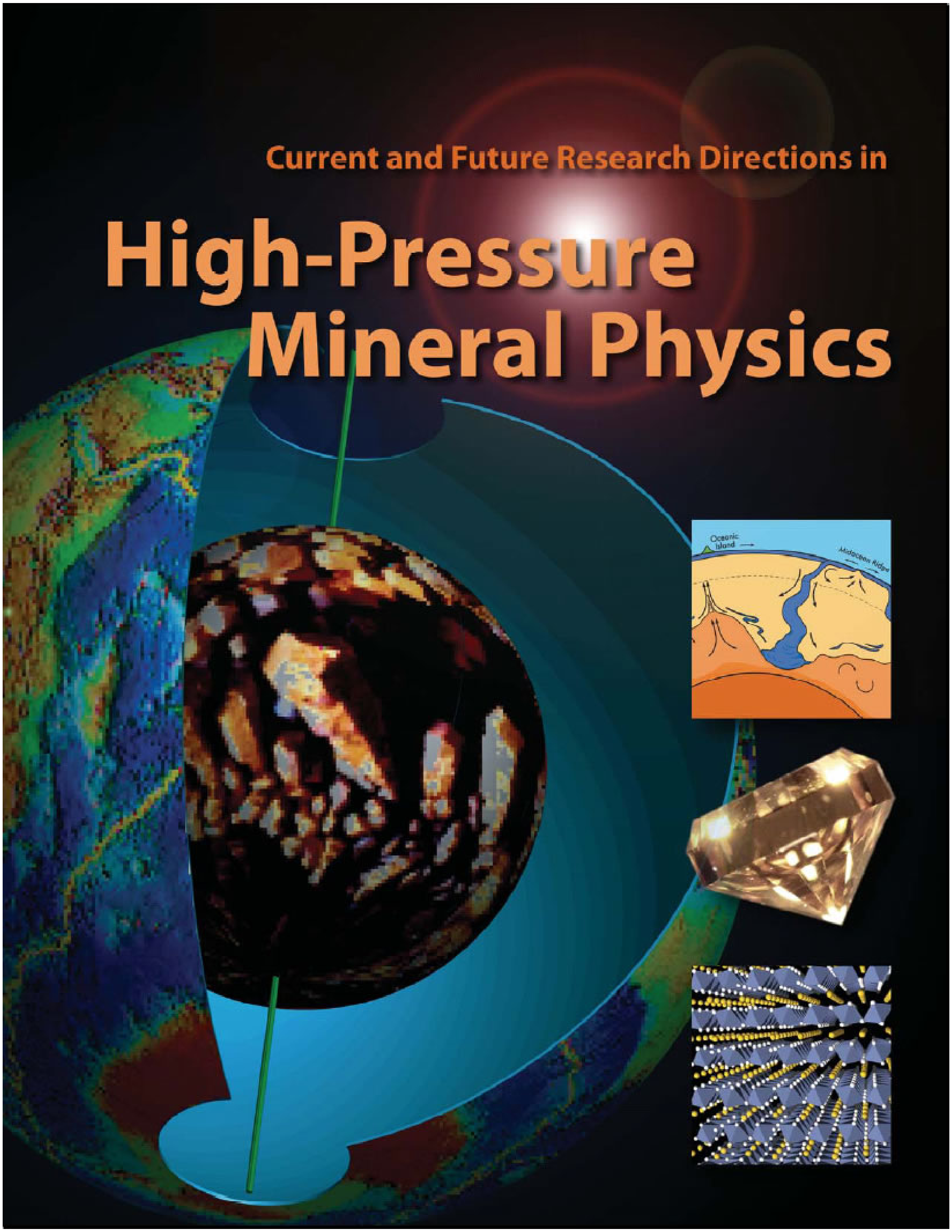
Year 3 Annual Progress Report of the Consortium for Materials Properties Research in Earth Sciences (COMPRES)

February 2005


Current and Future Research Directions in
High-Pressure
Mineral Physics
Oceanic Island
Midocean Ridge

A COMPRES YEAR 3: OVERVIEW

A.1 Executive Summary

In 2004, 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. As the consequence of a membership campaign, there are now 41 U. S. institutions which are voting members of COMPRES [the Electorate] and another 16 non-voting institutions overseas which have affiliate membership.

COMPRES has sponsored and/or organized many workshops and scientific meetings in the past year. These include the COMPRES Third Annual Meeting in Lake Tahoe, California in June and working group meetings for the Grand Challenge teams in "Ultra-High Pressure Rheology" at Yale University in May 2004 and "Elasticity of Mantle Minerals" at the University of Illinois at Urbana-Champaign in May 2004. Other workshops: (1) "Future Directions for the Laser-Heated Diamond Anvil Cell at the Advanced Photon Source, at the Argonne National Laboratory in March 2004; (2) Focused Ion Beam (FIB) Applications in Earth Sciences at the University of California at Riverside in March 2004; (3) SCEC/COMPRES Workshop on the "Science, Status and Future Needs of Experimental Rock Deformation" at Mt Holyoke College in August 2004; and (4) Structure Determination by Single Crystal X-ray Diffraction (SXD) at Megabar Pressures at the Argonne National Laboratory in November 2004.

The process of reviewing and revising the ByLaws of COMPRES, initiated at the 2003 Annual Meeting in Santa Cruz, was completed in September 2004. The revised ByLaws are posted on the COMPRES website at:http://www.compres.stonybrook.edu/AboutUs/Bylaws/index.html.

In September, COMPRES announced the publication of a new report entitled: "Current and Future Research Directions in High-Pressure Mineral Physics." The frontispiece of this Annual Report is from the cover page of this new report.

This report is an outgrowth of the discussions and results of a Workshop on "A Vision for High Pressure Earth and Planetary Sciences Research: The Planets from the Surface to the Center" which was held on March 22-23, 2003 in Miami, Florida. The NSF Division of Earth Sciences commissioned and supported this workshop, and

COMPRES organized it. Fifty-five scientists attended the Workshop, which was convened by Jay Bass and Donald Weidner.

The report was edited by Jay Bass using the materials presented at the Workshop or submitted soon thereafter. He collaborated with Ellen Kappel of Geosciences Professional Services, Inc. for the editing and design. In recognition of his work, we expect that this report will henceforth be known as the Bass Report.

This report can be viewed on the COMPRES website at: http://www.compres.stonybrook.edu/

If you would like to have a personal copy of the glossy version of this report, please write to Ann Lattimore at COMPRES: alattimore@notes.cc.sunysb.edu.

In this section of the Annual Report for Year #3, 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 #4 [May 1, 2005 to April 30, 2006]; 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.

- Theoretical studies using first-principles calculations confirmed the crystal structure, stability region in P-T space, and provided estimates of the elasticity of the post-perovskite phase of $MgSiO_3$, which was first discovered experimentally in Japan.

- Equation of state of fluid H_2O constrained to 80 GPa using the melting curve, bulk modulus, and thermal expansivity of Ice VII—see details in Sect. B.1. DAC at NSLS.

- Deformation of rocks and minerals: New experimental technologies:

  A new high pressure deformation apparatus D-DIA has been married to the synchrotron x-ray source. The new apparatus has typical cubic-anvil geometry and is currently operational to pressures about 8 GPa. details in Sect. B.2 MAC at NSLS.

  A rotational Drickamer-type apparatus [RDA] for high-pressure, temperature, large strain rheological experiments has been developed at Yale University and recently installed on the multi-anvil beamline at the NSLS. See details in December 2003 Newsletter of COMPRES.

- A new Brillouin spectrometer has been installed at the APS on GSECARS sector 13-BM-D. With the actual installation of Brillouin equipment into the synchrotron hutch, this infrastructure development project is nearing completion. Commissioning and the first scientific experiments will be performed during the coming year. See details in Sect. C.3 below.

- Upgrade of beamline at Advanced Light Source [ALS] for high-pressure research. The ALS Advisory Committee approved a guaranteed percentage of time on high-pressure beamlines to COMPRES users.

- Growth of CVD diamonds

  Collaboration between Carnegie Institution of Washington and Los Alamos National Laboratory scientists leads to major breakthrough in growing diamonds from chemical vapor deposition which are the hardest known crystals to date. See details in October 2004 Newsletter of COMPRES.

A.3 Meetings and Workshops

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

CSEDI Science Plan Workshop
February 21-24, 2004
Organizers: Guy Masters and Cathy Constable
Institute of Geophysics and Planetary Geophysics of the Scripps Institution of Oceanography at the University of California, San Diego in La Jolla, California. Among the 70+ attendees were 14 from the field of mineral physics.

This was an excellent venue for interactions and communications among the scientific disciplines of geodynamics, isotope geochemistry, magnetism, mineral physics, planetary studies and seismology. There were eight outstanding plenary lectures, including two from our colleagues in mineral physics [in the broadest sense], Marc Hirschmann from the University of Minnesota and David Walker from Columbia University.

In addition to the Hirschmann and Walker lectures, it was very gratifying to have the experimental and theoretical work in mineral physics highlighted in the other lectures by David Stevenson, Peter Olson, Louise Kellogg, Rob van der Hilst, Peter van Keken and Ed Garnero. Bob Liebermann gave a brief presentation on the new COMPRES consortium, as one example of organized research activities in Earth Sciences sponsored by the NSF.

Future Directions for the Laser-Heated Diamond Anvil Cell at the Advanced Photon Source
March 20, 2004
Advanced Photon Source, Argonne National Laboratory, Illinois.
Organizers: Thomas Duffy (Princeton University), Guoyin Shen and Dion Heinz (University of Chicago), who are leading the COMPRES Infrastructure Development Project on "Laser-Heated Diamond Anvil Cell." The Workshop was attended by 40 people. Copies of the presentations at the Workshop may be found on the COMPRES website and in the detailed report in Section C.2 below.

COMPRES Workshop on Focused Ion Beam (FIB) applications in Earth Sciences.

March 28-29, 2004.
Mission Inn, Riverside, California
Organizers: HW Green, L Dobrzhinestkaya, and K. Bozhilov of the Institute of Geophysics and Planetary Physics of the University of California at Riverside.

The Workshop was attended by over 50 participants, who were able to see a demonstration instrument set up by one of the manufacturers. A full report of the Workshop may be found at:
http://www.igpp.ucr.edu/Conferences_Geo_2004.htm

Rheology Grand Challenge Workshop on "Ultra-High Pressure Rheology"
May 1-2, 2004:
Yale University, New Haven, Connecticut
Convener: Shun-ichiro Karato [Yale University]
This meeting included all the principal members of the team for the Rheology Grand Challenge project. See details on the COMPRES website.

Elasticity Grand Challenge Workshop
May 8-9, 2004
University of Illinois at Urbana-Champaign [UIUC], Illinois.
Convener: Jay Bass [University of Illinois at Urbana-Champaign]

This meeting included all the principal members of the team for the Elasticity Grand Challenge project, including more than 29 graduate students, postdocs and faculty. See details on the COMPRES website.

Third Annual Meeting of COMPRES
June 19-22, 2004
Granlibakken Conference Center and Resort, Lake Tahoe, California

The 3rd Annual Meeting of COMPRES was held at the Granlibakken Conference Center in Lake Tahoe, California from June 19-22, 2004. There were 81 formal participants plus another 15 accompanying persons [including some young, but very promising future mineral physicists]. More than 28 of the 39 U. S. member institutions were represented, as well as one foreign affiliate [GeoForschungs Zentrum from Potsdam, Germany]. The program included Plenary Lectures, reports from the operators of the Community Facilities and directors of the Infrastructure Development projects, reports on past and future workshops, and exciting scientific results in the poster sessions. We were especially pleased that Sonia Esperanca, Program Director for Geochemistry in the Division of Earth Sciences at the NSF attended the entire meeting, and that Herman Zimmerman, Division Director for EAR paid a call at the end of the meeting. We all owe a special thanks to Ann Lattimore for organizing and coordinating such a successful meeting.

On June 18-19, 2004, just prior to the Annual Meeting, there was a meeting of the COMPRES Advisory Committee with the Executive Committee. All members of the Advisory Committee were in attendance for the first time: Bruce Buffett from the University of Chicago, Chi-chang Kao from Brookhaven National Laboratory, Guy Masters from the University of California at San Diego, Richard O'Connell from Harvard University and Paul Silver from the Carnegie Institution of Washington. The chairs of the COMPRES committees made brief presentations, followed by very useful discussions. Three of the Advisory Committee [Kao, Masters and O'Connell] also gave Plenary Lectures at the Annual Meeting.

On June 21-22, the Annual Business Meeting of COMPRES was held, including election of new officers and committee members as well as consideration of the report and recommendations of the ByLaws Committee [Bruce Buffett, Ronald Cohen (Chair), Charles Prewitt, Joseph Smyth, and Lars Stixrude].

The following new members of the current COMPRES committees were elected at the annual meeting:

Executive Committee:

Harry Green (University of California at Riverside); Chair 2004-2007
Donald Weidner (Stony Brook University); Member 2004-2007

Facilities Committee:

Abby Kavner (University of California at Los Angeles); Member 2004-2007

Infrastructure Development Committee:

Nancy Ross (Virginia Polytechnic Institute and State University); Chair 2004-2006
Sang-Heon Dan Shim (Massachusetts Institute of Technology); Member 2004-2007
Our deep appreciations to those committee members whose terms ended at Lake Tahoe for their voluntary services for the community. They are Donald Weidner (Chair of Executive Committee), Russell Hemley (Executive Committee), Harry Green (Facilities Committee), James Tyburczy (Chair of Infrastructure Development Committee).

See details at:

http://www.compres.stonybrook.edu/Meetings/2004-06-20/PostMeeting%20Info%20Page/index.html

Gordon Research Conference on Research at High Pressure
June 27-July 2, 2004.
Kimball Union Academy, Meriden, NH
Anastasia Chopelas of the University of Washington was the Chair of this year's conference with Reinhard Boehler serving as Vice-Chair [he will chair the 2006 meeting]; both Ann and Reini are card-carrying members of the COMPRES community. Of the 109 attendees, 25 were from mineral physics/geosciences, including many of the invited speakers: Yue Meng, Agnes Dewaele, Danielle Antonangeli, Przemek Dera, Ross Angel, Jennifer Jackson, Jonathan Crowhurst, and Yusheng Zhao. In addition, many of the poster presentations reported work done under the auspices of COMPRES support. The John Jamieson Award for the most outstanding lecture by a young post-graduate student was won by Jennifer Jackson of the University of Illinois at Urbana-

Champaign for her excellent lecture on "High-pressure investigations of deep Earth materials using Brillouin and X-ray spectroscopy."

SCEC/COMPRES Workshop on the "Science, Status, and Future Needs of Experimental Rock Deformation"
August 13-14, 2004
Mt. Holyoke College, South Hadley, Massachusetts
Conveners: Terry Tullis, Thomas Jordan and Robert Liebermann
SCEC and COMPRES jointly sponsored this workshop, which was attended by 38 scientists from around the world, including 80% of the members of the COMPRES Executive Committee. This workshop was tacked on to the end of a very successful Gordon Research Conference on Rock Deformation chaired by Andreas Kronenberg and Mark Jessell. The focus was on the current status and future needs of the community in experimental rock deformation Bob Liebermann attended and made a brief presentation about COMPRES, as a possible model for this related community.

Structure Determination by Single Crystal X-ray Diffraction (SXD) at Megabar Pressures
November 12-13, 2004
Advanced Photon Source, Argonne National Laboratory, Illinois
Organizers: Przemyslaw Dera (Carnegie Institution of Washington) and Charles Prewitt (University of Arizona).

Harry Green and Nancy Ross represented the COMPRES committees at this workshop. A report on this workshop may be found on the COMPRES website at:
http://www.compres.stonybrook.edu/Workshops/Structure%20Determination%20at%20a%20Megabar/sxd_meeting_report.pdf

Special Symposium in Honor of Jean-Paul Poirier
December 13-17, 2004
Fall 2004 AGU Meeting, San Francisco, California
Special Symposium in Honor of Jean-Paul Poirier convened by Falko Langenhorst, Robert Liebermann, G. David Price, and David Rubie.

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 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 2004, there were 38 U. S. institutions which were members of COMPRES and eight affiliate intuitions overseas. In the past year, three new U. S. institutions have become members of COMPRES:

California Institute of Technology
Massachusetts Institute of Technology
University of New Mexico.

With the revision of the COMPRES ByLaws, the three U. S. government institutions automatically became full, voting members of COMPRES.:

Argonne National Laboratory
Astromaterials Research and Exploration Science, NASA
Lawrence Livermore National Laboratory

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

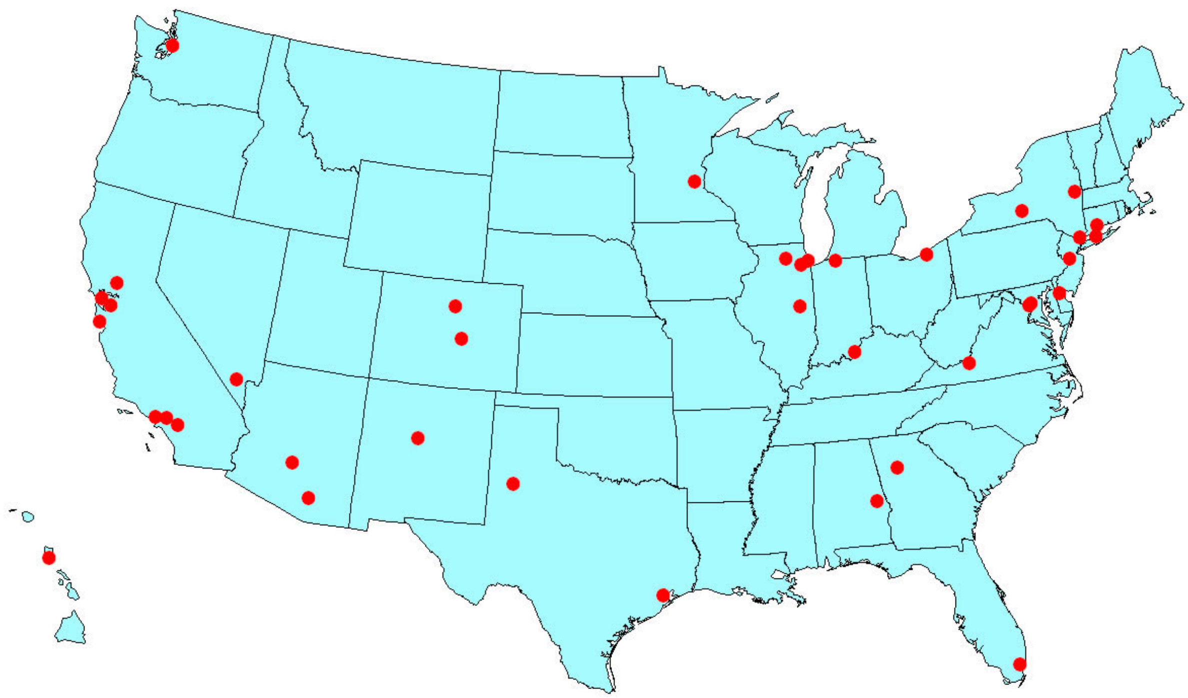
Bayreuth Universitat (Germany)
Eidgenossische Techniche Hochschule Zurich (Switzerland)
Institut de Physique du Globe Paris (France)
Royal Institution of Great Britain in London (United Kingdom)
Ruhr-Universitat Bochum (Germany)
Tohoku University, Sendai (Japan)
University of Manchester (United Kingdom)
University of Western Ontario (Canada)

This brings us to a total of 41 U. S. institutional members and 16 affiliated members of COMPRES. They are listed in the following table and indicated on the maps.

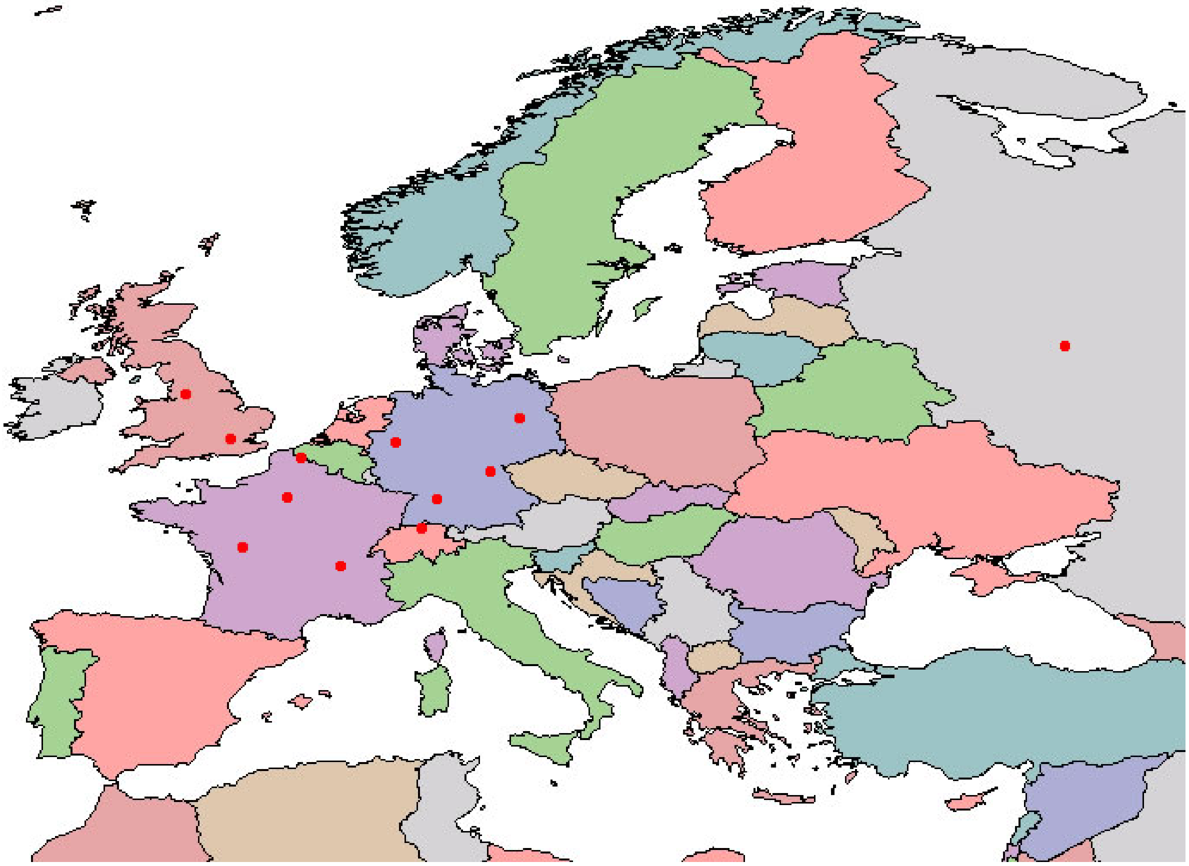
Institution	**Elector**	**Alternate**
Argonne National Laboratory	Wolfgang Sturhahn	Marcos Grimsditch
Arizona State University	Thomas Sharp	James Tyburczy
Astromaterials Research and Exploration Science, NASA	Kevin Righter	John Jones
Auburn University	Jianjun Dong	
Azusa Pacific University	Donald Isaak	
Bayreuth Universitat (Germany)	David Rubie	
California Institute of Technology	Paul Asimow	Thomas Ahrens

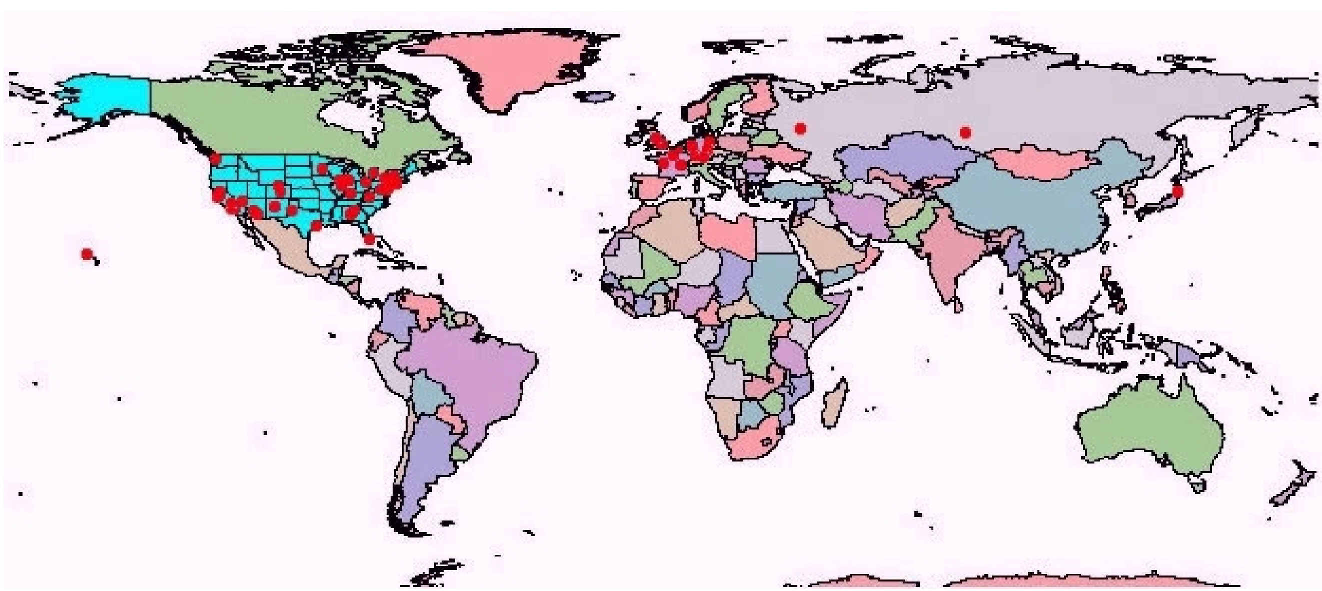
Carnegie Institution of Washington	Ronald Cohen	Yingwei Fei
Case Western Reserve University	James Van Orman	Nancy Chabot
Colorado College	Phillip Cervantes	
Columbia University	David Walker	Taro Takahashi
Cornell University	Chang-Sheng Zha	William Bassett
Delaware State University	Gabriel Gwanmesia	Al Sameen Khan
Ecole Normale Supérieure de Lyon (France)	Jan Matas	
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	
Lawrence Livermore National Laboratory	Daniel Farber	William Durham
Massachusetts Institute of Technology	San-Heon (Dan) Shim	Robert van der Hilst
Max-Planck Institute for Solid State Research, Stuttgart (Germany)	Paul Balog	
Northern Illinois University	Mark Frank	Jonathan Berg
Novosibirsk State University (Russia)	Elena Boldyreva	
Princeton University	Thomas Duffy	Guust Nolet
Rensselaer Polytechnic Institute	Anurag Sharma	John Schroeder
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	Mark Bukowinski	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	Andrew Campbell
University of Colorado at Boulder	Joseph Smyth	Hartmut Spetzler
University of Illinois	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	William McDonough	John Tossell
University of Minnesota	Renata Wentzcovitch	David Kohlstedt
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
Yale University	Shun-ichiro Karato	David Bercovici



U. S. Member Institutions of COMPRES





European (top) and World (bottom) Member Institutions and Affiliates of COMPRES

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].
- 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.
- **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 2004 issues have included reports on chemical vapor deposition of diamond, COMPRES use of facilities such as ALS, the Miami workshop, a call for infrastructure projects, the beamline internship program, membership updates, the 2004 COMPRES Annual Meeting, the pressure calibration project, and the DOD award for instrumentation.

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 2004 AGU Meeting

At the Fall 2004 Meeting of the American Geophysical Union in San Francisco in December 2004, 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 Mark Rivers of GSECARS.

A Powerpoint presentation created for the COMPRES Booth by Jiuhua Chen can be found at

www.compres.us/Meetings/2004-12-12-AGU-Powerpoint/COMPRESbooth04.ppt

A.6 COMPRES Publications

Papers of COMPRES

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Relevant dissertations

Jung, Haemyeong (2002) Effects of water on the plastic deformation and deformation microstructure of olivine, University of Minnesota (Advisor: Shun-ichiro Karato)

Lee . Kanani K. M. (2003) Exploring Planetary Interiors: Experiments at Extreme Conditions, University of California, Berkeley (advisor: Raymond Jeanloz),.

Li, Li, (2003) Rheology of olivine at mantle pressure, Stony Brook University (Advisor: Donald Weidner)

Speziale, Sergio (2003) Elasticity of Mantle Minerals, Princeton University (Advisor: Thomas Duffy)

A.7 Education and Outreach

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

In order to advance the practice of using digital tools to work with real Earth systems data, COMPRES is promoting the use of geographic information systems (GIS) and other data analysis tools in educational settings. At Stony Brook University, Glenn Richard co-taught a graduate-level course on using GIS as a research and educational tool with Dr. Glenn Smith of the Department of Technology and Society during the spring, 2004 semester. He has also been working with the Department of Geosciences to integrate the use of digital mapping and other data analysis tools into their field geology course.

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 2004, 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, COMPRES announced the opening of a searchable image library which is available on the web from its home page [see link at:

http://www.compres.stonybrook.edu:8080/COMPRESImageLibrary/index.html. This is designed to make images available to the academic community for education and research. This Library contains graphic images drawn from COMPRES meetings and workshops, with notes for referencing and appropriate attribution. We encourage members of the COMPRES and wider community to take advantage of this resource and to contribute to its growth. Anyone who would like to contribute material to the Library, please contact Glenn Richard, Educational Coordinator, at garichard@notes.cc.sunysb.edu

Future Plans

This summer, Glenn Richard plans work with the other members of the EarthScope Map Tools team to offer a one-week workshop that will provide teachers with an opportunity to develop curriculum materials that foster the exploration of EarthScope data in an educational setting.

The code for the COMPRES Image Library is being used as a basis for developing a digital library for the Center for Environmental Molecular Science (CEMS), which is an NSF-funded program. During the porting of the code to CEMS, upgrades are being made that increase the functionality of the library, with the help of undergraduate computer science majors. During the coming year, these improvements will be selectively incorporated into the COMPRES library to make it capable of serving a wide variety of digital formats, including images, movies, interactive applets, data and a catalog of mineral physics and high pressure research-related web sites.

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)
Shun-ichiro Karato, Yale University (2002-2005)
Donald Weidner, Stony Brook University)2004-2007)
Quentin Williams, University of California at Santa Cruz (2004-2007)

Previous members and affiliation (periods of service)

Thomas Duffy, Princeton University (2002-2003)
Russell Hemley, Carnegie Institution of Washington (2002-2004)
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)
Yingwei Fei, Carnegie Institution of Washington (2002-2005)
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)
Harry Green, University of California at Riverside (2002-2004)
Quentin Williams (Chair), University of California at Santa Cruz (2002-2003)
Infrastructure Development Committee

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 (2003-06).
Pamela Burnley, Georgia State University (2002-05)
Kevin Righter, NASA Astromaterials Laboratory (2003-06)
Yanbin Wang, University of Chicago (2002-05)

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)

ByLaws Committee

At the COMPRES Annual Meeting in Santa Cruz in June 2003, the Electorate passed the following resolution:

"A by-laws committee will be established to recommend changes in the by-laws. Timetable will be Oct 10 to Nov 1 for circulating to the COMPRES community. Target decision date is the 2003 AGU."

The following members were elected at 2003 Annual Meeting in Santa Cruz

Members

Ronald Cohen, Carnegie Institution of Washington
Bruce Buffett, University of Chicago
Charles Prewitt, University of Arizona
Joseph Smyth, University of Colorado
Lars Stixrude, University of Michigan

The process of reviewing and revising the ByLaws of COMPRES, initiated at the 2003 Annual Meeting in Santa Cruz, was completed in September 2004. The Electorate [36 U. S. institutions eligible to vote] cast its ballots, with 33 institutions voting. All of the proposed changes received more than the necessary number of votes [requires 2/3 of the Electorate, or 24 votes to approve changes]. The revised ByLaws are posted on the COMPRES website at:http://www.compres.stonybrook.edu/AboutUs/Bylaws/index.html. The Executive Committee instituted the changes in its procedures which are required by the revised ByLaws. As an example, the minutes of meetings of the Executive Committee are now posted on the COMPRES website [as of 14 September 2004] at: http://www.compres.stonybrook.edu/Publications/ExCommMinutes%20for%20Web%20site%20posting/ExCom%20Minutes%20Links%20page.htm
On behalf of the Executive Committee, we would like to thank the ByLaws Committee, the Electors and Alternates, and the wider COMPRES community for their participation and contributions to this important process.

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

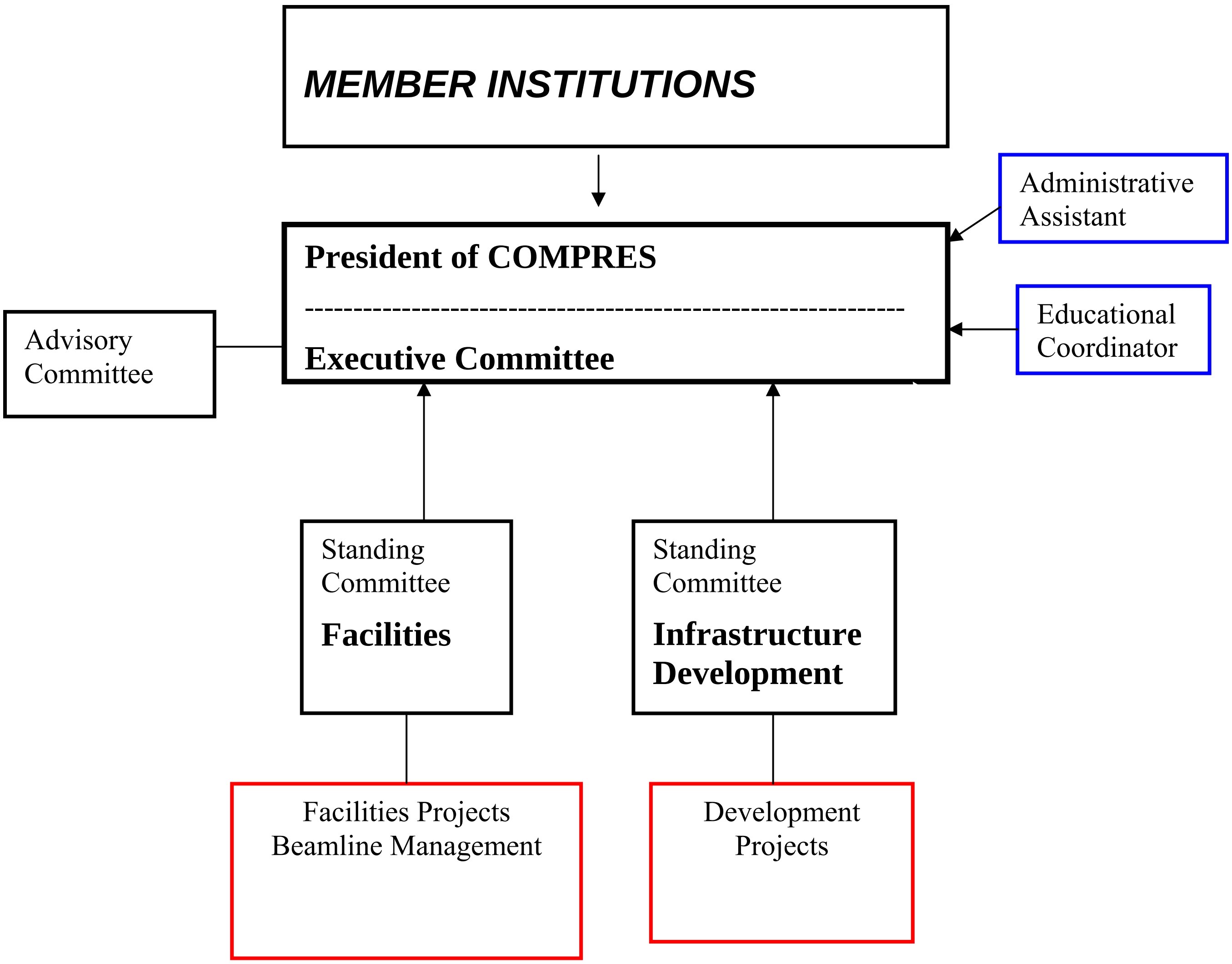
On 19 June 2004, the Advisory Committee met with the Executive Committee just prior to the start of the Third Annual COMPRES Meeting in Lake Tahoe, California.

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.

Organization of COMPRES Office



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

2004 has been a busy and productive year for COMPRES. Most of this progress is highlighted in Sections A, B and C of this Annual Report. I include in this narrative some additional news and highlights, largely drawn from my Monthly Messages to the COMPRES community and from the President's column in the Quarterly Newsletters.

The major activity of the Executive Committee in January 2004 was the preparation of the Year #2 Annual Report of COMPRES to the NSF, and the Annual Program Plan and Budget request for Year #3 [May 1, 2004 to April 30, 2005]. 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 5, 2004. The report, plan and budget for Year #3 [May 1, 2004 to April 30, 2005] was approved by David Lambert of NSF-EAR and the budget increment for Year #3 of $2.2 million authorized. The full Year #2 Annual Report can be viewed on the COMPRES website along with photos which accompanied these reports at the new url: www.compres.us.

The research team at the Carnegie Institution of Washington and the Los Alamos National Laboratory celebrated a major breakthrough in growing diamonds from chemical vapor deposition, which are the hardest known to date [see the separate email sent to the COMPRES community on 25 February and the NSF press release attached]. See also paper by C-s. Yan, H-k. Mao, W. Li, J. Qian, Y. Zhao and R. J. Hemley in phys. stat. solidi in Feb. 2004. This achievement is a product of one of the Grand Challenge collaborative research proposals which were submitted and funded by the NSF Division of Earth Sciences in 2002. While these collaborative projects are officially distinct from the COMPRES Core grant, they are closely linked on an intellectual level in that they provide some of the basic scientific rationale for developing and maintaining the experimental facilities overseen and operated under the auspices of COMPRES.

The Institut de Physique du Globe de Paris hosted a one-day symposium on "Physique des minéraux" in honor of Jean-Paul Poirier, who retired in May 2003. Convened by François Guyot and Philippe Gillet, the program included presentations by former French students and colleagues of Poirier [A. Nicolas, G. Fiquet, J. Ingrin, S. Labrosse, D. Andrault, C. Sotin, P. Gillet, and C. Allegre] as well as a few l'étranger [T.

Shankland, D. Price, F. Langenhorst, and R. Liebermann]. Details of the program may be found on the COMPRES website.

In April 2003, the bid for Approved Program (AP) status from High Pressure COMPRES team at the Advanced Light Source of the Lawrence Berkeley National Laboratory [R. Jeanloz, S. Clark, M. Kunz] was approved by the ALS Advisory Committee. Simon Clark was recently informed that the ALS will allocate 20 percent of the beamtime on beamlines 1.4 and 11.3.1 to their team for the period July 2004 until June 2007.

Jiuhua Chen and Donald Weidner of Stony Brook were recently informed that their proposal for "Instrumentation of Monochromatic X-ray Side-Station for Melt Property Studies' will be funded at a level of $200,000 by the Department of Defense through the Defense University Research Instrumentation Program. This new instrumentation will be installed on beamline X17B2 at the National Synchrotron Light Source of the Brookhaven National Laboratory.

As part of a program to visit experimental laboratories in mineral physics in the U. S. and overseas, I visited the diamond-anvil cell, high-pressure laboratory of Surendra Saxena at the Florida International University on April 5-6 and gave an invited talk on: "Sound Velocity Measurements in Minerals under Mantle Conditions." On April 23, 2004, I visited the Laboratoire des Mécanismes de Transfert en Géologie in Toulouse, France. While there I was able to observe the move of this lab from their current location on Allées Jules Guesde near the Jardin des Plantes to the Rangueil campus where most of the laboratories of the Université Paul Sabatier and the CNRS are located.

In April, the following members/friends of the COMPRES community have recently been elected to membership in the U. S. National Academy of Sciences:

Donald Helmberger--California Institute of Technology
Raymond Jeanloz--University of California at Berkeley
Dennis Kent--Rutgers, The State University of New Jersey at New Brunswick
David Stevenson--California Institute of Technology

At the 2004 Users Meeting for the Advanced Photon Source [May 3-6], Jennifer Jackson of the University of Illinois won an award for the outstanding student poster for her presentation on "(Mg,Fe)SiO_3 perovskite to 120 GPa using synchrotron Mossbauer spectroscopy". Jennifer was also recently awarded an MSA Grant for Student Research in Mineralogy and Petrology for her study of "Sound Velocities of aluminous $MgSiO_3$ perovskite under high-pressure and high-temperature conditions using Brillouin spectroscopy and laser heating."

In early May, Russell Hemley was invited to give the Third Annual Earth Day Distinguished Lecture at the National Science Foundation by the Geoscience Directorate. Rus spoke on recent developments in Earth science under the title: "Diamond Windows on a New Science."

On May 24-25, a "Workshop on Geoscience User Facilities—Enhancing Instrumentation Access" was convened in Gaithersburg, Maryland, under the auspices of the DOE Council on Earth Sciences by Steve Sutton, Richard Reeder and Marc Caffee.

The new report on "Current and Future Research Directions in High-Pressure Mineral Physics" was published in September 2004 in a glossy version which can be obtained by sending Ann Lattimore an email using the link on the Home Page at: www.compres.us. The report can also be downloaded from the Home Page at:

http://www.compres.stonybrook.edu/Publications/BassReport/Bass_Report_8_31_04.pdf

This report is an outgrowth of the discussions and results of a Workshop on "A Vision for High Pressure Earth and Planetary Sciences Research: The Planets from the Surface to the Center" which was held on March 22-23, 2003 in Miami, Florida. The NSF Division of Earth Sciences commissioned and supported this workshop, and COMPRES organized it. Fifty-six scientists attended the Workshop, which was convened by Jay Bass and Donald Weidner. It was edited by Jay Bass using the materials presented at the Workshop or submitted soon thereafter. He collaborated with Ellen Kappel of Geosciences Professional Services, Inc. for the editing and design. On behalf of the COMPRES and Mineral Physics community, I would like to thank Jay for his extraordinary and splendid efforts in bringing this important report to fruition. In recognition of his work, I expect that this report will henceforth be known as the Bass Report.

On September 21, Harry Green, Chair of the Executive Committee, and I visited the Division of Earth Sciences at the NSF for discussions with David Lambert and his colleagues. Our morning meeting with Dr. Herman Zimmerman, Division Director, centered on official presentation of glossy copies of the new report on "Current and Future Research Directions in High-Pressure Mineral Physics" from the 2003 Miami Workshop, which had been commissioned by Dr. Zimmerman; he had already downloaded it from the website and used it in presentations at NSF. In the afternoon in a meeting with Dr. Lambert and other EAR program directors [Russell Kelz, Robin Reichlin, Sonia Esperanca, and David Fountain]. I gave a presentation on "COMPRES at Age 2", followed by questions and discussion. Also attending was Nicholas Woodward from DOE-BES, who discussed the implications of new changes in DOE beamline operations at national laboratories and potential implications for beamlines operated by COMPRES and related programs [e.g., GSECARS]. In our separate meetings with Dr. Lambert, we discussed a number of budget issues, including the outlook for FY06 and funding for COMPRES in Year #4 [May 2005 to April 2006].

In November, we were informed of special double honors for Ho-kwang (Dave) Mao.
in being selected for two prestigious awards:

The Roebling Medal of the Mineralogical Society of America.

The Gregori Aminoff Prize in Crystallography from the Royal Swedish Academy of Sciences

In October and November, I spent two weeks at the Australian National University in Canberra, conducting a collaborative research project with Professor Ian Jackson in October and November. During these visits, he also gave a seminar on the topic of:
"Sound Velocity Measurements in Mantle Minerals under Mantle Conditions".

The major event of December 2004 for COMPRES was surely the Fall AGU Meeting in San Francisco.

Highlights included:

(a.) Exhibition booth jointly sponsored by GSECARS and COMPRES, which attracted lots of visitors, and which featured copies of the "Bass Report" on "Current and Future Research Directions in High-Pressure Mineral Physics", as well as COMPRES calendars for 2005.

(b.) 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 Mark Rivers for his cooperation.

(c.) We all took special pride in the award of honors and medals to our colleagues in Mineral and Rock Physics, including: Adolphe Nicolas [University of Montpellier]-Harry Hess Medal, Mervyn Paterson [Australian National University]-Walter Bucher Medal; New AGU Fellows: Brian Evans, David Green, Michael O'Hara, and Ernest Rutter.

(d.) The COMPRES Standing Committees held breakfast meetings to discuss the annual reports on the Infrastructure Development projects and Community Facilities. The Executive Committee met for breakfast on Dec 15 to begin the planning process leading to the submission of the Annual Report for Year #3 and Program Plan and Budget Request for Year #4 to the NSF on February 1, 2004.

(e.) The Physical Properties of Earth Materials group once again organized a fantastic dinner celebration at the Last Supper Club, a home-style Italian restaurant in the historic Mission district. Our congratulations to Brian Bonner and Bill Durham for discovering such a wonderful venue for this special evening.

(f.) The Mineral and Rock Physics Focus Group hosted a wine and cheese reception on Dec. 14, sponsored jointly by Almax and Technodiamant. During the reception, the 2004 Outstanding Student Awards in Mineral and Rock Physics were presented to:

Motohiko Murakami from the Tokyo Institute of Technology and

Sergio Speziale from Princeton University.

On Thursday, December 16, Shun Karato of Yale University was selected to deliver the Birch Lecture on the topic of "Where on Earth is the Ocean?"

(g.) Ronald Cohen, new Chair of the Mineral and Rock Physics Focus Group, organized two Town Hall Meetings [sponsored by IBM and Cray], on:

Petascale Computing in Earth Sciences [with Jeroen Trump, Frank Bryan and Luanne Thompson]
Computational Geoinformatics for Solid Earth Sciences [with Jeroen Trump, Dave Yuen, and Marc Spiegelman]

(h.) There were many special sessions organized by colleagues in mineral and rock physics. The structure, evolution, and properties of Earth's core was explored in a session honoring Prof. Jean-Paul Poirier and convened by F. Langenhorst, R. Liebermann, D. Price, and D. Rubie; this multidisciplinary session addressed the major outstanding questions surrounding core formation during Earth's early history, the identity of light elements in the core, coupling of the core with the mantle, and the ongoing crystallization of the inner core.

Other special sessions included:
Advances in Mineral and Rock Physics [H-J. Mueller, B. Li, S. Jacobsen]
Discovery of Post-Perovskite Phase Transition and the Deep Lower Mantle [K. Hirose, T. Lay, P. van Keken, R. Wentzcovitch]
The Earth's Deep Water Cycle [S. Jacobsen, S. van der Lee, L. Rupke, M. Koch-Muller, A. Pawley, J. P. Morgan, J. Smyth, and E. Ohtani]
Oxidation State of the Mantle [C. McCammon and C-T. Lee]
The Deep Earth Engine: Geophysics and Geochemistry

The European Association of Geochemistry has selected Alexandra Navrotsky of the University of California at Davis to be the 2005 Harold Urey Medallist. This medal will be presented to Alex at the annual Goldschmidt meeting in Moscow, Idaho in May 2005.

2005 Annual Meeting of COMPRES

The Executive Committee of COMPRES has made a final decision on the dates and site for the 2005 Annual Meeting of COMPRES.

Dates:
Arrival: Thursday, June 16 in afternoon or evening
Departure: Sunday, June 19 after lunch

Site: The Mohonk Mountain House in New Paltz, New York
[http://www.mohonk.com/frameset.htm]

Located 90 miles north of New York City on the spectacular Shawangunk Ridge and surrounded by thousands of acres of unspoiled forest and winding trails. Serviced by local airports in Newburgh, NY [Stewart Airport] and Albany, as well as the New York metropolitan airports in Newark, NJ, and La Guardia and Kennedy in New York City.

Details of the program and registration/logistics will follow early in the 2005 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 the Earth's Interior at Mt, Holyoke College in Massachusetts [June 12-17] to attend the COMPRES meeting with a minimum of extra travel.

A.10 Annual Program Plan and Budget

In preparation for the submission of the Annual Progress Report and Annual Program Plan and Budget to NSF in February, 2005, 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 2004, the two Standing Committees asked the project directors of each of the subawards to submit annual progress reports for Year #3 and budget requests for Year #4 by November 1, 2004. 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, 2004.

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 2004 AGU Meeting in San Francisco. Each of the Standing Committees gave oral reports on their deliberations to the Executive Committee at the Fall AGU Meeting, and then submitted their written report, with evaluations of progress and recommendations for funding in Year #4, to the Executive Committee. In the case of the Infrastructure Committee, this report included recommendations for initial funding of new projects and community workshops.

In January 2004, 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 #4. Following these meetings, the President prepared a budget plan which was discussed, revised, and approved by a majority of the Executive Committee.

B COMMUNITY FACILITIES

B.1 Diamond-anvil cell facilities at the National Synchrotron Light Source

[H-k. Mao, R. Hemley, Carnegie Institution of Washington]

Scientific highlights

Discovery of Pressure Induced Symmetric Hydrogen Bond formation as well as the Quantum Phase in Methane Clathrate by Synchrotron IR Spectroscopy.

Clathrate hydrates are compounds consisting of cages of hydrogen bonded water molecules surrounding guest molecules or atoms. Recent studies revealed the formation of new high-pressure phases of the CH4 clathrate and its possible implications for hydrogen bond research as well as providing a new model for the formation and evolution of the composition of Titan, a moon of Saturn. There has been an intense interest in this area of research. The CH4 clathrate is also of significant importance as a potential energy source. Since the clathrate is quite compressible, this raises the question of whether it may be possible to achieve the condition where the hydrogen bonds in the cages formed by the water molecules could be driven to a symmetric state as that observed in a high pressure form of pure crystalline ice, ice VIII. A series of far- and mid-IR measurements were carried out by Klug et al. to identify the predicted phase transition from non-symmetric to symmetric hydrogen bonds at both room and low temperatures up to 40 GPa. Pressure dependence of the C-H and uncoupled O-H stretching vibrational modes indicates that the possible center symmetric hydrogen bonds as well as quantum phase at about 20 GPa. It is well consistent with theoretical studies of the stability and phonons for this clathrate system.

Space weathering on airless planetary bodies: Clues from the lunar mineral hapkeite

The crystal structure of mineral hapkeite has been studied by in situ synchrotron energy-dispersive, single-crystal x-ray diffraction technique. (Anand, M. L et al, PNAS, 101, 6847–6851, May 4, 2004). It is confirmed that the crystal structure of hapkeite is cubic with a space group Pm3m (221) and lattice parameter of 2.831 (4) Å, similar to the structure of synthetic Fe2Si. This mineral and other Fe-Si phases are probably more common in the lunar regolith than previously thought and are directly related to the formation of vapor-deposited, nanophase elemental iron in the lunar soils. The rims of most lunar soil grains contain a myriad of minute (typically, _10 nm) metallic Fe grains dispersed in an amorphous glassy matrix. Similarly, the agglutinitic glass also contains these minute grains. This metallic Fe has been variously called single-domain, nanophase, superparamagnetic, and submicroscopic Fe0, all emphatic of the small size of these grains that are within the rims of soils and in agglutinitic glass that cements the soil aggregates. The formation of this nanophase elemental Fe0 (np-Fe0) is related to space weathering. Physical and chemical reactions occurring as a result of the high velocity impacts of meteorites and micrometeorites and of cosmic rays and solar-wind particles are major causes of space weathering on airless planetary bodies, such as the Moon, Mercury, and asteroids. These weathering processes are responsible for the formation of their regolith and soil.

Synchrotron Infrared Spectroscopy of Synthetic P21/m amphiboles at High-pressure.

Systematic mid-IR measurements of synthetic Na(NaMg)MgSi8O22(OH)2 amphiboles up to 30 GPa were carried out by Gianluca Iezzi et al. These minerals represent a key double-chain silicate to model the P21/m – C2/m phase-transition in A-site filled amphiboles. It has P21/m symmetry at room-T, and reverses to the usual C2/m space-group of monoclinic amphiboles at ~ 257 °C. The spectrum of the Na end-member shows three bands: (A) at 3740 cm-1, (B) at 3715 cm-1 and (C) at 3667 cm-1, respectively. The higher-frequency bands are assigned to two non-equivalent H atoms interacting with ANa; this pattern is typical of an amphibole with a P-lattice. The BLi-bearing amphiboles show in addition a fourth, minor band at 3690 cm-1. With increasing pressure, all bands linearly shift toward higher frequency. At 20.8 GPa, the peak centroid of the main (A) band is > 3800 cm-1. The A and B bands merge into a single, broad absorption band, and the P value at which the A-B doublet disappear is a function of the B-site occupancy. For the BNa end-member the A and B bands merge at around 18 GPa; for sample 406, with nominal B-site composition (Na0.2Li0.8Mg1), the A and B bands merge around 13 GPa. These results show that the Na(NaMg)MgSi8O22(OH)2 amphibole undergoes a P21/m – C2/m phase transition at high pressure, and that the transition pressure, PC, is a function of the aggregate dimension of the B-site.

Bioceramic hydroxyapatite at high pressure

Hydroxyapatite (HA), Ca10(PO4)6(OH)2, is an important bioceramic and it is the main mineral constituent of the bone tissue in humans. With advances of deposition techniques, various nanostructured ceramics including HA have become increasingly available for biomedical implant applications. The mechanical properties of HA coatings like hardness and elastic modulus are sensitive to the preferred orientation presented in the samples. It is not yet clear from the available data whether alignment of HA hexagonal grains is caused by the compressive stresses during laser deposition. A bioceramic hydroxyapatite, Ca10(PO4)6(OH)2 polycrystalline sample was studied under high pressure in a diamond anvil cell to investigate its structural, electrical, and mechanical properties under compression. (N. Velisavljevic et al. Appl. Phys. Lett. 82, 4271 , 2003). No phase transformation was observed in the pressure range of 0.1 MPa up to 32 GP. But its c/a ratio with pressure showed an anisotropic compression effect. Initially the c/a ratio is increasing up to 8 GPa suggesting that the c axis is less compressible than the a axis. Above 8 GPa, c/a reaches a steady value of 0.741, an isotropic compression persists up to the maximum pressure. These results imply that the least compressible c axis might align itself with the stress axis minimizing the elastic strain energy if a uniaxial stress applied. This experimental observation is consistent with the alignment of grains observed during PLD3 where the least compressible direction (c axis) will align along the stress axis due to impact of the laser-generated plume. The present studies demonstrate that a fully dense and translucent hydroxyapatite sample is attained above 10 GPa at 300 K.

High Pressure Far-IR Absorption Spectroscopy of Muscovite

Muscovite is a geologically-important hydrous mineral because it is common in both igneous and metamorphic rocks and is accordingly a significant host for mineralogic water storage in the Earth's crust. High-pressure x-ray diffraction studies suggested a loss of long range crystalline order starting at 18 GPa and pressure-induced amorphization by 27 GPa. To obtain a better understanding of the thermodynamic response of muscovite to compression, Henry Scott et al. have used infrared spectroscopy to sample vibrational modes spanning both the mid and far portions of the infrared spectrum using a diamond anvil cell as a both an optical window and pressure generating device up to 25 GPa. Nine FIR features between 100 and 550 cm-1 have been observed that have been previously documented in ambient pressure spectra. All modes shift monotonically to higher frequencies with increasing pressure; there are notable changes in relative intensities, but this is likely a result of enhanced preferred orientation due to the nature of compression in a DAC. Based on the lack of abrupt changes in the lattice modes, it appears that pressure-induced amorphization is not likely to occur over this pressure range and that muscovite can be compressed metastably well beyond its known stability field.

Lack of the critical pressure for weakening of size-induced stiffness in 3C-SiC nanocrystals under hydrostatic compression

The compressibility of 30 nm 3C–SiC nanocrystals was studied under hydrostatic conditions while helium was used as pressure transmitting medium, as well as under nonhydrostatic conditions without pressure medium. (H.Liu et al Applied Phys. Letters, Nov. 2004) No threshold pressure phenomenon was observed for the compressibility of the nano-crystals during compression in hydrostatic conditions, while the critical pressure around 10.5 GPa was observed during nonhydrostatic compression. These indicate that the threshold pressure phenomena, recently reported that the nanocrystals initially exhibited much higher bulk modulus below the threshold pressure during compression [Appl. Phys. Lett. 83, 3174 (2003); J. Phys. Chem. 107, 14151 (2003)], were mainly caused by the non-hydrostatic effect instead of a specific feature of nanocrystals upon compression. The bulk modulus of 3C–SiC nanocrystals is estimated as 220.6±0.6 GPa based on the hydrostatic compression data.

FTIR Spectroscopy of the mixture of N2 and H2O under High Pressure and Temperature Conditions

Accurate equations of state (EOS) for mixture reactions using a high pressure and high temperature diamond anvil cell (DAC) are essential for understanding the nature of inter-molecular forces and the behavior of simple molecules under extreme conditions.

The techniques used here to solve for pressure (P), temperature (T), and composition (X), and their results are relevant to a broad range of important processes. For example, interest in fluid-fluid phase equilibria at high pressures and in supercritical fluid mixtures has increased greatly over the last two decades for scientific and practical reasons: intermolecular interactions and general aspects of critical behavior can now be studied experimentally and computational capabilities to describe these systems have been improved. Models capable of accurately characterizing PXT properties can provide important tools for understanding many natural processes occurring in the earth's crust and mantle. Binary systems in which water is one component or systems that consist of one highly polar and one non-polar partner are also of particular interest. Becky Streetman et al. studied a mixture of N2 and H2O under high pressure and high temperature at U2A that focuses on measurements of phase separation boundaries of water and nitrogen mixtures over the range of experimentally accessible temperatures and pressures. An externally heated diamond anvil cell (EHDAC) was used for these experiments. At the coalescence temperature, initial results indicate that the mixture is homogeneous and that a clathrate is formed.

Constraining the equation of state of fluid H_2O to 80 GPa using the melting curve, bulk modulus, and thermal expansivity of Ice VII – The Equation of state properties of Ice VII and supercritical H_2O at temperatures of 300 - 902 K and pressures of 6 - 60.5 GPa have been studied using a Mao-Bell type diamond anvil cell with an external Mo-wire resistance heater. (M. Frank et al, Geochimica et Cosmochimica Acta, 68, 2781-2790, 2004) The unit cells of Ice VII and gold were monitored during the experiment with gold being used as an internal pressure calibrant. X-ray diffraction data of ice VII fitted to the third-order Birch-Murnaghan equation of state yield the isothermal bulk modulus KT0 = 21.1 ± 1.3 GPa, its pressure derivative K'T0= 4.4 ± 0.1and the volume V0 = 12.4 ± 0.1 cm3/mol at zero pressure, respectively. Additionally, the melting curve of Ice VII was determined to greater than 40 GPa by using the disappearance of the diffraction pattern of Ice VII to monitor melting in the system. The melting curve for Ice VII from 3 to 60 GPa was found to be accurately related by a Simon equation (P-2.17)/0.764) = (T/755)4.32-1. 4.32_1These results were used further to constrain the PVT properties of fluid H_2O at elevated pressures and temperatures by taking the pressure derivative of the Gibbs free energy difference between Ice VII and fluid H_2O along the Ice VII melting curve. Comparison of these results suggests that the previously stated equations of state of fluid H2O overestimate the molar volume of fluid H_2O at pressures greater than 20 GPa. These results can be used to constrain the internal order of icy satellites.

Future Beamline Upgrade Plans (not included in present budget)

U2A

High-pressure and high-temperature capability for general users: an EHDAC has been ordered from Prof. W. M. Bassett that will be solely used at U2A (purchased with CDAC funds). This cell will routinely cover the P-T range of up to 40 GPa and 1000 K.

New IR/Raman Microscope system (also supported by CDAC): this setup with higher spatial resolution will be completed earlier next year. Together with the EHDAC, 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.

New side station: measurements at this side station would provide an increase in the S/N by a factor of 5 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 (~$60 K). Combined with the new IR microscope discussed above, users could carry out both IR (down to 30 cm-1 with diffraction-limited spatial resolution) and Raman scattering experiments ROUTINELY under extreme conditions (i.e., up to >1000 K and >100 GPa). 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.

X17B3

- To setup YAG laser heating system working and upgrading its temperature measurement.
- To develop the 4-Laue monochromater and angle dispersive x-ray diffraction (ADXD) facility.
- To establish low temperature x-ray diffraction facility.
- To design and establish a single crystal XRD facility with mono and white x-ray beam.

X17C

- To develop single crystal diffraction program
- Upgrade VME control system
- Improve Monochromatic system
- Create the second ruby pressure calibration system.

2004 NSLS-DAC Publications

(The following publications are resulted, solely or partially, from using the x-ray, IR, or optical systems of the NSLS-DAC facility as noted.)

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B.2 Multi-anvil Cell Facilities at the National Synchrotron Light Source

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

Summary

The 2004 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.

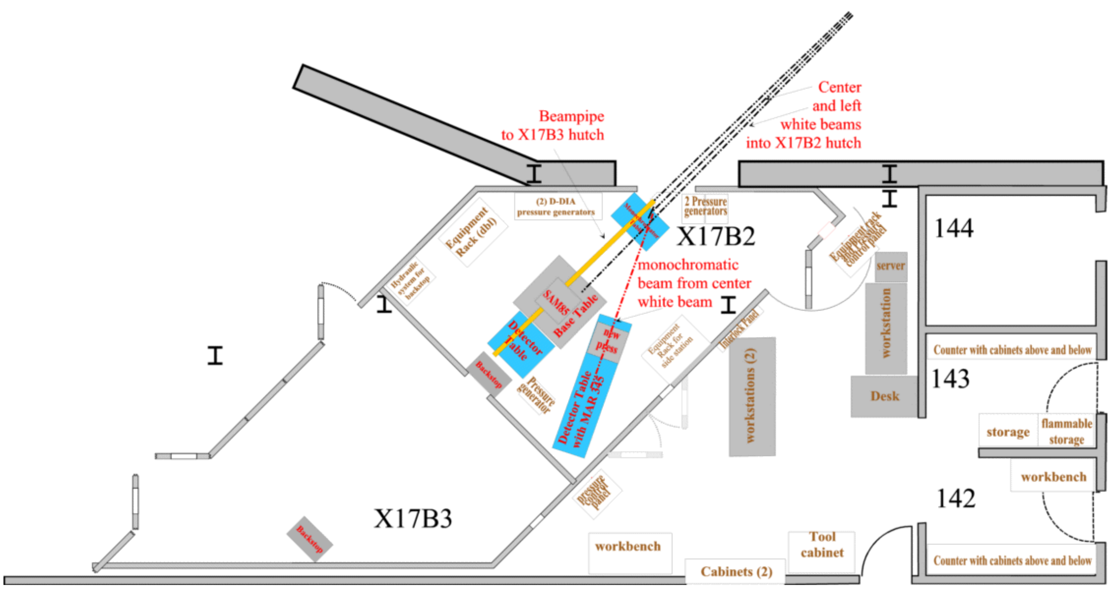
We have now begun development of a second phase designed to increase the available beam time in the multi-anvil hutch. We are building a monochromatic in-hutch-side-station. A single bounce monochromator will remove a thin slice of beam from the white beam and deliver it behind the main press to a second press equipped with a T-cup high pressure device. We have been funded by the DURIP program of the Department of Defense ($182,000) to purchase a significant portion of the equipment that is required. We have acquired the main detector, a MAR345 imaging plate system. We are designing the table and looking at presses. 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.

We are continuing our process of beam time allocation. Now all experiments must be submitted to NSLS review panel using the NSLS review process for general users. NSLS then assigns up to 25% of the standard mode beam time on the basis of their review. We reserve 10% for beamline development. We assign the remaining time following the rating of the NSLS review, but upgrading proposal that are consistent with a COMPRES agenda. assignment and the special considerations for the parasitic time.

This last year we took possession of a Deformation-DIA apparatus [D-DIA] that is being used for deformation experiments. This system is part of our long term push to include rheology experiments at synchrotron facilities. We feel that this opens the facility to a community that has not had a history using the synchrotron.

Hutch Layout



Science Highlights

- **Deformation experimental technique breakthrough and scientific research:** A new high pressure deformation apparatus D-DIA has been married to the synchrotron x-ray source. The 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.
- **Polycrystalline stress field:** Multi-phase aggregates have been the focus of recent studies, capitalizing on the D-DIA'
- **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. Measurements have been carried out on tin and promise to be quite interesting.
- **Metallic Glass:** By working in part at the multi-anvil beamline, X-17B2, scientists from Los Alamos National Laboratory have produced a new glass material by squeezing the metal zirconium under very high pressures. This glass may be stronger and more resilient than traditional glasses, and has the potential to be a better material for medical, sports, and electronics products. The research was published in the July 15, 2004, issue of Nature.

Beamline Usage - Calendar Year 2004 Summary

For the 2004 calendar year we received 24 General User beam time requests from 22 individuals totaling 161 days. NSLS awarded beam time to 7 of these users totaling 31 days. There were 59.5 Operations days assigned to X17B2, and 55 assigned to X17B3, of which we were able to use 50. Subtracting the 31 days assigned by the NSLS, 78.5 were left as PRT time. COMPRES assigned 69.5 of these days to 15 of the proposals evaluated and ranked by the NSLS Proposal Review Committee; 9 days were used for beamline development and other maintenance projects.

Major Support Personnel	**Source of Funding**
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.3 West Coast Synchrotron Facilities

[R. Jeanloz, University of California at Berkeley]
Report on COMPRES activities at the West Coast Beamlines for 2004-2005 by Simon Clark, Martin Kunz and Raymond Jeanloz.

Summary

West coast COMPRES activity has focused this year on providing experimental facilities at the Advanced Light Source (ALS) for COMPRES users. These include provision of facilities on existing beamlines for powder diffraction (beamline 11.3) and infra-red (beamline 1.4). Also, a new dedicated high-pressure beamline (beamline 12.2.2), incorporating both resistive and laser heated diamond cells, has been commissioned this year. COMPRES has achieved Approved Program status at the ALS guaranteeing COMPRES users 30% of the beam time on beamlines 11.3 and 1.4 and a similar amount on beamline 12.2.2. The first round of applications from COMPRES users has been completed with a total of 9 groups applying for 44 days of beamtime in the period from January to June 2005. The level of applications is expected to grow as the new beamline becomes available for users. New initiatives explored this year include small angle scattering and single crystal diffraction. Proposed activities for next year include completing beamline 12.2.2 development and installing a dedicated infrared end station. We also propose to continue to explore our potential for the development of facilities for single crystal diffraction and shockwave measurements.

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 30% 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. Projecting current contributions, we expect that COMPRES users will receive between 22 and 26 percent of the beamtime on 12.2.2 over the next five years. 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

High-Pressure Laboratory (Responsible: Arianna Gleason, Martin Kunz)

The high-pressure preparation lab was reorganized and completed with additional equipment such that users now have a versatile and ready-to-use lab including 7 diamond-anvil cells, a spark-erosion gasket-hole driller, 3 Druck pressure controllers, a cryogenic loading unit (to be operated with N2 or Ar), 2 preparation stereo microscopes including a digital camera for imaging, as well as an off-line ruby fluorescence pressure calibration system.

Diamond anvil cells (DAC) (Responsible: Arianna Gleason)

Six membrane driven DIACELL DACS and a screw-controlled DIACELL DAC are available for use. They can be equipped with 0.3 or 0.2 mm culet-diamonds. Load-pressure curves were established for all of them using the Ruby-scale. In collaboration with David Walker, an externally heatable DAC was constructed and tested. It operates with a resistive heater coil around the gasket assembly. Temperature is measured with a thermocouple touching the diamond facets. P-T conditions of 20-30 GPa and 450° C have so far been calibrated.

Beamline 12.2.2: (Responsible: Martin Kunz, Wendel Caldwell, Tony Yu, Simon Clark)

Construction of 12.2.2 was finished in late 2003; first beam was taken in early 2004. First test-experiments were performed in January / February 2004 on an improvised end-station. These experiments included high-pressure studies on white phosphorous (with Joe Zaug, Livermore) and a HP-HT study on garnet (together with Dave Walker, Columbia).

In May 2004, the final version of end-station-1 (ES-1) was installed. Commissioning experiments were performed between June and October. Commissioning included the following beamline characterizations:

- alignment of X-ray optics and optimization of focus point (0.15 mm horizontal x 0.09 mm vertical).
- Calibration of aperture slits and definition of aperture on focus point.
- Measuring of flux: ~ 75 % of calculated curve.
- calibration of monochromator and monitoring of long-term stability: ± 2-3 eV at 30 keV over the period of weeks including frequent wavelength changes.

- testing and calibration of Smart 6000 CCD detector with respect to dark-current, spatial distortion, distance calibration, pixel size.
- testing of sample centering routine (reproducibility within 0.01 mm)
- Ruby pressure scale vs. NaCl pressure scale.

Since June a variety of test-experiments involving the following user groups have been involved: UC Berkeley (Raymond Jeanloz and co-workers, Paul Alivisatos and co-workers), UC Santa Cruz (Elise Knittle), UCLA (Sarah Tolbert and Michelle Weinberger; Abby Kavner and Nathalie Conil), and Livermore (Joe Zaug and Alex Goncharev). These experiments were crucial in detecting existing weak links, and room for improvement for a user-friendly beamline. They also demonstrated the beamline's capability of performing high-pressure powder diffraction, combined high-pressure / high temperature studies using an externally heated DAC, radial- and axial-diffraction for stress-strain measurements as well as high-pressure small-angle scattering (will not be possible after installation of K-B mirrors).

On endstation-2 (ES-2), the on-line laser-heating system has been installed and tested in collaboration with Michael Walter (Bristol University). The goniometry has just been installed and we plan to install the K-B mirrors in December. Special attention was been given to establish a fool-proof safety procedure to operate the class 4 IR laser by general users.

Beamline 11.3.1: (Responsible: Martin Kunz, Sirine Fakra, Allen Oliver, Nobumichi Tamura).

In 2004 four shifts of 2-3 weeks of high-pressure experiments were performed. They were used for combined high-pressure – high-temperature experiments (Dave Walker, Arianna Gleason), high-pressure compressibility studies on super-hard materials (Michelle Weinberger), and an experiment testing the possibility to perform monochromatic single-crystal diffraction experiments at the ALS (Ross Angel, Oliver Tschauner, Martin Kunz).

Summary of proposed activities for next year

First priority in FY05/06 will be the optimization of the existing experimental high-pressure facilities at the ALS, namely the two end-stations at 12.2.2, the high-pressure laboratory as well as the use of 11.3.1 for high-pressure experiments. This will include continuous software upgrades based on user feedback, improvement of experimental procedures, further development of an externally heatable DAC, as well as improvement of the DAC-preparation environment (gas-loading-system). With this we hope to establish a reliable work-horse beamline that is able to produce high-quality P-V-T equation-of-state data for the mineral-physics and high-pressure community. Besides this, the art of in-situ laser-heating a DAC while centered on an X-ray beam shall be perfected. Here, we will mainly focus on reliably measuring temperatures and on safety issues.

Other development projects include:

- X-ray imaging in a DAC using an imaging camera to apply the rolling-sphere technique of measuring viscosity at higher P and T than currently possible in large-volume cells (in collaboration with UC Berkeley, Raymond Jeanloz).
- Axial X-ray diffraction to measure texture distribution as well as stress/strain behaviour of composite materials in diamond-anvil cells (in collaboration with UC Berkeley: Rudy Wenk, and UCLA, Abby Kavner)
- monochromatic and polychromatic single-crystal X-ray diffraction to extract a maximum of structural information, also at extreme conditions (in collaboration with VPI, Ross Angel and UNLV Oliver Tschauner).
- Feasibility tests for high-pressure EXAFS in order to complement our diffraction capabilities with a spectroscopic tool.
- Commissioning of a off-line Raman system.
- feasibility tests of interfacing synchrotron radiation with shock-wave experiments at LCLS (in collaboration with LLNL, Gilbert Collins, and BARC, India: B. Godwal).
- Commissioning of an in-hutch ruby fluorescence system.

Summary of Publications

Development of COMPRES activities on the West Coast are in an early stage. Given this, not many publications have yet come through. Nevertheless, some papers have come out this year. They are listed in the appendix.

Appendix : List of publications for this year

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B.4 Neutron Studies

[N. Ross, Virginia Polytechnic Institute and State University]

Introduction

The goals of the neutron initiative of COMPRES are to:

(a) Identify and broaden the neutron scattering community of Earth Scientists in the U.S.
(b) To stimulate and promote the use of neutron scattering, with emphasis on high-pressure research, in the Earth Sciences.
(c) To carry out educational activities that support the above goals.
(d) 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).

Activities

Support for Neutron Research in Year 3

The primary requirement for travel and subsistence support is that the researchers have obtained approval for beamtime at the neutron facility in question. Generation of neutrons is costly and therefore proposals for allocation of beamtime are carefully reviewed. Many facilities, however, do not provide travel and subsistence costs and COMPRES is therefore able to facilitate access to neutron facilities by providing these funds.

COMPRES provided funds to a number of researchers who performed neutron scattering experiments at facilities in the U.S. and abroad

Postdoctoral Research Associate

Funding was approved in Yr. 3 of COMPRES for a Postdoctoral Research Associate to help develop hardware, software, and instrument solutions for high-pressure neutron diffraction experiments, including:

- Assessment and testing of high pressure cells (and high P-T cells), with and without a focused beam and with different detectors;
- Determining the advantages and disadvantages of each cell for different types of experiments;
- Communication of these results to the community (once it is shown what can be done, it will help build the user community)

The search commenced in April 2004. There were 20 applications by June 1. The search committee, Ross Angel (VT), John Parise (Stony Brook) and Nancy Ross narrowed the short list to 4 candidates. Two of our top four choices accepted offers elsewhere – one opted for another postdoctoral position and the other accepted a permanent job in industry. All were reluctant to accept a 1-year position.

Two candidates were interviewed over the summer and an offer was made to Dr. Husin Sitepu in August 2004. Dr. Sitepu has a wealth of experience in neutron diffraction, originally at the ANSTO facilities at Lucas Heights, Australia, then at the Center for Neutron Research, NIST, Gaithersburg, U.S.A., and, most recently at the Institut Laue-Langevin, Grenoble. He has worked on the analysis of crystal structures, phase transformations in single crystals, and on the analysis of internal strains in crystals and shape memory alloys. Dr. Sitepu accepted the offer in September, 2004. Dr. Sitepu's current contract ends in 2005, and, depending on the progress H1-B visa application, Dr. Sitepu plans to start in late February 2005

Neutron Workshop Opportunities

- N. Ross is on the Program Advisory Committee for a NMI3 sponsored workshop on Neutrons in Earth Sciences and the Environment (NESE) to be held as a satellite meeting of EGU2005, April 24-29, 2005, in Vienna, Austria. This symposium is part of a joint US-European foresight studies series that is exploring directions for neutron scattering research in high profile technical areas. The aim of the workshop is to show where neutron scattering can have a major role/impact in research in Earth Sciences and the Environment and define future actions to further broaden application of neutrons in these fields. This workshop will be widely advertised to the COMPRES community.
- Professors R. Wenk (Berkeley) submitted a proposal to the Council of the Mineralogical Society of America for a MSA Reviews in Mineralogy Series on "Application of Neutron Scattering in the Earth Sciences". The proposal was approved and the suggested date of the short course is Fall 2006.

B.5 Student Interns at Beamlines of National Facilities

In 2004-2005, with supplemental funding provided by the IF Program of EAR, COMPRES supported the internships of two students working at beamlines of national facilities.

These included:

Arianna Gleason
Home Institution: University of Arizona
National Facility: Advanced Light Source of the Lawrence Berkeley National Laboratory.
Supervisors: Simon Clark and Martin Kunz

Christopher Young
Home Institution: University of California at Davis
National Facility: National Synchrotron Light Source of the Brookhaven National Laboratory
Supervisors: Jiuhua Chen and Michael Vaughan.

Both of these interns commenced their one-year appointments in late summer 2004. Following are reports from the interns and assessments by their supervisors on their progress in the first half-year of their internship.

Report of Arianna Gleason (December 2004)

As the COMPRES intern at the Advanced Light Source at the Lawrence-Berkeley National Laboratory, I am involved with a variety of projects and management tasks. I currently organize and maintain the High Pressure Lab at the ALS under the direction of Simon Clark and Martin Kunz. This involves helping beamline users with diamond-anvil cell [DAC] experiment preparation, high pressure equipment training and safety. These tasks not only facilitate refinement of my own skills, but also expose me to the wide variety of current synchrotron research. In tandem with this training, I participate in a weekly crystallography tutorial with Martin Kunz. To date, I have covered the following topics: space groups/ point groups, reciprocal lattice, bond lengths and angles, structure factor, temperature factor, and powder diffraction. I also maintain our new website for ALS High Pressure research at:
http://xraysweb.lbl.gov/bl1222/home.htm

My recent research focuses on development and implementation of a resistively heated DAC system. A resistively heated DAC system for high pressure and high temperature diffraction measurements has been developed at the ALS and tested on Beamlines 11.3.1 and 12.2.2. This system is placed in a controlled environment and consists of a commercial diamond cell supplied by Diacell Products heated by resistive

elements surrounding the diamonds. Temperature control is through PID feedback on a K thermocouple in contact with the diamonds and the gasket. To date, the system has operated to 450 ^{o}C and 24 GPa. Achieving these P/T conditions is important as we seek to understand more about physico-chemical properties of minerals as a function of pressure and temperature. Measurements at these temperatures are particularly crucial to study the behavior of minerals at subduction zones within the Earth where water content and phase stability are of great interest. Our pilot study involves the phase transitions of talc. I gave a poster presentation at the 2004 ALS Users' Meeting on
the progress of this talc project. The most recent talc data will be presented at the 2004 AGU Conference in San Francsico, CA. Once this pilot study is complete, I plan to investigate other hydroxides, such as diaspore, gibbsite, and goethite at subduction P/T conditions using this same experimental method. The overriding goal is to ascertain the equations of state for these materials and their role in deep earth water cycles.

The value of this project and my experiences at the beamline is multilayered. I am helping to generate a user-friendly heatable DAC for use at Beamline 12.2.2 which is advantageous for the larger high-pressure community and ALS users. A comprehensive understanding of the creation details and application of this heatable DAC system is a rich opportunity for me as a first-year graduate student. The training and skills acquired in this single year will be a ubiquitous benefit in pursuit of my Ph.D. and future scientific endeavors. I will integrate the techniques I have learned and the data I collect into a PhD thesis when I attend University of California, Berkeley in fall 2005. My experience here has been one of invaluable scientific involvement and immense opportunity. I feel honored to be apart of this group and look forward to the coming challenges.

Assessment of progress of COMPRES intern Arianna Gleason (December 2004)

By Martin Kunz and Simon Clark

Arianna Gleason started working as a COMPRES intern at the ALS high-pressure program in June 2004.
Her tasks are the following:

- Learn the theoretical basics in crystallography and mineral physics to enable her the reading of the relevant literature.
- Collect a background in the most important literature on the role of hydrous phases in the deep Earth.
- Learn about the basic experimental skills to perform X-ray diffraction experiments in combination with diamond anvil cells.
- Manage the preparation lab. This includes maintaining the necessary equipment and consumables; train, assist and supervise users of the preparation lab as well as characterization of the pressure cells.
- Continue the development of an externally heatable cell, originally started by Dave Walker, Columbia University.
- Help with commissioning work on 12.2.2; this includes operating the beamline and performing commissioning experiments in connection with the externally heatable cell.

Arianna is fulfilling all her tasks in an exemplary way. Her progresses in theoretical and practical knowledge of the various issues surrounding a high-pressure beamline at a synchrotron source are remarkable. She very quickly picks up the essentials of her tasks hand fully takes responsibilities to get them completed as good as possible. Her approach in problem solving is exemplary in that she is able to find possible solutions independently but is also not shy to find the necessary help from outside if needed.
All in all, Arianna, although an intern to be trained, has quickly grown to a very competent collaborator within the high-pressure group of the ALS and therefore is a big help!

We feel that this program is an excellent win-win opportunity for the trainees and the personal running the high-pressure program. The trainee gets a very realistic practical insight into the tasks and problems of doing Science in the realm of high-pressure physics, which is supplemented by some theoretical training. The high-pressure group on the other hand strongly benefits from the practical work performed by the intern. We strongly recommend to continue this program on at least the same level. An expansion of the program would be desirable so that all Synchrotron sources with COMPRES stations could benefit from it.

Report of Christopher Young (December 2004)

<u>Background:</u>
I received my Bachelor's degree in chemical engineering/materials science and engineering from UC Davis in June 2004. I served as an undergraduate research assistant at LLNL under the direction of Joe Zaug. At LLNL I studied the physical properties of high-explosives under extreme conditions in a diamond anvil cell. I also performed preliminary studies with the pressure induced band-gap transition of CdTe nanocrystalline semiconductors.

Now as the current intern for COMPRES at the NSLS I have the oppurtunity to explore an entirely new field. I have been working with Jiuhua Chen (SUNY-SB) and other visiting scientists on a variety of projects. The main focus has been on high pressure and high temperature melt properties, synchrotron capability development, and deformation experiments using the D-DIA. Below is a summary of the projects that I have been working on.

<u>Density of Molten FeS:</u>

Studying the liquid properties of metals at earth core conditions has long been a difficult task. The SAM-85 large volume press at X-17B2 provides us the opportunity to study melt density at high pressure and temperature. The density measurements are made using an x-ray imaging plate. The density can be calculated using the radiograph intensity and known x-ray absorption properties of the absorbing metal. Using a modified Beer's law, accounting for spherical geometry, we find the density as follows with a constant x-position:

$$B(x_c, y) = Ce^{-[\mu_{FeS}\rho_{FeS}(D(x_c,y)-l(x_c,y))+\mu_{Al_2O_3}\rho_{Al_2)_3}l(x_c,y)]} \tag{1}$$

$$l(x_c, y) = 2[r^2 - (x - x_0)^2 - (y - y_0)^2]^{1/2} \tag{2}$$

$$D(x_c, y) = (D_0{}^2 - x^2)^{1/2} \tag{3}$$

Where μ is the mass absorption constant, ρ the density, I_0 the intensity of the entering x-ray, D_0 the diameter of the cylindrical sample chamber, r is the radius of the Al_2O_3 sphere, x and y are the coordinates of the pixels, x_0 and y_0 are the center coordinates of the Al_2O_3 sphere. Using two dimensional fitting provides an approximate result, however it is much more desirable to constrain the fitting to the entire image. A 3-D model for the intensity across the sphere is as follows:

$$B(x, y) = I(x, y)Ke^{-[\mu_{FeS}\rho_{FeS}(D(x,y)-l(x,y))+\mu_{Al_2O_3}\rho_{Al_2)_3}l(x,y)+\mu_0\rho_0 d_0]} \tag{4}$$

In equation 4, μ_0 ρ_0 d_0 is a correction factor for the absorption of the surrounding materials. Using a 3-D model to find the density of the molten FeS should provide a much more accurate result. Figure 1 is a representative x-ray radiograph used for the density measurement.

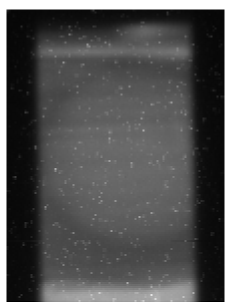

Figure 1 An Al203 sphere placed in an FeS sample

Performing a non-linear regression with Equation 1 we obtain the following fitted intensity profile:

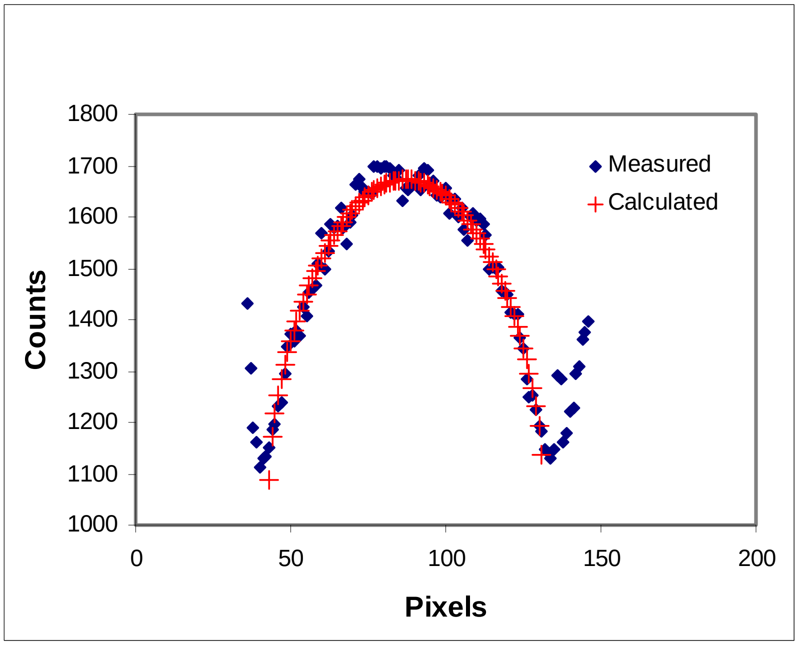

Figure 2 2-D fitting of the intensity of a radiograph across the sphere

The red points are the fitted data and the blue points are the experimental data obtained from the image. Figure 2 is a good fit, but performing a 2-D fitting only fits approximately 90 data points (an 80 pixel slice from the original image). Fitting in 3-D allows the fitting to be constrained by the whole image (approximately 90 pixels X 90 pixels providing 8100 points). Figure 3 is a representative image of the 3-D fitting that has been performed:

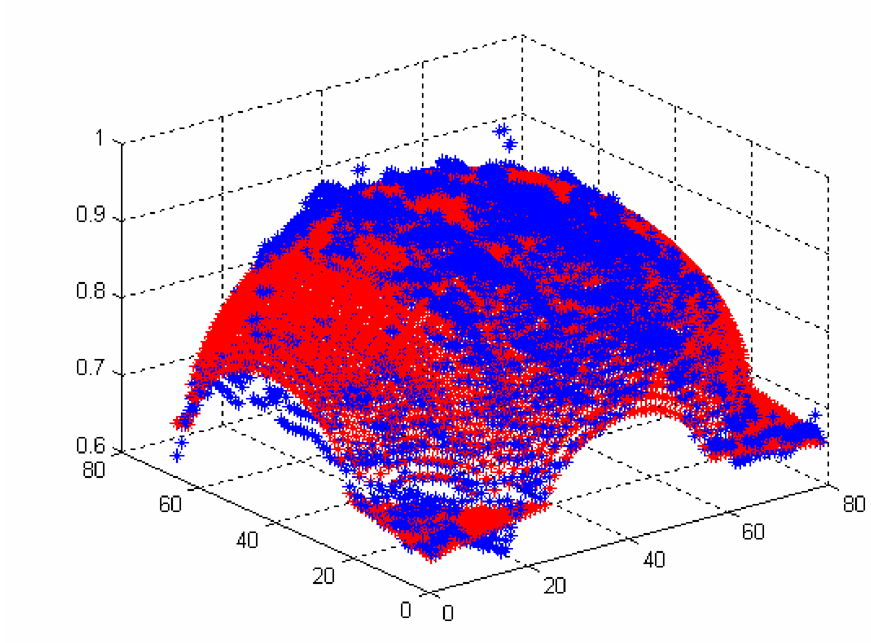

Figure 3 3-D fitting of the intensity of a radiograph across the sphere

Here in figure 3 the blue points are the experimental data and the red points represent the fitted points from the non-linear regression. Further revision to the code needs to be added to achieve a better fitting for the 3-D pattern. The density measurement provided by the 3-D fitting is much lower than the density measurement from the 2-D. It is also lower than the expected value for the FeS. However, with further revision of initial conditions and constraining of parameters a more accurate density can be calculated.

Viscosity of Sn:

X-ray radiography at X-17B2 also provides the opportunity to measure the viscosity of melts at high pressure and temperature. In these experiments a small Al_2O_3 sphere is placed in a sample. As the temperature rises and the sample melts the Al_2O_3 sphere will move vertically in the sample. The speed that the Al_2O_3 sphere descends through the material can be tracked using the radiographs. The acceleration of the Al_2O_3 sphere can then be related to the viscosity of the material. As the viscosity of the material decreases the speed of the Al_2O_3 sphere will increase. Figure 4 shows the motion of an Al_2O_3 sphere with time:

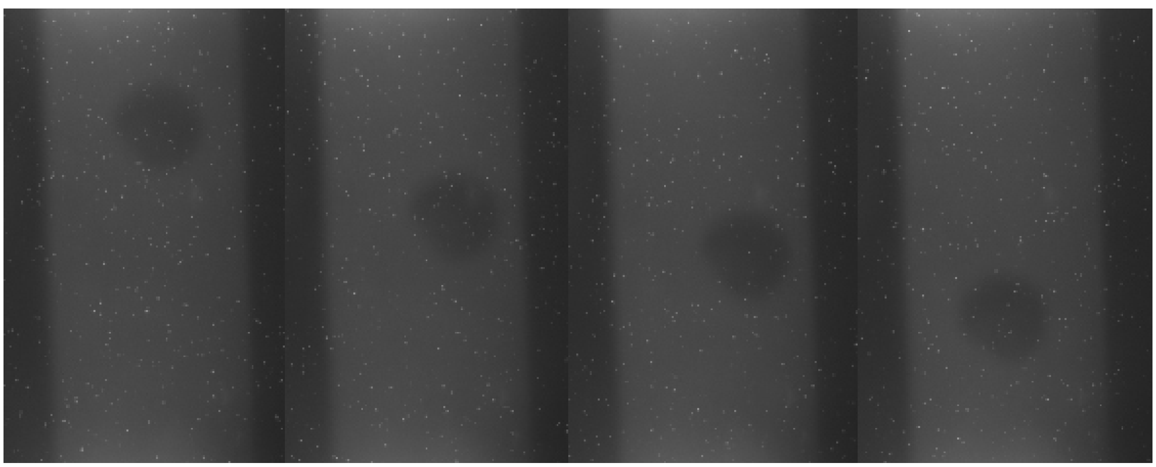

Figure 4 The dark circle is the sphere. Vertical motion is tracked

Each image is taken over a specified time interval. These 4 images are only representative and are not spaced equally over tine. Figure 5 is a graph showing the motion of the sphere over a complete time series. We can see that the motion of the Al_2O_3 sphere is non-linear.

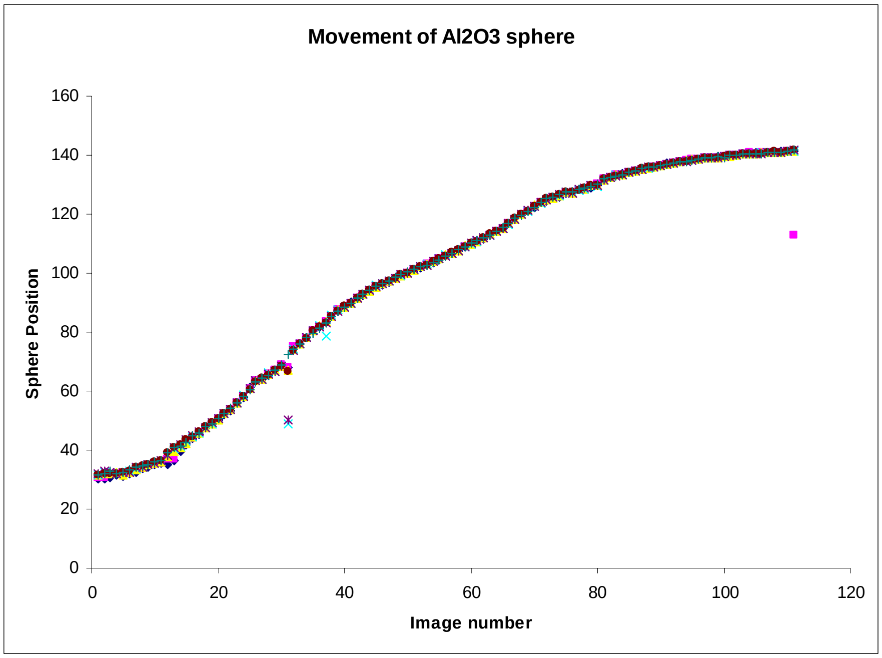

Figure 5 The position of the sphere is non-linear

Diffraction Enhanced Imaging (DEI):

Diffraction enhanced imaging aids in enhancement of resolution of x-ray radiographs. With diffraction enhanced imaging two materials of similar Z number can be resolved using computer analysis of surface features. The intensity of an image from DEI can be related to the density of a material, much like the use of x-ray absorption to obtain the density of a material. DEI can be used as a confirmation of the density measurements obtained from the x-ray absorption calculations of the x-ray radiographs. The density is directly proportional to the intensity of the image:

$$\frac{I}{I_0} = \frac{\rho}{\rho_0} \qquad (5)$$

I_0 is the intensity of the surrounding material, I is the intensity of the sphere, ρ_0 is the density of the surrounding material, and ρ is the density of the sphere. As long as the density of the sphere is known at the particular high temperature and pressure conditions, we can find the density of the surrounding sample.

Assessment of progress of COMPRES intern Christopher Young (December 2004)
By Jiuhua Chen.

Chris has shown great interest in material properties study (especially melt related) at high pressure. He is very strong in analytical data processing, little weak on experimental aspect. The COMPRES beamline intern program is perfect to develop trainees' hands-on capabilities and excite their interests of high pressure research in conjunction with synchrotron radiation sources. The program is greatly beneficial to a participant like Chris. Although Chris came with his material/engineering background, he is now very interested in Earth related material. He is making satisfactory progress on the training track. In addition to the progress in the scientific research project, he has been also involving beamline development and user support. We believe that the beamline intern program meets the current urgent needs of training/preparing the young generation for future beamline scientists or attracting them to the Earth science research field. It should be continued at an expanded level.

C. INFRASTRUCTURE DEVELOPMENT

C.1 Multi-anvil Cell Assembly Development

[K. Leinenweber, J. Tyburczy-Arizona State University]

Introduction

With the COMPRES Multi-anvil Cell Assembly Development project we were able to develop many new ceramics and other parts for high-pressure research. Over the three-year period, we established contacts with ceramics companies and other outside sources for fabricating parts for multi-anvil pressure cells. We built a machining facility consisting of a safe, dust-free lathe and tooling, with ready access to an entire preexisting shop for other work such as milling and EDM. We hired a machinist, Brian Nagy, who in cooperation with others in the shop solved many of the technical problems and figured out how to produce high-quality ceramic parts for multi-anvil work at low cost. We worked with other laboratories on testing and evaluating new cell assembly designs. Many designs as well as individual components were tested around the country and unavoidably, around the world as well as laboratories in other countries caught wind of the project.

COMPRES paid for all this but got the involvement of K. Leinenweber in the project for free. Also, the expertise of many researchers at ASU and around the country was utilized for the project, and many people put long hours into testing the assemblies in their own laboratories with their own carbide. In the end, the results have been worth the investment, because we have developed an overall cell design scheme that can be used for multi-anvil high-pressure work in general. We have developed four cell assemblies based on this scheme that will continue to be used and many components and new ceramics that will also be used well into the future. There are 15 or so individual projects that are currently active in various locations, and all of them are contributing greatly to our overall understanding of these cell assemblies as they relate to our scientific goals and the attainment of pressure and temperature.

Cell assembly design principles

We started with an overall design scheme for the cell assemblies. We began designing from the "outside in," taking each component and finding ways to make enough of them at a low enough price that we could supply them to collaborating labs to do the evaluation. We also had to make the components very easy to assemble with obvious geometries, because otherwise they would be too difficult to use by other laboratories, or use consistently. We wanted to eliminate all the parts that are done by hand, so that the geometry of the cell assembly would be well-defined and the same for every user, but we didn't want this to result in high costs. At each step there were obstacles that were encountered, and we dealt with all of them.

We began with the gasketing of the assemblies. ASU had developed a paper backing (Fig. 1) that was cut at a local laser-cutting shop, to replace the razor-blade cut paper used in Japan and Bayreuth assemblies. This paper backing has the effect of reversing the order that the gasketing is attached to the cubes, and eliminating the differences between the gasket placement of different researchers. It also makes assembling the cubes much faster. This paper is placed first instead of last, and it guides the placement of the pyrophyllite gaskets, aligns them and allows them to be easily positioned. Combined with a set of aluminum "nesting plates" that we have supplied, the gaskets can be accurately placed and the nest of cubes easily assembled without the danger of gaskets falling out, which was a common problem before.

The gaskets themselves were presented to the machine shop as a challenge – we wanted them to be pre-made precisely to trapezoidal shape. In the end, after several other techniques were tried over a one-year period, we adopted the technique from Daresbury, which is to stick a pyrophyllite layer onto double-sided tape and mill it on a numerically controlled milling machine. The whole slab of pyrophyllite can be machined in one run without human intervention. The trick we found is to machine most of the way through in one pass and then remove the last 30 microns or so at the very end – this prevents the pieces from breaking loose from the tape. We also found out that the material can be laser-cut extremely precisely, but the company that we worked with did not come through when we ordered 2000 pieces, and we never received them. We would like to reopen this avenue of investigation because it is potentially the best way to make gasket pieces if it can be done inexpensively enough.

Following this came the octahedron, which was deemed to be the most critical part of the whole project. At $30 a piece, the commonly used octahedra from Mino Yogyo or Ceramic Substrates would quickly consume the budget of a project such as ours. One could argue that a Walker-style castable octahedron could be used, but that technology is fully developed and can already be used by any laboratory; also, the gasketed assemblies were desired by many laboratories to fill out the high-end of the pressure. We settled on the technique of injection-molding as the solution to this problem (Fig. 2). ASU had encountered an interesting ceramic formula in working with injection-molding during its MRSEC. It was based on copying the composition of castables, which is 66% MgO and 33% Al_2O_3 by weight, but the molding company fires their ceramics at 1500 C, which resulted in all the alumina reacting to form $MgAl_2O_3$ spinel. At that time the formula failed, because we had tried to cast on the fins as in a Walker-style assembly, and the material was too hard. However, it occurred to us that it should work in a gasketed assembly. We procured blocks of the material at first and machined it into octahedra. When those worked, we began to order molds. The molds are $2500 each but can be used basically forever, and produce octahedra that are only $6, meaning they pay for themselves after only about 100 octahedra are made. They also have the sample holes molded in, which saves money and assures excellent centering of the hole, but means the hole size also has to be pre-selected. We now have 7 octahedral molds in 5 different edge sizes (8, 10, 14 x 3, 18 and 25 mm); the five sizes together are shown in Figure 2. These form the basis for our series of assemblies, both the ones that are already developed and the ones we would like to develop.

After this, the inner parts of the assemblies: furnaces, thermal insulating sleeves, sample sleeves, etc. had to be developed. We had requested and received funding from COMPRES for a CNC lathe for machining ceramic parts, and we obtained the lathe with live tooling and set it up with a vacuum line for removing dust and covered all the sensitive parts. The vacuum line creates a net pull into the lathe chamber, which prevents airborne dust from getting into the gearing of the lathe, and more importantly the dust is removed from the building so it does not present a hazard to the machinist. The lathe automatically drills and turns parts, but what has turned out to be the biggest advance for us is that the live tooling on the lathe (which resembles little air-driven Dremel tools that are computer controlled; Figure 4) can be used to cut notches or drill side-holes in the parts, eliminating the need for researchers to cut thermocouple trenches by hand. Another useful technical development was cutting foil furnaces (Figure 3) by wire EDM, another ASU-driven development. The thermocouple notches can be made during the cutting. At $10 plus $3 material cost per furnace, these are the most expensive pieces we have. However, for the small assemblies it saves a great deal of time. Also, there is very little rhenium scrap left over, whereas when furnaces are cut by hand there is a pile of scraps left after the cutting, making it hard to quantify the price for the handmade furnaces.

The thermocouple itself was also changed. Jim Van Orman suggested that the failure rate of thermocouples in one of the assemblies would be reduced if we could use thermocouples between .005 and .010 inches diameter (type C). We looked into it, and the major thermocouple companies did not sell intermediate sizes, but Rhenium Alloys, the supplier for some of those companies, would sell us the intermediate size, and at a much lower price. The thermocouple wire is not calibrated, but we decided to go with it anyway since the calibrations do not vary much for our purposes, and in theory we could calibrate the wire after we have verified its usefulness, if desired. Our .007 thermocouple wire has turned out to virtually eliminate thermocouple failures in that assembly, as well as being easy to work with, and we are also using it in all the other sizes so far.
The last pieces are the small ceramic pieces for the thermocouple (alumina and mullite). We now have these pre-cut, at some 35 cents to 50 cents each, these can be cut very precisely by an outside grinding company and there is no longer any good reason to destroy our own diamond saws cutting these pieces. Also, variations in pressure calibrations have been blamed on variations in these pieces (Jie Li, pers. comm.), so we decided to make the pieces uniform in size.

All of this left only the thermocouple grooves in the octahedron that have to be made by hand. This has also been blamed for problems in reproducibility (Tony Withers, pers. comm.) and is time-consuming and troublesome especially for the small assemblies, so we very recently had a jig built in the machine shop for holding ten of the 8 mm octahedra at a time and cutting slots in them. The resulting thermocouple slots are excellent – far better than we have been able to cut by hand, and very reproducible. We still have a problem with breaking diamond tools on them – currently the slots are running $3 per piece in tooling, and we would like to reduce that to $1 per piece – but the concept is at least working. We are now supplying all the 8 mm octahedra with the slots cut and will see how the response is (note, although this is a "final" report, the 3-year project actually is not over yet).

Designing and Testing

The first series of specific designs were arrived at through an open community discussion at AGU in the fall of 2002. The Fei 8/3 was considered a good target for the first complete COMPRES assembly. It had a good record at the Geophysical Lab and it filled out a pressure range that several laboratories had not reached but had a desire to reach. There were also no objections to a Bayreuth-style 14/8 assembly. We set about applying the design principles outlined above to these assemblies.

For the Fei 8/3, we did testing in our lab and sent out some batches of assemblies to Canberra, and when those tests were promising, we sent out batches to many other laboratories. We have sent about 25 batches of 10 assemblies, with 35 parts per assembly. These assemblies are complete and there are no parts left to be made by the researcher, unless they have special sample containment or other issues which means they might have to change out the center of the assembly. The COMPRES version of the Fei 8/3 assembly is now calibrated at several laboratories, with 3 room-temperature runs at APS (Fig. 5); high temperature runs at APS are planned in our November 2004 beam-time session.

The Bayreuth 14/8 $LaCrO_3$ step-heater assembly was designed and tested by Jed Mosenfelder at Caltech. He used the COMPRES gasketing and octahedron, and built the inner parts based on the Bayreuth design. The design has been calibrated at Caltech and in 3 runs at APS (Fig. 6). We will start producing this assembly for testing by Minnesota and other interested laboratories in winter 2004.
A Stony Brook-style 14/8 assembly was adopted, designed and tested at ASU, and has been sent out to a few labs for trials. About 5 batches of this assembly have been sent out so far. Gabriel Gwanmesia has made large samples of Mg_2SiO_4 wadsleyite with this assembly.

The COMPRES 10/5 assembly is under testing at ASU by Tamara Diedrich. We are in the prototyping phase with the first 35 assemblies made with the full numerical control. It is now at the stage where it is ready to go out for testing by other laboratories, and is considered to be the fourth COMPRES assembly. We have also sent out batches of the "bare" 10 mm octahedra, about 50 in total, for testing with other configurations.
For the 18 mm and 25 mm sizes, designing is just underway. A batch of the 25 mm octahedra has been provided to Jed Mosenfelder who is developing the first COMPRES 25 mm assembly based on a Bayreuth design. This is meant to be a workhorse assembly for making large samples of materials at pressures below 10 GPa. The 18 mm octahedra are waiting for an assembly to be developed, we plan to initiate this at ASU in early 2005 assuming the other developments all go smoothly.

Beamline projects

We are also developing a series of ceramics for beamline applications; these have been a component of the project from the beginning. We desire to turn these into complete beam line assemblies, and the concept of a “hybrid” assembly that can be used both on and offline with equal effectiveness is very appealing. Such a hybrid assembly would become extremely familiar and well-characterized and it is easy to see how it would improve experiments both at the beam line and in the conventional laboratories. However, it presents severe challenges and requires the replacement of many components in the assembly with lower-Z materials. We have been developing and testing these components one by one, because that is more tractable than trying to develop a full assembly with new and untested materials.

We have a mullite injection-molded ceramic that Stony Brook became interested in when we sent them some 6 mm test cubes. We subsequently had a cubic mold made (6 mm with a 3 mm hole) and 100 cubes are being tested by Hongbo Long at Stony Brook who is presenting the results at the Fall 2004 AGU meeting. The basic interest in them is that they have excellent thermal insulating capabilities, which is needed for high-temperature applications at the beam line, but without the furnace and sample contamination problems caused by boron epoxy. The Stony Brook group reached record temperatures (some 1800 °C) with the assembly they tried, and were able to hold the temperatures stably, something that was never possible with boron epoxy combined with a graphite furnace. We tested an octahedron with this ceramic as well, and although it gave the best power curve we have ever seen, using only half as much power as any other assembly, it did not produce as much pressure as the MgO-spinel ceramic. We are awaiting the results from the beamline project before deciding whether to use the mullite ceramic for any of our in-house or hybrid assemblies.

We have also tried new insulating sleeves, to replace zirconia, and new furnace materials, to replace $LaCrO_3$. For insulating sleeves, we obtained a batch of finished forsterite sleeves at a cost of $1 each form an outside ceramics company for the 14/8 box furnace. These insulate similarly to zirconia and hold pressure well in preliminary tests. However, the sleeves were contaminated with $MgSiO_3$ pyroxene, and we are working with the company to have a cleaner batch made. These would be excellent for a hybrid assembly, since they are far more x-ray transparent than zirconia. For the furnace, we have tested a machinable BN/TiB_2 composite that failed at 1300 °C; a similar composite that does not fail is currently being searched for. When we can replace $LaCrO_3$ with such a material, the hybrid design will be ready. We also expect to greatly reduce thermal gradients if we replace graphite with a low-conductivity furnace, because that will eliminate the need for large current rings that cause heat loss out the ends. Thus instead of making the hybrid assemblies “as good” as preexisting assemblies, we are aiming for an improvement for both beamline and offline applications.

A new rhenium furnace design we have recently made is a “hybrid” design – we have simply rotated the seam in the furnace by 30 degrees so that the x-ray beam passes through the slit in the furnace, cutting the rhenium absorption in half. This is being tested at APS in November 2004. If this is combined with MgO plugs in the $LaCrO_3$, and possibly with a second slit in the back of the furnace, we could have a basically transparent 8/3 assembly; however, the latter modifications are not suitable for a "hybrid" assembly but would only be desirable for online experiments.

Community.

We have developed contacts with a broad community of high-pressure laboratories, and we believe we have helped foster a further dialogue on high-pressure techniques between these laboratories. A list of involved laboratories is attempted at the end of this report. Because we are now accelerating our production rates and have solved many of the technical problems with the basic production of cell assemblies, we think this dialogue will increase because we will now be able to supply test batches in greater quantities. We are also receiving more inquiries because, although we have not heavily advertised this effort, it has been getting word-of-mouth advertising. We have avoided a vast announcement because we were still learning to produce assemblies; however, now we can make broader announcements and hopefully live up to the expectations created by them.

One way we will accomplish this is with a workshop on cell assemblies and in-situ techniques, in collaboration with Yanbin Wang at APS. We are planning a 3-day workshop in Spring 2005 and have applied for 2 days of beam time for the workshop. The main purpose of this workshop is to show the new technologies for multi-anvil experiments and the use of the beam lines, and to create discussions and new ideas. However, we also intend for the preparation and the workshop itself to help bring our cell assembly development effort to a wider audience who may be interested in participating. Now that the development burden has been removed for the first four assemblies, we will in the remainder of the project be able to fully realize the community involvement and the community service that was built into the project from the outset. It is very exciting to have these fully functioning assemblies and very unique ways of making them that have been developed over the 3-year period of this grant. We are looking forward to being able to work with all of the interested laboratories in turning these assemblies into a permanent part of the high-pressure tools that are available to researchers.

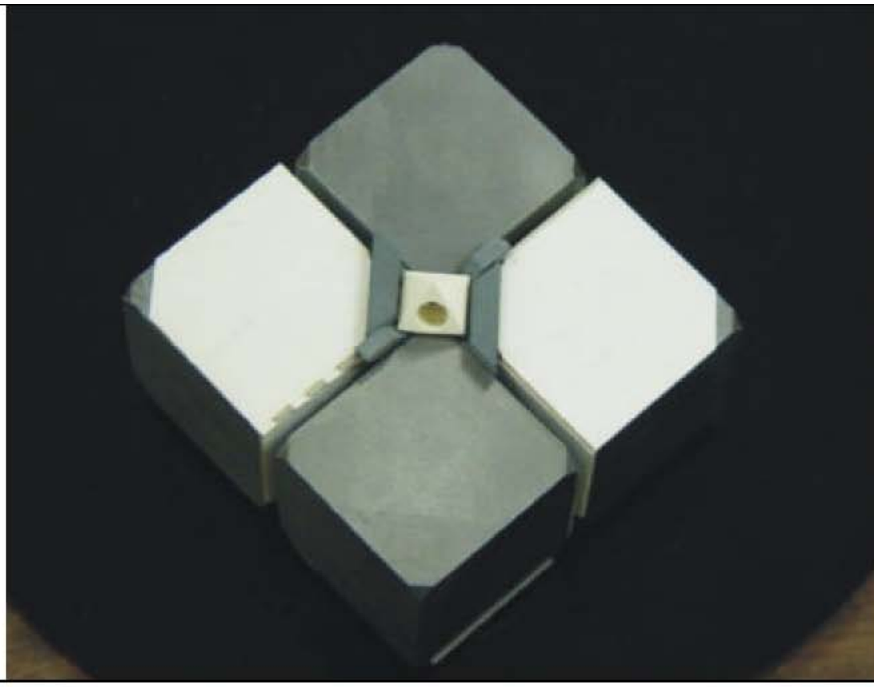

Fig. 1: Laser-cut paper glued to cubes. One piece of the paper folds over 3 sides of a cube and attaches to itself with the small tabs, a row of which are visible to the left of the octahedron. The gasket pieces are glued on after the paper, so the paper helps to position them. An injection-molded octahedron is shown at the center.

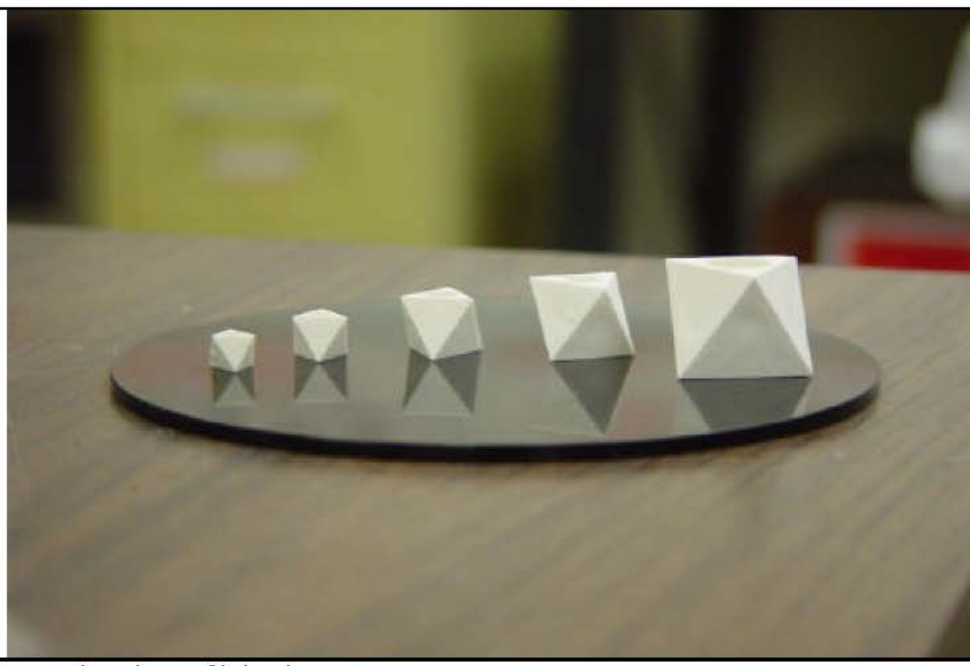

Fig. 2. Five sizes of injection-molded MgO/spinel octahedra made for the COMPRES project (L to R): 8 mm, 10 mm, 14 mm, 18 mm and 25 mm.

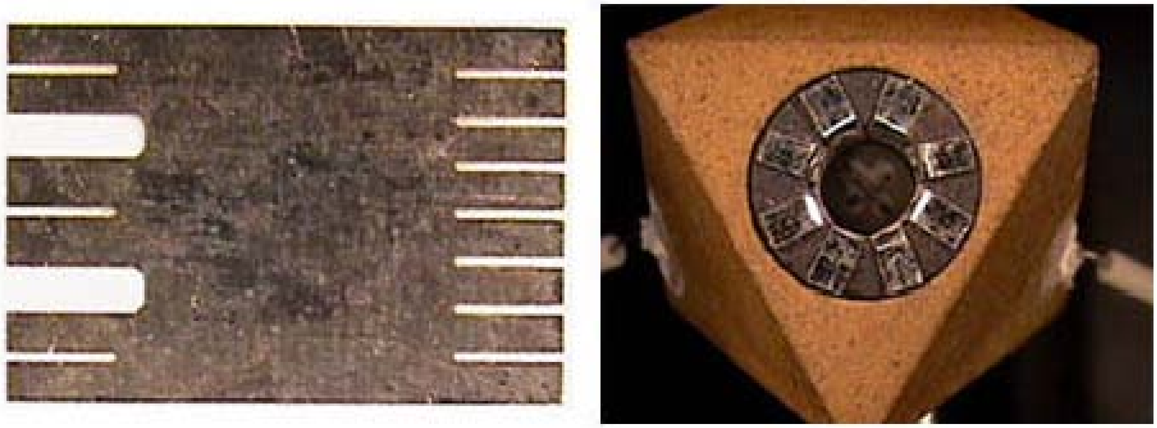

Fig. 3: Rhenium furnace rectangle (left) about 8 mm across, cut by the wire EDM technique, with narrow slits and two thermocouple slots. The rhenium is wrapped and placed into an 8/3 assembly (right – shown with a conventional octahedron from Mino Yogyo).

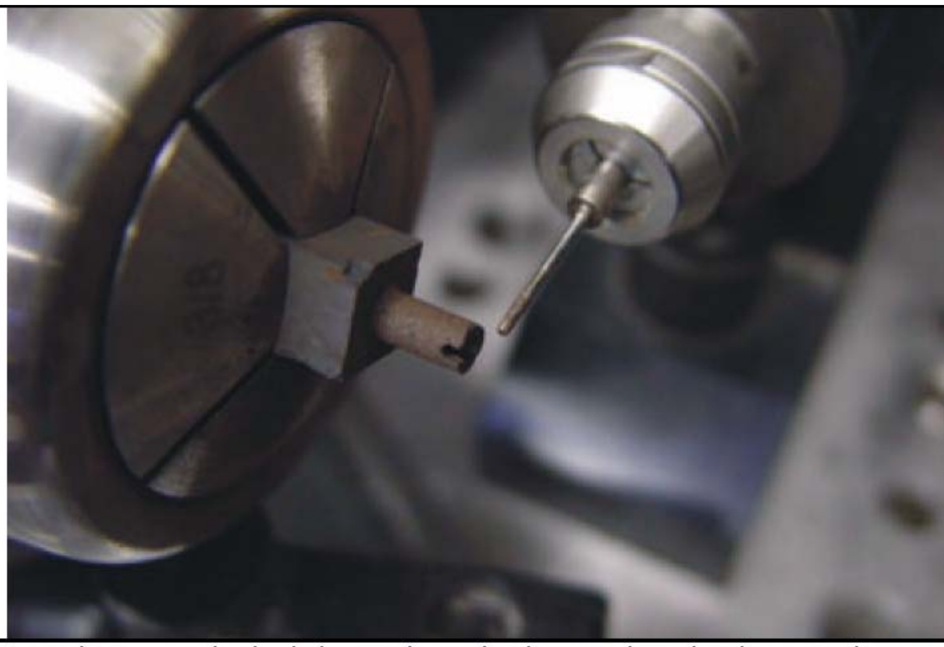

Fig. 4: A thermocouple slot being cut into a lanthanum chromite sleeve on the automated lathe. The hole has already been drilled in the middle and the outside turned down to the correct diameter. After this, the sleeve will be parted off and is ready to use. All these steps are done automatically; the ceramic can also advance for the next sleeve automatically thanks to a compressed air advancer designed by Brian Nagy and Zoltan Farkas.

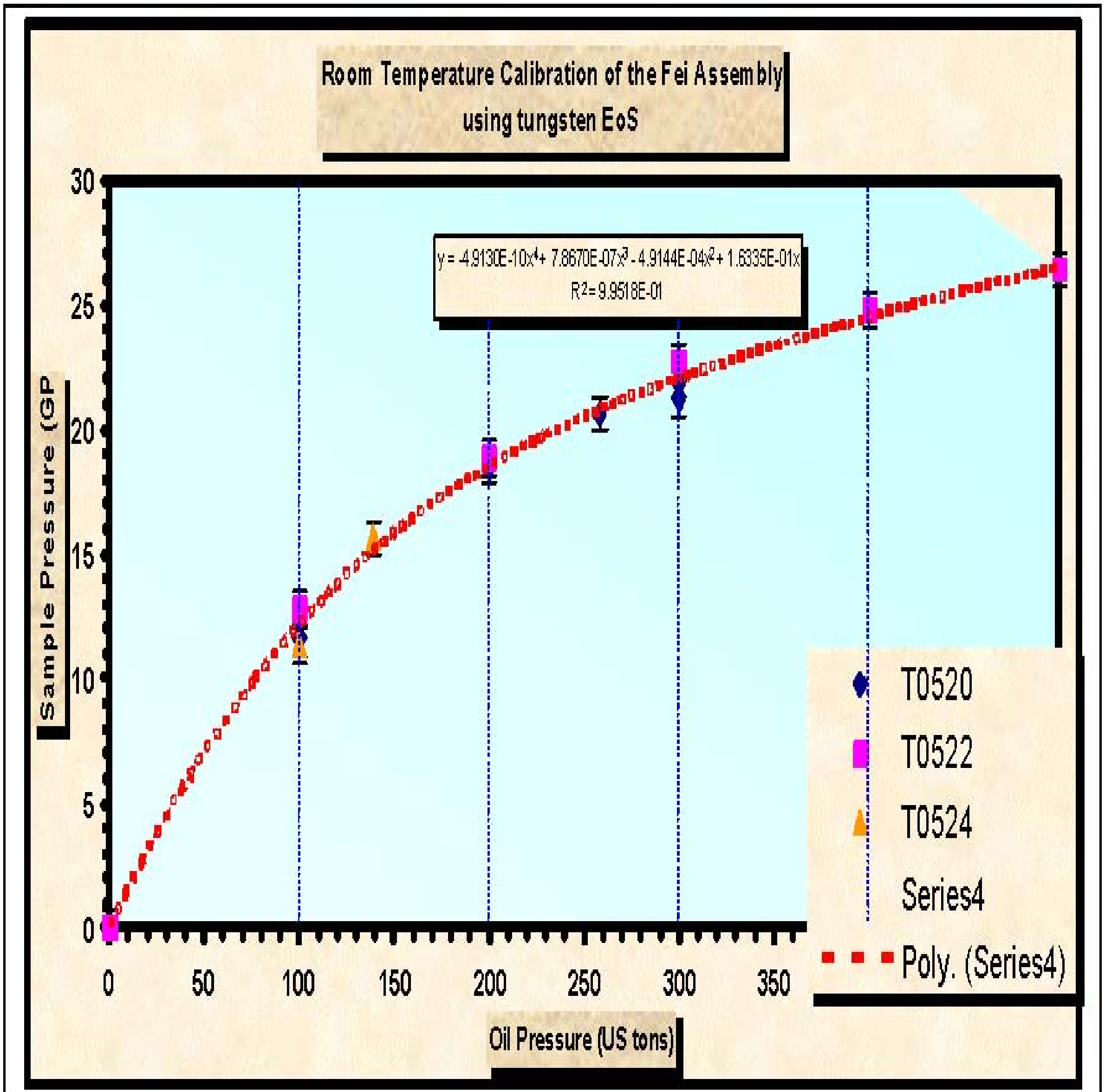

Fig. 5. Three room-temperature pressure curves of the 8/3 assembly, measured at the APS beamline, are superimposed in this Figure.

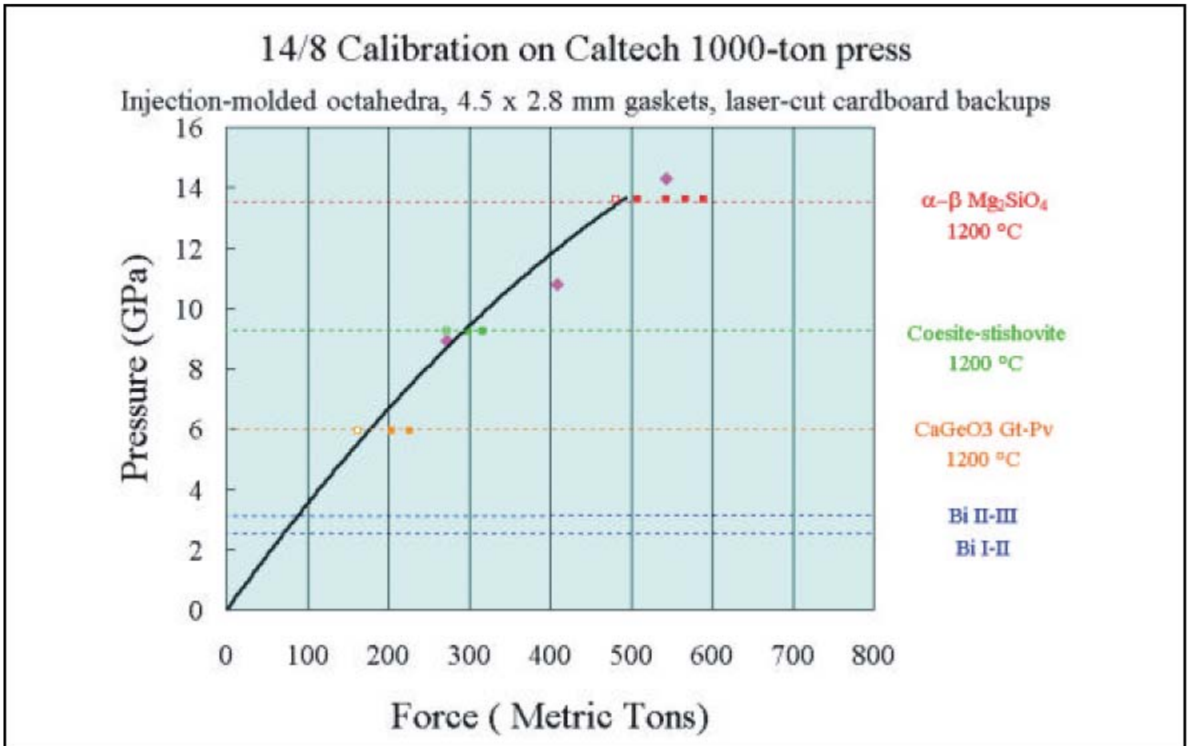

Fig. 5: Calibration of the COMPRES 14/8 $LaCrO_3$ step-heater assembly at 1200 °C. Fixed-point measurements were made by Jed Mosenfelder in the Caltech press with a Walker module. The purple diamonds are 3 points from the beam line at APS.

List of collaborating laboratories and individuals (experimental facilities are shown in parentheses when different from the home institution). (Persons at the same institution are listed separately if they are collaborating on different projects or assemblies).

Gabriel Gwanmesia, Delaware State University (Geophysical Laboratory)
Rondi Davies, American Museum of Natural History (Lamont-Doherty)
Jie Li, University of Illinois at Champaign-Urbana
Jed Mosenfelder, California Institute of Technology
Dean Scott, and Tom Sharp (on sabbatical), Research School of Earth Sciences,

Australian National University, Canberra, Australia Yingwei Fei and Shantanu Keshav, Carnegie Institute Geophysical Laboratory Jim Van Orman, Case Western Reserve University Darren Locke, University at Stony Brook Jennifer Kung, University at Stony Brook/BNL David Dobson, University College London, U.K. Emmanuel Soignard, Arizona State University Ed Bailey, Royal Institute of London, U.K. Baosheng Li, University at Stony Brook Jiuhua Chen and Hongbo Long, University at Stony Brook (APS and NSLS)

Recent inquiries and smaller exchanges:
Bill Durham, Livermore National Laboratories Kevin Righter, NASA Takeyuki Uchida, APS Ray L. Jones, Daresbury Synchrotron, U.K. Tony Withers, University of Minnesota

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

[T. Duffy, Princeton, University, G. Shen and D. Heinz, University of Chicago]

Workshop on "Future Directions for the Laser-Heated Diamond Anvil Cell at the Advanced Photon Source" May 19-20, 2004

We organized a workshop on the laser-heated diamond anvil cell that was held on May 19-20, 2004 at the Advanced Photon Source. A total of 41 persons attended the workshop including participants from Japan, Europe, and the US. The workshop (see appendix) included presentations from leading researchers in the field, as well as a series of open-ended discussions regarding future needs for high-pressure laser heating science. A broad cross-section of the high-pressure laser-heating and synchrotron communities was represented. The appendix provides a detailed summary of the workshop discussion. Individual presentations are posted on-line at the COMPRES website (http://www.compres.stonybrook.edu/Meetings/index.html). A central conclusion of the workshop is that there is strong support across the community for community-based and interdisciplinary efforts to improve laser-heating technology at synchrotron facilities. More specifically, plans for further development of laser heating and x-ray capabilities at the GSECARS sector received strong support from the community.

Personnel

Dr. Andrew Campbell joined our project in July 2004. Dr. Campbell, who is a Senior Research Associate at the University of Chicago, is supported by this project at the 50% level. Dr Campbell has extensive experience in high-pressure research and laser heating techniques. He is leading the effort to develop the new laser heating system at the GSECARS sector of the Advanced Photon Source. We consider ourselves very fortunate to have found someone with Dr. Campbell's expertise and experience for this position. He has already made considerable progress in design and procurement of components for our laser heating system in just a few short months.

CO_2 Laser Selection and Acquisition

A Synrad f201 CO_2 laser has been purchased for the laser heating system being developed at GSECARS. This system will be installed online at beamline 13-IDD. Several laser systems were considered, and most deliberation revolved around models from Coherent, PRC Lasers, and Synrad. Several factors were considered, including power, CW output, power control, mode quality, and stability.

The Synrad f201 is rated at 200 W of output power, which is anticipated to be sufficient for heating even samples that have been compressed up to ~100 GPa pressure or higher. Its CW output avoids problems related to thermal fluctuations inherent in pulsed laser heating, and its linear polarization will permit external power control by, for example, using a rotating Brewster window device. The mode quality of the Synrad f201 is very high for a CO_2 laser (98% TEM00), which not only enhances the fraction of the output power that will be directed into the diamond anvil cell, but also minimizes the amount of laser light that is dumped unnecessarily into the hutch. Finally, the Synrad f201 was very competitive in terms of cost. A summary table, showing a comparison of several other lasers to the selected model, is attached in the appendix.

The laser was recently received (in late October). The next several months will be devoted to testing the laser and system designs on the benchtop in the GSECARS optical laboratory. Some off-line experiments can also be carried out during this period. After thorough testing of design and performance, the system will be transferred to the 13-ID-D hutch. After a short period of further in-house testing on the beamline, the system will be opened to outside users in about one year from now. A detailed proposed schedule is given below. Dr Campbell and Dr. Shen have been working together to meet all applicable ANL safety procedures for the use of this high-powered laser system both in the laboratory and at the beamline. Presently under development is a Standard Operating Procedure authorized by the Laser Safety Officer at ANL, regarding such issues as shielding of the optical table to reduce stray laser light, and interlock systems.
Consultation with Other CO_2 Laser Users in the COMPRES Community

Since joining the project, Dr. Campbell has visited some diamond cell laboratories in which a CO_2 laser is actively being used for laser heating of samples at high pressure. In addition to the University of Chicago, Dr. Campbell visited the Geophysical Laboratory of the Carnegie Institution of Washington and the Department of Physics at the University of Nevada, Las Vegas, to discuss technical details of their CO2 laser heating systems and to obtain advice on optical designs, materials, suppliers, safety considerations, etc. Campbell was hosted by J.-F. Lin and Y. Song at the Geophysical Laboratory on August 26, 2004, and by O. Tschauner at UNLV on October 20, 2004. These visits were very beneficial in the design and selection of beam delivery optics for the CO_2 laser to be installed at GSECARS. In addition, earlier phone discussions with these CO_2 laser users yielded important input into the laser selection.

Preliminary Optical Design

A sketch of the preliminary optical design for the CO_2 laser beam delivery system is shown in the appendix. The strategy to be followed is to test the suitability of each component in this design, and to evaluate the effectiveness, reliability, and ease of use of the design, in the GSECARS laser laboratory before transferring the system into the 13-ID-D x-ray station.

In this design, the Synrad f201 laser will be emitting its full 200 W continuously, as this is the only power level at which it produces true CW output. The power will then be controlled using an external attenuator, which is likely to be a motorized Brewster window device. Feedback from a power meter can be used to stabilize the laser power incident onto the sample. The beam will be focused with a ZnSe lens onto the sample. Our initial design calls for entry at an angle with respect to the cell axis; this will permit the existing optical system for temperature measurement to be used. The laser and most of the optical components will be located on an enclosed optical table above the plane of the x-ray diffractometer; only the final beam delivery mirrors and focusing lens will be outside the enclosure. All aspects of this design are subject to modification based on the results of our bench-top testing in the GSECARS laser laboratory. In the initial stage, the CO_2 laser heating system will share the temperature measurement, sample stage alignment, and related components with the existing Nd:YLF laser heating system, but subsequent upgrades to these systems, including independent systems, are being actively pursued.

Finite element models of the laser-heated diamond anvil cell

This work has been carried out in collaboration between Dr. Duffy and Dr. Boris Kiefer (New Mexico State University). Detailed simulations of the thermal structure of the laser-heated diamond cell were carried out using finite element calculations over a wide range of initial conditions. An initial manuscript focusing of the effects of thermal conductivity and sample thickness variations has been submitted for publication to Journal of Applied Physics. A second manuscript that compares in detail a variety of experimental geometries currently in use or proposed for laser heating is in preparation.
Development of Pressure Standards for the Laser-Heated Diamond Anvil Cell
We have begun project to augment the number and type of materials that can be used as internal pressure standards for laser heating experiments. There are very few materials that are widely accepted for this purpose, with Pt and MgO being the most commonly used, and this selection is inadequate for some geophysically important sample materials (Fe being a good example) that may alloy or otherwise react with the pressure standard. We have been allocated beamtime at GSECARS Sector 13-ID-D to inter-calibrate the high-P,T equation of state of Pt with several alkali halides using X-ray diffraction in the laser heated diamond anvil cell. These experiments will begin on November 20, 2004, and will include the participation of scientists from both the University of Chicago and Princeton University. In a related project being carried out by Dr. Atsushi Kubo, we are conducting an on-going study of thermal pressure effects in the laser-heated diamond cell. We have collected experimental data in two runs and analysis of the data set is in progress. The specific goals of this project are to examine pressure changes before, during, and after laser heating using a variety of both cold (e.g. ruby, argon) and heated pressure standards (MgO, Pt). This will lead to a better understanding of the effects of thermal pressure, pressure gradients, and deviatoric stress on pressure measurements in the laser-heated DAC.

Publications supported fully or in-part by this grant:

Heinz, D. L., G. Shen, and T. S. Duffy, Development of laser-heated diamond anvil cell, COMPRES third annual meeting, Lake Tahoe, CA, June, 2004.
Kiefer, B. and T. S. Duffy, Finite-Element Modeling of the Thermal Structure in Laser-Heated Diamond Anvil Cell Experiments, Eos Trans. AGU, 84(46), Fall Meet. Suppl., Abstract V31D-0968, 2003.
Kiefer, B. and T. S. Duffy, Finite element simulations of the laser-heated diamond anvil cell, Journal of Applied Physics, submitted, 2004a. Kiefer, B., and T. S. Duffy, Finite element analysis of sample geometries for the laser-heated diamond cell, in preparation, 2004b.

Kubo, A., T. S. Duffy, S. R. Shieh, B. Kiefer, V. B. Prakapenka, and G. Shen, Synthesis and equation of state of $MgGeO_3$ post-perovskite phase. AGU Fall Meeting, MR23A-0181, 2004.
Shieh, S. R., T. S. Duffy, A. Kubo, G. Shen, and V. B. Prakapenka, Synthesis of post-perovskite phase from a natural orthopyroxene, AGU Fall Meeting, MR23A-0182, 2004.
Shieh, S. R., T. S. Duffy, and G. Shen, In situ x-ray diffraction study of SiO_2 at deep lower mantle conditions, Earth and Planetary Science Letters, submitted, 2004.
Shim, S.-H., T. S. Duffy, R. Jeanloz and G. Shen, Stability and crystal structure of $MgSiO_3$ perovskite to the core-mantle boundary, Geophysical Research Letters, L10603, doi: 10.1029/2004GL019639, 2004.

Appendices:

I. Report on "Future Directions for the Laser-Heated Diamond Anvil Cell at the Advanced Photon Source" Workshop.
II. CO_2 laser summary table
III. Preliminary design of IDD laser heating system
IV. Year 4 Work Schedule

Appendix I

GSECARS/COMPRES High-Pressure Workshop "Future Directions for the Laser-Heated Diamond Anvil Cell at the Advanced Photon Source" Saturday, March 20, 2004 Advanced Photon Source, Argonne National Laboratory Final Program

Morning Session:

Welcome and Introduction
Tom Duffy, Princeton

What experiments should we be doing?
Dion Heinz, Chicago

Vibrational spectroscopy on laser-heated materials in DAC
Choong Shik Yoo, LLNL

An overview of CO_2-laser heating technique and recent accomplishments
Oliver Tschauner, UNLV

What are the key ingredients for a successful laser heating experiment at the synchrotron?
Guoyin Shen, Chicago

Temperature measurement in the laser-heated DAC
Abby Kavner, UCLA

Finite element models of the laser-heated DAC
Boris Kiefer, New Mexico State

Application of laser heated diamond cell technique for lower mantle phases - phase equilibria, phase boundary, and crystal structure
Dan Shim, MIT

Nanosecond pulsed laser heating
Dan Shim, MIT (for Sandeep Rekhi, MIT)

Using laser-heated diamond anvil cell technique to understand planetary interiors Jung Fu Lin, Carnegie Institution

Internally heated diamond anvil cell
Chang-sheng Zha, Cornell

Laser heating activities at sector 3 of the APS
Wolfgang Sturhahn, APS

Overview of HPCAT
Yue Meng, HPCAT

Overview of laser heating at ALS
Simon Clark, LBNL

The laser heated DAC system at the BL10XU of SPring-8
Nagayoshi Sata, JASRI

Magnesiowustite stability in the lower mantle
Leonid Dubrovinsky, Bayreuth Geoinstitut

Afternoon Session:

Discussion Forum I: What features are required in the next generation laser heating system at GSECARS?

Moderators: Duffy, Yoo

T. Duffy opened this discussion by outlining preliminary plans for laser heating development at GSECARS over the next few years. The plans call for a system that will include a diffractometer redesigned to reflect the emphasis on angle-dispersive diffraction. A two-tiered laser heating system will be constructed, following the demonstrated success of this approach at sector 3. The system will include both YLF and CO_2 laser heating systems to provide the widest flexibility in heating capabilities. The two systems will use separate delivery optics, but will, at least initially, share spectroradiometry systems.

C. Yoo provided a thorough overview of the relevant questions. Among the most important experiments: melting and phase diagram studies above 100 GPa; structural studies on ordered and disordered systems; novel materials applications, and study of mechanical properties (e.g. strength, elasticity, microstructures). Also important are x-ray spectroscopic studies and real time structural studies. It was emphasized that the system should be simple and easy to operate with optimized alignment and calibration procedures; this will maximize efficient use of limited synchrotron beam time. The system should also be compatible with various types of diamond cells.

D. Heinz emphasized the importance of thermal conductivity measurements for geophysical applications. The potential for making transport property measurements using a pulsed laser together with the time structure of the ring was discussed. It was agreed that this is a fruitful area for future investigation.
A question was raised as to why CO_2 laser heating systems were not widely used at synchrotrons presently. In response, it was pointed out that the GSECARS-design for double-sided YLF heating has become dominant at both the APS and synchrotrons around the world. It was also emphasized that development of a CO_2 system at GSECARS will provide users with the flexibility to choose the type of laser heating most appropriate for each sample. It was felt that the problems that have limited CO_2 heating to some extent at user facilities could be overcome. While CO_2 heating has not been widely adopted at synchrotrons, it is being successfully pursued at many individual laboratories around the world. V. Prakapenka showed a preliminary design for a CO_2 laser heating system that complements the existing YLF design at GSECARS. It incorporated the existing spectroradiometry system but involved separate beam delivery optics.

E. Alp and W. Sturhahn both emphasized that mechanical stability of the system is the most important consideration, even if this meant some loss in flexibility in the types of experiments that can be performed. It was pointed out that the new combined diffraction-laser heating system is expected to be considerably more stable than the existing system due to replacement of two-circle goniometer. In the ideal case, we would like to perform laser heating both for radial and axial diffraction experiments, if this can be accomplished without paying too high a price in mechanical stability.

M. Rivers asked whether it would be useful to have an off-beamline laser heating system at APS. It could be used for annealing pressure gradients or for sample synthesis. T. Duffy added that this would allow users to practice loading styles and sample geometries, and to evaluate the 'heatability' of their samples before mounting the cell on the beamline. S. Clark commented that off-line facilities have a history of not being maintained properly at synchrotron facilities, and that use of a nearby university facility might offer advantages.

Discussion Forum II: What are the key technical issues for next-generation laser heating?

Moderators: Prakapenka, Dubrovinsky

There was a discussion of the relative merits of imaging plate and CCD detectors for laser heating experiments. CCD detectors are most compatible with the timescales of laser heating experiments whereas imaging plates are superior in terms of dynamic range and resolution. It was emphasized that the resolution of current detectors is just borderline, and that efforts towards higher resolution detectors are greatly needed. It was pointed out that mosaic CCD detectors could be useful for laser heating experiments. These detectors have active areas comparable to imaging plates, and hence can be moved further away from the sample. However, M. Rivers also pointed out that resolution in x-ray patterns is also limited by the x-ray beam divergence introduced by the KB mirrors, and so users already have the ability to improve resolution at the cost of some loss of x-ray intensity on the sample, just by closing the slits upstream of the KB mirrors.
The advantages and disadvantages of diode pumped near-IR lasers was discussed. While having increased stability, they suffer from the disadvantage of higher cost per watt, although operating costs are lower.

A question was raised as to whether the community should be directing more efforts towards single-crystal diffraction. G. Shen explained that GSECARS is developing a side station on the bending magnet beamline that will be equipped for diamond anvil cell experiments including single-crystal diffraction. There are no plans for laser heating facilities at this station, but off-line heating will be available.
There was general agreement about the importance of sample loading and attaining a good sample environment for laser heating. It was suggested that the high-pressure user community work to develop new methods such as thin film deposition techniques to improve the quality and reproducibility of the sample loading.

The development of a high-pressure gas loading capability at GSECARS was also considered to be a priority. It was felt that there would be considerable demand for such a facility, if available. While it was pointed out that such a facility may soon be in operation at NIU, the availability of such a facility at ANL was still considered to be desirable. This might be a good area for collaboration between GSECARS and HPCAT

Discussion Forum III: What community-wide efforts are needed to advance laser heating capabilities at synchrotrons?

Moderators: Heinz, Tschauner

It was agreed that there is a strong need for greater efforts at cross-correlation and inter-laboratory comparisons for temperature determination. The lack of appropriate standards was discussed, and a number of possible solutions proposed. These include: focused cm-sized temperature gradient source; appropriate solid-solid transition, intersecting melting curves, miscibility gap that disappears at high temperature. It was agreed that the first required step is a systematic evaluation of the possible standards. Another issue that has become increasingly important is the absence of a supplier of NIST traceable standard lamps. This is a good area for a community initiative, perhaps involving NIST as well. D. Heinz suggested that blackbody cavities could be constructed for use as emission standards.

Outside the diamond cell, detection of ambient pressure melting points of pure metals remains the best calibration tool. It was emphasized that distortion introduced by the diamond window is a potentially significant problem for which creative means are needed to address.

To making progress in the study of melting at high pressure, objective, reproducible melting criteria are the greatest need. G. Shen described his work on detection of diffuse scattering from Fe in the diamond anvil cell above 50 GPa. It was agreed that this method is promising in that it provides a positive signature of the melt. However, several questions about the technique were also raised that will require some further efforts to answer.

Over the long term, the use of sound velocity measurements through Brillouin scattering and other techniques also offers much promise for a positive means to detect melting at high pressures. Brillouin spectroscopy also may help establish pressure calibration in the laser heated diamond cell. J. Bass summarized COMPRES-supported progress in development of a synchrotron-based Brillouin system. A. Kavner advocated making pressure calibration to ± 1 GPa a priority.

The importance of better software tools was also emphasized. These are needed not only for improving and accelerating data processing at the home institution but perhaps even more importantly for the "dynamic" or on-line evaluation of the data that is crucial for understanding the progress of the experiment while at the synchrotron. Because of the limited size of our community, it was concluded that the best approach was to seek ways to plug into the larger community at APS for data processing development. There was also discussion of specific software tools such as FIT2D, and concern was expressed that our reliance on this software is problematic because of lack of support and undocumented bugs.

It was recommended that the laser-heating community meet on an annual basis to assess further technical progress.

Adjournment

ATTENDEES FOR COMPRES/GSECARS LASER HEATING WORKSHOP
ADVANCED PHOTON SOURCE, ARGONNE NATIONAL LAB
MAY 20, 2004

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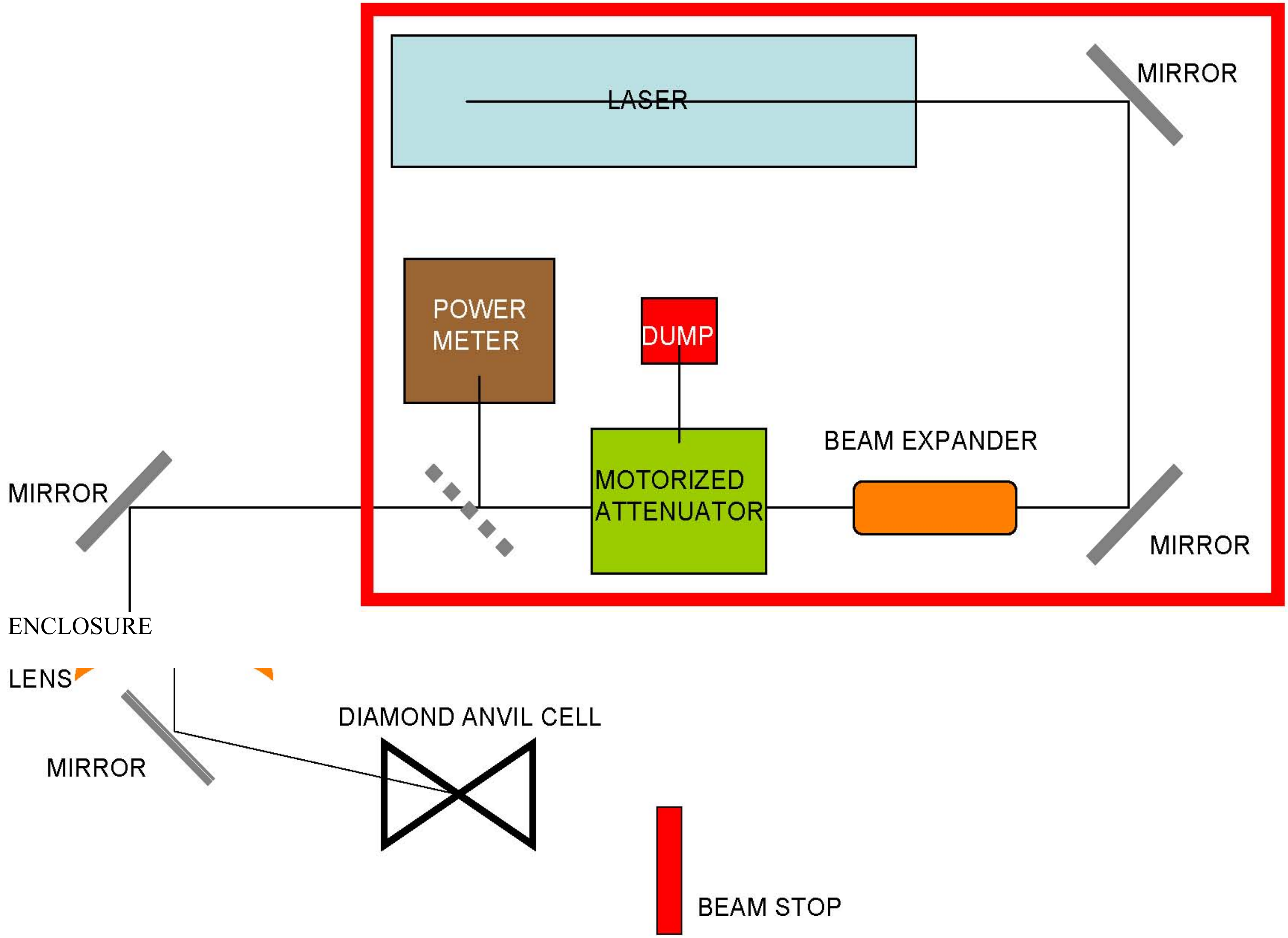
Appendix II

Summary of CO2 lasers						
Company	Coherent	PRC	Synrad	Synrad	Synrad	Synrad
Model	K-300	XL 1000	Evo 240	f200	f201	f400
Price	70000	89000	44593	32100	32100	59212
Tube type	sealed	gas-flow	sealed	sealed,double	sealed	sealed, double
Power, W	300	1000	240	200	200	400
Polarization	linear	linear	linear	crossed	linear	crossed
Mode, quality	M2 < 1.3	M2 < 1.5	TEMoo 90%	TEMoo 95%	TEMoo 98%	TEMoo 98%
Beam diameter, mm	8.8	13	4.4	3.5	4.5	4.5
Divergence, mrad	2.1	1	3.2	4.0	4.0	4.0
Stability	8%	0.50%	5%	6%	5%	5%
Max repetition rate	100 kHz	CW / 1 kHz	CW / 20 kHz	CW / 25 kHz	CW / 25 kHz	CW / 25 kHz
Pulse rise time, usec	40	n.a.	150	100	100	100

Notes:
Synrad lasers require an additional controller, such as the UC-2000 for $712.50.
The PRC XL 1000 includes a chiller, which would be an additional cost for Coherent and Synrad lasers.

Appendix III

SETUP FOR CO_2 LASER HEATING SYSTEM IN GSECARS SECTOR 13-IDD



Appendix IV

Schedule of Work on Development and Installation of CO_2 Laser Heating System
November 2004 – August 2005: Installation and bench-top testing of optical components and design in GSECARS laser laboratory. Safety features must first be put in place in accordance with APS guidelines. Concurrently, work on the beamline hutch (interlock, safety enclosure, utilities, and control systems) to prepare it for installation of the CO_2 laser system.
September 2005: Install CO_2 laser and optical system in Sector 13-IDD hutch during APS maintenance period. If testing and hutch preparation proceed very smoothly then installation may occur as early as the May 2005 maintenance period.
October 2005 – December 2005: Commissioning of the system during 2005-3 APS run.
January 2006: Modify system, if necessary, and open to general users for 20061 APS run.
February 2006 – June 2006: CO2 laser team members will complete collaborative projects using the new instrumentation, and publish results

C.3 Brillouin Spectroscopy at the Advanced Photon Source

[J. Bass-University of Illinois at Urbana-Champaign and G. Shen-University of Chicago]

Accomplishments

This past year has been a very active and productive on this project. In short, a new Brillouin spectrometer has been installed at the APS on GSECARS sector 13-BM-D. Photographs of the new system are attached. The Fabry-Perot interferometer and all associated optics are installed. The only major missing components is the Coherent Verdi laser, which has been ordered - but due to delivery delays has not arrived yet.

With the actual installation of Brillouin equipment into the synchrotron hutch, we are far along toward completion of this project. Commissioning and the first scientific experiments will be performed during the coming year.

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 could be provided by resistance and/or laser heating techniques. Our initial experiments in the coming year will include investigations of several materials along room temperature isotherms. The first materials to be studies are single-crystal NaCl, MgO, and Al2O3.

A second major goal of this proposal was to provide a centralized facility for Brillouin scattering studies. We will 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).

During years one and two, we ordered equipment and considered a number of different designs for the spectrometer. 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 that are 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. Out of several possible designs, we ultimately decided that most of 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 (that are near the sample during an experiment) to be easily moved in and out of position for Brillouin work. 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. Very detailed designs of the APS Brillouin system were made at the end of year 2 and in year 3, and an enormous amount of time went into choosing the optimal components. Drawings needed to be made for parts that could not be purchased but were made at the University of Illinois. Finally, on September 30, 2004, we moved the Brillouin system from Champaign to the APS-GSECARS, and installed it.

Work Remaining to be Performed:

- Install laser (Verdi 2W, Coherent)
- Perform final optical alignments of the system. Many critical alignments cannot be done without the laser in place.
- Order and install components that have been borrowed from either the UIUC lab, or GSECARS, or manufacturers.
- Write software for remote operation of the Brillouin system, from outside the hutch.
- Install shielding panels for protecting optics and the interferometer from radiation damage.
- Install some options onto the system, such as the ability to perform 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 will be needed. Provisions for this option need to be put into place.
- Test and commission the instrument. Debug problems.
- Install a safety interlock system and enclosure panels to construct a laser controlled area (LCA) which conforms to the stringent APS laser safety requirements. It will be necessary for this LCA to provide absolute safety for users, yet allow experts to access optical components for periodic maintenance and alignment.
- Perform first scientific experiments.

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)

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.

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.
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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.

To the public welfare beyond science and engineering?

Figures

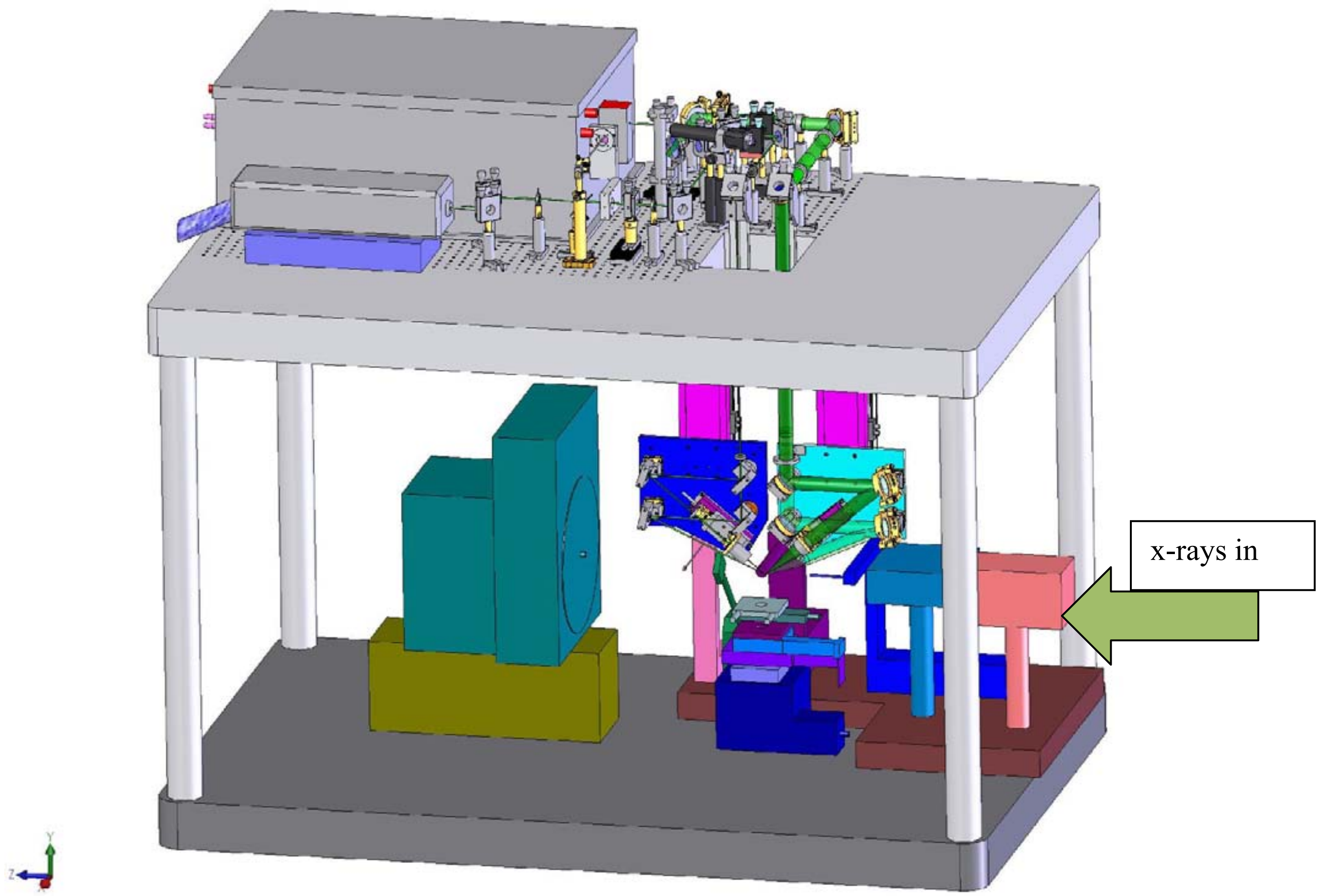


Fig. 1. Schematic diagram of the Brillouin spectrometer at sector 12-BM-D of GSECARS, Advanced photon source. Most of the Brillouin optics are on the upper level, whereas the sample is in placed in the x-ray beam for all experiments on the lower level.

Figure 2: Schematic diagram of the Brillouin system at the APS.

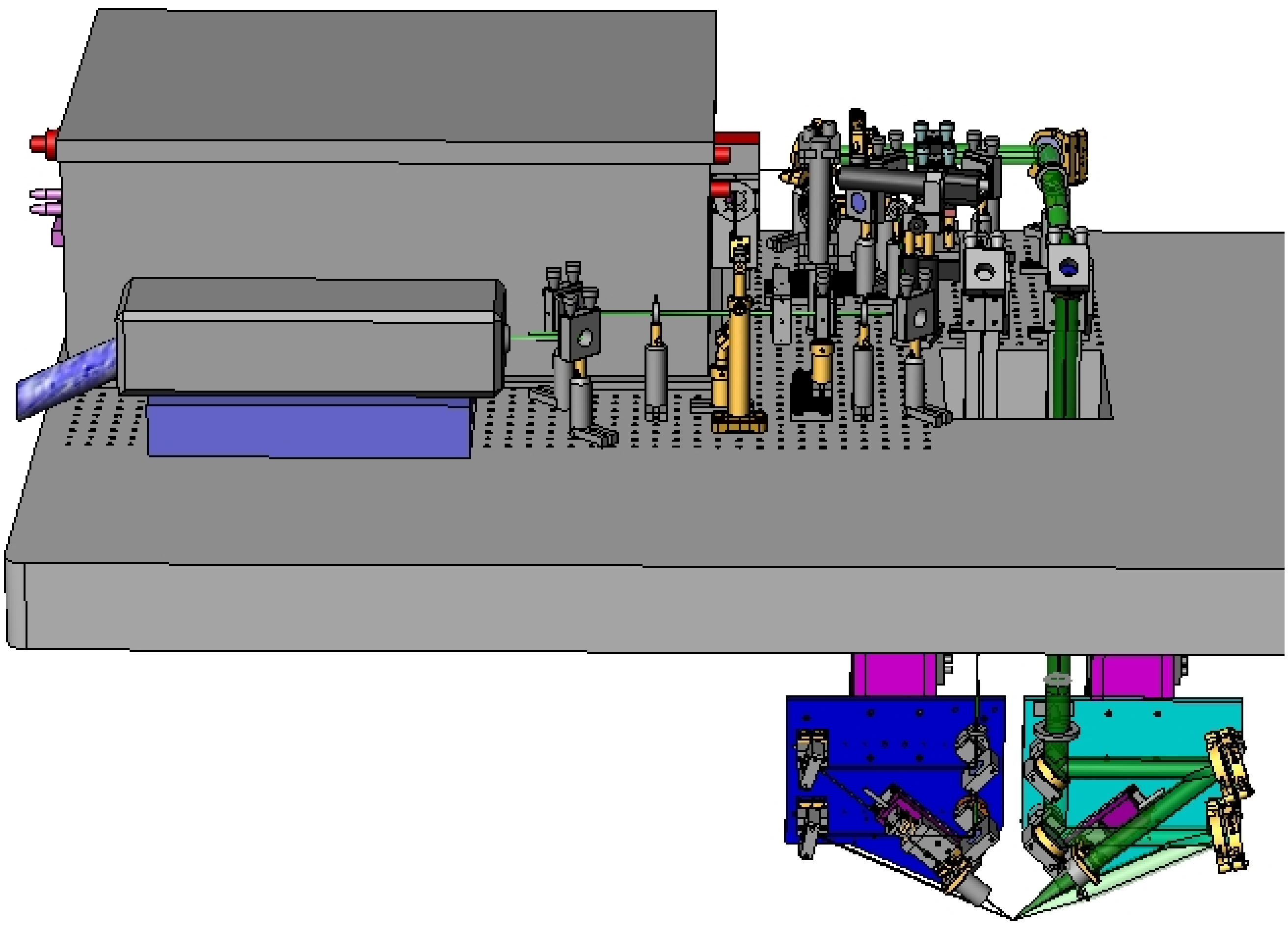


Figure 3: Schematic plan drawing of the upper Brillouin optics.

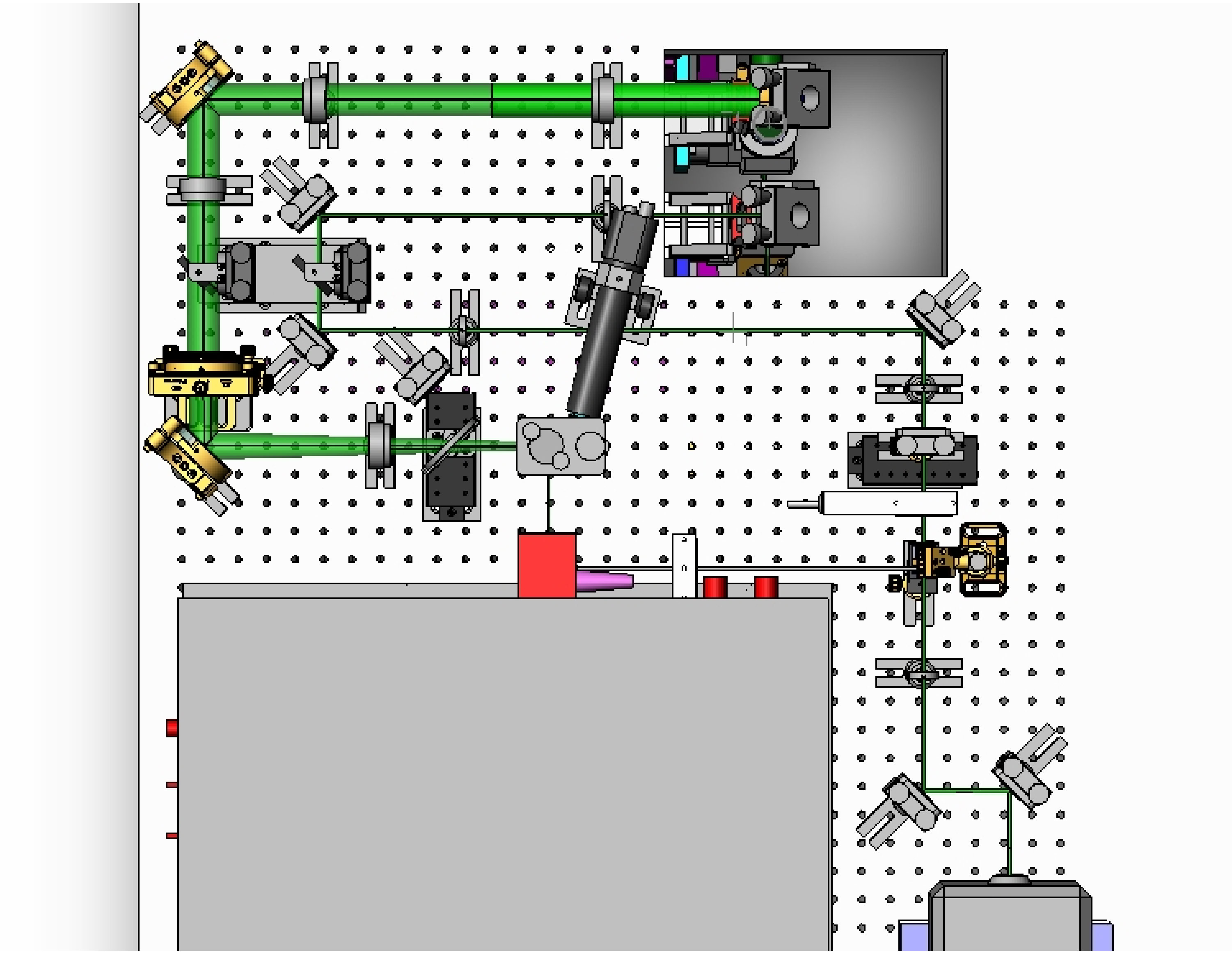


Figure 4: Installation of the Brillouin spectrometer at the APS.

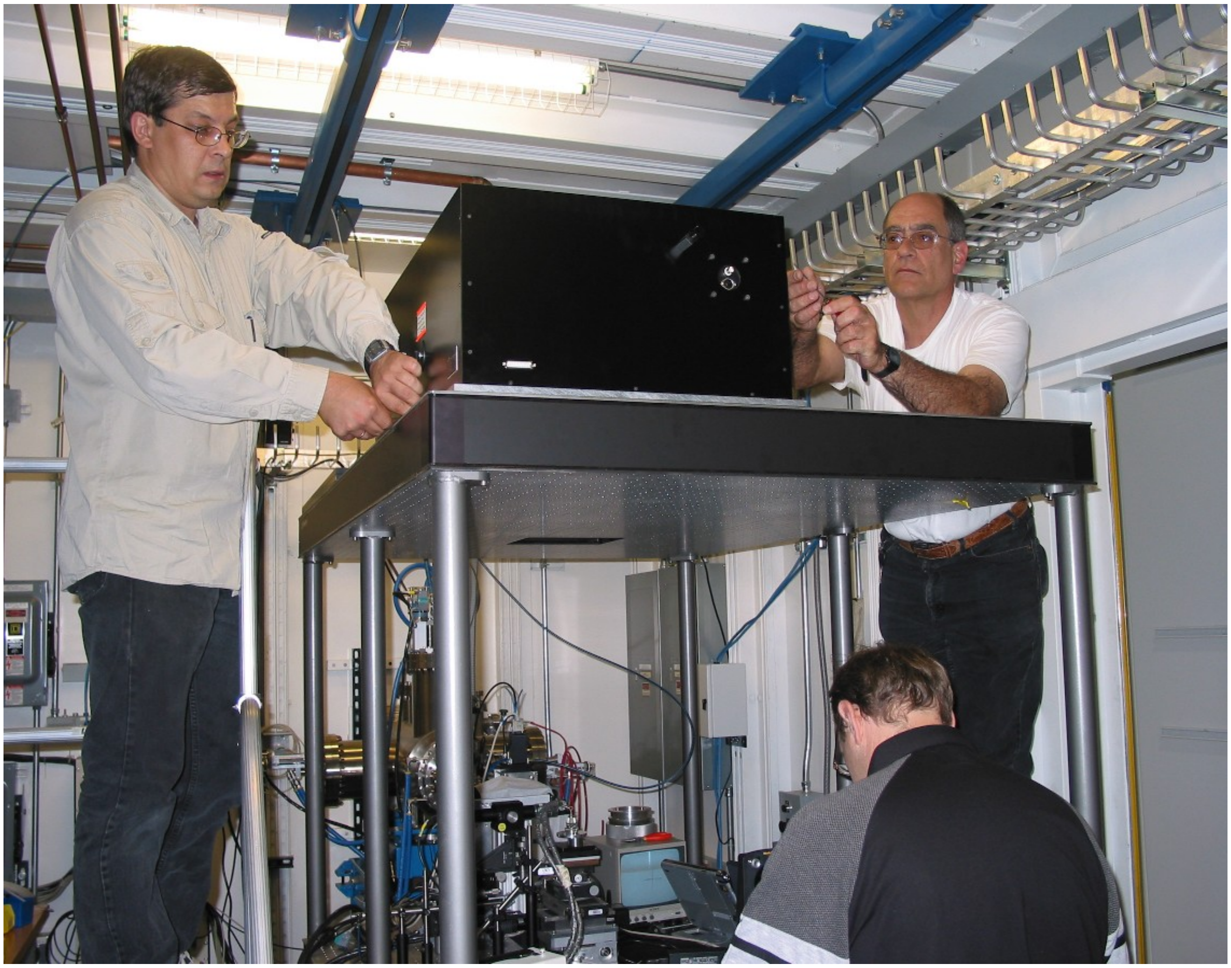


Figure 5: Upper level Brillouin optics installed, and Fabry-Perot Interferometer.

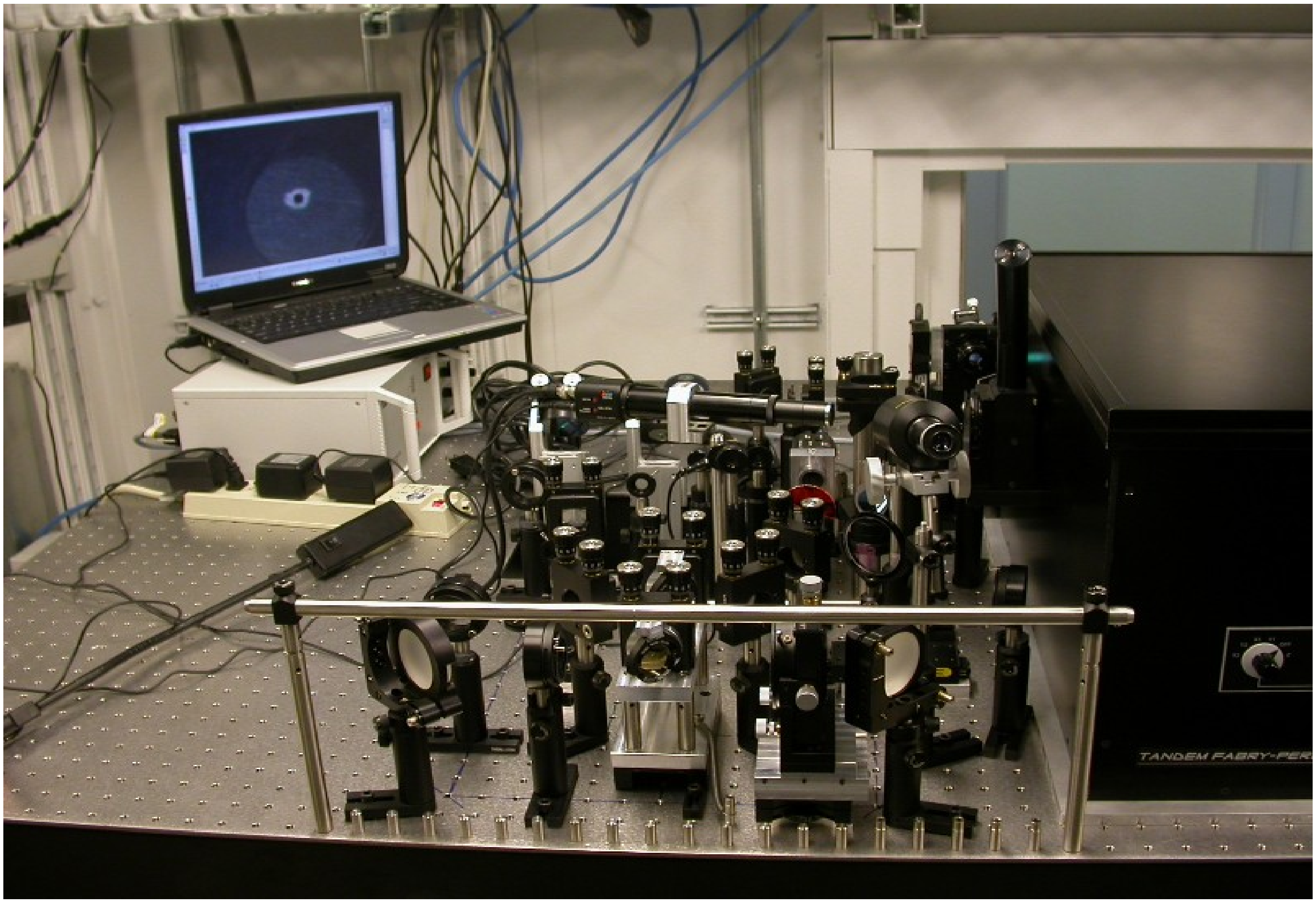
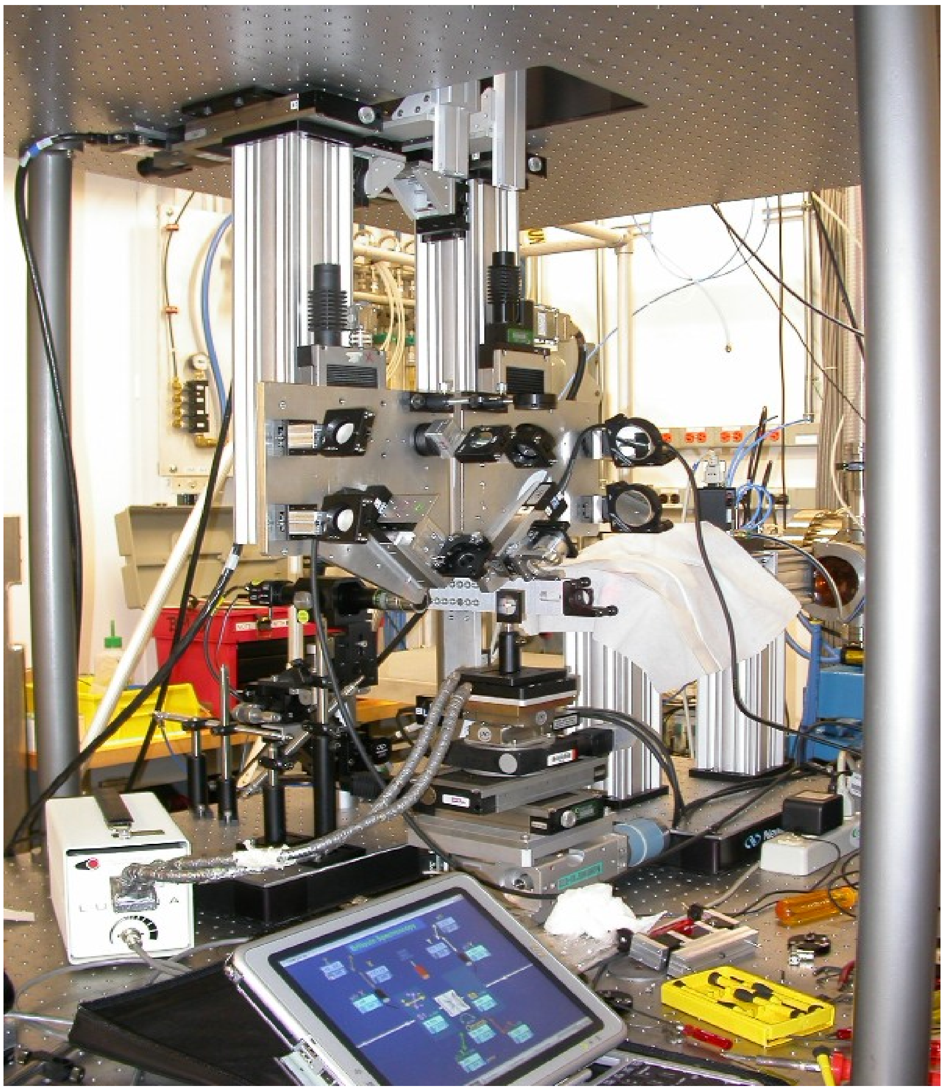


Figure 6: Lower level of 13BMD, with optics for Brillouin scattering in place. These optics slide in and out for Brillouin experiments on motorized rails. Thus they can be rapidly put into place for Brillouin, and retracted so as not to interfere with other types of X-ray experiments.



C.4 Absolute Pressure and Temperature Calibration

[I. Getting, University of Colorado]

This component of the COMPRES Infrastructure Development program sought initially to establish accurate temperature and pressure measurements within the high pressure community based sound metrological practice. In light of reduced manpower and funding it was agreed to concentrate on the accurate determination of temperature.

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 determine 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 ηV. This is an 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 I approached Dr. John Hall, a colleague at the University of Colorado. John is a world renowned metrologist at JILA (http://jilawww.colorado.edu/), a NIST co-sponsored research institute at the University of Colorado. John has provided all the critical circuit design for this project. Over several years we have constructed a Johnson noise thermometer for use at high pressure.

Signal Correlation

The Johnson noise thermometer consists of a sensing resistor and circuitry to measure its noise voltage. The noise voltage across the resistor is amplified, filtered, digitized, and then correlated and averaged numerically. The signal of interest is comparable to the input voltage noise of the quietest amplifiers which would make high resolution temperature determinations impossible. In our design two amplifiers are used in parallel and their outputs correlated to eliminate the contributions from amplifier noise. Each amplifier adds its own random noise.

$$E_A = E_R + E_a$$

$$E_B = E_R + E_b$$

where E_A and E_B are the total outputs of the two amplifiers. Each consists of a contribution form the resistor noise voltage, E_R, and the noise introduced by each amplifier, E_a and E_b. Each of these terms is a random time series consisting in our design of one million samples.
Correlation consists in finding that part of the two signals with is common to both, namely E_R. The two time series are multiplied point by point and averaged.

$$C = \frac{1}{N}\sum (E_R + E_a)(E_R + E_b)$$

$$C = \frac{1}{N}\sum \; (E_R E_R + E_a E_R + E_b E_R + E_a E_b)$$

where N is the number of samples.
Each voltage time series is a sequence of random values. The product of two random numbers is random and therefore averages to zero. Thus, all the terms above average to zero except for the term $E_R E_R$ in which the two factors are identical. Each term is positive and therefore contributes to a positive definite average:

$$C = \frac{1}{N}\sum \; (E_R E_R) = \langle E_R^2 \rangle$$

which is just the term in the original noise equation.
Slight non-idealities in the amplifiers and the vague definition of the band-width make it extremely difficult to build a Johnson noise thermometer with intrinsic calibration at the ~1 Kelvin level. The thermometer we have built will be calibrated against NIST traceable thermocouples at one atmosphere where the thermocouples are correct.
A layout diagram of the instrument is shown below.

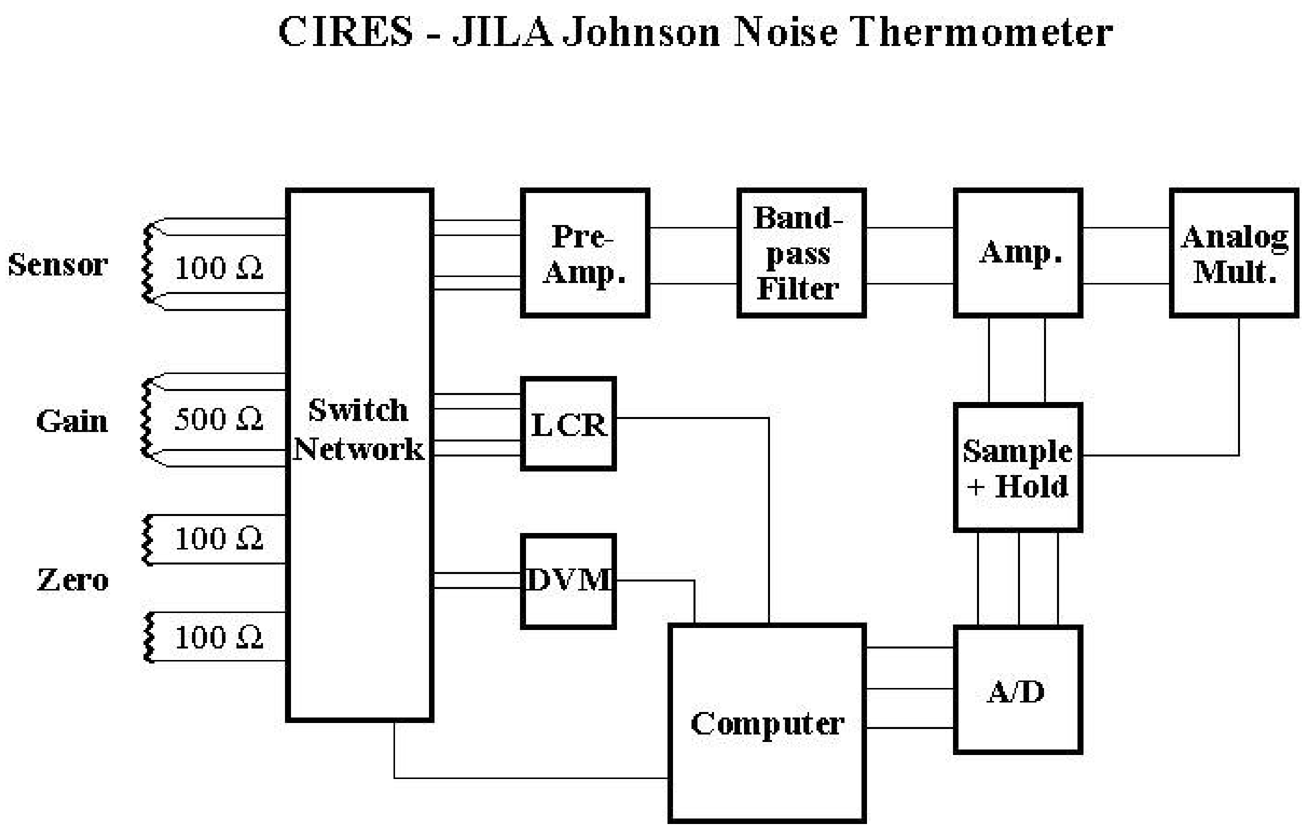


Figure 1. Layout of the Johnson noise thermometer.
The 100 ohm sensor resistor is connected to the two pre-amplifier inputs by a very quiet switching network. Amplifier gain and zero values are monitored by periodically connecting a 500 ohm gain resistor or two uncorrelated 100 ohm resistors to the amplifiers. The wires to the sensor and to the gain resistors are actually pairs of thermocouples. They are appropriately connected by the switching network to a digital volt meter (DVM) to determine the thermocouple outputs. The sensor resistance is determined by connecting the four sensor leads to a commercial Inductance-Capacitance-Resistance meter (LCR) with the switching network. All switching operations are done with prescribed sequencing and timing under computer control.

The outputs of the two pre-amplifiers are band-pass filtered, further amplified, directed to a sample and hold device, digitized, and stored in the computer. They are then numerically filtered and averaged to determine the value of $\langle E_R^2 \rangle$. The analogue multiplier provides the ability to correlate and average the signals without recourse to digital manipulation. This procedure, while simpler, has proven less useful because of longer averaging times, lower stability, and lack of any ability to inspect the signals graphically.

As it turns out, the ability to inspect and analyze the time series it critical. Both time domain and power density spectra plots are available in the data reduction scheme. The typical RMS magnitude of resistor noise voltage is well below 1 μV. It is a demanding task to preserve this delicate signal which originates in a furnace heated by electric current. Special shielding and transmission line considerations have been used to protect the noise signal. Inspection of the time series and its power density spectrum is vital in this process. Therefore, the more sophisticated digital method is used. Examples of synthetic and real data spectra are shown in the next figure.

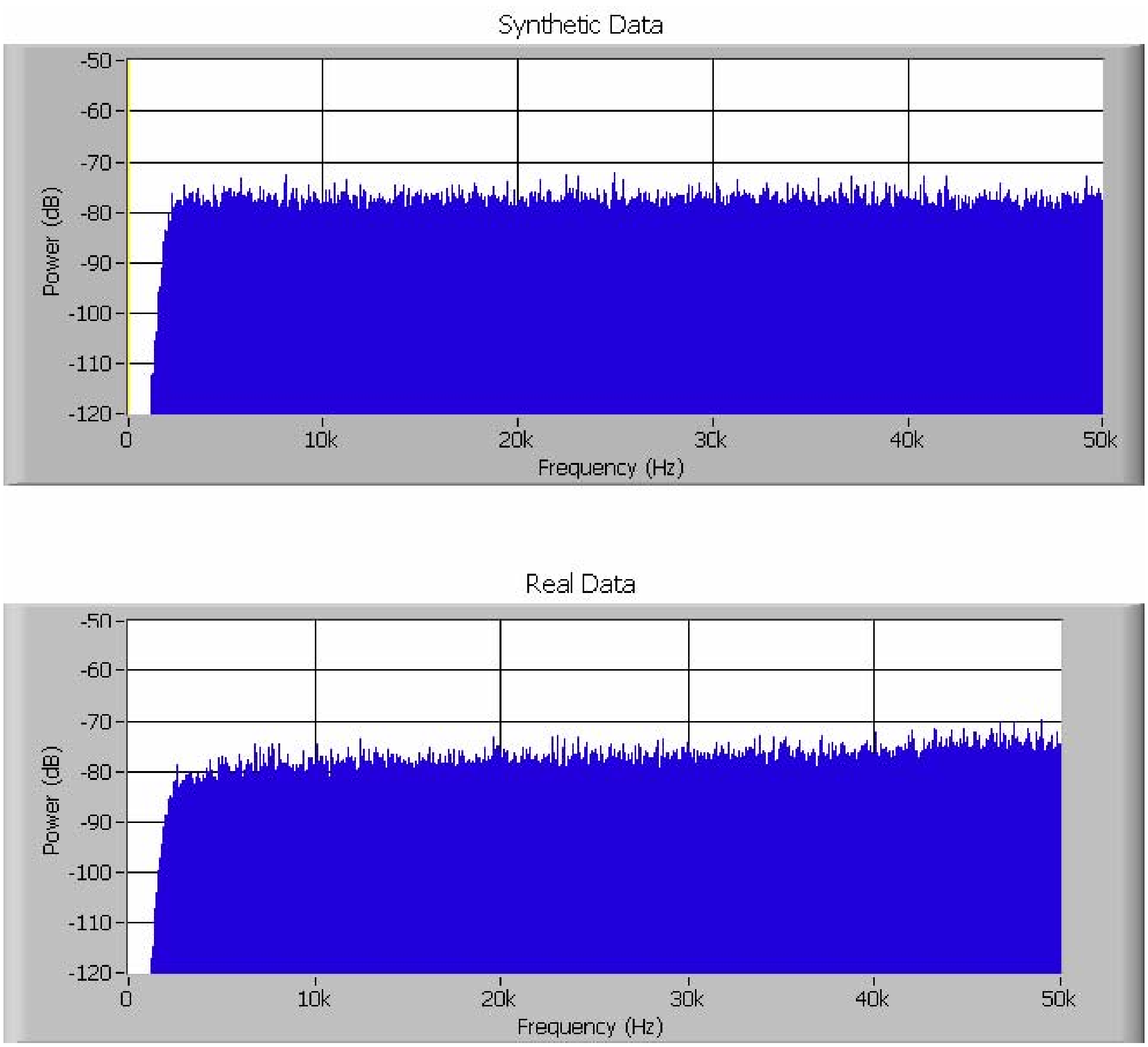


Figure 2. Power density spectra of synthetic and real data.
Johnson noise is a random Gaussian signal. Its amplitude exhibits Gaussian distribution characterized by a standard deviation and having a zero mean. Its power density spectrum is "white"; it has the same power density at all frequencies. It is critical to

know that the signal measured in this instrument is Johnson noise sufficiently uncontaminated by electrical interference. The spectrum of synthetic data with the desired properties is show in the upper plot. The spectrum of the real data in the lower plot differs only in minor detail. The lower corner is slightly less abrupt because the digital filter used in the synthetic data does not exactly simulate the analogue filter in the amplifiers. Also, the region above ~30 kHz increases slowly by about 6 dB. This appropriately reflects power between the Niquist frequency of 50 kHz and the corner frequency of the low-pass filter, 70 kHz, in the under-sampled time series. All circuit resonances and external interference spikes have been successfully eliminated.

The value of $\langle E_R^2 \rangle$ depends only on several constants and the product RT. We are now making fully automated readings of all the relevant electrical parameters simulating high temperatures by changing resistance at room temperature. One million samples of this random noise requires 10 seconds sampling time and results in an equivalent temperature resolution ~1.5 K at 1000 K. The time to sweep through a complete set of all the required measurements is 15 seconds. Higher resolution is achieved by additional sampling. The current performance of our instrument is on a par with that of a second Johnson noise thermometer developed independently over the same time period by NIST personal for temperature standards measurements.

Recent progress has recently been made on three fronts: 1.) reduction of susceptibility to ambient electromagnetic noise, 2.) ambient electromagnetic noise testing, and 3.) fabrication techniques for a multi-anvil sensing resistor.

1.) Susceptibility to ambient electromagnetic insult

Very good progress has recently been made on shielding and isolation. We have reduced the magnitude of the noise power measurement by a very significant 4 %. This 4 % came from ambient insult: power line coupling, ground loops, and the radiation from local radio stations, computer monitors, fluorescent lamps, etc. This spurious component of the signal was not Johnson noise. Its time dependence was manifest as scatter in our measurements.

There is a theoretical limit to the reproducibility of these noise power measurements give by the Rice equation:

$$\frac{\sigma_{\langle E_R^2 \rangle}}{\langle E_R^2 \rangle} = \sqrt{\frac{1}{\tau_m B}}$$

where τ_m is the measurement time, and B is the correlation bandwidth of the thermometer. For a discussion see, for instance, White *et al* (1966) who introduce this limiting equation in the context of Johnson noise thermometry or the original reference, Rice (1944).
On bench tests the amplifier inputs are connected to a adjustable precision resistor whose resistance is accurately measured to 0.1 % with an LCR meter and whose temperature is measured with NIST traceability to 0.1 K. Output values of $\langle E_R^2 \rangle$ are determined as a function of the product *RT* and fit with a polynomial. The relative residuals of this fit are plotted vs. *RT* in the figure below. Prior to the recent elimination of spurious noise the amplifier gain and zero were measured for each determination. Since all of these measurements exhibit scatter, as described by the Rice equation above, using redetermined values of amplifier gain and zero in the data reduction increases the scatter in the final value of $\langle E^2 \rangle$. In the absence of time dependent spurious noise the gain and zero values are so stable that they no longer need be redetermined during the measurements. Well-determined, constant values can now be used reducing the scatter. The thermometer was originally designed to achieve a type A standard uncertainty (precision) of 0.2 % for a single reading of one million samples in 10 seconds. This is slightly more conservative than the Rice equation limit of 0.15 %. With the elimination of spurious noise our instrument now comes very close to the Rice equation limit and well within the original design limit. This is somewhat analogous to building an optical telescope which is diffraction limited. It is not possible to make it any better. This is the best possible condition from which to progress to temperature measurements in a real high pressure
furnace.

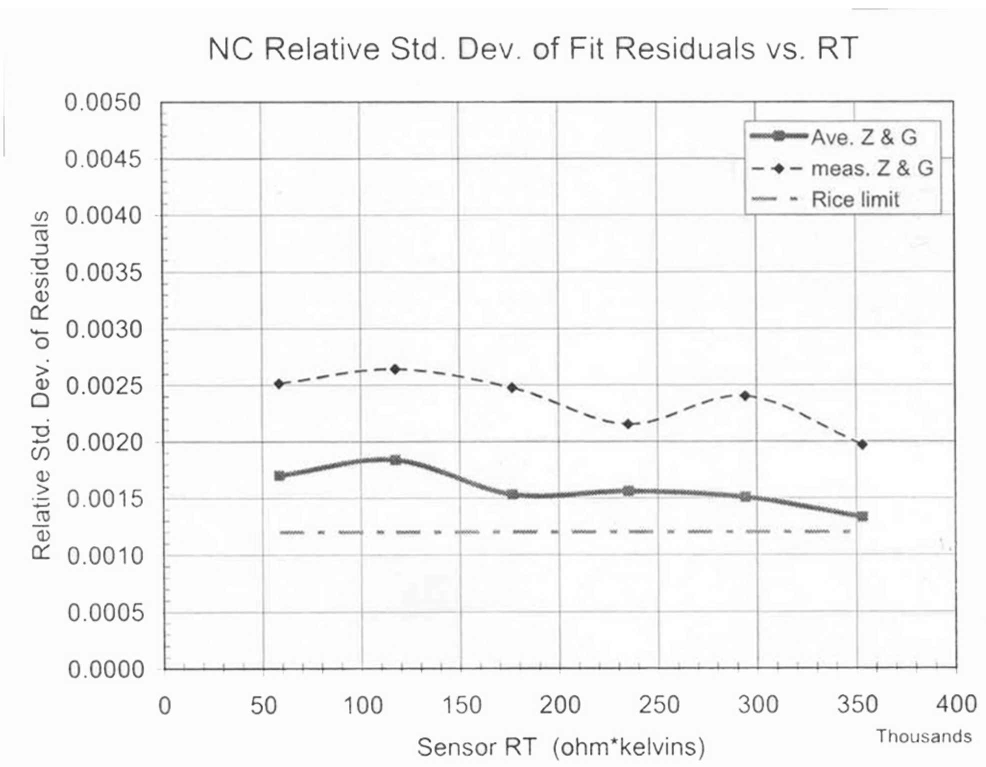


Figure 1. Relative standard deviation of the residuals. The top dashed curve indicates the precision of the thermometer using redetermined amplifier gain and zero values for each measurement. The use of pre-determined values reduces the scatter to the solid curve very near the Rice equation limit shown by the lower dashed curve.

2.) Ambient electromagnetic noise testing

Of course, these delicate measurements could still be corrupted by sufficiently powerful electromagnetic insults from the ambient environment. Ultimately, we seek to install this thermometer in another lab making it available to the community. Towards this end we have developed a method of testing the electromagnetic ambient. We use a commercially available signal analyzer with a very low noise pre-amplifier to measure the voltage spectral noise density over the relevant bandwidth under several input conditions. A 50 ohm termination on the pre-amplifier input terminal reveals the "noise floor", the low signal limit set by the nature of the high quality electronics under the local conditions. Secondly, we connect a shielded resistor to the pre-amplifier through a 6 foot coaxial cable. The cable acts as an antenna and senses the electromagnetic ambient. The Johnson noise from the resistor is calculated and compared with the increase in voltage spectral density observed on the signal analyzer. The Johnson noise should rise uniformly above the observed noise floor by a prescribed amount over the full bandwidth. The voltage spectral density should also be free of spurious spikes and time dependence.

Such measurement were made in John Hall's electro-optics laboratory at Colorado. The noise floor was established at about -166 dB, -120 dB indicated minus 46 dB for the pre-amplifier gain. Tests with a conventional RG58 coaxial cable and a probe resistor revealed many local spikes from nearby electronic instrumentation. The cable was not sufficiently well shielded relative to the ambient. Tests with a more effectively shielded RG55 cable gave a good, clean spectrum. With a resistor connected the observed rise in the voltage spectral density was appropriate to the value of the resistor in both cases.

I plan to terminate my work on this project in the spring of 2005. The Johnson noise thermometer must be applied in high pressure devices and moved to a laboratory where it can serve the community. Toward this end, a collaboration with Mark Rivers and Yanbin Wang of GSECARS at APS has been established as a result of conversations between myself and Mark Rivers at the June, 2004 Annual COMPRES meeting. Mark brings a sophisticated electronics background to the project and Yanbin an remarkable talent with multi-anvil instruments. I could not have wished for a better team. Ambient noise tests have now been begun at the large volume high pressure hutch at GSECARS. The first results are very encouraging. They are very much like the results at Colorado. With the same model instruments the noise floor was again observed to approach -120 dB indicated at the high frequency end of the band using the same pre-amplifier gain. These tests were conducted with a RG58 cable and a shielded 6 kohm probe resistor. The results are comparable to those at Colorado with an RG58 cable. The Johnson noise from the resistor was readily observed, but, like the Colorado tests, various spikes are seen in the spectrum from local sources. The predominant spikes occur at intervals of 60 Hz and ~15.7 kHz. The first are power line frequency harmonics which die off by the lower end of the noise thermometer bandwidth at 2 kHz. The second are likely to be harmonics of the 15.75 kHz frequency of CRT computer monitors which reside just outside the open door of the hutch.

This is very good news. The spectrum is relatively clean, except for the spikes whose origin we think we understand. The proximity of the synchrotron does not seem to introduce any disturbing electromagnetic noise into the hutch. This is extremely encouraging for the prospects of setting up the Johnson noise thermometer at GSECARS with Mark and Yanbin.

I have just sent to GSECARS a RG55 cable with better shielding and both a magnetic and an electrostatic probe for use with this new cable. The ambient noise measurements will be repeated with the better shielded cable. We anticipate that the spikes observed in the first tests will be significantly reduced, as they were in the Colorado tests. The shielding in the Johnson noise thermometer cables and circuits is probably considerably better than that in the RG55 cable. A significant reduction in the spikes with the RG55 cable would portend very well for use of the thermometer in the GSECARS hutch. If local sources of insult remain, they can be located using the probes which I have provided. Effective electrostatic shielding of local sources can be achieved with a wrap of grounded aluminum foil. Effective magnetic shielding of local sources can be achieved by placing a 1 mm thick sheet of mild steel between the source and the susceptible instruments. A closed loop surface of mild steel around the source or around the instrument would be even more effective.

At this point, I am extremely encouraged about the prospects of setting up the Johnson noise thermometer at GSECARS. The collaboration with Mark and Yanbin is likely to be particularly fruitful. This would be an excellent facility for community access and support.

3.) Probe resistor fabrication

The Johnson noise thermometer requires a resistive probe in the high pressure cell assembly. The resistance must be around 100 ohms. The probe must survive the highest pressures and temperatures of interest. The space for such a probe in a small-scale multi-anvil cell is on the scale of 1 mm. A method of fabricating such a probe must be found. In typical high pressure experiments it is important to have uniform stress on the sample. In this case, the stress state on the resistor is not particularly important. Of course, the resistor must be at the same temperature as the adjacent thermocouples being calibrated. The change in calibration of the thermocouples at high pressure depends on the stress and temperature distribution on the thermocouple wires as well as their electrical and chemical environment. These must be typical of the cells in which thermocouple measurements are to be made without the noise thermometer. In short, we have gained one degree of freedom, but must maintain typical conditions on the thermocouples.

I have just explored resistor probe fabrication with David Alchenberger, manager of the JILA Keck Laboratory at the University of Colorado. This lab is part of the same institute where John Hall, the designer of the thermometer circuits, is stationed. The most critical thermometer circuits were built in the JILA electronics shop. Now it looks as though we are likely to be able to fabricate the probes in JILA as well. Collaboration with this first class metrology institute has contributed immeasurably to this project.

The resistor probe will likely consist of a refractory metal grid bonded to an insulating substrate. The metal grid would be established by electron-beam physical vapor deposition through a contact mask. In this technique the source metal is heated by an electron beam in a vacuum of about 10^{-7} Torr. A metallic vapor stream emanating from the hot source metal deposits solid metal on the much cooler substrate. The form of the grid is controlled by a mask placed against the substrate to block the vapor stream from hitting the unwanted portion of the substrate. The grid is likely to be similar in geometry to those used in strain gages in order to achieve sufficient resistance. The JILA Keck Laboratory is set up to do this work. David has had experience depositing Tantalum, Titanium, Molybdenum, Platinum, and Tungsten, which is more difficult due to the extremely high temperature required. At this dimensional scale the mask would probably be made by photolithographic techniques. Either a photo-resist layer could be applied directly to the substrate with the desired portion removed by chemical development or a separate metallic mask could be made using photo lithography followed by etching away the desired portion. Preliminary grid design consists of a deposited layer 200 ηm thick in a folded ribbon 100 μm wide with a total length of 5 mm. Room temperature resistance of such a grid would be in the range of 10 to 50 ohms depending on which metal is selected. Over the temperature range of interest, ~2000 K, the resistivity of the candidate metals increases as much as an order of magnitude making such a resistor a good match to the Johnson noise thermometer.

The substrate could be a ceramic disk, possibly Lucolox (ultra high purity, polycrystalline alumina), a single crystal insulator, or boron nitride if the metal will adhere to it. The mechanical properties of boron nitride are very different from the hard oxides giving us a significant range of mechanical options. The substrate, like the thermocouple wire insulators, must maintain high electrical resistivity at the highest temperatures of interest.

Electrical contact must be made at each end of the resistor to a thermocouple junction. Contact pads will be built into the geometry of the mask and will be an integral part of the resistor. My first suggestion is to establish the electrical and thermal coupling by mechanical contact in the high pressure cell using appropriate design of the adjacent components. This is an area in which Yanbin Wang's expertise will prove very valuable.

Plan

During remainder of this third year Johnson noise thermometry will be migrated to solid media, large-volume high pressure devices. A year ago I envisioned calibrating many types of multi-anvil cells at Colorado. This strategy has been abandoned in favor of what I believe to be a much better plan. The best way to pursue our objectives will be to bring a single multi-anvil tooling set to Colorado. Under the collaboration with Yanbin

Wang and Mark Rivers, we will bring a compact multi-anvil tooling set from GSECARS to Colorado. Migration of the noise thermometer to the multi-anvil environment will be made in my laboratory. This phase of the work will start very early in 2005 when Yanbin becomes available. Issues of electrical noise pollution from the high pressure cell heater will have to be solved. The collaboration of John Hall, at Colorado, may be very important in this step. A specialized power supply may be required for cells in which the Johnson noise thermometer is used as the electrical noise from typical SCR power supplies may be intolerable. Special digital filters, currently under development by John Hall, may be required in the data reduction process. The accomplished LabView programmer who wrote the data reduction code, Benjamin Manthey, is available at Colorado. Both Ben and this project have benefited from our work together. The code which Ben wrote works extremely well. Ben, who has an electronics background, learned a lot about subtle, state-of-the-art electronic techniques.

Once the noise thermometer is established in a multi-anvil tooling set we will move it to GSECARS, assuming the ambient electromagnetic noise measurement have proven to be as encouraging as I anticipate. There we will have a new set of electrical problems to solve in the new environment. With the best of luck these problems will be trivial, but in case they are not, we will have Mark's strong electronics background locally to help solve them. The result should be a unique temperature calibration facility readily available to high pressure community. If successful, we will have solved the 100 year old problem of temperature measurement in large volume high pressure environments. Researchers from other labs can bring there typical cells to this facility and compare the accurately determined temperature with that indicated by their thermocouples. Once this relation is established the relevant corrections can be applied to all subsequent, and probably much prior, work without further dependence on the Johnson noise thermometer itself.

References

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Appendix 1: Colorado ambient noise test and instructions for measurements at GSECARS

August 26, 2004 To: Yanbin and Mark,

Here is an explanation of the ambient electrical noise test to see if your hutch is a likely place to implement the Johnson noise thermometer.

We wish to inspect the noise voltage spectrum between 1 Hz and 100 kHz using a 6 k resistor as a source. I have sent two such resistors and one cable.

Test equipment used at Colorado

Stanford Research Systems Model SR 560 Low-noise Preamp Stanford Research Systems Model SR780 Signal Analyzer (100 kHz max. frequency)

The preamp was set as follows: Coupling: AC Channel: A High Pass Filter: 1 Hz with a slope of -6 dB/octave Loss Pass Filter: 100 kHz with a slope of -6 dB/octave Voltage Gain: 200x (46 dB)
Note: Definition of dB as used in this work:

$$x \text{ [dB]} = -20\log_{10}(E/E_{ref})$$

with the voltages measured in the same units. For absolute measurements E_{ref} is taken as 1 volt.

Connect the resistor in the zinc (rectangular) box to the input of a low noise preamp using the supplied (RG58) cable and the BNC connectors on each. Observe the voltage spectral density on the signal analyzer. You should expect significant noise at low frequencies starting at 1 Hz with a fairly rapid decrease (1/f noise) to a nearly flat noise floor well below the 100 kHz top end. We are looking for the level of this noise floor and for the presence of any local spikes or other hash protruding above the floor and the low frequency 1/f noise.

Next try shorting the input of the preamp using a BNC shorting cap or a BNC 50 ohm terminator, no 6 k resistor, no cable. You should see a noticeable drop in the noise floor, ~-10 dB if all is well. If you see this drop without significant spikes in the spectrum we are in pretty good shape.
The copper canister offers better shielding than does the zinc box. Try it as well. The cable I provided (RG58) is the lowest grade coax cable to consider for this task. If it works we are in good shape. If it does not there are better shielded cables we can use. Shortly I will also provide a RG55 cable which is double shielded with BNC connectors.

Observations at Colorado

We saw the noise floor at about -120 dB indicated with a 500 ohm resistor (not the 6 kohm which I sent you) and a gain of 200x. The input noise floor was therefore at -120 - 46 for the gain = -166 dB real. This implies 5.0 $nV_{rms}/\sqrt{Hz}$. The voltage is calculated from the equation above with E_{ref} = 1 V. With the preamp input shorted we observed the noise floor at ~-124 dB indicated => -170 dB real. This is equivalent to ~3.2 $nV_{rms}/\sqrt{Hz}$. Thus, we observed at 4 dB increase in signal from the 500 ohm resistor and the cable at ~100 kHz from -124 dB indicated to -120 dB indicated.

At room temperature the thermal noise voltage density of a 50 ohm resistor is 0.9 $nV_{rms}/\sqrt{Hz}$ (standard, well known, every day number for the folks who do this stuff all day). It goes up as the square root of the resistance. Thus our 500 ohm resistor at room temperature should have a thermal noise voltage density of ~2.8 $nV_{rms}/\sqrt{Hz}$. We saw ~5 $nV_{rms}/\sqrt{Hz}$ still decreasing with frequency at 100 kHz. The true noise floor, at higher frequency, would be slightly lower. Five dB above the theoretical noise floor limit is not too bad at these low levels and includes the absolute contribution from amplifier noise.

To make your life easier, I have provided you with a 6 kohm resistor. This is 120 times 50 ohms. The thermal noise voltage density should be √120 = ~11 times that of a 50 ohm resistor or ~10 $nV_{rms}/\sqrt{Hz}$. Expressed in dB this should be ~-160 dB. If you have a preamp gain of 200x (46 dB) you should observe ~-114 dB on the signal analyzer. This is about 10 dB higher than our, and hopefully your, noise floor and should be easy to observe.

Table of relevant values

						Indicated
Res.	Voltage	Voltage	Voltage	Gain	Gain	Voltage
at room	Noise Density	Noise Density	Noise Density			Noise Density
temp.						
(ohm)	(nV/√Hz)	(V/√Hz)	(dB)		(dB)	(dB)
50	0.9	9.0E-10	-180.9	200	46.0	-135
500	2.8	2.8E-09	-170.9	200	46.0	-125
5000	9.0	9.0E-09	-160.9	200	46.0	-115
6000	9.9	9.9E-09	-160.1	200	46.0	-114
10000	12.7	1.3E-08	-157.9	200	46.0	-112

Appendix 2: GSECARS test results

Report on Electronic Noise Level Test Inside GSECARS 13-ID-D For the Development of Johnson Noise Thermometry

(in part)

Yanbin Wang and Mark Rivers

Oct. 18, 2004

1. Test Equipment:

Stanford Research Systems Model SR560 Low-noise Preamp Stanford Research Systems Model SR770 Signal Analyzer

2. Setup:

2.1 Preamp: Coupling: AC Channel: A High Pass Filter: 1 Hz with a slope of -6 dB/octave Loss Pass Filter: 100 kHz with a slope of -6 dB/octave Voltage Gain: 200x (46 dB)

2.2 Signal analyzer:

Frequency spans: 0-1.5625 kHz, 0-12.5 kHz, and
0-100 kHz Vertical unit selection: dB V/√Hz
2.3 Load testers:
Short (0.1 Ohm shorted BNC connector shielded
with Al foil) 50 Ohm terminator
6.02 kOhm resistor with copper canister shield and 70" RG58 cable (low grade cable provided by Getting)
6.02 kOhm resistor with zinc box shield and 70" RG58 cable
Connect the resistor in a load tester to the input of the low noise preamp using a BNC connector (and the supplied RG55 cable in cases of 6.02 kOhm testers). Observe the voltage spectral density on the signal analyzer at various frequency spans.

3. Hutch Electronic Environment:

There many instruments in the hutch: stepper motors (for both LVP and DAC setups), detector electronics (HV power supply, NIM bin, etc), Keithley multimeters, SRS preamps, TV monitors, cameras, cooling fans, heater power supplies, etc. Preliminary tests indicated that the most electronic noise came from the "chopper" stepper motors driving the 7-ton LVP. Therefore, tests were conducted and results are compared with most of the electronics turned on and off, with the exception of hutch cooling fans and CCD cameras.

4. Summary of Results

The white noise floor is about -120 dB with both the 50 Ohm resistor and shorted input. This level is similar to Colorado test environment. The 6.02 kOhm resistors pick up some thermal noise that is about 8 dB higher than the terminator. These noise levels are not affected by hutch electronics. However, turning them on introduces spikes at certain frequencies. Even when the motors were turned off, there are still certain sources of noise at ~15.7 kHz increments. The source of this noise has not been located.

It appears that the 13-ID-D environment is similar to that at U. Colorado, and therefore it is possible to continue the JN project in the 13-ID-D station at GSECARS.

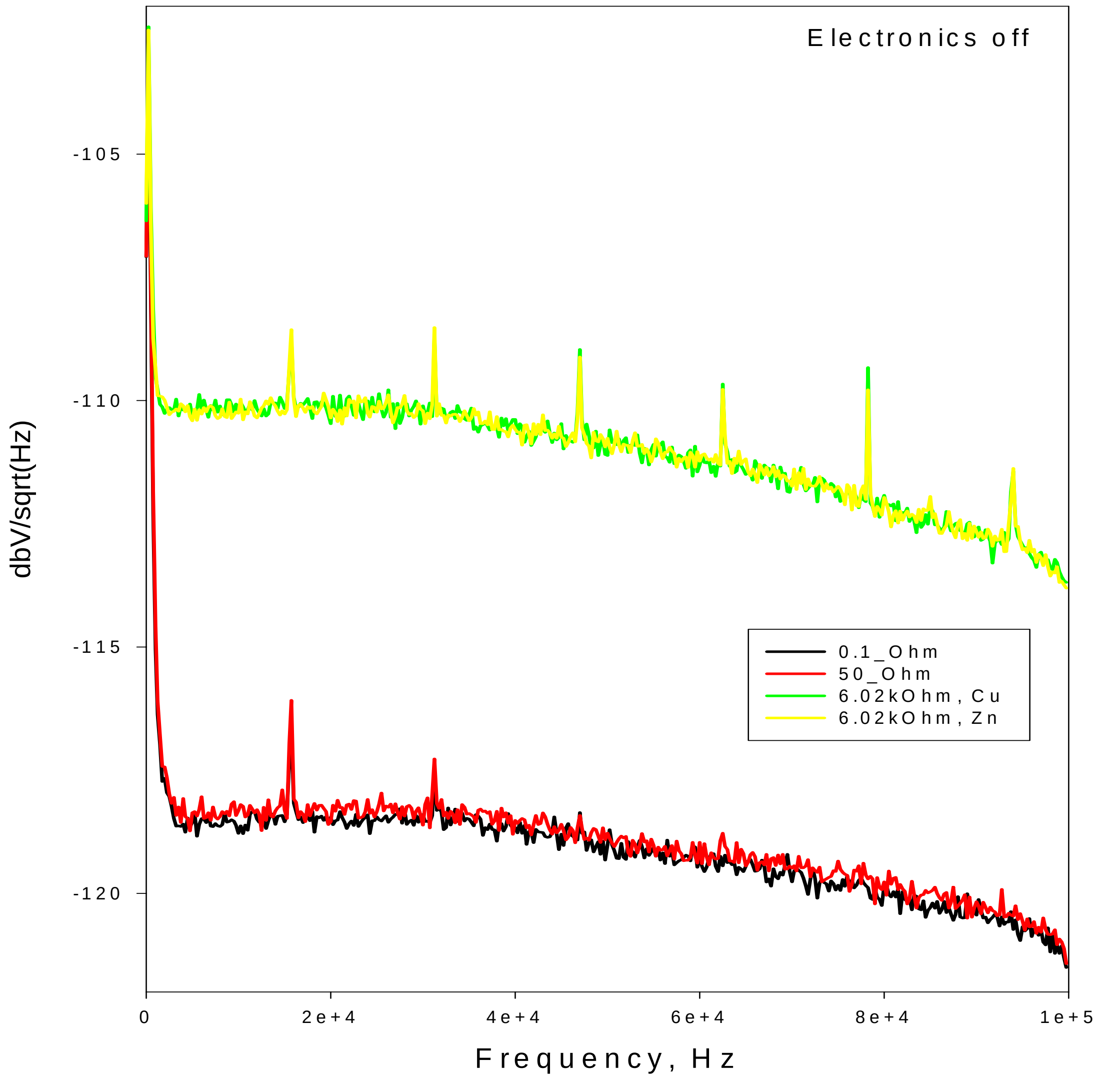


Figure 1. 0 - 100 kHz spectra with hutch electronics turned off. Only the 15.7 kHz repeated peaks are present.

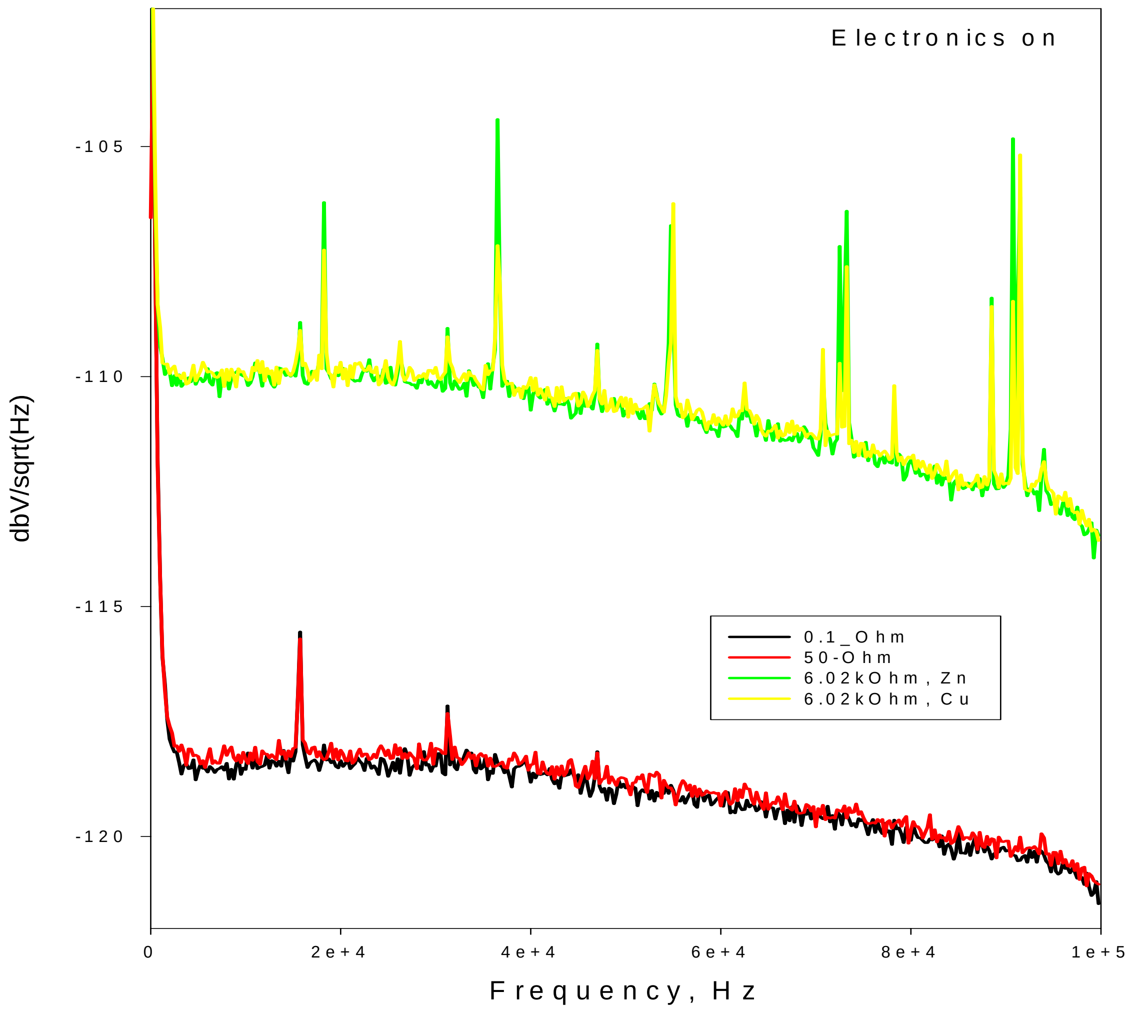


Figure 2. 0 - 100 kHz spectra with hutch electronics turned on. Note repeat spikes every 15.7 kHz - compare to Fig. 1 with electronics off. Also note additional spikes due to chopper frequencies.

Unwanted spikes are anticipated to be dramatically reduced with the use of a better shielded, RG55, cable. The GSECARS ambient appears to be generally similar to that at Colorado where the thermometer now resides.

Appendix 3: GSECARS test results

Cell Design for Testing of Johnson Noise Thermometer in Multi-Anvil Apparatus of the Kawai-type

Yanbin Wang and Ivan Getting

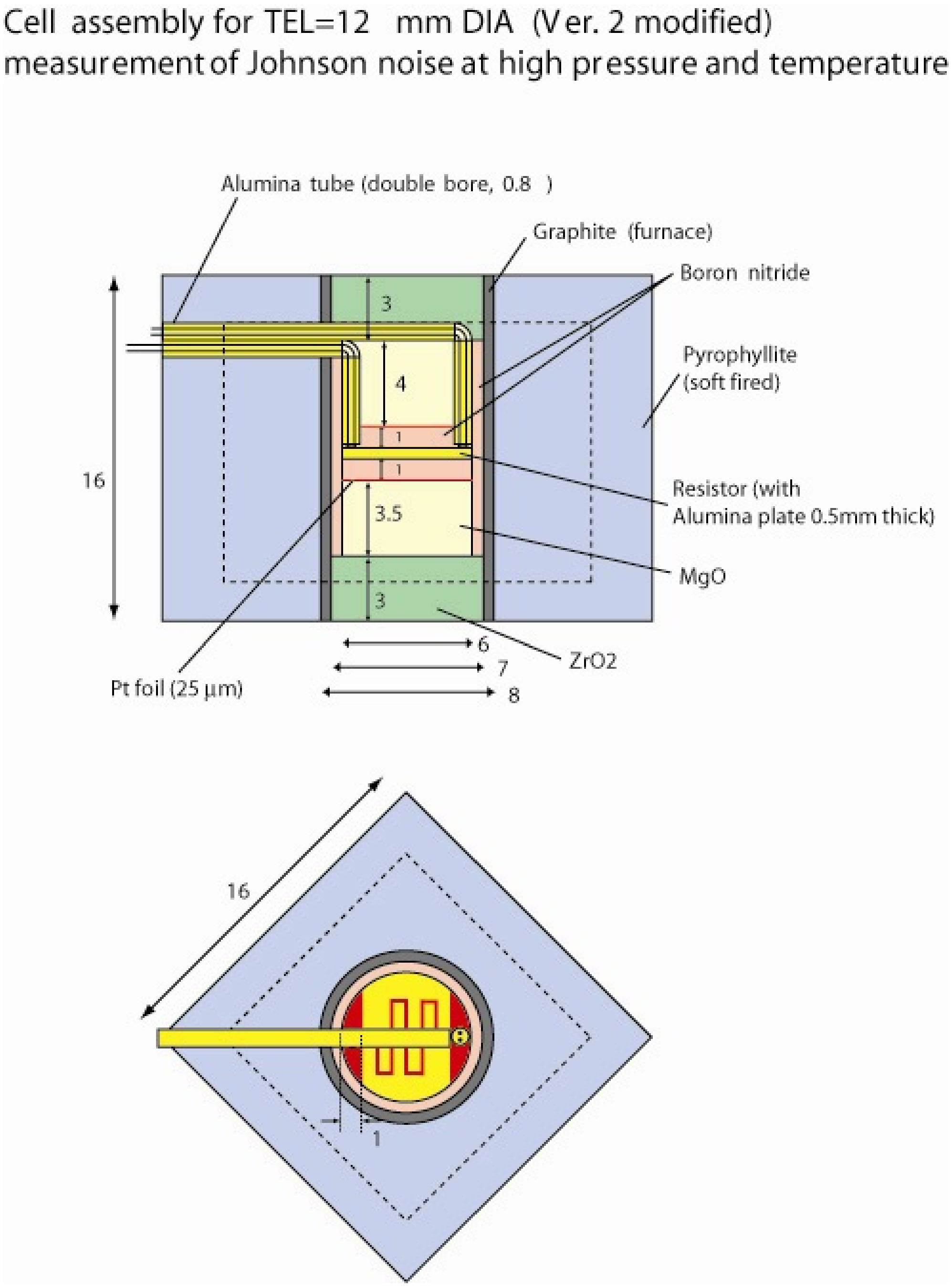


Figure Caption:

Cubic multi-anvil cell design for Johnson noise thermometry. The cell contains a metallic grid resistor and two thermocouples. The resistor is vapor deposited an alumina disk positioned in the center of the heater. To minimize temperature variations the resistor and thermocouple contacts with lie in the central plane normal to the heater axis and are surrounded by high thermal conductivity boron nitride. Low thermal conductivity pyrophyllite and zirconia are in the outer regions of the cell further reduce temperature gradients around the central resistor. In addition to serving as the thermocouples under test, the thermocouple wires are used to measure the Johnson noise and the resistor resistance. The four thermocouple wires are led out of the cell along the same path to minimize inductive coupling to the furnace currents. The cell is to be tested mechanically and electrically at CARS prior to the first Johnson noise thermometry tests at Colorado planned for Feburary, 2005.

C.5 Nuclear Resonant Scattering at High Pressure and Temperature: A New Capability for the COMPRES Community

[W. Sturhahn, Advanced Photon Source; J. Bass, University of Illinois at Urbana-Champaign; G. Shen, University of Chicago]

Summary

We report here on the activities to date of Year 1 of a 3-year infrastructure development project on Nuclear Resonant Scattering (NRS) at high P and T. The full three year proposal was submitted last year to COMPRES, and it was funded for the initial year with the 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 2 of the project.

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 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 first year of our infrastructure development project, we focused on the hiring of a full-time postdoctoral researcher to support the goals laid out in the original proposal text. We also improved the experimental capability of the NRS beam line (sector 3-ID) 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 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:

- hiring of a full-time postdoctoral researcher;
- development of refined high-pressure equipment for NRS;
- improvement of the laser-heating system at sector 3-ID of the APS;
- organized the workshop "Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation", February 12-13, 2005 at the APS.

The individual items are described in more detail below.

Hiring of Postdoctoral Researcher

The position for the postdoctoral researcher was advertised in EOS and through the COMPRES email system. We received six applications from suitable candidates. The position was then offered to Dr. Michael Lerche who accepted the offer and started on

August 16, 2004. We decided to offer this position to Michael because of his experience of working with synchrotron radiation in general and with nuclear resonant scattering techniques in particular. Michael is located full time at the APS and has already improved the laser-heating setup at sector 3-ID (see Fig.1). He is also co-organizing a workshop on nuclear resonant scattering.

Development of Refined High-pressure Equipment

The requirements of SMS and NRIXS with respect to the type of high-pressure cell used are quite different. Whereas SMS operates in a transmission geometry, the NRIXS technique relies on the detection of incoherently scattered x-rays, e.g., Fe K-fluorescence radiation, in a solid angle as large as possible. Special wide-angle diamond anvil cells (DAC) were developed to permit close placement of detectors to the pressurized sample. Now we started work on an enhanced design of this type of DAC to also allow x-ray diffraction experiments. Such a DAC would offer wide-angle access of the sample radially and also a wide-angle opening axially. The added diffraction capability can provide us with structural confirmation as well as with an equation-of-state during NRIXS data collection in the laser-heated DAC.

Improvement of the Laser-heating System

A laser-heating system was purchased earlier and integrated at sector 3-ID of the APS. The logical continuation of this effort now consists of the full integration of this system with NRIXS experiments using the DAC. We added several automated controls, e.g., the heating power distribution over the two sides of the DAC, to obtain a more user-friendly system. The integrated laser-heating system was tested with metallic iron samples. Stable conditions were achieved over 12h and more depending mostly on sample temperature and pressure.

Many high-pressure experiments require a very well-defined x-ray focus to minimize background due to unwanted scattering contributions. We accommodated such situations by the addition of clean-up slits into the x-ray beam path as visible in Fig.1b. A set of two orthogonal tungsten apertures is mounted on high-precision stages which are controlled remotely. This instrument upgrade facilitates the removal of scattering contributions that originate from the tails in the intensity distribution of the x-ray focus very effectively.

Workshop Organization

We are organizing the first workshop on “Nuclear Resonant Scattering on Earth Materials using Synchrotron Radiation” to take place on February 12-13, 2005 at the APS. Participants will learn about the capabilities and the theoretical background of NRS methods, visit sector 3 at the APS where NRS is performed, and obtain some hands-on experience. The goals are formulated as follows:

(a) provide a basic introduction of NRS to the Earth science community;
(b) define the state-of-the-art of NRS especially at high pressure;

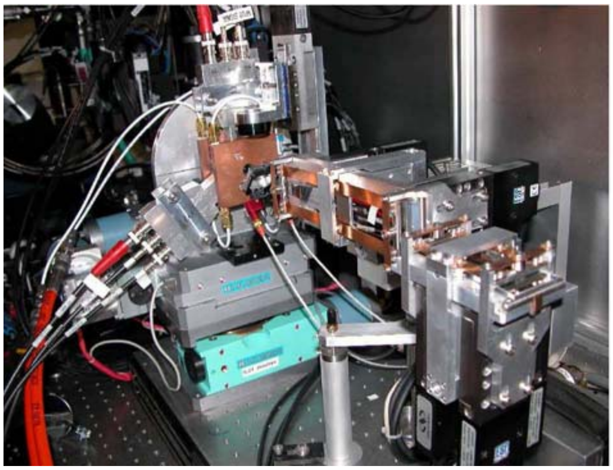
(c) discuss the applications to important geophysical problems;
(d) develop productive collaborations;
(e) address common experimental issues confronting users.

This workshop provides an ideal format to collectively address possible solutions to experimental problems and will help to build a viable COMPRES user base for this facility. Details on the workshop agenda can be obtained on the internet at http://www.nrs2005.aps.anl.gov.

Planned Activities

In Year 2 of our infrastructure development project, we will continue the outreach effort to the COMPRES community by assisting interested groups in design, preparation, execution, and evaluation of NRS experiments. We will focus on the manufacturing of high-pressure cells that conform to the special needs of the NRIXS technique. For improvements of the laser-heating system, we plan to include two-sided temperature readout via the conventional radiometric method, and depending on APS capital equipment funding we intend to enhance the system by adding an x-ray diffraction capability. 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. The successful completion of all these tasks depends on a dedicated postdoctoral researcher like Dr. Michael Lerche who we have hired recently. We expect that proposals for NRS experiments on sector 3 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 have it's own expert to help write proposals, consult on technical aspects of experiment design, and to help run experiments. This should be a significant fraction of his workload in Year 2.

Illustrations



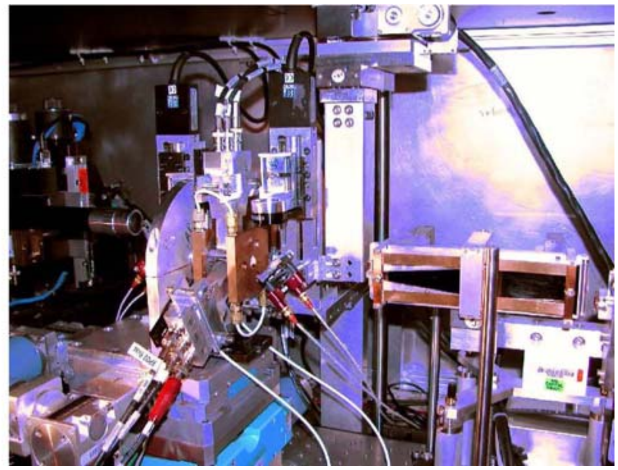


Figure 1a: DAC environment for NRS experiments with laser heating after the addition of clean-up slits.

Figure 1b: DAC environment for NRS experiments with laser heating before the addition of clean-up slits.

The distance between x-ray focusing mirrors (right) and DAC (middle) was increased, and a clean-up slit assembly was inserted. On the left, a microscope for DAC alignment is visible.

C.6 New Projects and Workshops

New Projects

In September 2004, 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.

Eight proposals for initiating new projects were reviewed and four were recommended for funding in Year #4. Workshops will be sponsored for several other initiatives.

(a) Development of CEAD (COMPRES Environment for Automated Data analysis) (Simon Clark and Paul Adams, LBNL; John Parise, Stony Brook; Mark Rivers, Univ. of Chicago, ANL; Ross Angel and Nancy Ross, Virginia Tech)
Note: Nancy Ross at Virginia Tech to be the PI.

(b) Technical Support for a Dual Beam Focused Ion Milling Facility for TEM Foil Preparation + 3D Chemical Analysis and Imaging (Harry W. Green, II, Univ. Calf. Riverside)

(c) Proposal for the Second COMPRES Cell Assembly Initiative: New Developments and Production (Kurt Leinenweber, James Tyburczy, Thomas Sharp, Arizona State

(d) A Gas Loading System for Diamond Anvil Cells at the APS (Mark Rivers, Guoyin Shen, Vitali Prakapenka, Univ. of Chicago and GSECARS)

Workshops:

COMPRES has proposed funding for several Workshops in 2005-2006, including:

Development of CEAD (COMPRES Environment for Automated Data analysis)
Organizers: S. Clark Lawrence Berkeley National Laboratory and Nancy Ross, Virginia Polytechnic Institute and State University.

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

Physiochemical Properties of Melts at High Pressure.
Organizer: Carl Agee, University of New Mexico.

D BUDGET REQUEST FOR YEAR #4

Budget Request for Year #4 [May 1, 2005 through April 30, 2006]. Details may be seen in the NSF 1030 Forms and the associated budget justification pages which are in the appendices to this report.

The COMPRES budget request for $2,100,000 for Year #4 [May 1, 2005 to April 30, 2006] is comprised of three major components (units of $K, which include fringe benefits and indirect costs):

D.1 Community Facilities

West Coast Synchrotron Facilities (R. Jeanloz, University of California at Berkeley)
$215K Operational budget

Diamond-anvil cell facilities at the National Synchrotron Light Source [M. Rivers, University of Chicago, H-k. Mao and R. J. Hemley, Carnegie Institution of Washington]
$352K Operational budget

Multianvil Press Facility at the NSLS [D. Weidner and M. Vaughan-Stony Brook University]
$333K Operational budget

Neutron Studies [N. Ross, Virginia Polytechnic Institute and State University]
[$85K] Operational budget [no new monies requested in Year #4].

D.2 Infrastructure Development Projects

$93K Development of the Laser-Heated Diamond Anvil Cell [T. Duffy, Princeton University, G. Shen and D. Heinz, University of Chicago]. Two subawards: $34K to Princeton and $59K to Chicago.

NC Absolute Pressure and Temperature Calibration [I. Getting, University of Colorado]. NC=No-cost extension

NC Brillouin Spectroscopy at the Advanced Photon Source [J. Bass, University of Illinois and G. Shen, University of Chicago].

$60K Nuclear Resonant Scattering at High P & T:A New Capability for the COMPRES Community [W. Sturhahn, Advanced Photon Source, J. Bass, University of Illinois and G. Shen, University of Chicago]

$84K Development of CEAD (COMPRES Environment for Automated Data analysis) [S. Clark and P. Adams, Lawrence Berkeley National

Laboratory; John Parise, Stony Brook University; M. Rivers, University of Chicago; Ross Angel and Nancy Ross, Virginia Polytechnic Institute and State University]

$70K Technical Support for a Dual Beam Focused Ion Milling Facility for TEM Foil Preparation + 3D Chemical Analysis and Imaging [H. Green, University of California at Riverside]

$112K Second COMPRES Cell Assembly Initiative: New Developments and Production [K. Leinenweber, J. Tyburczy, T. Sharp, Arizona State University]

$118K A Gas Loading System for Diamond Anvil Cells at the Advanced Photon Source [M. Rivers, G. Shen, V. Prakapenka, University of Chicago and GSECARS]

D.3 Other COMPRES Activities

This component of the budget is devoted to two principal areas of activities:

$202K **Workshops, Meetings, Education & Outreach, Publications** which includes:

- $80K Annual Meeting
- $102K Workshops (see list below*)
- $20K Education & Outreach

$461K **Central Office** which includes:

- $378K Salaries and fringe benefits
- $41K Materials and Supplies
- $42K Travel (including that of Advisory Committee, Executive Committee and Standing Committees)

$663K Total for Other COMPRES Activities

*COMPRES has proposed funding for several Workshops in 2005-06, including:

$20K Development of CEAD (COMPRES Environment for Automated Data analysis) Organizers: S. Clark Lawrence Berkeley National Laboratory and Nancy Ross, Virginia Polytechnic Institute and State University.

$20K Application of "Calorimetry-on-a-Chip" Technology to Heat Capacities and Transitions in Quenched High Pressure Samples Weighing Less than a Milligram. Organizers: A. Navrotsky, University of California at Davis and Frances Hellman, University of California at Berkeley.

$20K Physiochemical Properties of Melts at High Pressure. Organizer: Carl Agee, University of New Mexico.

SPECIAL NOTE:

The annual budget for COMPRES in Year #3 [May 1, 2004 to April 30, 2005] is $2.2M.

The scheduled budget level for Year #4 [May 1, 2005 to April 30, 2006] was anticipated to be $2.3M based on the original 2002 Cooperative Agreement with the NSF.

In early January 2005, we were informed by Dr. David Lambert of EAR-IF, the cognizant Program Director for COMPRES, that budget target level for Year #4 for COMPRES was to be $2.1M. This budget target represents a 5% cut over the current funding level for Year #3, or 10% lower than anticipated for Year #4.

Over the past few weeks, the Executive Committee has considered the reports and recommendations of the Standing Committees on Community Facilities and Infrastructure Development and prepared a Program Plan and Budget Request for Year #4 in the context of this reduced budget target.

As a consequence, several important programs had to be curtailed or temporarily put on hold. These include:

1. Beamline intern program [see Section ??? above]. This program provided funding for two full-time beamline interns who worked in 2004-2005 at the COMPRES-supported facilities at the National Synchrotron Light Source and the Advanced Light Source. Cost of these two interns was $126K in Year #3 (includes salaries of $35K per person, plus fringe benefits and indirect costs).

2. Equipment upgrades at COMPRES-supported facilities at the National Synchrotron Light Source. Sufficient funds were not available for this purpose in either Year #3 or Year #4.

3. High-pressure crystallography tools for the future: Combined white beam and monochromatic single-crystal microdiffraction. Funds to initiate this promising infrastructure development project were not available in Year #4.

4. Technical Support for a Dual Beam Focused Ion Milling Facility for

TEM Foil Preparation + 3D Chemical Analysis and Imaging. Funds were not sufficient to provide full funding of this technical position in Year #4.

D. 4 Other Funding Initiatives Related to COMPRES Core Program

In the past two years, there have been a number of important initiatives that have been funded by the National Science Foundation, the Department of Energy and the Department of Defense, that are not formally connected to the COMPRES Core Program, but which are scientifically and technologically related to the activities of the COMPRES community. These include:

2003:

- SNAP proposal funded by DOE-BES.
- The SNAP proposal, Spallation Neutrons And Pressure (PI's: J. Parise (Stony Brook University) , R. Hemley, H-k Mao (Carnegie Institution of Washington) and C. Tulk (Argonne National Laboratory)) was approved for funding by the Department of Energy, Office of Basic Energy Sciences in July 2003. The funding for SNAP includes construction of a high-pressure beamline at the SNS and funds for high-pressure cell development and totals $11.8 million over 5 years.
- NSLS provides funds to rebuild high-pressure hutches.

  In 2003, the National Synchrotron Light Source invested $1.44M to build new high-pressure hutches on the superconducting wiggler beamline for the COMPRES facilities for both multi-anvil and diamond-anvil cell apparatus.

2004:

- Award of DURIP grant to Chen and Weidner
  J. Chen and D. Weidner (Stony Brook University) were awarded a grant for $182K from the DURIP program of the Department of Defense to construct a monochromatic X-ray side station at X17B2 at NSLS. See details in Sect. B.2 MAC at NSLS.

- Award of IF grant to Eng, Rivers and Sutton at GSECARS
  P. Eng, M. Rivers and S. Sutton (GSECARS and University of Chicago) were awarded a grant for $550K from the Major Research Instrumentation Program at the NSF for the construction of a for X-ray side-station at bealmine 13BM of the APS.

- Award of ITR grant to Wentzcovitch team for Virtual Lab
  R. 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: Yousef Saad, Ilja Siepman, Donald Truhlar, D. Yuen, all at Minnesota.P. Allen [Stony Brook], G. Erlebacher [Florida State], B. Karki [Louisiana State], M. Marlon Pierce [Indiana], F. Spera [UC Santa Barbara]

Proposals from the COMPRES community to the NSF's Major Research Instrumentation Program for the January 27, 2005 deadline.

As announced at the 2005 Annual Meeting in Lake Tahoe, we had been informed by the NSF's Office of Integrative Activities that COMPRES was eligible to submit proposals directly to the NSF's MRI program. Consequently, on 28 September 2003, COMPRES issued a call for preproposals for potential proposals to be submitted in January 2005 to the MRI Program under the banner of COMPRES eligibility. In response to this call, we received three excellent preproposals from outstanding teams of principal investigators for new initiatives on behalf of the COMPRES community. On 4 January 2005,we wrote to Dr. D. Brzakovic, Senior Staff Associate in the Office of Integrative Activities at the NSF [the office that oversees the MRI program], to inform her of the plans to submit these three proposals under the banner of COMPRES eligibility:

(1) "Development of a capability for improved stress resolution using white synchrotron X-rays"
(2) by D. Kohlstedt, W. Durham, H. Green, S. Karato, Y. Wang and D. Weidner
(3) "Development of a universal detector system for high-pressure single-crystal and powder diffraction and thermal diffuse scattering at the Diamond-Anvil Facilities of COMPRES at the National Synchrotron Light Source"
(4) by H-k. Mao and R. Hemley
(5) "Development of a New Generation of Single-Crystal X-ray Diffraction Infrastructure for Materials Structure Research at the National Synchrotron Sources"
(6) by P. Dera, R. Downs, M. Rivers, M. Kunz, M. Nicol and B. Denton

When we were informed in early January 2005 by the NSF's Office of Integrative Activities that COMPRES was NOT eligible to submit proposals directly to the NSF, we encouraged the proposal teams to pursue avenues via other host institutions to do so. During the period January 6-10, the following alternative strategies evolved for these three initiatives:

(1) **"Development of a capability for improved stress resolution using white synchrotron x rays"** This proposal is being submitted by Georgia State University as the host institution with Pamela Burnley as the Principal Investigator. Co-Principal Investigators include: Harry Green (University of California at Riverside), Shun Karato (Yale University), Yanbin Wang (University of Chicago), and Donald Weidner (Stony Brook University). Additional collaborators include William Durham (Lawrence Livermore National Laboratory) and David Kohlstedt (University of Minnesota).

(2) "Development of a universal detector system for high-pressure single-crystal and powder diffraction and thermal diffuse scattering at the Diamond-Anvil Facilities of COMPRES at the National Synchrotron Light Source" by Mao and Hemley   A variant of this proposal will be submitted to the regular Instrumentation and Facilities Program for the July 16, 2005 deadline.

(3) "Development of a Five New Approaches for Micro-focus Single-Crystal X-ray Diffraction for Materials Structure Research at Synchrotrons" This proposal is being submitted by the University of Nevada Las Vegas as the host institution with Malcolm Nicol as the Principal Investigator. Co-Principal Investigators include: Przemek Dera (Carnegie Institution of Washington), Robert Downs (University of Arizona), Mark Rivers (University of Chicago), Martin Kunz (Lawrence Berkeley National Laboratory), and Bonner Denton (University of Arizona).