Powder Diffractomer) Instrument Scientist at Los Alamos, about using this beamline for high pressure neutron research .
- Administering COMPRESS financial aid ( *M. Kunz,S. Jacobsen, W. Mao, S. Clark*).
- Helping members of COMPRES community to apply for beam time at neutron facilities (see below).

**Neutron Proposals:**

- Sitepu H, Ross NL *"Combined neutron powder diffraction and texture study of calcite at high pressure and temperatures"*. Submitted to Los Alamos Neutron Science Center (LANSCE) April, 2005 (declined July 2005)
- Sitepu H, Wenk HR, Ross NL *"Quantitative texture analysis of R-phase in Ti50.75.Ni47.75.Fe1.50 shape memory alloy using MAUD Rietveld refinement with WIMV method"*. Submitted to Los Alamos Neutron Science Center (LANSCE) April, 2005 (declined July 2005)
- Sitepu H *"Compressibility of layered molybdite (MoO3) powders determine from neutron diffraction studies at high pressure*" Submitted to Laboratoire Leon Brillouin (LLB), CEA, France, September 29, 2005. Sitepu H *"Compressibility of layered molybdite (MoO3) powders determine from neutron diffraction studies at high pressure*" Submitted to Laboratoire Leon Brillouin (LLB), CEA, France, September 2005.
- Sitepu H *"Compressibility of layered molybdite (MoO3) powders determine from neutron diffraction studies at high pressure*" Submitted to Laboratoire Leon Brillouin (LLB), CEA, France, September 29, 2005. Sitepu H *"Compressibility of layered molybdite (MoO3) powders determine from neutron diffraction studies at high pressure*" Submitted to Laboratoire Leon Brillouin (LLB), CEA, France, September 2005.
- Tschauner O, Sitepu H, Ahrens, TJ and Asimov, PD *"Investigation of Mg-Al site disorder in shocked MgAl2O4 spinel using neutron diffraction*" Submitted to The ISIS Facility, CLRC Rutherford Appleton Laboratory, Chilton ISIS, Didcot,

Oxon, OX11 0QX, United Kingdom, submitted October 2005.

**Presentations:**

- Ross NL (2005) *Insights into Mineral Behavior from Neutron Diffraction* (invited). Neutrons at the Frontier of the Earth Sciences and Environment (NESE) symposium, Vienna, Austria, April 25th-26th, 2005 NESE Symposium, European Union of Geosciences Meeting, Vienna, Austria, April 25-26, 2005.
- Sitepu H, Ross NL, Hansen T, Brokmeier H.-G, Chateigner D *Quantitative texture analysis of isostatically-pressed molybdite powders by means of neutron diffraction*. Geophysical Research Abstracts, Vol. 7, 08430, 2005.
- Sitepu H., Wright J.P, Ritter C. (2005). *Combined synchrotron and neutron structural refinement of two stages martensitic transformations during thermal cycling of the Ti50.75.Ni47.75.Fe1.50* ***and*** *the aged Ni-rich Ti49.30Ni50.70. shape memory alloy*. Proceedings of the seventh LANSCE User Group Meeting", Los Alamos, NM, September 11–13, 2005.
- Ross NL (2005) *Neutrons in the Earth Sciences* (invited). American Chemical Society Meeting, Washington, DC, August 29-31, 2005.

**Publications:**

Ackermann S, Kunz N, Armbruster T, Schefer J and Hänni H (2005) Cation distribution in a Fe-bearing K-feldspar from Itrongay, Madagascar. A combined neutron- and X-ray single crystal diffraction study**.** *Schweiz. Mineral. Petrogr. Mitt.*, in press.

Breger J, Dupre N, Chupas PJ, Lee PL, Proffen T, Parise JB, and Grey CP (2005) Short-Short- and long-range order in the positive electrode material, Li(NiMn)(0.5)O - 2: A joint X-ray and neutron diffraction, pair distribution function analysis and NMR study. *J. Am. Chem. Soc*., 127: 7529-7535.

Sitepu H, Wright JP, Hansen T, Chateigner D, Brokmeier H.-G., Ritter C and Ohba T (2005). Combined synchrotron and neutron structural refinement of R-phase in Ti50.75.Ni47.75.Fe1.50 shape memory alloy. *Mat. Science Forum*, 497: 255-260.

Sitepu H and Brokmeier HG (2005). Use of neutron diffraction for describing texture of isostatically-pressed molybdite powders. *Solid State Phenomena*, 497: 83-88.

Sitepu H, O'Connor BH, and Li DY (2005). Comparative evaluation of the March and generalized spherical harmonic preferred orientation models using X-ray diffraction data for molybdite and calcite powders. *J. Appl. Crystallogr*., 38: 158-167.

Sitepu H, Brokmeier HG, Chateigner D and Wright JP (2005) Crystallographic phase composition and structural analysis of Ti-Ni-Fe shape memory alloy by synchrotron diffraction. *Solid State Phenomena*, 105:139-144.

**Plans for Year #5 include the following:**

We will continue to work with the COMPRES community to broaden the base of neutron researchers by providing financial assistance for researchers to carry out

experiments at neutron facilities and by helping with preparation of proposals.

Dr. Sitepu will follow up on conversations with LANSCE personnel to explore new opportunities for high-pressure research on the HIPD beamline to complement high-pressure activities on the HIPPO beamline (which is oversubscribed). This will also require coordination with LANSCE and the SNAP team for use of Paris-Edinburgh cells.

H. Sitepu will coordinate efforts with S. Clark (LBNL) and Y. Zhao (LANSCE) to explore the use of neutron resonance techniques to obtain temperature at high pressure in high PT cells.

Professor R. Wenk (Berkeley) and N.L. Ross (Va. Tech) are organizing a Mineralogical Society of America Short Course on "Application of Neutron Scattering in the Earth Sciences" that will be held in December 2006 adjacent to the Fall AGU meeting.

We will work with Y. Zhao (LANSCE) to develop a Winter School to be offered in early 2007 that will focus on high-pressure neutron diffraction and involve a "hands-on" experience for participants.

# *C. Infrastructure Development*

## C.1 Multi-anvil Cell assembly Development Project.

[K. Leinenweber, J. Tyburczy, T. Sharp; Arizona State University]

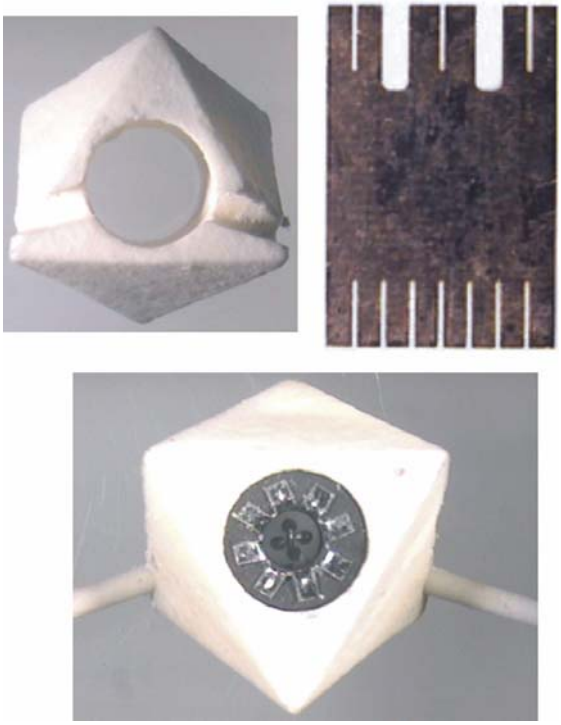
This report describes progress on the COMPRES multi-anvil cell assembly development initiative in Year #4.

**Current status of the project**

The first four years of this initiative have resulted in the development of cell assemblies that are now available to the community. In order to offset the costs of these assemblies, members of the community are now paying for them in cases where the development is far along and the proper functioning of the assemblies has been demonstrated. In order to set up the fee scale, we have analyzed the cost of producing the assemblies carefully, piece by piece. For new designs that are under testing, or when a laboratory simply needs a few samples of an established assembly to test, the assemblies are still being distributed free of charge. The assemblies are available in their entirety – i.e. everything for multi-anvil runs except the carbide – in order to enable other laboratories to do their research more easily. The materials can also be ordered separately.

We have identified outside sources for a significant fraction of the parts. We have tested many new sources that are capable of providing well-functioning pieces of assemblies, and have paid special attention to price breaks that occur when larger numbers of parts are made. A typical number that we use as a benchmark is one thousand pieces. We find in practice that if a company can successfully manufacture this many of a particular part - for example, a thermal insulating sleeve or a furnace - at a good price, then it can be used effectively as a source for this project. With such sources for the majority of the parts, we can easily provide a large number of multi-anvil laboratories with working assemblies. We can also expect better short-term reliability and reproducibility because the batches tend to be internally consistent. Long-term reliability is ensured by fully inspecting new batches when they arrive. This sourcing also allows the price to be more easily known, since there are fewer hidden costs associated with outside sources.

This year we have developed outside sources for molybdenum and TZM contact rings, and for the various MgO inner sleeves in all the assemblies. These were all made by the COMPRES-supported machinist before, which took time away from the important task of doing prototyping of new designs. We also initiated the first use of laser-cut Re furnaces to replace our furnaces made by EDM, a significant new step that allows large quantities of very clean, precisely cut and well-functioning furnaces to be made at a low cost. It also creates new technical capabilities because holes and slits can now be cut within the furnaces as well as around the edges (such slits are used for the in-situ assemblies; see below).



(Figure 1. Basic construction of the octahedron, foil furnace, insulating sleeve and thermocouple for the 8/3 COMPRES assembly, showing a furnace made by EDM).

Many of the parts for the standard assemblies, however, are still made in-house by the COMPRES-supported machinist. Currently, we are still doing the full fabrication of all the parts made of zirconia (thermal insulation; 1 to 3 parts per typical assembly) and lanthanum chromite (thermal insulation or furnace; 1 part per typical assembly) in-house. This involves cutting raw ceramic blocks into square strips and turning them on the COMPRES lathe to produce the parts, a labor-intensive process. We are also still milling the pyrophyllite gasket trapezoids (twelve parts per assembly). In addition, although the ceramic octahedra are injection-molded at an outside company, we are grinding the thermocouple notches into them ourselves on a computerized mill. These are the major functions that our shop is performing on the production end of the COMPRES project, along with the distribution and packing of the materials to all the laboratories, the firing or cleaning of some parts from outside sources, and the checks of quality between batches.

**Needs for 2005-2006 that are not covered by recharge**

The 2005-2006 funding is to be used to make improvements that will be necessary for this project to function effectively on a recharge basis, and to continue multi-anvil technique developments that are useful to the community but are not covered by the fees charged for the assemblies.

A primary need is in proving a new source for zirconia parts, fully made in final form and significantly less expensive than the current parts. We have recently identified

a promising source for this material: we have developed a provisional formula and technique for injection molding zirconia parts in collaboration with an outside company and made test boules. We will need to order batches of finished parts, using the funding for the final year, and do calibrations of assemblies made using this new zirconia. This will be a significant development because of the widespread use of zirconia ceramic in our field and the current expense and difficulty of procuring and machining it. The existing COMPRES assemblies currently have a total of eight different parts made of this material, and they occupy a significant part of the fabrication time at present.

In order to outsource the task of cutting pyrophyllite gaskets, we will be testing an outside source of pyrophyllite plates of the correct thickness and a laser-cutting source that has provided excellent samples of trapezoids in the past numbers (the laser-cut gaskets have better tolerances and more perfect shapes than the milled ones) but only in small numbers so far.

Another important group of parts not made outside are those made from LaCrO3, again starting with ceramic blocks. We will continue making these parts ourselves while seeking outside fabricators, although we have not yet identified a candidate, and LaCrO3 is a much less common industrial material than zirconia.

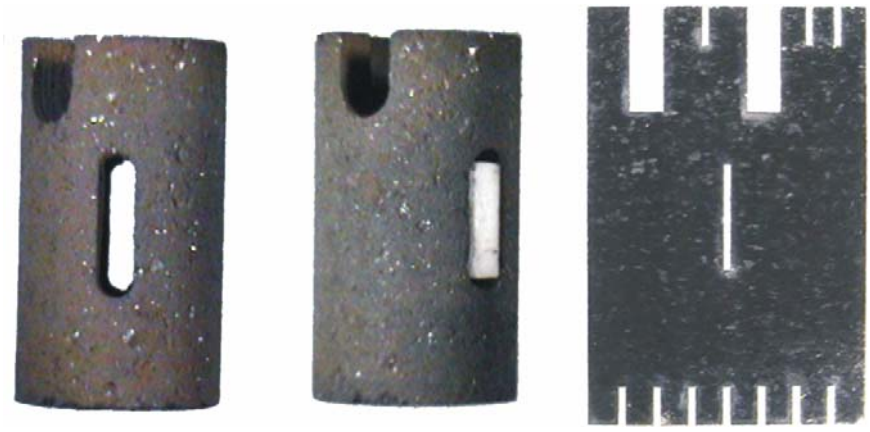
We will set up a facility for welding type C thermocouples, with a small CCD camera and microscope, a welding box using argon/hydrogen mixtures, and tungsten welding electrodes (the combination recommended by the company that makes the thermocouple wires). The camera will be used because the arc is too hot to view by eye through a filter and still be able to see the thermocouple. We would like to try providing welded thermocouples because the current method of crossing the thermocouple through a 4-hole ceramic, although easy to set up, sometimes does not lead to a connection until the pressure is increased first. This has the undesirable consequence that a thermocouple connection cannot be proven until the pressure is already increased, when it is too late to modify the circuit if there are problems external to the assembly but internal to the multi-anvil module. We feel that welded thermocouples will further increase success rates in our system.

**Other developments**

We will continue to sell full assemblies at costs from $40-55 each depending on the assembly, as well as separate parts or raw materials as needed or requested, and will continue to work on reducing the prices as new sources are found and/or larger batches are made. The effect will be to continue to reduce the overall labor and material costs for high-pressure research, because laboratories will not have to develop materials or assemblies if they don't choose to, and because the procurement of larger quantities and the use of better fabrication techniques will result in savings.

We will also work on further establishing the new in-situ assemblies, which have relied on several recent developments: slitted Re furnaces (laser-cut), LaCrO3 sleeves with windows (in-house machining), special mullite octahedra (injection-molded), and in

one case forsterite thermal insulation sleeves for x-ray access. These assemblies have generated a surge of interest in various groups and are being thoroughly tested and used at APS and Daresbury not only by us, but by several other groups whose in-situ work is being enabled in part by these designs.



(Figure 2. Slit system for allowing x-ray access to samples in the 8/3 assembly, for in-situ x-ray diffraction studies. The zirconia sleeve with thermocouple slots and windows (left) is machined by us, while the rectangular alumina pieces (inserted in the windows, center) are cut at a ceramics company, and the slitted rhenium furnace (right) is commercially laser-cut. )

Finally, we will continue testing the assemblies in our laboratory, in collaborating laboratories, and at APS and Daresbury where in-situ testing and calibration of the standard cells (not just the specialized in-situ cells) is ongoing.

## C.2 Development of the Laser-Heated Diamond Anvil Cell

[T. Duffy, Princeton University, V. Prakapenka, University of Chicago, G. Shen, Carnegie Institution of Washington, D. Heinz, University of Chicago, A. Campbell, University of Maryland]

**Timeline of 2005 Activities**

February 2005. Safety hardware installation completed for use of CO2 laser system in GSCEARS laser lab. Laser safety protocol established and approved for use by APS administration.

March 2005. Princeton/Chicago collaborative beamtime at 13-ID-D. Measurements of thermal pressure and calibration of new pressure standards.
February 2005-July 2005. Equipment procurement and bench-top testing of laser heating system design and sample configurations in GSECARS laser lab.
July 2005 Andy Campbell becomes Asst. Prof. at U. of Maryland
June – August 2005 Finite element modeling calculations carried out by B. Kiefer (New Mexico State) and T. Duffy (Princeton)
June-September 2005 Search for Campbell's replacement. Post-doctoral position formally offered to Alexei Kutznesov in November 2005.

**Accomplishments**

$CO_2$ laser heating system: The bench-top layout of the $CO_2$ laser heating system is shown in Figs. 1 and 2. The system has been tested using diamond cell samples of $SiO_2$ and San Carlos Olivine. Figures 3 shows a screen shot of the CCD monitor during in situ heating whereas figure 4 shows the quenched sample with clear evidence that a high-pressure phase transition has been achieved.

**Some of the technical considerations that have been addressed are as follows:**

The heating of different optical components when placed in the $CO_2$ beam path was measured using a thermocouple. Laser-induced heating was usually measured over a range of laser powers, and as a function of time. A key issue is the amount of heating of the glassy carbon laser mirror near the DAC through which the x-ray beam passes (Fig. 5). The Ag/C mirrors that are currently used for 1 μm heating in 13-IDD are a poor choice for $CO_2$ laser heating. In fact, the reflectivity was measured as only ~90% for this mirror at 10.6 μm. An Au/C mirror, which was prepared by Campbell and Shen by Au-coating the existing glassy carbon mirror, was far superior to the Ag/C mirror, and did not exhibit significant heating even at high laser powers.
Power regulation of the $CO_2$ laser is carried out using a variably attenuated using a rotatable brewster window device. In CW mode there is no power regulation available at the laser head; it must be done externally. The attenuator system has a measured extinction ratio is about 160:1 which is more than adequate for our purposes. The next step is to motorize this device so power can be varied remotely or a feedback system used.

Beam alignment is currently carried out with a 633-nm diode laser together with a beamcombiner. With the beam nearly centered through all of the ZnSe optics, and with an incident angle close to the DAC axis, there was only minor deviation (maybe 10-20 μm) between the positions of the alignment laser and $CO_2$ laser inside the DAC. We are investigating IR-sensitive CCD cameras to improve our ability to image the sample and heating spot simultaneously inside the diamond cell.

Several different DAC heating geometries have been tested. Delivering the $CO_2$ laser beam into the DAC at an off-axis incidence angle was tested but abandoned because alignment turned out to be cumbersome. This will be re-investigated in the future. On-axis delivery on one side with viewing optics on the other side was the arrangement used for most tests to date (Fig. 1). This design should be relatively easy to integrate with existing optics in 13-ID-D.

$CO_2$ laser heating of DAC samples could be carried out with either type I or type IIa diamond anvils. Type I diamonds absorb quite a bit more, and therefore require 2-3 times higher laser powers to heat the samples. In these cases, cooling of the diamond anvil cell is critical. Type II anvils transmit considerable radiation through the cell, and this necessitates attention to stray beams and protection of sensitive components. A arrangement that uses a Type II anvil on the delivery side and a Type I anvil on the transmitting side might eliminate this problem. To date, we have heated at maximum pressures of about 30 GPa with type IIa anvils and 40 GPa with type I anvils and we do not appear to be close to any pressure or laser power limits.

There are a number of further technical developments necessary in the bench-top mode. In addition to power control, motorization of several translation and tilt stages isneeded as is development of a computer-based user interface. An external shutter system (water-cooled) needs to be developed as does a DAC water-cooling system. A feedback system to compensate for slow drifts of laser power is also needed. Long term stability of optics (including mounts) needs to be tested and, if necessary, cooling systems included. A series of systematic studies using a variety of diamond anvil types and sample types will also be carried out.

Finite element models of the laser-heated diamond cell: We expanded our study of finite element simulations in the diamond anvil cell (Kiefer and Duffy, 2005) to consider a range of realistic sample geometries that are used in practice for $CO_2$ and Nd:YLF laser heating. This work is currently being written for publication and selected figures (Fig. 6-10) for different geometries are shown. The results in some cases confirm preconceptions, but in several cases rather surprising results are obtained. As examples, we have simulated single- and double-sided hot plate geometries (Figs. 6,7), single- and double-sided heating of metallic samples (Fig. 8,9) and the micro-furnance geometry of R. Boehler (Fig. 10).

**Future Plans**

This is our proposed timeline for future work on this project.

- February 2006 -- A. Kuznetsov joins project.
- Until April 2006 - lab work/testing and complete equipment purchases
- May 2006 - final optical design of $CO_2$ laser heating in the 13-IDD station completed.
- July 2006 - hardware design and laser safety operation procedure
- 2006-3 APS run (October-December 2006) - $CO_2$ system installation in 13-IDD station and testing
- 2007-1 APS run (February-April, 2007) - commission time
- 2007-2 APS run (June-August, 2007) - commission time
- 2007-3 APS run (October-December, 2007) - open for general users

**Publications**

Kiefer, B. and T. S. Duffy, Finite element simulations of the laser-heated diamond anvil cell, Journal of Applied Physics, 97, 114902, 2005.

Duffy, T. S., Synchrotron facilities and the study of deep planetary interiors, Reports of Progress in Physics, 68, 1811-1859, 2005.

Shieh, S. R., T. S. Duffy, and G. Shen, X-ray diffraction study of phase stability in SiO2 at deep lower mantle conditions, Earth and Planetary Science Letters, 235, 273-282, 2005.

A. Kubo, T.S. Duffy, S.R. Shieh, G. Shen, V.B. Prakapenka, Thermal pressure in the laser-heated diamond cell, Advanced Photon Source Activity Report 2003, ANL-04/16, December 2004.

Kiefer, B and T. S. Duffy, Effect of sample geometry on thermal structure of the laser-heated diamond anvil cell, in preparation, 2005.

**Figures**

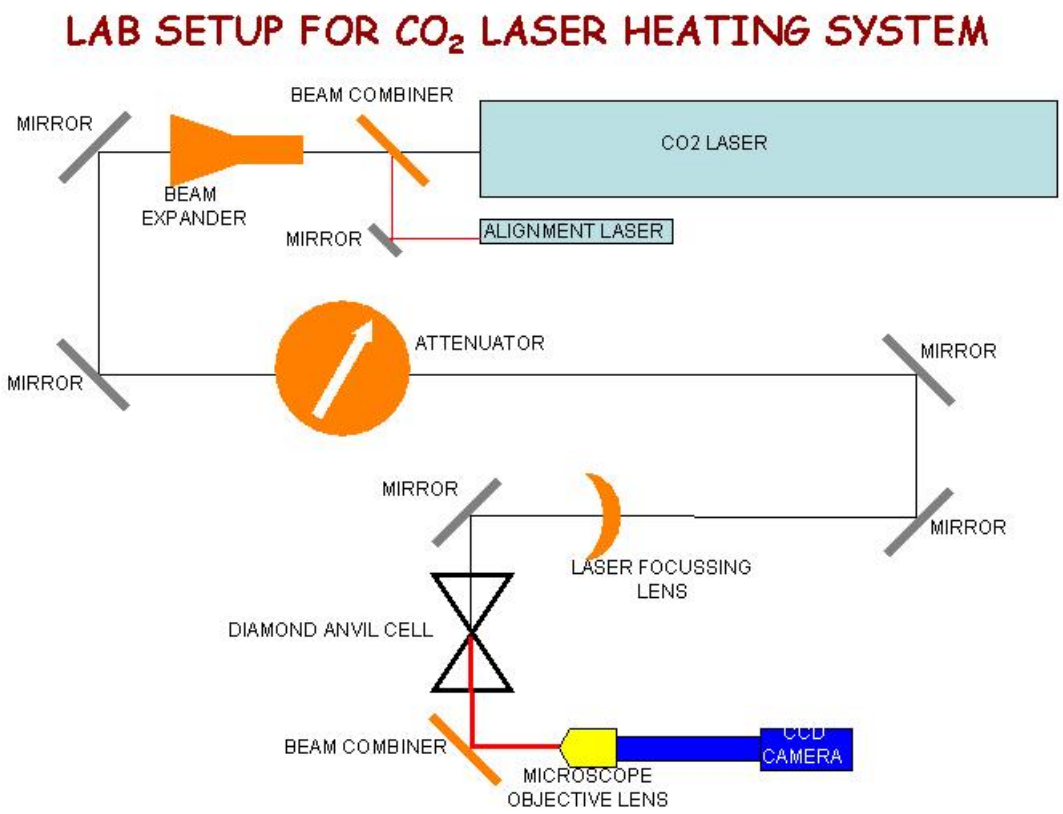



Figure 1. Bench top set-up of $CO_2$ laser heating system.

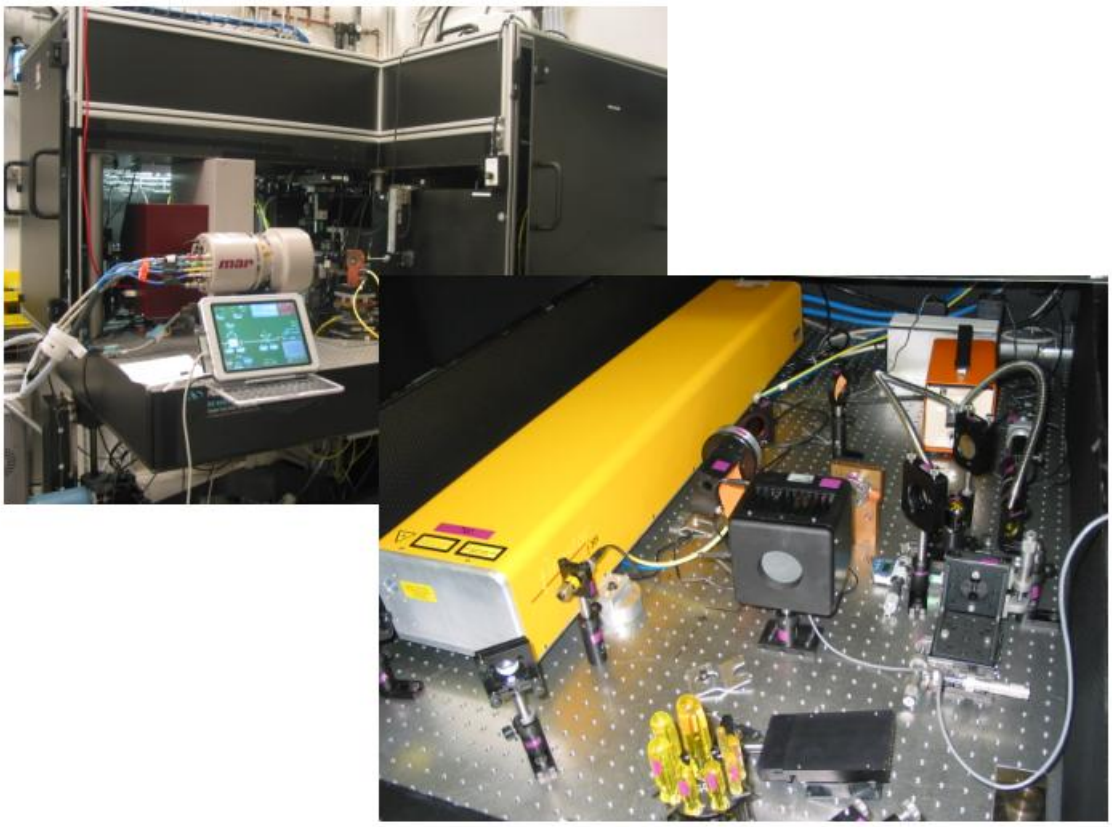


Figure 2. Upper left. Diamond anvil cell set-up at 13-ID-D, GSECARS. The $CO_2$ laser heating system will share space with the existing Nd:YLF system in the upper deck of the recently re-designed set up. Lower right. Photo of breadboard setup of $CO_2$ heating system.

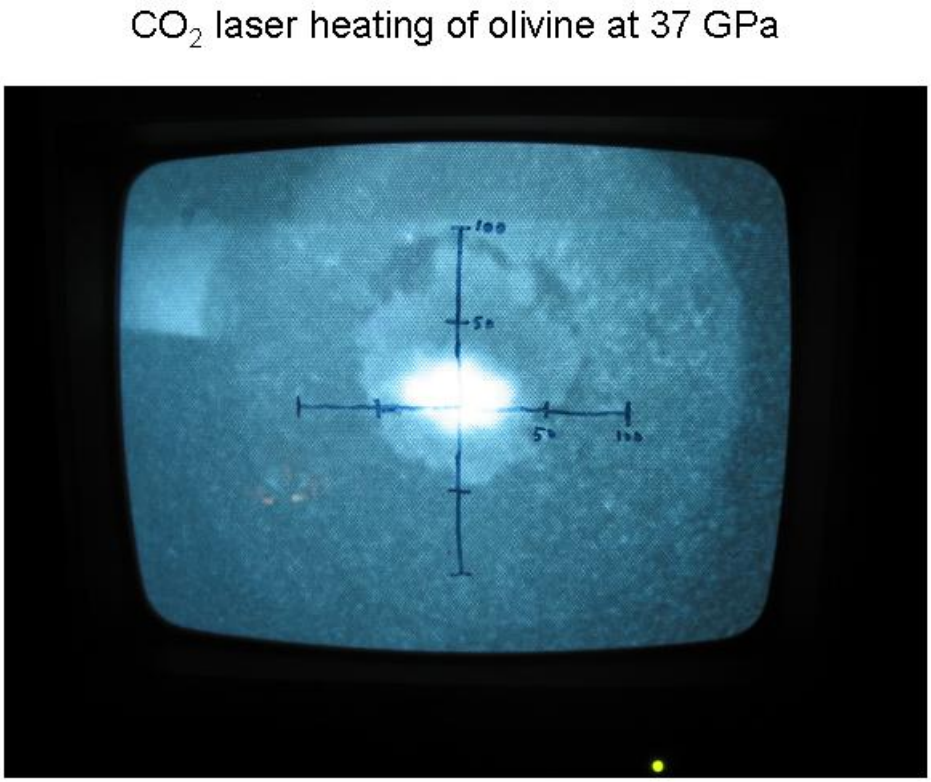



Figure 3. Screen shot of CCD monitor showing $CO_2$ laser heating in situ.

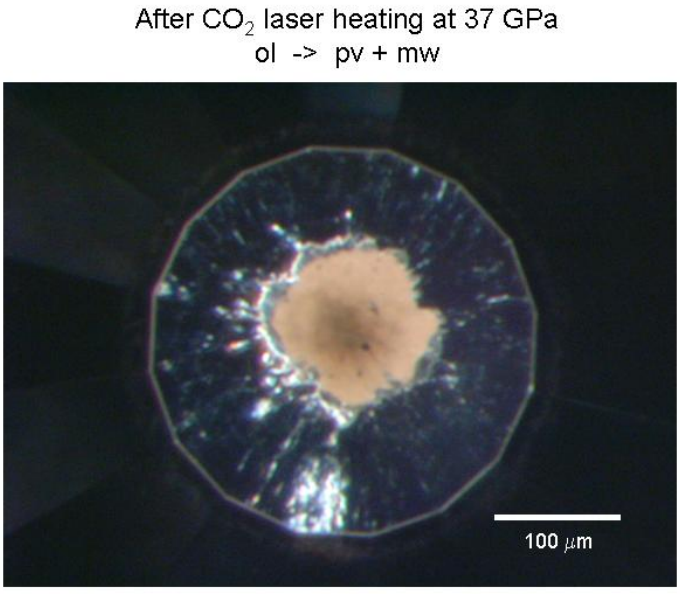



Figure 4. Quenched sample of San Carlos olivine after $CO_2$ laser heating at 37 GPa. The dark region in the center is where olivine has been transformed to a mixture of $(Mg,Fe)SiO_3$ perovskite and (Mg,Fe)O ferropericlase.

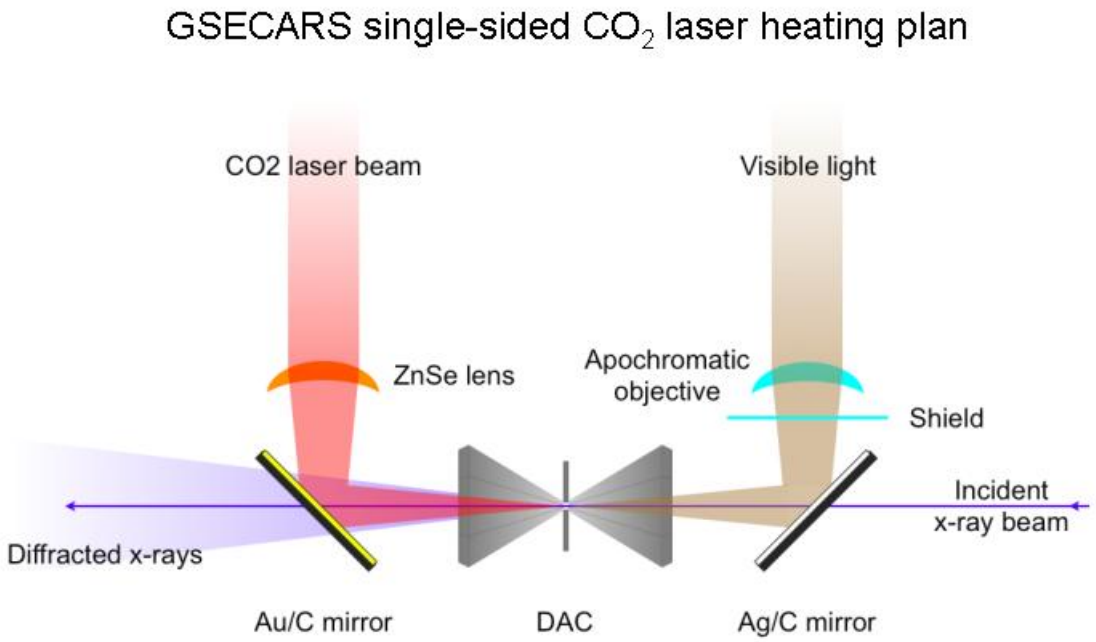



Figure 5. Beamline layout of CO2 laser heating system. (Shape of the apochromatic objective is for visible radiationand will be modified for IR)

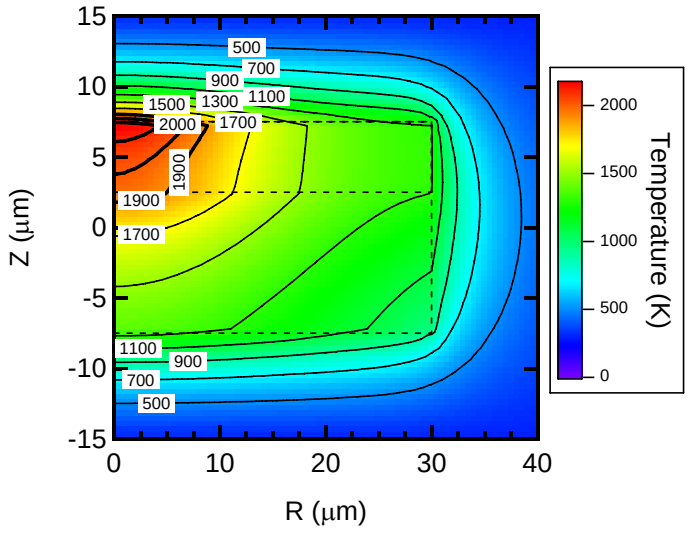



Figure 6. Thermal structure for single-sided hot-plate geometry using TEM00 laser.

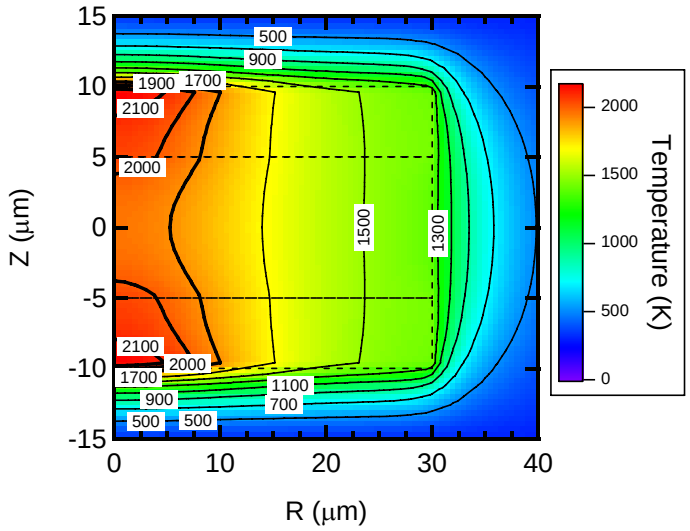



Figure 7. Thermal structure for double-sided hot plate geometry using TEM00 laser.

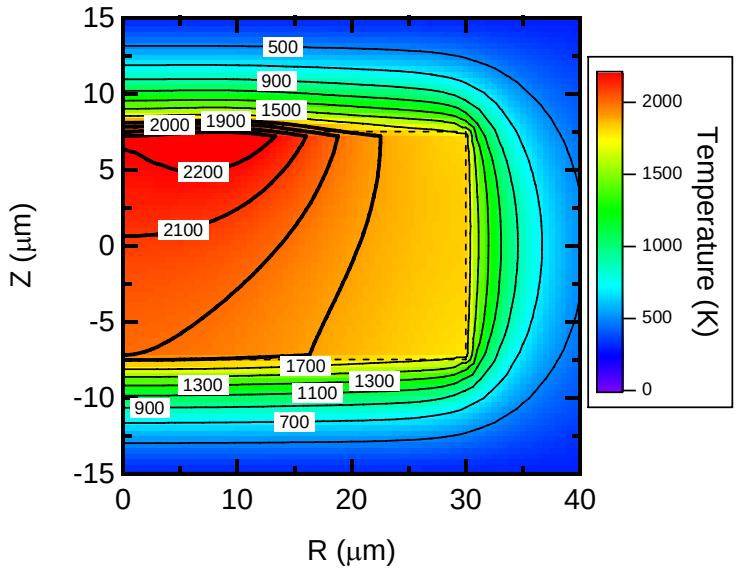



Figure 8. Thermal structure developed by single-sided laser heating of a metallic sample with a TEM01 laser beam. In this case, the axial thermal gradient is much reduced when a TEM01 laser is used compared to a TEM00 laser, for which lateral heat flow is more important and thus results in a strong axial gradient.

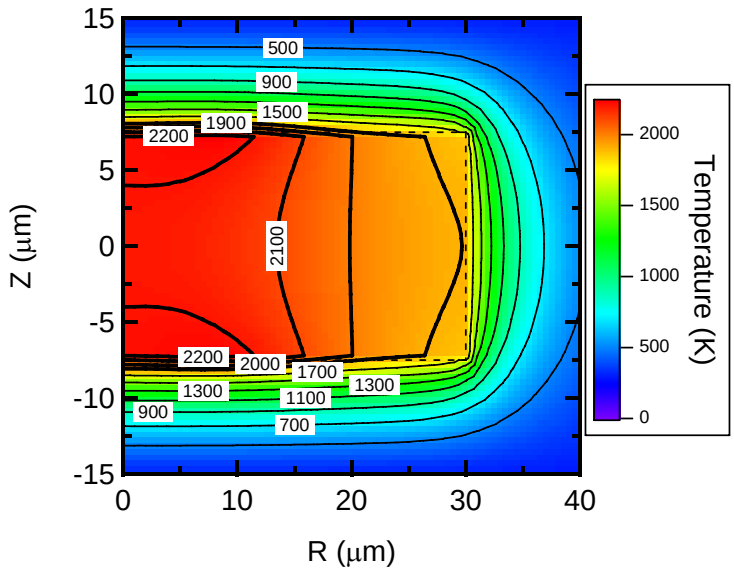



Figure 9. Thermal structure of a metallic sample heated on both sides using a TEM01 laser beam. The axial gradient is much reduced compared to single-sided heating.

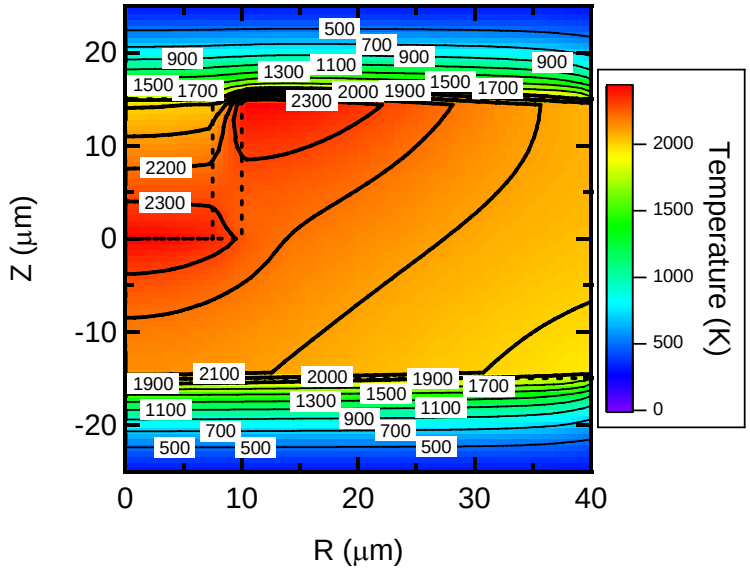



Figure 10. Thermal structure for microfurnace geometry.

## C.3 Brillouin Spectroscopy at the Advanced Photon Source

[J. Bass, University of Illinois, Urbana-Champaign and G. Shen, Carnegie Institution of Washington]

Editor's Note: A feature article on this Infrastructure Development Project appeared in the November 2005 issue of the COMPRES Newsletter and may be found at: http://www.compres.stonybrook.edu/Newsletter/V4N3/Newsletterv4n3.pdf

During past year, a great amount of progress has been made on the installation and commissioning of a Brillouin spectrometer has been installed at the APS on GSECARS sector 13-BM-D. In short, a working system is now in place and the first data have been collected. Photographs of the new system are attached. Initial testing and our first commissioning experiments of the Brillouin spectrometer was carried out during two beam time allocations during the last year, and these tests were successful. The first data collected are presently being analyzed and will be written up for publication. With the installation and testing of Brillouin system in the synchrotron hutch, we are far along toward completion of this project.

As described in the original COMPRES proposal, one of the main purposes of this project was to simultaneously determine the density and sound velocities in a variety of materials that could be useful as calibration standards in high P-T experiments. By simultaneous velocity and density measurements, one obtains the pressure on a sample absolutely. Thus, one of our primary goals is to determine a number of primary pressure standards for use in high-pressure-temperature research. Our long range goals are to perform such velocity-density measurements under a wide range of P-T conditions. The high temperatures can be provided by resistance and/or laser heating techniques.

**Our initial experiments this year included the following:**

1. NaCl in B1 phase to 30 GPa in a diamond anvil cell.
2. MgO to 30 GPa with the DAC.
3. Aggregate acoustic velocities, elastic moduli and equation of state of polycrystalline NaCl in B2 phase to 70 GPa.
4. MgO and NaCl at high pressure and high temperatures (by resistance heating) up to 400°C.

In all absolute pressure scale experiments gold + ruby (+ platinum + powdered NaCl) were added to experimental charges to cross calibrate these pressure standards against absolute equations of state of NaCl and MgO.

A second major goal of this proposal was to provide a centralized facility for Brillouin scattering studies. We have provided a state-of-the-art facility that is open to the entire scientific community and not widely available elsewhere (except in a few specialized labs). We are already working with other groups that have expressed interest in using the system (e.g., U Nevada Las Vegas, Arizona State).

Up to the present we have designed the system, ordered equipment, built a much-simplified protype at Illinois, and tested the main components. In year 2 and 3 we were

building up various prototype optical configurations that might be used at APS, and working on ways of making the optical set up more compact. We tested the Fabry-Perot interferometer that would be moved to APS. Note that the APS Fabry Perot and control electronics differed substantially from the system we used in Urbana (which was purchased 20 years ago), and we spent time gaining experience with the new components. Over the last year the system to sector 13 and installed the full and more complex optical configuration that is now in place, worked on controls for remote operation of the spectrometer, and performed initial testing/commissioning of the system on samples of MgO and NaCl in the diamond cell.

Some key design considerations are 1) the restricted space in a synchrotron hutch, 2) making sure that the Brillouin system does not interfere with other experiments performed on the beamline, 3) the need for quick set up/break down of Brillouin experiments, and 4) the safety requirements due to the use of the class-IV laser. We ultimately decided that the Brillouin system should be on an elevated optical table so that it does not interfere with other x-ray experiments. In addition, we decided to use a vertical scattering plane, which is different from all Brillouin systems we have seen before. This novel design allows the focusing and collecting optics to be easily moved in and out of position for Brillouin work.

**Work Remaining to be Performed:** The following tasks will be worked on until the end of our current COMPRES support on April 30, 2006.

1. Simplify procedures for optical alignments of the system.
2. Implement hardware and software for additional and easier remote operation of the Brillouin system, from outside the hutch.
3. Augment the system with for backscattering experiments. Right now, the system can perform experiments in either a 50° or 90° scattering geometries. These should be the most desired options. However, for some experiments a 180° geometry may be needed. Provisions for this option need to be put into place.
4. Continue with testing and commissioning of the instrument. Debug problems.
5. Begin writing a set of instructions for the system
6. Work with GSECARS on transfer of the system's management to them.
7. Writing up a description of the facility (a manuscript is written and being revised for submission to Rev. Sci. Instruments), and writing up research done thus far for publication.

**Participants:**
**Who has been involved? What people have worked on the project?**
Jay D Bass (University of Illinois, Urbana-Champaign (UIUC))
Stanislav V Sinogeikin (research scientist, UIUC)
Dmitry Lakshtanov (grad student, UIUC)
Guoyin Shen (University of Chicago, GSECARS)
Vitali Prakapenka (University of Chicago, GSECARS)
Carmen Sanchez-Valle (post doc at UIUC)

**What other organizations have been involved as partners?** None

**Have you had other collaborators or contacts?** No

.

**Activities and Findings: What have you done? What have you learned?**

**What were your major research and education activities?**

Designed, built, and installed a Brillouin spectrometer at the APS synchrotron. This is the first such facility of its kind and the only place worldwide where Brillouin and synchrotron x-ray diffraction can be performed simultaneously.

**What are your major findings from these activities?**

That Brillouin spectrometer can be successfully interfaced with a synchrotron x-ray beam line for simultaneous density and velocity measurements.

**What opportunities for training and development has the project helped provide?**

This project is an integration of Brillouin spectroscopy and synchrotron x-ray measurements by two groups with expertise in each area. People in both groups will be trained in the other area. This project also provided for the training of a graduate student.

**What outreach activities have you undertaken?**

We have given talks on this subject at several major conferences, workshops, and at COMPRES annual meetings. Input provided by attendees was valuable for the development of this project's concept. We have also identified the nucleus of a user base for the instrument once it is fully tested and commissioned.

**Products: What has the project produced?**

**What have you published as a result of this work?**

No journal publications thus far, but several conference abstracts. A description of the system is almost ready for submission to Rev. Sci. Instr.

**Major Journal Publications** None

**Books and other one-time publications** None

**What Web site(s) or other Internet site(s) reflect this project?**

COMPRES website. A website describing this project is being developed, to be accessed via Bass' university webpage. A GSECARS website describing the Brillouin scattering facility is also being developed.

**What other specific products have you developed?** None

**Contributions: How has the project contributed?**

**To the development of the principal discipline(s) of the project?**

This project will allow accurate pressure scales to be developed for high-pressure-temperature experimentation. It will thus allow more accurate determination of phase boundaries in Earth materials and more accurate equations of state. Thus this project will have a great impact on our understanding of deep planetary interiors.

**To other disciplines of science or engineering?**

The pressure scales developed as an outgrowth of this project will be used by all the physical sciences in which high-pressure research is performed. To the development of human resources?

**To the development of human resources?**

This project has involved a graduate student who is obtaining advanced training in spectroscopy and synchrotron x-ray techniques.

**To physical, institutional, and information resources that form the infrastructure for research and education?**

This project makes a powerful and highly specialized facility available to the entire scientific community. It will be open to all for research and education.

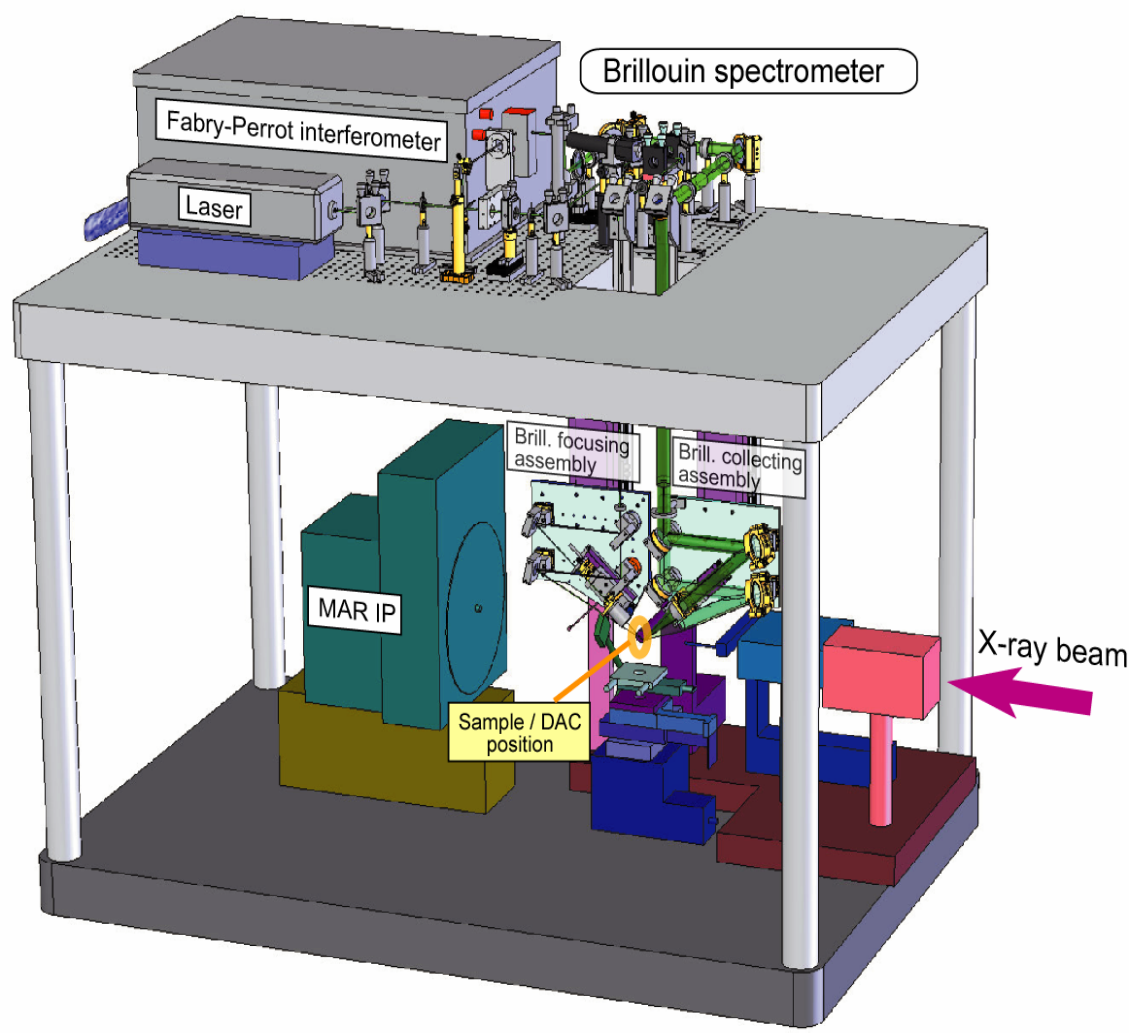



Fig. 1. Schematic diagram of the Brillouin spectrometer at sector 12-BM-D of GSECARS, Asvanced photon source. Most of the Brillouin optics are on the upper level, whereas the sample is in placed in the x-ray beam for all experiments on the lower level.

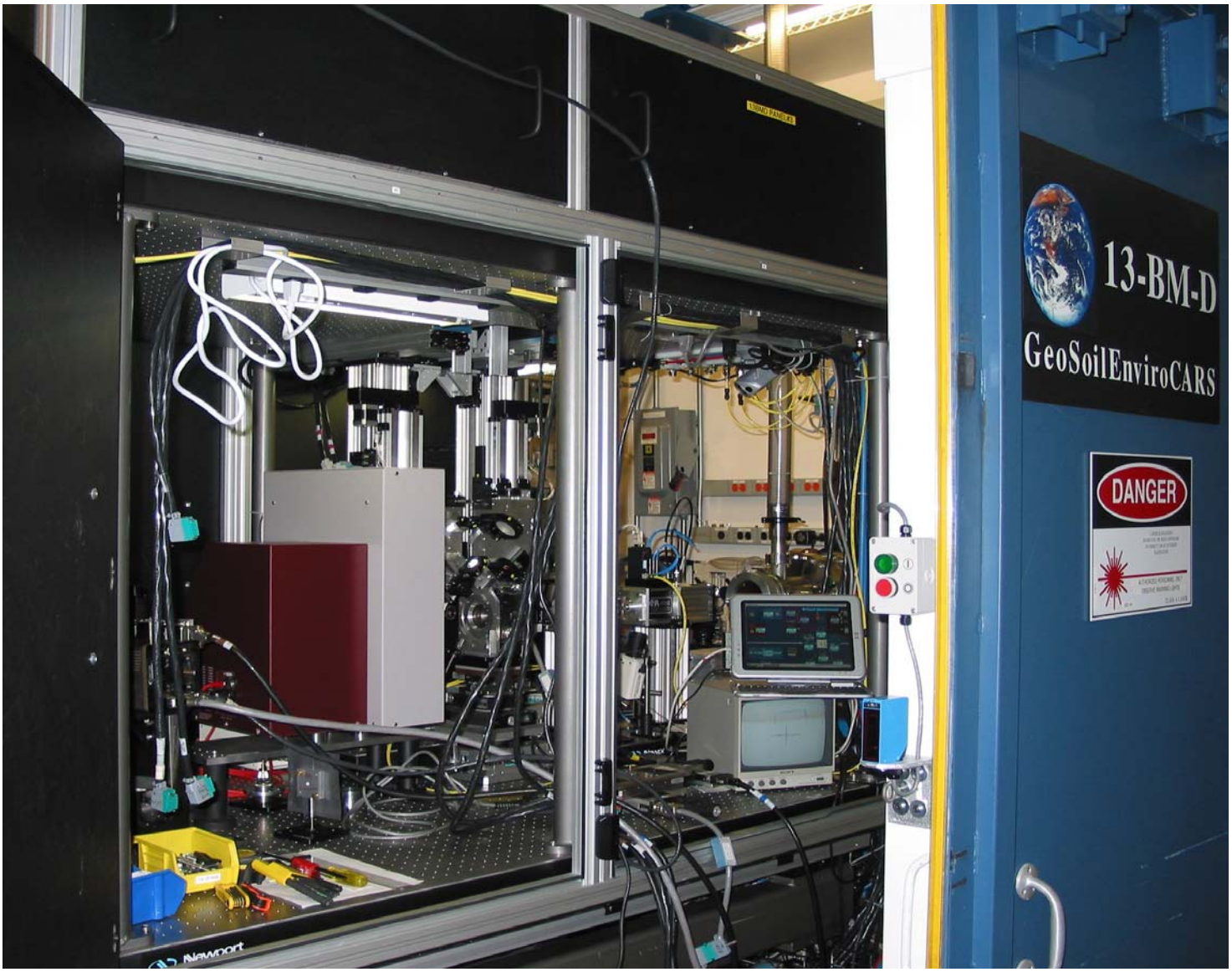
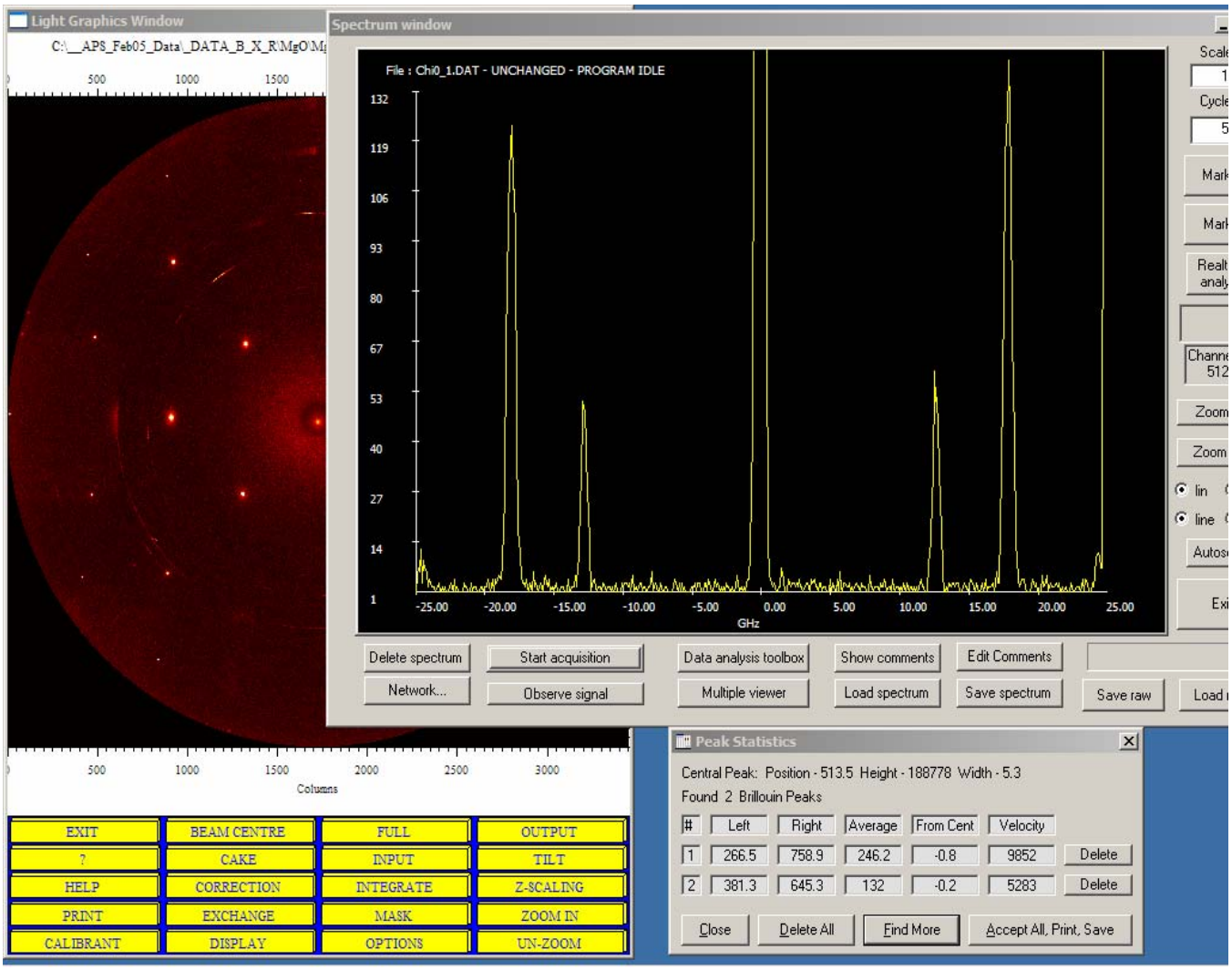



Figure 2: Side view of the Brillouin system at the APS. The upper optics are in the black enclosure at the top of the photo, to comply with APS laser safety regulations.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## C.4 Absolute Temperature Calibration

[Y. Wang and M. Rivers, University of Chicago and I. Getting, University of Colorado]

### Introduction

This component of the COMPRES Infrastructure Development program sought initially to establish implement accurate temperature and pressure measurements within the high pressure community based sound metrological practice. In light of reduced manpower and funding it was agreed in 2004 to concentrate on the accurate determination of temperature. After Ivan Getting's retirement in June 2005, it was decided by the COMPRES Executive Committee on Oct 3 that the program be transferred from University of Colorado (with Getting as PI) to the University of Chicago (with Wang as PI). This report summarizes progresses made thus far in the development of the Johnson noise thermometry in the multianvil apparatus, in order to provide absolute temperature calibrations under high pressure.

### Absolute Temperature Calibration

Temperature measurements have proven very difficult in high pressure environments. Decades of consideration have failed to yield realistic calibration for thermocouples as used at high pressure. Temperature can be measured accurately by Johnson noise thermometry in a high pressure environment, however. Johnson noise is the very small, fluctuating voltage noise which appears across any resistor at temperature above absolute zero. For an open circuit resistor in thermal equilibrium, the relation between the mean square noise voltage across the resistor, $\langle E_R^2 \rangle$, the resistance, R, and the absolute temperature, T, is given by $\langle E_R^2 \rangle = 4kBRT$, where k is Boltzmann's constant and B is the electrical bandwidth over which the noise voltage is observed. This random fluctuating voltage has Gaussian-distributed amplitude, a zero mean, and a white power spectrum. All of the effects of pressure, strain, and any chemical reactions on the resistor sensor are cast into the resistance term. The resistance is measured separately for each reading thereby accounting for all such effects. Very subtle electrical measurements are required to the value of $\langle E_R^2 \rangle$.

The Johnson noise signal in a practical noise thermometer has a typical RMS value of less than one μV. To achieve the desired temperature resolution of ~0.1 % this signal must be resolved to about one part in a thousand, or about one nV. This is a demanding electronic challenge. The measurements must be restricted to the Johnson noise itself. Any spurious noise in the signal would corrupt the measurements by reducing the sensitivity and by introducing time varying errors. These errors must be eliminated by making the thermometer circuits and cables sufficiently insensitive to the ambient electromagnetic environment. This is achieved by having sufficiently good isolation and shielding of the circuits and cables and by having an electromagnetic ambient which is sufficiently quiet.

In an effort to address this long-standing high pressure temperature measurement

problem Getting approached Dr. John L. Hall. John is a world renowned metrologist at JILA, a NIST co-sponsored research institute at the University of Colorado, and recipient of the 2005 Nobel Prize in Physics for his outstanding contributions to the development of laser-based precision spectroscopy, frequency/time standards, determination of the speed of light, and the optical re-definition of the meter. John has provided all the critical circuit design for this project. Over several years' effort, a Johnson noise thermometer (JNT) has been constructed for use at high pressure. In last year's report, Getting provided detailed information on the operation principles and laboratory performance of the JNT under ambient conditions.
Progress made in 2005

***1. Fabrication of resistors for high pressure testing:*** The resistors have been successfully built on the planner end of Lucolox (pure, polycrystaline alumina) disks 5 mm in diameter and 1 mm thick. They are fabricated by vapor deposition of metals (Ti and Pt) through a mask to produce a serpentine metal ribbon. The initial resistance of ~20 ohms is expected to increase several fold at the target pressures and temperatures to ~100 ohms maximum to match the design of the JNT circuits.

***2. Development of high pressure cells for JNT testing:*** Several runs were conducted at GSECARS using the DIA apparatus to develop a cell that will accommodate the 5-mm diameter resistor with four thermoelement leads. These four wires serve as:

1 Four-wire access to the resistor for the JNT measurements,
2 Two independent thermocouples (for comparison with the JNT measurements), and

A four-wire probe for measuring resistance of the resistor under high P and T. The cell design for a subsequent test at Boulder (see 3 below) is show in Fig 1.

3

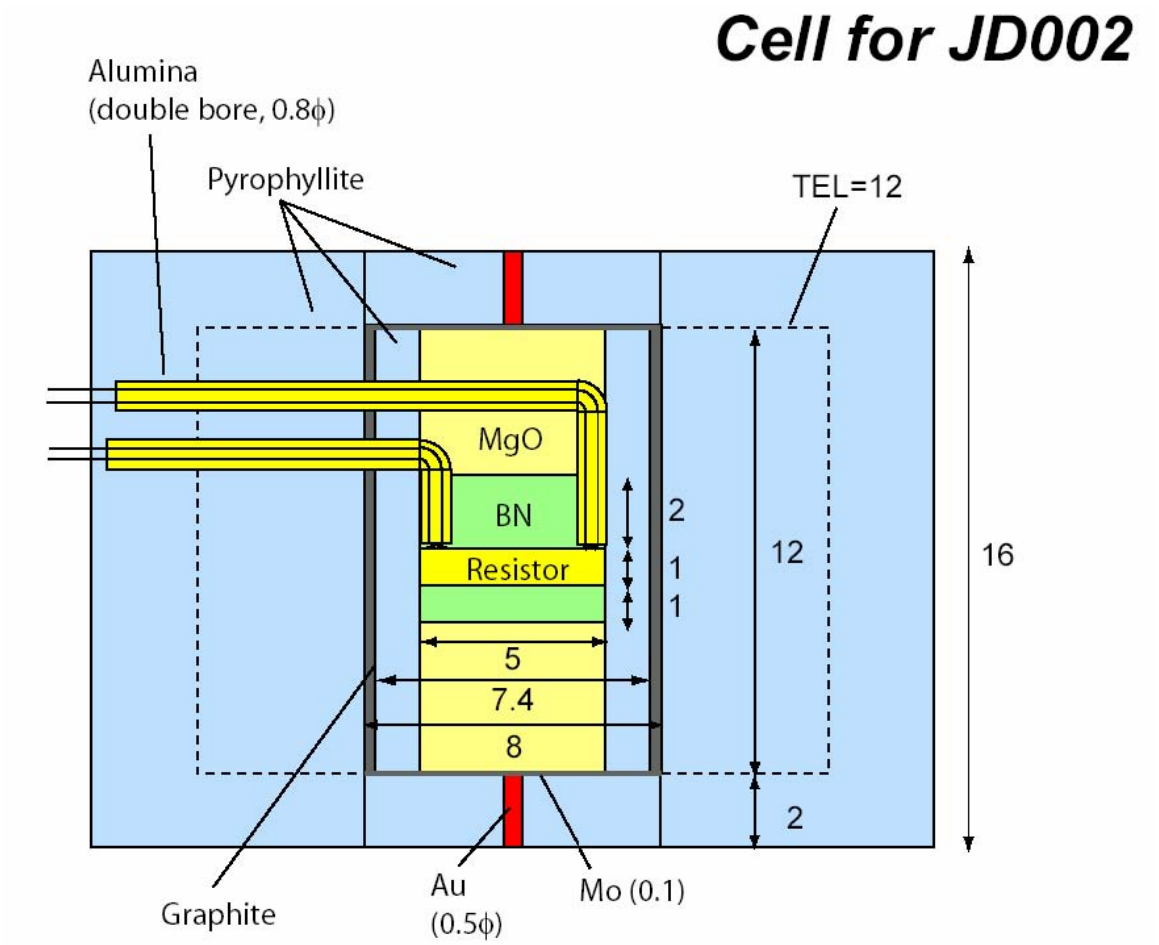



**Figure 1**. The 16 mm DIA cell used for test in Colorado, in June 2005. Dimensions are in mm.

***3. An in-situ test at University of Colorado:*** Based on these developments at GSECARS, Yanbin Wang and Nori Nishiyama traveled to Boulder in June of 2005 and worked with Ivan Getting to conduct the first high P-T test of the JNT cell with the emphasis on cell electronic noise characterization. For this purpose, the JNT was not connected to the cell; rather, an oscilloscope was used to examine the noise across all thermocouple wires during heating. The resistor behavior at high temperature was also studied. For the test, the DIA module was shipped from GSECARS to the CIRES lab, where environmental electronic noise has been carefully characterized (see 2004 report).

In this test, we have achieved the following:

1 The two thermocouples made excellent contact to the resistor, so that TC emfs and JNT probe resistance could be measured and recorded.
2 The furnace was successfully heated to 1000 °C
3 AC noise levels on the W/Re thermocouples as well as on the resistor were measured and recorded. This was the first detailed observation of AC noise on a thermocouple known to us in ~35 years. AC voltage noise can cause significant systematic errors in thermocouple measurements and could make the Johnson noise measurements very difficult. Both the thermocouples and the JNT probe

are vulnerable to inductive coupling to the heater because the leads are separated from each other in part of the cell in the presence of a strong, alternating magnetic field. The observed values are surprisingly low (Fig. 2). The AC voltage levels, 0 - 4 mV on the JNT probe and 0 - 2 mV thermocouples to 1000°C, are about an order of magnitude lower than approximate values recently reported to one of us (Getting) observed in other multianvil cells. They are non-threatening to the very sensitive JNT pre-amplifier and to the accurate measurement of thermocouple voltages (See technical note by Getting distributed to COMPRES members in July 2005 and attached hereto as Appendix A).

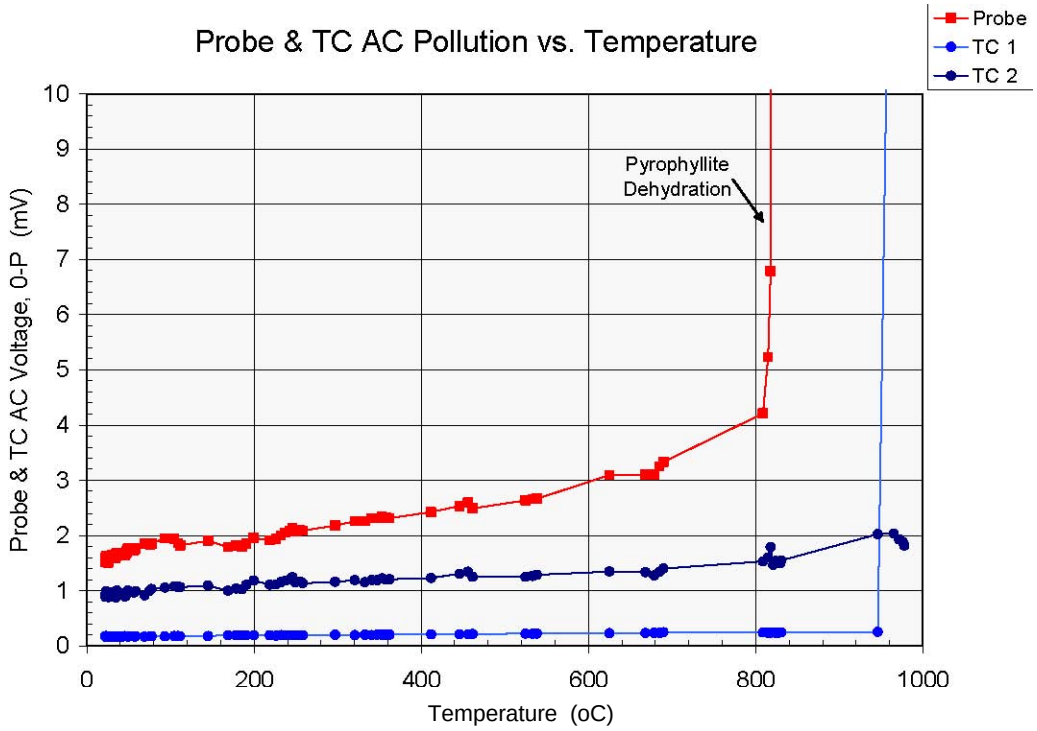



**Figure 2.** AC voltage noise on the JNT probe and thermocouples. The levels on the JNT probe are non-threatening to the very sensitive JNT pre-amplifier.

At about 800°C, AC noise levels jumped by more than one order of magnitude. This was observed on both the thermocouples and the resistor. This temperature is close to the dehydration temperature of pyrophyllite, which was likely the cause of the increase in AC noise. The JNT probe apparent resistance increased by about two orders of magnitude around that temperature and one of the TC failed at about 1000 °C.

Overall, this was a very successful run. The signals we observed indicate that JNT measurements in this type of cell look very feasible. Modification of the cell design is being carried out at GSECARS, to eliminate the pyrophyllite dehydration and improve temperature distribution on the probes.

The report is attached as Appendix B.

**Future plans**

Progress in 2005 has been relatively slow, due to Ivan Getting's retirement and the lack of manpower at GSECARS. Now the project is in the process of being transferred to GSECARS, with the agreement that a post-doc will be hired under joint support of COMPRES and GSECARS. This person will commit at least half of his or her time working the JNT project, and will bring the project back to the fast track. The following is a tentative plan:

**1) Remaining 2005:**

- Build and test the modified cell at GSECARS.
- Continue tests similar to that performed in June at University of Colorado, reduce AC noise across thermocouples and the resistor.
- Refine JNT circuitry and software as warranted to accommodate AC noise.
- Seek a post-doctoral research associate to carry out future development work. Target starting date: 1/1/06.
- Support for the post-doc comes from Getting's remaining funds (~$20,000), with additional COMPRES commitment, and GSECARS, for two years (see plan below).

**2) Jan/Feb 2006:**

- Initial post-doc training at GSECARS, to familiarize current cell design and operation.
- Post-doc begins full time commitment. Cell part preparation and testing
- Connect JNT to proven cell at Colorado; first JNT measurements in the 16 mm DIA cell at Boulder.
- Ship JNT to GSECARS. Install JNT in 13-BM-D.

**3) March - May 2006:**

- Test and installation of JNT at GSECARS (post-doc, Yanbin, Mark, Ivan; ~3 person days x3, Ivan at no cost). Noise characterization in 13-BM-D (location of 250 ton press and DIA), locate noise sources and develop techniques for noise reduction.
- First JNT measurements complete in the 16 mm DIA cell at GSECARS.

**4) May 2006 - Dec 2007:**

- Submit the first paper based on the results obtained from the first test.
- Transfer technical development from DIA to T-25.
- Design, fabricate, and test T-25 cells, starting from large truncations (~ 12 mm).
- Design, fabricate, and test resistors suitable for smaller cells.
- Design, fabricate, and test smaller cell assemblies for higher pressure JNT measurements.
- Conduct systematic measurements of pressure effects on emf for various thermocouples: W/Re, Pt/Rh, etc.
- Conduct JNT measurements in a few selected community "standard cells", e.g., ASU developed COMPRES cells.

- Report results to the COMPRES community, publish obtained results and, if necessary, hold a workshop in Dec., 2007 or early 2008. Complete the project.

**Community Involvement and Outreach**

Once we reach stage 3) in the above plan, we need to calibrate a serious of multianvil cells, with community inputs. Possible collaboration with the ASU cell development project is critical in identifying COMPRES "standard cells" to begin such calibration. The JNT technique may be an additional component in future multi-anvil workshops (like the one held in March, 2005, at GSECARS) or it may even deserve an independent workshop on effects of pressure on thermocouple emf and how to use the JNT to calibrate thermocouple in various cells. In any event, the JNT will remain a community instrument for those interested in calibrating their cells to use.

## C.5 Nuclear Resonant Scattering at High P & T: A New Capability for the COMPRES Community

[W. Sturhahn, Argonne National Laboratory, J. Bass, University of Illinois at Urbana-Champaign, G. Shen, Carnegie Institution of Washington,]

We report here on the activities to date of Year 2 of a 3-year infrastructure development project on Nuclear Resonant Scattering (NRS) at high P and T. The full three-year proposal was resubmitted last year to COMPRES, and it was funded for the second year with the Executive Committee's expectation of continued funding for the full term of the project. We include here a description of activities to date, planned activities for the coming year, and a budget request for Year 3 of the project. The recent move of Guoyin Shen from GSECARS to HPCAT is a positive factor in that it will allow us to coordinate NRS capabilities between sector 3 and sector 16 (HPCAT) even more effectively.

Nuclear resonant scattering techniques are relatively new applications of synchrotron radiation for determining the properties of condensed matter. Our infrastructure development project is aimed at outreach to the COMPRES community on the capabilities and use of this technique and at creating state-of—the-art NRS 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: Synchrotron Mössbauer Spectroscopy (SMS) and Nuclear Resonant Inelastic X-ray Scattering (NRIXS). The applications include (but are not limited to) determining the valence states of iron, the phonon density of states, sound velocities, detection of melting, and detection of high-spin low-spin transitions, all for iron-bearing compounds of geophysical interest.

In the second year of our infrastructure development project, we focused on improvements of the experimental capabilities of the NRS beam line (sector 3ID) of the Advanced Photon Source (APS) to enhance its performance in high-pressure research and made it more accessible to the COMPRES community. Outreach activities, e.g., an upcoming workshop on NRS data evaluation and various presentations at meetings and

conferences, have broadly disseminated information on applications of NRS to understand Earth materials. In particular, we accomplished the following tasks:
Organization of the workshop "Evaluation of Synchrotron Mössbauer Spectroscopy Data using the CONUSS Software", October 2930, 2005 at the APS.
Procurement of a new focusing mirror for increased X-ray intensity;
Installation of a DAC loading facility for users of the NRS beam line;
Procurement of image plate device for NRS with X-ray diffraction;
Generation of numerous new proposals for sector 3-ID of the APS by COMPRES members.

The individual items are described in more detail below.

**Workshop Organization**

We are organizing a workshop on "Evaluation of Synchrotron Mössbauer Spectroscopy Data using the CONUSS Software", to take place on October 2930, 2005 at the APS. Participants will learn about the strategies to successfully evaluate and interpret SMS data collected at sector 3-ID or sector 16-ID. The goals are:

1. Provide a basic introduction of SMS to the Earth science community;
2. Introduce the CONUSS software for SMS data evaluation;
3. Provide "hands on" training in the use of the CONUSS software;
4. Address common experimental issues confronting users.

This workshop provides an ideal format to collectively address data evaluation problems and will help to train COMPRES members to fully utilize the SMS technique. Details on the workshop agenda can be obtained at http://www.aps.anl.gov/News/Conferences/2005/Mossbauer_Data_Workshop. This workshop is a natural follow-up to the introductory workshop on NRS held in year 1.
Procurement of a New Focusing Mirror

Experiments with small samples require a small x-ray beam. In particular, high-pressure studies with sample sizes of 50 μm 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 is about 300 μm and 700 μm, respectively, but the size of the SR beam at the mirror location is about 350 μm vertical and 2 mm horizontal. Therefore, an improvement of photon flux incident on a pressurized sample mounted inside a diamond anvil cell can be achieved by a longer horizontally focusing mirror.

With funds of the High Resolution X—ray Scattering (HRX) group at the APS (W. Sturhahn is leading this group) amounting to about $200k, we procured a horizontally focusing mirror of 60 cm length (see Fig. 1). This mirror has a piezo-electric bending mechanism build into the mirror itself for optimal shape adjustment and will capture most of the X-ray beam at 14.4 keV. We expect an increase the X-ray flux on the

sample by a factor of two to three. 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. Also the persistent oversubscription of sector 3-ID can be more effectively addressed.

**Installation of a DAC Loading Facility**

A facility for loading diamond cells is indispensable if sector 3-ID is to be used regularly for high- P studies by the entire COMPRES community. This is especially true for SMS and NRIXS experiments since they require special types of highpressure cells and loading techniques that are quite different from other X-ray methods, e.g., the development and implementation of Be gaskets for NRIXS. We set up a DAC loading facility in one of the laboratories of HRX group near sector 3. The facility is now available to COMPRES members working at the sector 3-ID beam line.

**Procurement of Image Plate Device**

With $120k in funds from Sturhahn's High Resolution X-ray Scattering (HRX) group at the APS we procured an image plate device. This is the key component for the planned enhancement of the NRS beam line by adding an X-ray diffraction capability. Once operational, the added 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.

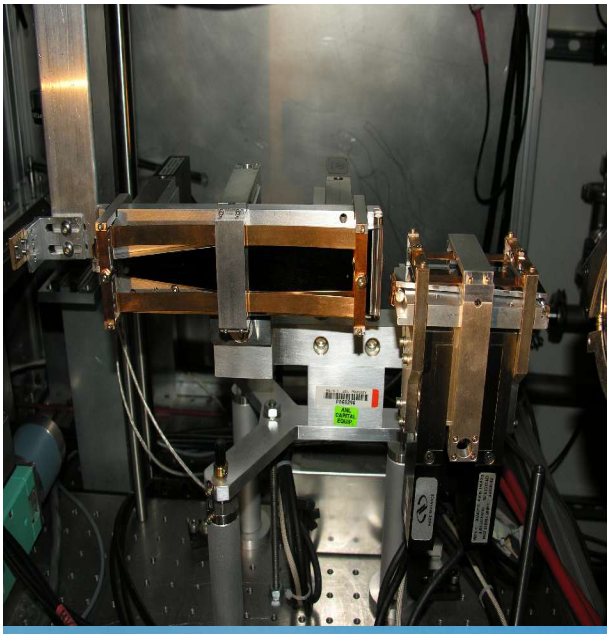
**Generation of New Proposals**

In large part as a result of the first workshop on "Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation" that took place on February 12-13, 2005 at the APS. we were able to catalyze nine new beam time proposals for NRS studies at sector 3-D from COMPRES member institutions for the October-November-December operations cycle of the APS. Experiments based on proposals over the last year have produced novel results, e.g., to be presented in "Novel melting investigations of iron at high-pressure using synchrotron Mössbauer spectroscopy" by J.M. Jackson et al., Abstract for Fall 2005 AGU meeting, San Francisco. A paper on this topic is in preparation, and the manuscript "The equation of state of MORB-related (Al,Fe)$MgSiO_3$-perovskite" by C.B. Vanpeteghem et al. has been submitted to Phys. Chem. Minerals. Other work that benefited from COMPRES support through this proposal is in progress. 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. The HRX group also plans to effectively increase the total amount of NRS beam time in sector 3-ID by 20 % with the beginning of operations at the new IXS beamline 30-ID.

**Planned Activities**

In Year 3 of our infrastructure development project, we will continue the outreach effort to the COMPRES community by assisting interested groups in design, preparation, execution, and evaluation of NRS experiments. We will organize a second tutorial workshop introducing NRS 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 installation of the new focusing mirror system for increased X-ray intensity and the integration of the capability of X-ray diffraction with NRS experiments. The added diffraction capability will 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. The successful completion of all these tasks crucially depends on a dedicated postdoctoral researcher like Dr. Michael Lerche who was hired in 2004. We expect that more proposals for NRS experiments on sector 3-ID will likely result from the workshop, and that Michael will work with the PIs to develop effective proposals that will be very competitive for beam time. In effect, COMPRES will continue to have its own expert to help write proposals, consult on technical aspects of experiment design, and to help run experiments.

**Illustrations**



## C.6 Development of CEAD (COMPRES Environment for Automated Data analysis)

[S. Clark and P. Adams, Lawrence Berkeley National Laboratory, J. Parise, Stony Brook University, M. Rivers, University of Chicago, R. Angel and N. Ross, Virginia Institute of Technology and State University]

In Year 4 of COMPRES, funding was approved for the first year of a two-year project to develop an automated data analysis environment aimed specifically at the needs of the COMPRES community in a code named CEAD (COMPRES Environment for Automated Data analysis). The environment will allow the automation and linking together of existing computer codes, providing a massive gain in efficiency of data processing and analysis. It will also allow the direct comparison of data processing strategies and software and enable the rapid development of new data analysis procedures and computer codes. In our original proposal, we proposed to build on an existing automated crystallographic computing environment, PHENIX, in order to allow rapid and cost-effective development. The resources that we outlined for this infrastructure development project were salary for one post doc with knowledge of crystallography and programming skills, support for two workshops and travel funds for management meetings and site visits. The duration of the project was to be for two years. In that time frame we proposed to recruit a suitable programmer, hold a community workshop, build the software environment, integrate a range of existing program packages, roll out the software to the COMPRES community with a "hands on" workshop and to apply to NSF for funds for the maintenance and the further development of CEAD. This proposal offers the opportunity for COMPRES to show leadership not only to the high-pressure Earth Science community but also to the wider Earth Science and crystallographic communities and beyond. In this report, we include a description of activities to date, planned activities for the coming year, and a budget request for Year 2 of the project.

### Recent Software Developments

Ross Angel attended the International Union of Crystallography General Congress in August, 2005. He learned of several new developments in data processing software that could be employed to address some of the issues we were planning to tackle with CEAD:

1. Robert Dinnebier's group (MPI, Stuttgart, Germany) has developed automated integration software to reduce 2-dimensional powder pattern images (CCD, image plate) down to one-dimensional patterns. Unlike Fit2d, this software handles masking, outlier pixel rejection, and the treatment of aberrations completely automatically, and can be run in batch mode to handle a set of diffraction images. The group is still developing the software, and we expect that it will be distributed in the next year. Robert is very keen to collaborate with us to bring the software to a broader user base.
2. The Rietveld refinement package Topas (university version) is driven by scripts that can be set up to refine a batch of powder patterns simultaneously, and to constrain and chain-refine parameters common to all patterns. John Evans of the

University of Durham, England gave an excellent demonstration at IUCr of how one can directly refine the thermal expansion coefficients of a material to a set of diffraction patterns collected over a range of temperatures. It appears that we might be able to employ Topas to do a similar thing to refine EoS parameters to a series of high-pressure powder diffraction patterns. All that would be required is the development of a series of high-pressure scripts.

**Plan of Action**

Since it appears that many of the issues we identified in our original proposal (batch integration, batch refinement) may be addressed in newly-developed software packages such as those described above, we have modified the plan of action in our original proposal to include:

1 Establish collaboration with Robert Dinnebier (Stuttgart) and John Evans (Durham, Topas).
2 Test and integrate and develop Dinnebier's integration package and Topas for high-pressure work in collaboration with code developers.
3 Review the need for Phenix aspects once item 2 complete.
4 Produce the prototype package based on 1-3 above along with website to gather community input.
5 Schedule a "hands on" workshop in Year 5 of COMPRES for testing of the prototype package.
6 Make revisions and produce documentation, manuals, scripts and tutorials.
7 Distribute to the national facilities.

## C.7 A gas loading system for diamond anvil cells at APS

[M. Rivers, and V. Prakapenka, University of Chicago, G. Shen, Carnegie Institution of Washington]

**Introduction**

A gas-loading system is under construction at the Advanced Photon Source, which allows for loading diamond-anvil cells (DAC) with various kinds of high-pressure gases, gas mixtures, or liquid-gas mixtures at room temperature and at low temperatures down to –30 oC. The main features include:

The system is able to accommodate various types of diamond-anvil cells
The design of the system suits the community's various needs, with documents available to the community to avoid redundancy in reinventing designs.

Safety issues are streamlined as best as possible – in both achieving the safest designs and facilitating the approval for use at various places

.

The system will be available to anyone willing to travel to the APS, and it not restricted to users performing experiments at APS beamlines.

**Benefits of a gas loading system**

- The ability to load gases, gas mixtures, or gas-liquid mixtures
- The ability to load gases (e.g., $H_2$, He) whose boiling temperatures are below liquid nitrogen temperature
- Loading at room temperature without a large temperature cycle
- The sample assembly remains relatively intact during loading, while in the cryogenic loading the boiling liquid sometimes disturbs the sample configuration.
- Providing a better hydrostatic pressure medium

**Project progress**

We have not made as much progress as we had hoped on this project, because GSECARS has a single design drafter (Clayton Pullins), and he has been working on the design of the mirror and monochromator for the 13-BM-C side station, under the NSF-MRI grant that Peter Eng received last year. However, these tasks are nearly complete, and Claytons next project will be the gas-loading facility.

In October'04, we conducted an email survey to the community and received overwhelmingly supportive inputs.

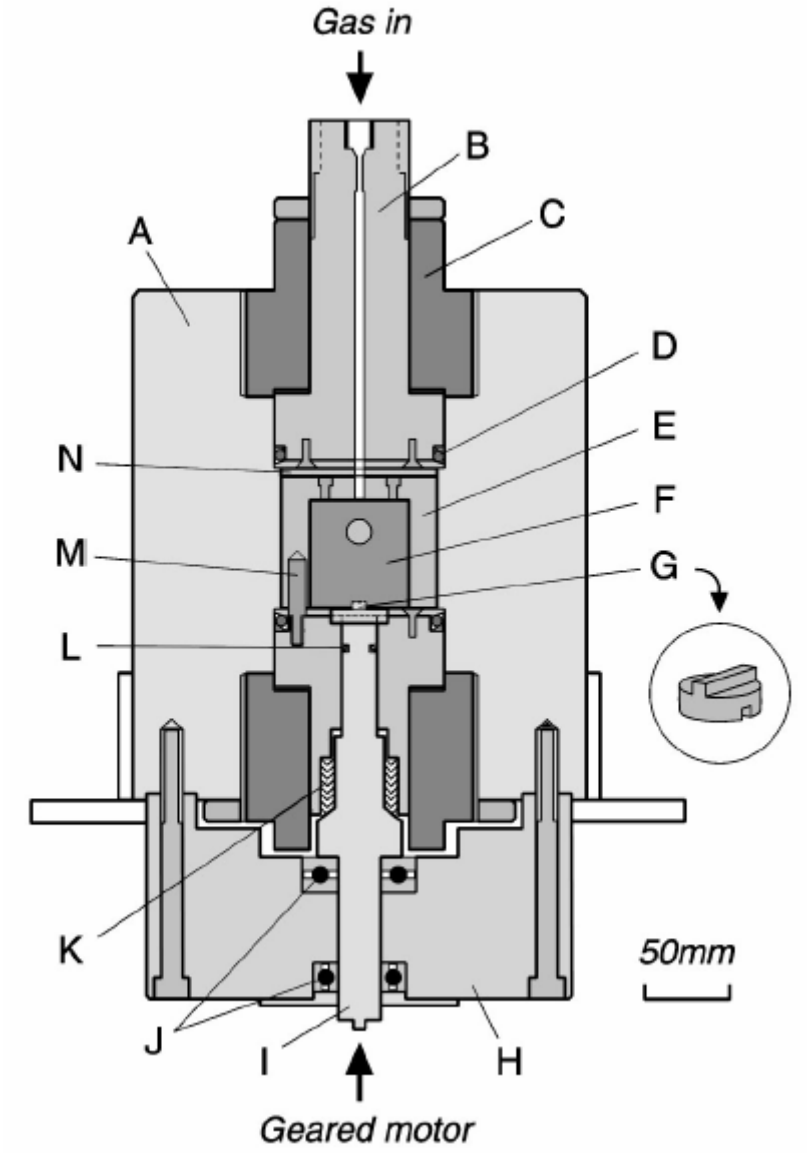
It has been agreed that APS will provide a room for the system in the chemistry lab at sector 3.

Guoyin visited Spring-8 in June'05 and operated a gas loading system there. The conceptual design is to have a pressure vessel that combines both Takemura's design (Takemura et al 2001) and Mao's design (Mao et al 1986). The vessel will be in a refrigerator in order for low-temperature operation. The first detail design will be ready by March 2006.

A workshop is planed to have the community inputs and to discuss an optimal design. (Probably February 2006 after the GSECARS renewal proposal submissions) We anticipate that the completion of the system by the end of 2006, and that within a year after that an optimal design for gas-loading will be available to the community.

**Project budget**

There have been no funds expended on the project to date.




High pressure vessel (from Takemura et al 2001)

References:
Mao HK, Xu J and Bell PM, (1986). Calibration of the ruby pressure gauge to 800 kbar under quasi-hydrostatic conditions. J. Geophys. Res., 91: 4673-4676.
Takemura K, Sahu PC, Yoshiyasu K and Yasuo T, (2001). Versatile gas-loading system for diamond anvil cells. Rev. Sci. Instrum., 72: 3873-3876.

## C.8 Dual Beam Focused Ion Milling Facility for TEM Foil Preparation

[H. Green, University of California, Riverside]

Progress on this new initiative in Year #4 has been restricted by delays in installation of the new FIB in the nanofabrications center at UC Riverside. Green was

successful in obtaining funds for technician support from the Instrumentation and Facilities Program in EAR at NSF, so that the seed monies provided by COMPRES in Year #4 will be leveraged and provide funding for the technician [and access by the COMPRES community] for a total four-year period.

## C.9 New Projects and Workshops

### New Projects

In September 2005, the Infrastructure Development Committee issued a call to the COMPRES community for proposed new initiatives for technological projects that would contribute to the COMPRES mission.

Seven proposals for initiating new projects were reviewed and four were recommended for funding in Year #5.

Development of Next Generation Multi-anvil Module for Megabar Research [Y. Wang-University of Chicago, and others].

Completion and Commissioning of the Monochromatic X-ray Side-Station at the X17B2 Beamline of the NSLS for the COMPRES Community
[J. Chen-Stony Brook University].

Application of "Calorimetry-on-a-Chip" Technology to Heat Capacities and Transitions in Quenched High Pressure Samples Weighing less than a Milligram
[A. Navrotsky-University of California at Davis, F. Hellman-University of California at Berkeley].

Brillouin Scattering at the Advanced Photon Source
[J. Bass, University of Illinois at Urbana-Champaign]