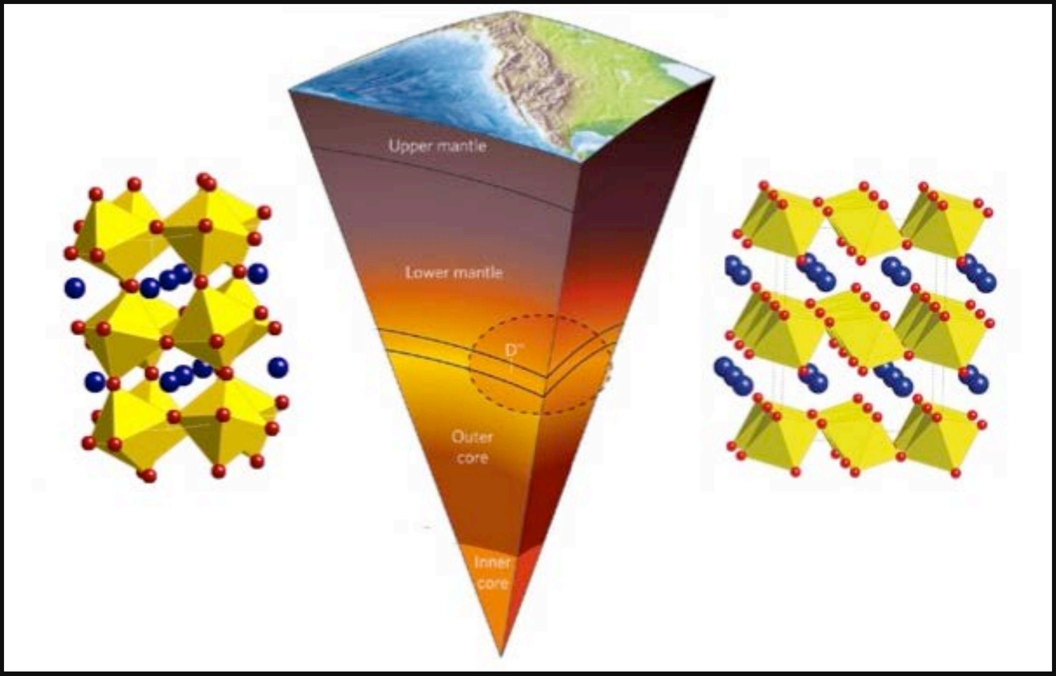
Understanding the Building Blocks of Our Planet: The Materials Science of Earth Processes



COMPRES:

The Consortium For Materials Properties Research in Earth Sciences

National Facilities and Infrastructure Development for High-Pressure Geosciences Research

Proposal to NSF 2012-2017

Volume I
Part A: Project Overview
Part B: Program Reports

COMPRES
2012-2017

Volume 1 – Project Description

Submitted to
National Science Foundation
Division of Earth Sciences
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About the title page: The center cover image is modified from T. S. Duffy, *Nature, 451*, 269-270 (2008). Crystal structure illustrations are courtesy of Susannah Dorfman.

This proposal is submitted by COMPRES on behalf of the Executive Committee, which represents the 56 U.S. universities and research institutions that are members of COMPRES. This proposal evolved through a year-long process involving public forums, the 2010 and 2011 COMPRES annual meetings, a town hall meeting at the 2010 Fall AGU meeting, and public solicitations for new initiatives. This process has allowed the COMPRES community to provide input on the form and content of this proposal. All community input and proposals were reviewed and discussed by the COMPRES standing committees, with decisions on the projects to include in the proposal and on budgets by the Executive Committee. The materials provided by PI's of COMPRES facilities and infrastructure development projects, include input from the numerous faculty members and researcher at U.S. institutions who are engaged in research projects at COMPRES facilities.

The proposal and supporting materials are contained in two volumes. Volume I includes the Project Summary, Project Description, and Budget (Section A). Section A is written to be a self-contained proposal. More detailed descriptions of the facilities and infrastructure programs that represent the main activities of COMPRES can be found in Section B, in case the reader wants additional information on a particular program or project. Volume II is a summary of scientific achievements that have emerged from use of COMPRES facilities and infrastructure development projects.

The Project Description gives an overview of the COMPRES Consortium and facilities, followed by a section on Results from Prior NSF Support, summarizing some of the scientific and technical accomplishments facilitated by COMPRES. The Project Description also includes a description our vision for activities over the next five years to support state-of-the-art research in mineral physics, and a brief outline of our funding request. The Budget provides our estimates of costs to carry out the activities that are summarized in the Project Description and detailed in the Program Descriptions. The Program Descriptions in Section B are summaries of the infrastructure and operation of COMPRES core facilities and several related programs. Each report includes an overview of the program's current activities, and a description of plans and resources requested to continue meeting the needs of the research community and support new opportunities.

Volume II Accomplishments starts with an introductory narrative that provides an overview of accomplishments in some of the main scientific and technical areas. This is followed by approximately 180 one-page research summaries, contributed by the COMPRES community, and based on research that has been enabled by COMPRES, through use of one or more of the core COMPRES facilities or infrastructure projects.

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Project Summary

<u>Intellectual merit</u>

Experimental investigations of the properties of Earth materials at elevated pressures and temperatures are of fundamental importance for interpreting observational data from geophysics and geochemistry to further our understanding of the structure, composition, and evolution of the Earth. The Consortium for Materials Properties Research in Earth Sciences (COMPRES) is a community organization with 56 current U.S. member institutions and 39 foreign affiliates. COMPRES provides for (1) operation and support of dedicated beamlines for high-pressure research at national synchrotron X-ray facilities; (2) support for development of new technologies for high-pressure research; (3) educational and outreach programs at the graduate and undergraduate levels.

This proposal reports on the advances and achievements of COMPRES over the previous five and one half years, and describes the goals and needs of the community for the upcoming five years (June 2012 – May 2017). This period offers exciting opportunities as new and upgraded synchrotron facilities will dramatically improve experimental capabilities and allow for novel experiments. Infrastructure and facility developments supported by COMPRES are at the same time creating a new generation of tools and techniques for attaining and interrogating deep interior conditions in the laboratory. This will enable COMPRES users to address key geophysical questions in the following areas: (1) rheological properties at *in situ* mantle pressure-temperature conditions with applications to understanding mantle dynamics and plate tectonics; (2) elastic properties, anisotropy, and equations of state for determining the composition of the earth; (3) effects of water on mineral properties and the deep Earth water cycle; (4) the physical and chemical properties of mantle minerals such as the post-perovskite phase to understand chemical heterogeneity in the deep Earth and the core-mantle boundary region; (5) the properties of iron and iron alloys representative of core compositions and their relevance for understanding the bulk Earth chemistry, magnetic field generation, planetary temperature structure, and the mechanism of core formation.

<u>Broader Impacts</u>

COMPRES is a community organization that operates facilities at national laboratories and develops new technologies for high-pressure research in Earth sciences for the benefit of undergraduate students, graduate students, postdoctoral scientists, and faculty and staff of U.S. educational and research institutions. These facilities are open to all potential users in the Earth Sciences and all other areas of high-pressure science. In addition to its initiatives in developing new techniques, one of the major interests of COMPRES is to ensure that all members of the U.S. Earth Sciences high-pressure community, irrespective of whether they are at solely undergraduate institutions, top-ranked Ph.D.-granting departments, or research/governmental institutions, have access to facilities, infrastructure, and technical support to conduct state-of-the-art research in our discipline. In addition, COMPRES conducts activities directed at dissemination of the scientific advances that emerge from COMPRES projects to students and professionals. Examples of the range of these activities include the COMPRES annual meeting, multiple workshops each year, educational development projects, and the COMPRES Distinguished Lecturer Series. COMPRES supports and promotes the advancement of students, postdocs, and other young scientists through making facilities available for their research, educational programs, community activities of various types, and some employment opportunities.

In many cases, the results of research facilitated and supported by COMPRES reach far beyond the Earth Sciences, and have significant impact in materials science, chemistry, and condensed matter physics. COMPRES has provided a new collaborative model for research in experimental geophysics that serves as a model for other branches of Earth Sciences.

Project Description

1. Introduction

In this proposal we intend to address four questions: 1) What is COMPRES and what types of activities is COMPRES engaged with; 2) How does COMPRES operate (management and organizational structure); 3) What has COMPRES achieved over the past 5 years; 4) What does COMPRES propose to do in the next five years.

This proposal requests continued NSF support of COMPRES activities for a five-year period from June 2012 to May 2017. We propose to continue operation of the four COMPRES-supported synchrotron beamlines, three of which are located at the National Synchrotron Light Source (NSLS, Brookhaven NY), and one at the Advanced Light Source (ALS, Berkeley CA). During year 3, the NSLS beamlines will transition to the newest US synchrotron, the NSLS-II. We request support for a new COMPRES program, a COMPRES Technology Office, to be located at both the Advanced Photon Source (Argonne, IL) and at the NSLS-II. We propose to continue the COMPRES Infrastructure Development program, which funds smaller projects, often of short duration, to develop new instruments, methods, and services for the COMPRES community. Finally, we request support for COMPRES workshops, meetings, educational initiatives, and outreach. The broad range of activities we propose have been defined by the COMPRES community, and reflects a collective view of priorities of the high-pressure Earth science community for the future.

Part A of this proposal is written as a self-contained proposal, with sufficiently detailed descriptions of each aspect of COMPRES to evaluate the various components, the consortium as a whole, and plans for the next five years. In Part B, we present lengthier descriptions of each COMPRES component, with additional technical details.

Overview of COMPRES and its Activities

COMPRES, the Consortium for Materials Properties Research in the Earth Sciences, supports and advocates for research on the materials properties of Earth and planetary interiors with a particular emphasis on high-pressure science, technology, and related fields. COMPRES is charged with the oversight and guidance of several high-pressure laboratories at national synchrotron facilities. These have become not just important tools in Earth science research, but essential facilities for carrying out the research activities for a large portion of the mineral physics community. COMPRES supports the operation of beam lines, the development of new technologies for high-pressure research, and develops educational and outreach programs.

COMPRES is community based. Educational and not-for-profit US Institutions with research and educational programs in the properties of Earth materials at high pressure are eligible to become members, and each institution is entitled to one vote in decision-making processes. 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. As of July 2011, there were 56 U. S. institutions that were members of COMPRES, and 39 affiliate institutions overseas.

COMPRES manages and provides financial support (accounting for the bulk of its budget) for four synchrotron beamlines, referred to as the COMPRES facilities. These are:

- Beamlines X17B3 and C at the National Synchrotron Light Source (NSLS), Brookhaven National Laboratory (BNL), NY. These beamlines are dedicated to diamond anvil cell (DAC) research, with high temperatures through laser heating and resistance heating. Many techniques for diamond-cell research were pioneered at these beamlines, including laser heating.
- Beamline X17B2 at the NSLS, dedicated to large-volume multi-anvil press (MAP) research. It is best known for research in the areas of rheology and ultrasonic sound velocity measurements at high pressures and temperatures. X17B2 is a world leader in these fields. Many techniques for elasticity and deformation measurements were first developed at this beamline, including sound

velocity measurements in the MAP, and rheology measurements using the "Deformation DIA" or D-DIA apparatus, and the rotational Drickamer apparatus.

- Beamline U2A at the NSLS, dedicated to high-pressure infrared (IR) measurements using the diamond-anvil cell. This was the first IR beamline dedicated to high-pressure studies. Many of the techniques used at IR beamlines worldwide were developed at U2A, and it is still the world leader in this area of research. Capabilities at U2A include studies of thermodynamic properties at extreme conditions, the presence and structural state of water in minerals, electronic structure, and thermal conductivity.
- Beamline 12.2.2 at the Advanced Light Source (ALS), Berkeley CA. This beamline enables X-ray diffraction experiments at high pressures and temperatures using the diamond anvil cell. 12.2.2 has become particularly well suited for studies of deformation and texture development at ultra-high pressures using the radial diffraction technique in the diamond cell, innovative resistance heating methods, and a developing program in single-crystal X-ray diffraction.

All of these COMPRES synchrotron facilities are in high demand and are, on average, oversubscribed by a factor of 1.5-2.6 or more (defined as the ratio of beamtime shifts requested to those available; there are sometimes much higher oversubscriptions for certain run periods). Thus, most beamtime requests at these facilities receive less time than requested and many are declined. All requests for beamtime are submitted through the General User proposal system at each synchrotron. Proposals are rated by a review panel and beamtime is assigned to the highest-ranking proposals, regardless of discipline.

In addition to operating facilities, COMPRES has, from its inception, viewed part of its mission as fostering the development of new technologies and methods for high-pressure Earth science research, making new capabilities at synchrotrons accessible to the entire COMPRES community, providing services that make research more efficient, productive, accurate, and cost effective, and providing education and outreach to inform our community of emerging opportunities. These goals are achieved through the Infrastructure Development program of COMPRES. This program builds into the structure of COMPRES a means for responding to community initiatives and needs. When COMPRES invests in a new technology or facility, the consortium follows through with education and outreach to inform the community and to build a user base. Summarized below are projects that have been funded via the Infrastructure Development program over the past 5 years. Detailed descriptions of each project are given in part B of this proposal.

- Multi-anvil Cell Development: Designs and produces cost-effective sample assemblies and inserts for large-volume multi-anvil presses, and distributes them to home-based laboratories and synchrotron facilities. The PIs work with users to design new sample assemblies for specialized applications. They also assist with accurate pressure and temperature calibrations of sample assemblies.
- Inelastic X-ray Scattering: Aimed at developing the inelastic X-ray scattering (IXS) techniques at Sectors 3 and 30 of the Advanced Photon Source (APS) for the COMPRES community. Techniques include nuclear resonant inelastic X-ray scattering (NRIXS), synchrotron Mössbauer, and momentum-resolved inelastic X-ray scattering (IXS) (to measure phonons and sound velocities). Partial support for a postdoctoral scientist is provided to develop high-pressure techniques at the beamlines, grow the Earth sciences user base, and organize education and outreach.
- Gas Loading DACs at GSECARS: COMPRES funded a project to build an apparatus for loading inert gas pressure-transmitting media (e.g., Ne, He) into diamond cells, with matching funds from GSECARS. COMPRES continues to provides 50% support for a postdoctoral fellow to train and assist users in loading DACs, to maintain the apparatus, and to load DACs that are mailed to GSECARS.
- Mössbauer spectroscopy: Provided support for a conventional (energy domain) Mössbauer facility at the Advanced Photon Source that is open to the entire high-pressure community. A

common use is to determine the valence state of Fe in mineral samples. No other Mössbauer facilities that are open to the community are available in the USA.

- Applications of Focused Ion Beam/Scanning Electron Microscope (FIB/SEM) Technology: Provides training for new users in FIB/SEM methods as applied to high-pressure research. Workshops with hands-on instrument instruction for small groups are held at the Carnegie Institution of Washington.
- Portable Paris-Edinburgh (PE) Apparatus: Partial support for developing a PE high-pressure apparatus at GSECARS and HPCAT at the APS. This type of apparatus is particularly well suited for experiments on melts and other fluids at high pressures and temperatures.
- Mineral Physics Educational Modules: Development of web-based courses on mineral physics at the upper-level undergraduate and graduate level.
- HEETDAC: Development of novel resistance heating technologies for diamond anvil cell research.

In addition to the above projects, each year COMPRES supports a number of workshops, and sponsors a Distinguished Lecturer Series that sends prominent members of our community to colleges and universities to deliver colloquia and to meet with students. Details on the Facilities, Infrastructure Development projects, and Education & Outreach projects that we propose to continue in a next phase of COMPRES are described in the project plan later in this section.

The community aspects of COMPRES cannot be overemphasized. The community defines all the activities of COMPRES and its future directions. Each year there is a call for new Infrastructure proposals to the entire COMPRES community. Any group or individual can propose a technology, service, or community activity for development by COMPRES. Two committees evaluate all proposals before deciding whether to fund or decline. Often workshops will be held to gauge the level of support for a particular technology or activity. Once COMPRES commits to a facility or technology, workshops are often held to inform the community and/or for training. Through this process we build user groups for the best experimental tools available and raise the level of our science. An excellent example of community building is given by the IR beamline U2A at the NSLS. Until 2002, this beamline was operated by a Participating Research Team (PRT). In 2002 when U2A became a COMPRES-supported facility, a total of four General User proposals were submitted for the year (Fig. 1). Since that time, the number of GU proposals has grown by more than a factor of 10. This has come about through COMPRES sponsored and organized workshops, open forums and yearly presentations by Dr. Zhenxian Liu at the COMPRES Annual Meeting, and a great number of informal discussions between members of the Executive and Facilities Committees with potential users. As a result, there is now a large and highly diverse user base at U2A; it is thriving, and the science of our community has benefited. For example, the capabilities of this beamline allow the water content and speciation of minerals to be determined, and U2A has been a key factor in the growth of studies on the volatile content of Earth's interior.

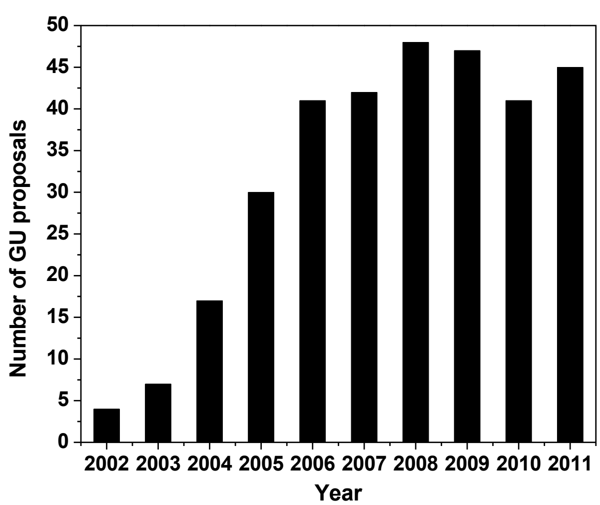


Fig. 1: Annual number of user proposal from community at beamline U2A at NSLS since it became a COMPRES facility in 2002.

2. Scientific Goals and Research Themes

COMPRES does not fund specific scientific projects. Rather, the role of COMPRES is to enable scientific investigations by providing world-class facilities and the best infrastructure possible for the high-pressure geosciences community. The intellectual focus of COMPRES is defined by the scientific goals of the mineral physics community it serves, which spans a diverse range of sub-disciplines including (but not limited to) mantle petrology, geochemistry of the mantle and core, the thermodynamic properties, bonding, and electronic structure of minerals, rock rheology, elasticity, and the transport properties of minerals.

High-pressure geoscience examines the properties of the materials within the Earth's interior, which are generally inaccessible to direct sampling and compressed to extraordinary pressures. *The overall goal of the field is to understand the state of Earth's interior, and the ongoing physical and chemical evolution of the planet.* Mineral physicists approach this goal through understanding various properties of the materials that comprise the Earth at all depths and comparing them with geophysical observations. The extreme pressure and temperature conditions within the Earth give rise to phenomena that can *only* be understood through high-pressure experiments and theory. Examples include phase transitions to denser structures, novel rheological and electronic properties, and changes in melting behavior and liquid structure. High-pressure mineral physics is highly interdisciplinary and has direct applicability to seismology, geodynamics, geomagnetism and geochemistry among other fields. For example, elastic wave speeds in Earth materials are necessary to interpret the seismic images; experimental studies of the rheology of mantle minerals are crucial for the geodynamic modeling of the convective flows that drive plate tectonics; and studies of iron and its alloys at high pressures are essential to understand the energetics driving the geodynamo in the Earth's core. It is also notable that the deep interior likely contains more water, carbon and certainly sulfur than exists at Earth's surface. Our oceans and atmospheres originated from degassing of the interior of the planet early in Earth history, and they continue to be cycled through the interior via subduction. All of the scientific issues that have driven much of high-pressure Earth science research also apply to other planets in our solar system and their moons. These broad motivating themes for the research of the COMPRES community are developed in detail in a planning document *Understanding the Building Blocks of the Planet: The Materials Science of Earth Processes* (edited by Q. Williams), which is the outcome of a long-range planning workshop held March 2-4, 2009 in Tempe, Arizona. This planning workshop, which was funded by NSF and organized by COMPRES, had the goal of identifying key scientific questions and future opportunities for high-pressure Earth sciences research; it can be downloaded from the homepage of the COMPRES website (www.compres.us).

The overarching scientific goal of the COMPRES community can be divided into a number of Grand Challenges (with types of laboratory measurement needed to address an issue given in brackets):

How did the Earth and other planets form, and how have they evolved?

- How did elements (including volatiles) partition among various regions through planetary formation? [element partitioning and separation under cosmochemical environment]
- How do various elements (including volatiles) partition among various regions by partial melting and/or solidification through the geological history? [melting relationships, compositions and densities of melts and co-existing solids]
- How does the mantle and core interact? [diffusion, non-diffusive mass transport]
- How did a magma ocean evolve? [melting temperature, adiabatic gradient (Grüneisen parameter)]
- How does a core evolve? [melting temperature, adiabatic gradient (Grüneisen parameter)]

What is the composition of Earth's interior?

- Is the mantle chemically layered? [elastic and anelastic properties of minerals under extreme conditions]

- What are the origins and significance of seismic "discontinuities"? [elastic and anelastic properties, anisotropy]

How does mantle convect?

- What is the viscosity stratification of the mantle? [rheological properties at extreme conditions]
- How can we map mantle convection? Is seismic anisotropy a map of flow directions? [elastic and velocity anisotropy; texture formation in deformed rocks]

Technological Grand Challenges: The Tempe Report outlines a number of technical advances of high priority for mineral physics that can realistically be achieved in the coming 5 years. These include: The ability to measure rheological properties at top-of-the-lower-mantle pressures; expand the pressure range over which multi-anvil experiments can be routinely performed; IR spectroscopy at simultaneous P-T conditions in the DAC; measurement of elastic properties and anisotropy at high P-T conditions using X-rays (momentum resolved IXS); enhance our ability to create and utilize nano-scale chemical and structural probes of high-pressure samples; provide access and expertise to routinely utilize nanofabrication techniques for constructing high-pressure sample assemblies.

Historically there has been a very close tie between the fields of seismology and mineral physics, largely because seismology is the main probe of the deep interior. Thus, much of the early activity in mineral physics was aimed at providing a laboratory database for interpreting and utilizing seismic information for understanding the Earth. As the capabilities of both fields have improved with time, this tie has grown stronger. The document "Seismological Grand Challenges in Understanding Earth's Dynamic Systems" (Lay, T. (ed.) 2009), that came out of a 2008 workshop on a Long-Range Plan for Seismology, lists many goals in common with those of the COMPRES community. All of the 10 Grand Challenge research questions listed in this document require mineral-physics input to answer.

In order to exploit the new capabilities of modern synchrotron and neutron facilities to advance our science, we must simultaneously create a new generation of tools and techniques for sustaining and interrogating deep interior conditions. Based on community discussion, we perceive the most promising new directions to include: (1) reaching higher pressure and temperature conditions, and achieving high pressures and temperatures within larger sample volumes; (2) improving the ability to probe samples, both *in situ* at high pressures and temperatures and quenched from these conditions, at the nanoscale; (3) making the transition from 'point' measurements on high pressure and temperature samples to full-scale imaging of the spatial variations in sample properties; (4) augmenting the ability to address issues of extrapolating between different timescales (e.g., from the experimental, in the femto- to megasecond range to those of planetary processes in the 0.01 to 100 petasecond range); (5) enhancing capabilities to probe the properties of heterogeneous phases and complex assemblages (in particular, interfaces and grain boundaries); and (6) achieving the same precisions, accuracies and resolutions in high pressure and temperature work as at ambient conditions. While these represent an ambitious set of goals, considerable progress has been made on each of these challenges in the first ten years of COMPRES, and this proposal outlines our plan to continue and advance this rate of progress in the coming years.

3. Accomplishments: Results of Prior NSF Support 2007-2011

Through its support of community facilities and infrastructure development projects, COMPRES has enabled major advances in experimental studies of the physical and chemical properties of Earth and other materials over the past five years. Scientists at many member institutions, both large and small, in the U.S. and around the world have benefitted from access to COMPRES facilities and infrastructure. As examples of the vitality and excitement of COMPRES science, Volume II of this proposal gives approximately 180 community-submitted one-page summaries of research ("one-pagers") that fall into eleven categories:

Rheology of the Upper Mantle

Elastic and Anelastic Properties of Mantle Minerals: Keys to the Structure and Composition of the Upper Mantle
Earth's Deep Water and Carbon Cycles
New Insights into the Deep Mantle
Iron, Iron Alloys and Earth's Core
New Techniques Enabled by COMPRES
Anvils and More: Essential Materials for High-Pressure Research
Planets and Planetary Materials
Mineralogy, Crystal Chemistry, and Phase Transitions
Equations of State and Elastic Properties
Physics and Chemistry of Materials

A large number of technological innovations were pioneered at COMPRES-supported facilities, leading to entirely new classes of experimental capabilities. For example, developments in ultrasonic interferometry in the large-volume press were pioneered at X17B2 of NSLS (e.g., Li and Liebermann, 2007) and provide the only means to measure elastic properties directly at the pressure and temperature conditions of the upper mantle and transition zone. A combination of support from COMPRES (for equipment), GSECARS, and funding through an Elasticity Grand Challenge grant (Bass, Illinois) led to the development of a Brillouin spectroscopy system on GSECARS beamline 13-BMD at the Advanced Photon Source. This first-of-a-kind facility has opened up capabilities to combine X-ray diffraction measurements with Brillouin spectroscopic determination of the complete elastic tensor (Sinogeiken et al., 2006). The COMPRES partnership with Sector 3 at the APS has led to novel studies of elastic properties at extreme pressures and temperatures using emerging techniques such as nuclear resonant inelastic scattering (NRIXS) and phonon inelastic x-ray scattering (IXS) (Sturhahn and Jackson, 2007; Jackson et al., 2009; Lin et al 2010). The gas-loading system developed through a COMPRES Infrastructure Development project in partnership with GSECARS (Rivers et al., 2008), has become the standard design for loading soft, inert pressure media in diamond cells and is being reproduced in other labs and synchrotron facilities. As a testament to the pioneering success of COMPRES in initiating major advances in our ability to characterize elastic properties, we note that other facilities around the world have adopted the COMPRES lead and are adapting Brillouin systems for synchrotron facilities (SPring-8, Petra-III) and the development of ultrasonic elasticity in combination with large-volume press facilities (SPring-8, DESY). All of the technology developed by COMPRES has been made openly available to the broader scientific community on an international scale and have helped scientists from other laboratories, both domestically and internationally, in reproducing our instruments and techniques. Although COMPRES instrumentation is being duplicated around the world (e.g. Murakami et al., 2009; Higo et al., 2009), COMPRES facilities are the beamlines of choice for many types of experiments, remaining at the forefront in their respective capabilities and attracting an international clientele on a regular basis.

Publications: For the period from 2006 through July 2011, there are 541 peer-reviewed publications and theses that have resulted from COMPRES facilities and infrastructure projects. Tables 1and 2 show the number of publications for each facility and infrastructure development project by year. These numbers are one indication of the strong demand for COMPRES facilities, their productivity, and the broad use of the services COMPRES provides through its infrastructure programs and facilities. Tables 1-2 show that the COMPRES publication rate has increased for many of our facilities and projects over the COMPRES II period. In particular, our investment in the ALS West Synchrotron Facility has seen a strong payoff in growth, and this facility is well represented among the COMPRES scientific highlights. The number of publications from infrastructure development projects is also rising.

The synchrotrons where COMPRES facilities are located were built, are operated, and funded by the Department of Energy, and COMPRES-supported beamlines are subject to DOE access policies. All proposals for beamtime are submitted through the General User (GU) Program and evaluated by a review panel. The highest ranked proposals are assigned beamtime regardless of discipline. From 35-50% of the beamtime is assigned with an advantage for Earth science proposals related to COMPRES themes if proposals have equivalent panel rankings. Although COMPRES proposals account for over 50% of the beamtime allocated at all facilities, significant GU beamtime is allocated to strong proposals from fields other than Earth science, primarily high-pressure materials sciences, chemistry, and physics. This is reflected in the publication list. There is a strong synergy between the high-pressure Earth science community and these allied disciplines, with regular exchange of ideas and techniques.

Table 1. Total COMPRES Publication Statistics (2006-2011).

	2006	**2007**	**2008**	**2009**	**2010**	**2011***	**Total**
ALS	7	5	19	22	23	12	**88**
U2A	11	14	13	21	20	8	**87**
X17B2	11	19	25	19	25	6	**105**
X17C/B3	31	33	30	39	32	31	**196**
Infrastructure	15	15	16	24	26	22	**118**
Total	**75**	**86**	**103**	**125**	**126**	**79**	**594**

Includes peer –reviewed publications and theses. Publications that used more than one facility/project are counted under each. The total number of unique publications from January 2006-July 2011 is 541. *Through July 2011

Table 2. Publications of Infrastructure Development Projects (2006-2011).

Project	2006	2007	2008	2009	2010	2011*	Total
Sector 3, APS	6	3	4	7	8	2	**30**
Gas Loading	-	-	2	6	10	7	**25**
Multi-anvil cells	3	2	5	8	7	6	**31**
Other Infrastr.	2	6	5	2	1	4	**20**
Central	4	4	0	1	0	3	**12**
Total	**15**	**15**	**16**	**24**	**26**	**22**	**118**

Includes peer –reviewed publications and theses*. Publications that used more than one facility/project are counted under each. *Through July 2011

In the following paragraphs, we describe some representative results and publications resulting from use of COMPRES-supported facilities and Infrastructure Development projects.

Rheology of Olivine and Transition Zone Minerals: A team led by Shun Karato of Yale has measured the creep strength of anhydrous olivine, wadsleyite, and ringwoodite to >20 GPa at high temperatures. These results help understand the stability of deep continental roots, and energy dissipation from deep slab deformation. The relative strengths of olivine and its high-pressure polymorphs can be compared quantitatively for the first time. (Nishihara et al., 2009; Kawazoe et al., 2010).

Deformation mechanisms in post-perovskite (pPv) and anisotropy in the lowermost mantle: $MgSiO_3$ pPv is thought to be a major phase in the Earth's lowermost mantle (D" region). An understanding of pPv deformation behavior is necessary to interpret seismic anisotropy in the deep mantle. In radial X-ray diffraction measurements on pPv under non-hydrostatic stress in a DAC at beamline 12.2.2 of the ALS (Miyagi et al., 2010), it was observed that at large strains a texture evolves which is consistent with (001) slip. The new (001) slip system is compatible with observed seismic anisotropy in the D" zone, i.e. fast S-waves polarized parallel to the core-mantle boundary and an opposite anisotropy behavior for fast S-waves and P-waves. These results open new possibilities for modeling anisotropy evolution during convection in the lowermost mantle, linking microscopic properties to macroscopic observations.

Strength of the Lithosphere and Subducting Slabs: Measurements of the activation volume of olivine up to 10 GPa indicate there is a substantial pressure effect, representing a pressure-induced viscosity increase of nearly 7 orders of magnitude from the base of the lithosphere to the bottom of the upper mantle (Dixon et al., MIT). Experiments on olivine at lower temperatures by Mei et al. (Minnesota) and Long et al. (Stony Brook) result in a better understanding of slip systems and deformation behavior under lithospheric conditions. New methods for deformation studies on single crystals at high pressures and temperatures have been employed to understand the effect of water on olivine deformation (Girard, Florida International). Water is shown to have an important effect on the pressure of transitions from one slip system to another. These results suggest models of mechanical and mineralogical layering needed to explain the dip angle of slabs and slab penetration through the 660 km discontinuity (Mei et al., 2010).

Phase Transitions in Stishovite: Stishovite is expected to be abundant in deep subducting slabs, and will likely contain dissolved Al and water. Lakshtanov and colleagues (Illinois) determined the effect of these elements on the transition from the rutile structure to a denser PbO_2 structure using the Brillouin spectrometer built at GSECARS under an Infrastructure Development project of COMPRES (Bass, UIUC) with simultaneous X-ray diffraction. Al and H dramatically lower the transition pressure by a factor of 2, making the rutile- PbO_2 transition a candidate for seismic reflections in the top of the lower mantle, and affecting the buoyancy of slabs (Lakshtanov et al. 2007).

Thermal Diffusivity at High Pressure: A new method was developed to measure thermal diffusivity at elevated pressure and temperature using the D-DIA on X17B2 at NSLS (see X17B2 section below). With this technique thermal diffusivity can now be measured for many materials relevant to the Earth's interior. Measurements under upper mantle conditions help constrain heat flow, mantle dynamics, and the triggering of deep seismicity (Dobson et al. 2010).

Simultaneous Ultrasonic Velocities and X-ray Diffraction at X17B2 of NSLS to 20 GPa 1773K: A team led by B. Li and R. Liebermann (Stony Brook) have developed techniques to conduct simultaneous ultrasonic interferometry, X-ray diffraction and X-ray imaging measurement on solids and liquids at high pressures and temperatures using NSLS beamline X17B2. Experiments on minerals relevant to the Earth's mantle and core (e.g., MgO, olivine, Fe-S-Si alloys), as well as functional materials, have been performed. These techniques have been implemented at other synchrotron facilities around the world, all patterned after the X17B2/NSLS model. A great advantage of the NSLS setup is ability to obtain both ultrasonic velocity and X-ray diffraction data on crystalline materials, providing a way to determine thermo-elasticity and to directly determine pressure independent of any secondary standard. These techniques can also: (1) determine the equation of state for glass/amorphous materials; (2) establish absolute pressure scales, and (3) conduct *in situ* investigation of time-dependent processes such as phase transformations and melting. The newest developments enable us to conduct these measurements up to P=20 GPa and T=1773 K (Li, B. et al. 2006; Whitaker, M. L. et al., 2009; Li and Liebermann, 2007).

Origin of Microdiamonds in UHPM rocks: A team led by L Dobrzhinetskaya (UC-Riverside) used beamline U2A at the NSLS to investigate the origin of metamorphic diamonds from Erzgebirge, Germany. The results suggest that crystallization from a C-O-H supercritical fluid is the most likely explanation for the origin of diamonds from ultrahigh-pressure metamorphic (UHMP) terranes. IR spectroscopy can distinguish Erzgebirge diamonds from kimberlitic sources and suggest very fast exhumation for these UHMP rocks. Dobrzhinetskaya et al., 2006).

Superhard Alternative to Diamond Discovered: Chung et al (UCLA) found that rhenium diboride (ReB_2) is a candidate superhard material. Using facilities at beamlines X17B3 at NSLS and 12.2.2 at ALS, they determined that the bulk modulus rivals that of diamond, and that ReB_2 is able to support a remarkably high differential stress. This material can scratch diamond, and may be more suitable than diamond or cubic boron nitride in certain industrial and research applications. Chung et al., 2007).

Post-Perovskite High-Temperature Elasticity: Shim and co-workers (MIT) used beamline 12.2.2 at the ALS to determine the crystal structure and thermoelastic properties of $(Mg_{0.91}Fe_{0.09})SiO_3$ post-perovskite up to 135 GPa and 2,700 K. Their results help explain some of the seismic properties of this region, and the stability of post-perovskite lenses on the core-mantle boundary (Shim et al. 2008).

Sound Velocities Across the Spin Transition in (Mg,Fe)O: Marquardt et al (Potsdam) used the COMPRES Brillouin spectrometer at GSECARS to measure the elastic properties of ferropericlase across the high-spin low-spin transition. The HS-LS transition increases elastic anisotropy considerably, and likely accounts for most lower mantle seismic anisotropy (Marquardt et al., 2009).

Carbonatites from the Transition Zone and Lower Mantle: Measurements from ALS beamline 12.2.2 provide experimental evidence that silicate mineral inclusions in diamonds from Juina, Brazil, crystallized from primary and evolved carbonatite melts in the mantle transition zone and deep upper mantle (Walter, et al., 2008).

Pyrochlore under Pressure: Pyrochlore, $A_2B_2X_6Y$, has over 500 different compositions and applications from radiation resistant materials to fast ionic conductors. Zhang et al. (2010, Michigan) have demonstrated a new method for quantitatively measuring the degree of pressure-induced atomic disordering in pyrochlore ($La_2Zr_2O_7$) using synchrotron XRD (NSLS-X17C), IR spectroscopy (NSLS-U2A) and Raman scattering. Anomalous lattice expansion was confirmed at 10 GPa in experiments where the pressure medium contained some water. This is the first report of anomalous expansion via incorporating water into the structure.

Spin Transitions in MgSiO3 Perovskite: Catalli et al (MIT) used COMPRES-supported facilities at Sector 3 of the APS to determine the spin state of ferric iron in $(Mg,Fe)SiO_3$ perovskite and its effect on elastic properties. The spin transition in Fe^{3+} makes perovskite more compressible, which could be diagnostic of Fe variations in the lower mantle (Catalli et al., 2010).

Wet Olivine in the Upper Mantle? The effect of water on the elasticity of wadsleyite can provide constraints on the water content in the Earth's transition zone. Researchers from Princeton, Northwestern, and Bayreuth measured the elastic properties of wadsleyite, β-Mg2SiO4, with 0.84 wt.% H_2O, up to 12 GPa from Brillouin scattering and single-crystal x-ray diffraction (X17C, NSLS). They found that hydrogen reduces the elastic properties of wadsleyite at ambient conditions, but that the pressure derivatives of the bulk and shear moduli are indistinguishable between hydrous and anhydrous wadsleyite. They estimate that ~1 wt.% H_2O in wadsleyite at 410-km depth may reconcile seismic bulk sound velocities with a pyrolite composition mantle (Mao et al., 2008).

(Mg,Fe)O-rich Ultra-Low Velocity Zones at the Core-Mantle Boundary? A team from Caltech used Nuclear Resonant Scattering at the APS and X-ray diffraction at the ALS beamline 12.2.2 to determine the sound velocities in $(Mg_{0.16}{}^{57}Fe_{0.84})O$ at high pressures. Their measurements showed very low velocities, suggesting that iron-rich (Mg,Fe)O can explain the characteristic sound speeds of ultra-low velocity zones (ULVZs) near Earth's core-mantle boundary. (Wicks et al., 2010).

High-Performance Low-Cost Cells for *In Situ* Multi-Anvil Experiments: A COMPRES Infrastructure Development project serves the US multi-anvil community by producing optimized cells for multi-anvil high-pressure work, with low cost through economies of scale. These cells are becoming the standard in many multi-anvil press labs in the USA and overseas (Leinenweber et al., 2006).

Effect of phase transitions on P wave velocities in the Earth's mantle: Using the deformation apparatus at NSLS beamline X17B2, Li and Weidner (Stony Brook) showed that the bulk modulus is significantly lowered if the pressure of a seismic wave drives a volume-reducing phase transformation. Their experiments demonstrate softening of the bulk modulus within the two-phase loop of olivine-ringwoodite at a time scale of 100 seconds. Scaling to seismic amplitudes and grain sizes expected in the Earth, the P wave velocities within the discontinuities at 410, 520, and possibly 660 km are likely significantly lower than otherwise expected. This opens the possibility of large velocity perturbations throughout the upper 1000 km of the mantle (Li and Weidner, 2008).

Rheology of Post-Perovskite and seismic anisotropy of the deep mantle: A team from University College London and Stony Brook determined the relative strength of the perovskite and post-perovskite forms of a structural analogue, $CaIrO_3$, that is stable at low P-T conditions. The experiments at NSLS

X17B2 show that the post-perovskite phase is significantly weaker than the perovskite phase, possibly explaining the properties of the D" region at the base of the Earth's mantle. (Hunt et al., 2009).

Water in the Mantle and the X Discontinuity: S. Jacobsen and colleagues (Northwestern U.) used high-pressure synchrotron IR spectroscopy, X-Ray diffraction (XRD), and Raman spectroscopy, to show that just 1300 ppm variation of H_2O content in $MgSiO_3$ can displace the transition of low-pressure clinoenstatite to high-pressure clinoenstatite by up to 2 GPa. 30–45 km (1.0–1.5GPa) of deflection could occur per 0.1 wt.% H_2O. If the mantle X-discontinuity at~300 km depth results from pyroxene transitions in depleted harzburgite, the depth of the X-discontinuity could serve as an indicator of upper mantle water content. This study demonstrates that synchrotron-based IR at NSLS-U2A is suitable for studies on mantle silicates containing relatively low concentrations of water (10's to 100's of ppm by weight).

Radiation Damage and Zircon Stability: A group led by Lang and Ewing (Michigan) used NSLS beamline X17C to show that radiation damage dramatically modifies the phase stability of crystalline zircon at high pressure, specifically the high-pressure transformation to a scheelite-structured polymorph, reidite (Lang et al. 2008).

Melting in the Fe-C system to 70 GPa: A group from Bristol and Columbia determined high-pressure melting curves for Fe_3C, Fe_7C_3 and the Fe–Fe_3C eutectic using laser-heated diamond anvil cell techniques at beamline 12.2.2 at the ALS. They found an expanding field of Fe_7C_3 + liquid with pressure. In situ X-radiographic imaging shows a rapid drop in carbon in the eutectic composition above 20 GPa, and predicts that the eutectic lies close to pure iron by ~ 50 GPa. Results indicate that Fe_3C is replaced at the solidus by Fe_7C_3 at ~ 120 GPa. Fe_3C is unlikely to be an important crystallizing phase at core conditions, whereas Fe_7C_3 could become an important crystallizing phase (Lord et al., 2009).

Paris-Edinburgh Press Provides Keys to High Pressure Melt Structure: A Paris-Edinburgh high-pressure apparatus, partially funded by COMPRES, was commissioned at Beamline 16-BM-B at HPCAT and adds a new technique for research at extreme conditions. Using white beam diffraction methods with energy up to 100 keV, researchers from Ehime Univ., Univ. of Chicago, and HPCAT investigated the structure of liquid albite, $NaAlSi_2O_8$. Diffraction profiles can be interpreted as a combination of structure factor S(Q) and the effective source intensity. The structure factor yields the radial distribution function G(r) of the liquid, which gives the number of near neighbors in successive coordination shells. Further technical developments in high-pressure x-ray micro-tomography, absorption mass density and ultrasonic interferometry will be explored using this apparatus (Yamada et al., 2011).

4. Scientific Opportunities for the Next Phase of COMPRES

The tools of high-pressure mineral physics: Creating the conditions of planetary interiors

At the crux of high-pressure geosciences is the ability to both generate and simulate the high pressures and temperatures associated with the interiors of the Earth and planets. The conditions of planetary interiors are extreme: compression equivalent to a material under thousands of km of rock while at temperatures far in excess of ambient melting temperatures. To achieve these extraordinary conditions, a wide-range of experimental technologies and computational approaches have been pioneered towards addressing our fundamental questions: What resides within, and how does our interior govern the evolution of the interior and surface?

Achieving extreme P-T conditions is only half the task: the other half is to interrogate geomaterials either after they are quenched or under *in situ* conditions. To this end, the high-pressure community, led by COMPRES, has development specialized probes including spectroscopy, acoustic interferometry, calorimetry, elemental analysis, measurements of electrical and thermal conductivity, deformation, and state-of-the-art diffraction and scattering techniques to address the broad suite of chemical, elastic and dynamic issues associated with planetary interiors.

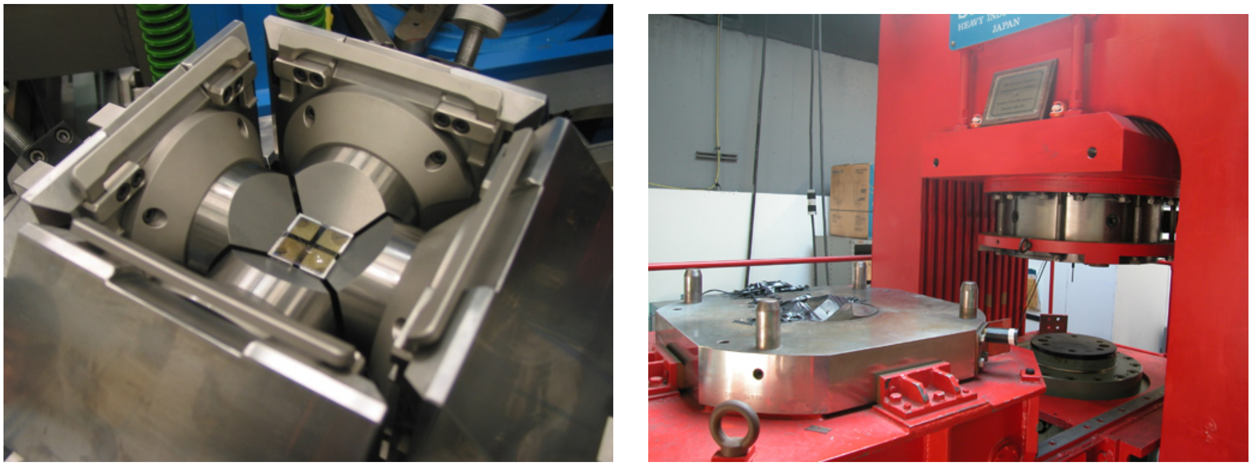


Figure 2. (Left) View from above, with top anvil assembly removed, of a multi-anvil press. The sample assembly is sitting in the square region between the four visible hydraulically-driven anvils (a fifth provides the base of the central square). Scale across the picture is approximately 0.7 meters. Photo courtesy Y. Wang, APS. (Right) Representative hydraulic press in which multi-anvil assemblies are compressed. Bottom anvil assembly (steel-colored object on left) has been slid out of the press. This is a 2000-ton Sumitomo Industries Press installed at Stony Brook Univ. Photo courtesy of R. Liebermann.

The COMPRES community uses two main static compression techniques to achieve the extreme conditions of deep interiors: the multi-anvil press and the diamond-anvil cell. The multi-anvil (or "large-volume") press relies on simultaneous hydraulic compression of a cubic or octahedral assembly composed of tungsten carbide or sintered diamond blocks with truncated corners. The advantages of this technique include: (1) a fairly uniform high pressure and temperature environment; (2) high-intensity x-ray beams can be directed between the blocks (if separated by low absorbance material), and the sample can be x-rayed for either imaging or diffraction/spectroscopy during a high-pressure–temperature experiment; (3) small (~1 mm^3) but macroscopic high-pressure samples can be quenched from high-pressures and high-temperatures and characterized at ambient conditions, allowing determinations, for example, of phase assemblages and chemical transport properties; (4) by applying differential stress to the sample, deformation experiments designed to probe the viscous flow of Earth's interior (and hence the mechanisms of lithospheric plate motions) are conducted; (5) by introducing transducers into the sample assembly, ultrasonic sound wave velocities can be measured; (6) electrical conductivity can be characterized by introducing electrical leads into the samples; and (7) liquid density and viscosity are constrained by imaging falling (or rising) spheres using radiography. With this broad suite of capabilities, the multi-anvil press has produced much of the insight into the phase transitions and melting processes undergone by Earth material down to ~700 km depth (or ~25 GPa), and there are significant possibilities that this range could be extended in the future.

More extreme conditions of pressure and temperature can be achieved using the opposed anvil configuration of the diamond anvil cell (DAC, Fig. 3). With this apparatus, pressures in excess of those within Earth have been generated, albeit not routinely. However, pressures in excess of 1 million bars (100 GPa), corresponding to depths of roughly 3000 km in Earth are being achieved regularly in a number of labs.

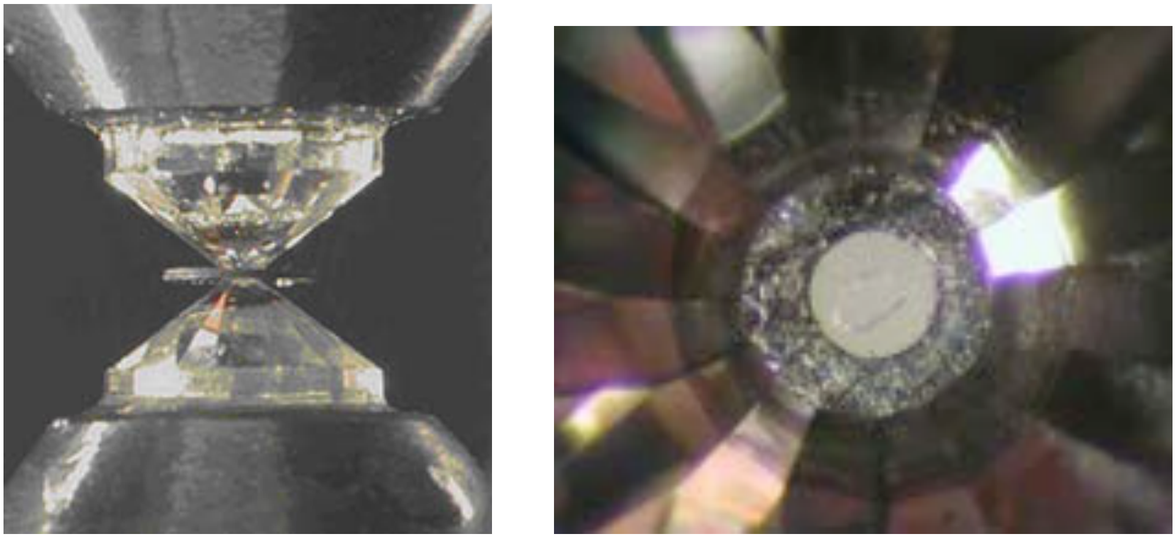


Fig. 3: (Left) Close-up view of the diamonds and metal gasket (center) within a diamond anvil cell. Vertical dimension of picture is ~1 cm; total flat portion of the anvil tips is ~ 500 microns. Photo courtesy R. Wenk; (Right) View through the diamond anvil into a pressurized sample. Grey speckled annulus is the metal gasket; the mineral sample (wadsleyite) (center oblong feature) is held within a liquid pressure medium. Sample diameter is ~200 μm. Photo courtesy of Z. Mao and T. Duffy.

The transparency of diamond allows the ability to probe the sample using various types of radiation, including X-rays, IR radiation, and visible light. The high-pressure geosciences community pioneered the application of x-ray diffraction and scattering techniques, as well as Mössbauer, infrared, Raman and Brillouin spectroscopies on samples at extreme conditions. Using such techniques, the crystal structure, elastic wave velocities, thermodynamic behavior, and electronic structure of materials throughout the pressure range of much of the planet's interior can be determined. Heating the sample with an infrared laser allows temperatures up to 1000s of degrees to be attained. The laser-heated DAC enables study of materials at conditions spanning the crust through the core of our planet, and hence produce an unprecedented level of insight into the physical and chemical properties of the deepest reaches of our planet.

There are many challenges in diamond cell research: to improve the ability to characterize pressure and temperature at extreme conditions; optimize capabilities to maintain and characterize single-crystal samples (which often shatter under differential stress) under extreme conditions; and to extend the achievable pressure and temperature range even further. Future development also hinges on making better measurements at smaller scales. Improving our ability to characterize and interrogate samples at the nano-scale is one of the community's highest priorities. Many in situ probes require the use of complex cell assemblies, such as microcircuitry deposited on the diamond tip (so-called "designer anvils") or embedded in multi-anvil assemblies. Improvements in fabrication techniques have allowed such cell assemblies to become increasingly useful. The high-pressure geosciences community expects a greatly enhanced need for nanofabrication of intricate diamond-cell assemblies and diamonds themselves in the future. Therefore, characterization of smaller samples, along with reasonably routine access to micro-fabrication facilities and training in related techniques is an area of emphasis.

New Probes of Planetary Interior Conditions

In recent years, synchrotron-based techniques have played an ever-increasing role in experimental efforts to understand geological materials at high pressures and temperatures. Over last decade, development of new 3rd generation synchrotrons augmented by improvements in x-ray optics and detectors have led to dramatic advances in material property measurements at high pressure and, hence, in our ability to interpret geophysical observations of the deep Earth and planetary interiors. The last few years have also witnessed rapid, synergistic development of advanced pressure-generating capabilities and new synchrotron techniques. Established techniques such as x-ray diffraction are being used at higher pressures and temperatures with increased precision and accuracy of measurement. New techniques in high-pressure x-ray spectroscopy and scattering have greatly advanced capabilities for studying thermodynamic, elastic, and electronic properties. During the next five years we plan to capitalize on these new experimental capabilities, and to broaden their use within the COMPRES community.

5. Research Plan

Over the last decade, COMPRES has leveraged access to national synchrotron facilities to develop a wide array of state-of-the-art techniques for high-pressure experimentation. This has enabled our user community to produce novel discoveries and new insights into the internal structure of the Earth. As new facilities are constructed and older facilities upgraded (or in some cases, replaced), it is critical to enhance our access to this improving set of high-intensity X-ray sources and to continually develop new innovative technologies to expand the range and quality of experiments our community can perform.

Here we outline the capabilities that COMPRES provides to our community, our vision for developing these capabilities at existing facilities, and our plan for taking advantage of the opportunities at new and upgraded facilities over the next five years. The infrastructure-oriented aspects of the plan include (1) maintaining, upgrading and replacing national X-ray and other facilities; and (2) ensuring appropriate support and access for high-pressure experimental needs at these facilities.

The scientific problems that this plan will enable us to address span a broad range of first-order problems in solid-earth geophysics and planetary science, including the current chemical and dynamical state of Earth's deep interior, the rheological properties of minerals at high pressures and temperatures, the thermal structure and dynamics of lithospheric slabs, the volatile distribution of the mantle, the properties of magmas, and understanding processes occurring now or in the past on other bodies in our solar system.

5.1 COMPRES Facilities

West Coast Synchrotron Facilities (Beamline 12.2.2, Advanced Light Source)

The Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL) is a third generation synchrotron that through a series of upgrades and a focus on its strengths has attracted a strong domestic and international user base. It provides capabilities for a range of high-pressure X-ray experiments to pressure and temperature conditions of the Earth's deep mantle and core. Specific areas of focus include in-situ laser heating at high-pressures; well-developed radial diffraction capabilities for deformation and rheologic experiments; and state-of-the-art in-house external heating infrastructure. High-pressure experiments are conducted on a beamline that uses a superbend source, with energies in the 6-40 keV range.

The investment made by COMPRES in 12.2.2 at ALS over the previous funding cycle has paid major dividends. COMPRES benefits from strong institutional support for staffing (2.33 FTE supplied by ALS) and equipment, such as new X-ray detectors obtained in 2010, and a gas-loading apparatus based on the GSECARS design that is now under construction (all of these items paid for in full by the ALS as an institutional match for COMPRES support). The COMPRES Facilities committee conducted a review of the management of the COMPRES program in December 2009. Based on the recommendations of this committee, the management of the ALS program was shifted to Quentin Williams at the University of

California at Santa Cruz in June 2010. Prof. Williams has developed and implemented an ambitious program of beamline upgrades and improvements as described below. In large part due to the change in management and upgraded infrastructure, beamtime at 12.2.2 is now in great demand and highly competitive, with an oversubscription rate of 2.6. There has been a marked increase in the number of publications, including high-profile publications. The ALS facility is emerging as one of our top facilities and is a testament to COMPRES's effective investment and stewardship.

Beamline Overview

Beamline 12.2.2 at the Advanced Light Source offers a broad range of capabilities for the high-pressure geosciences community. These include readily interchangeable axial and radial X-ray diffraction geometries using both CCD and MAR detectors, two-sided laser heating and associated spectroradiometry, external heating capabilities, and nascent single-crystal diffraction capabilities Sample preparation facilities include a computer-controlled laser-milling machine (Oxford Laser) for micro-machining of gaskets, as well as the full suite of tools and equipment to carry out diamond-anvil cell experiments to Mbar pressures at high temperatures.

Recent hutch improvements include automated and rapid 2-D scanning for sample location and a gas-driven online pressurization system for using membrane-driven diamond cells. Recent scientific achievements at 12.2.2 include radial diffraction on laser-quenched samples of magnesium silicate post-perovskite (pPv) at pressures in excess of 180 GPa (Miyagi et al., *Science,* 2010), and markedly enhanced temperatures of externally-heated diamond cell apparatuses, with temperatures in the region of 2000 K being achieved at high pressures in radial geometries, and 900 K in axial diffraction geometry (Raju et al., JAP, submitted). Beamline 12.2.2 has developed an identity as the preferred facility for radial-diffraction deformation experiments and for external resistance heating experiments using the diamond cell.

New Capabilities

S. Clark (ALS), P. Dera (GSECARS) and O. Tschauner (UNLV) and co-workers have recently established high-pressure single-crystal X-ray diffraction capabilities (see part B for a description of this effort). The recent development of synchrotron beamlines optimized for single-crystal diffraction experiments enables better determinations of crystal structures and compression properties, especially for low-symmetry systems, to pressures reaching up to 100 GPa (Dera, 2010). Other future directions include: further improvements and upgrades in our laser-heating system; benchmarking and refining the external heating achievements for both axial and radial geometries; augmenting the successes in radial diffraction by exploring mixed-heating (laser-plus-external) approaches to these experiments; interfacing single-crystal capabilities with heating approaches; and enhancing interactions between users of the 12.2.2 High Pressure beamline and those of other beamlines at ALS. For example, recent users have taken advantage of the tandem abilities of micro-diffraction beamline 12.3.2 and 12.2.2 to both synthesize and characterize their samples following laser-heating at high-pressures, and subsequently chemically characterizing different phases present in their quenched samples at 12.3.2 (e.g., Friedrich et al., 2010).

A gas-loading system of similar design to the COMPRES/GSECARS system (Rivers et al., 2007) is under construction is expected to be on-line in 2012. High-pressure loading of inert gases in the sample chamber is the optimum means to provide quasi-hydrostatic stress conditions at >10 GPa and to obtain uniform laser heating to >2000 K by insulating the heated sample from the surrounding diamond anvils. This will thus provide a significant upgrade in the capability to provide high-quality sample environments on-site to enable users to carry out the most robust and reliable high-pressure experiments.

ALS Upgrade

The Advanced Light Source is planning a lattice upgrade for 2012 that will reduce the horizontal emittance and improve source brightness by a factor of 3. With suitable upgrades to the beamline optics (to be funded by the ALS), a flux increase of about a factor of 10 is expected at the sample. The current focus spot size of 10x10 μm FWHM will also be reduced to 5x5 μm FWHM. Shorter collection times and better spatial selectivity will be a feature of high-pressure capabilities as the ALS facility moves forward (see the ALS Strategic Plan at http://www-als.lbl.gov/index.php/about-the-als/strategic-plan.html).

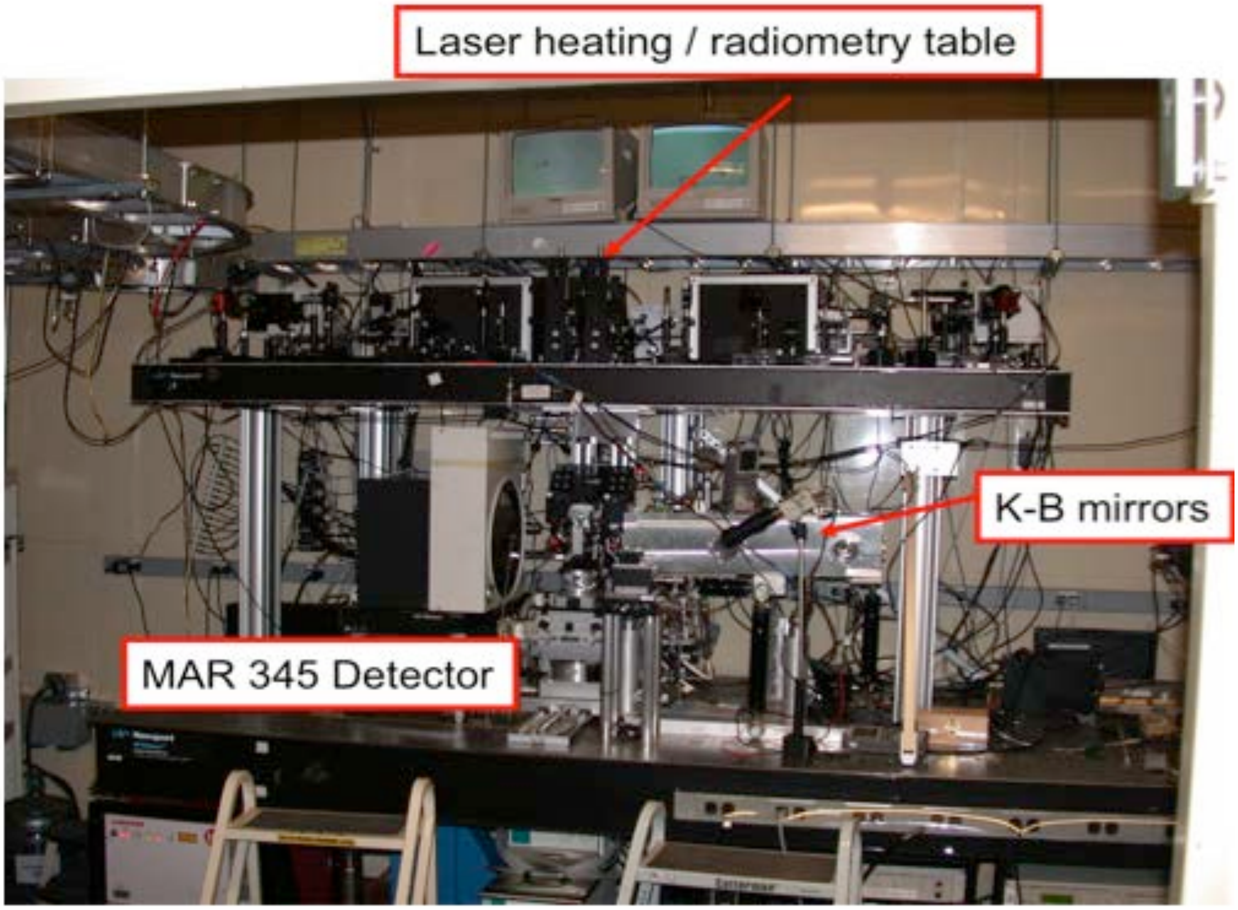


Figure 4. Experimental station at beamline 12.2.2 at the ALS; samples are typically positioned to the right of the MAR detector, and the laser heating system primarily occupies the upper table, with the beam being steered into the sample area through holes in the table.

National Synchrotron Light Source (2012-2014)

The National Synchrotron Light Source is the home of the first US dedicated high-pressure diamond-cell beamline in 1990, the first multi-anvil beamline in 1992, and the first IR beamline in 1999. These beamlines continue to foster creative science and spawn new techniques. X-ray diffraction and imaging capabilities enable a wide range of experimental studies at the NSLS. Our current portfolio at NSLS includes X17-LVP and X17-DAC, which encompass the stations X17B2, X17B3, and X17C, all located on a superconducting wiggler beamline of the X-ray ring. The DAC-IR program operates on beamline U2A of the vacuum ultraviolet (VUV) ring. All three are operated under a Cooperative User agreement with the NSLS.

X-Ray Diamond Anvil Cell Facility (X17-DAC, Beamlines X17C and X17B3)

The diamond-anvil cell X-ray (X17-DAC) facility at the National Synchrotron Light Source consists of two stations (X17C and X17B3) and a sample preparation/spectroscopy laboratory. Over the last 5 years, COMPRES has undertaken a comprehensive effort to enhance the infrastructure and upgrade many components throughout this facility. This has resulted in major enhancements in experimental quality and user experience. From Jan. 2009-April 2011, X17C had more than 204 person-visits representing 44 separate universities and institutes while X17B3 had 57 person-visits representing 18 separate universities and institutes. From Jan 2010 – May 2011, as one of the most productive beamlines at NSLS, X17-DAC beamlines have recorded a total of 57 publications (peer-reviewed journal publications and theses).

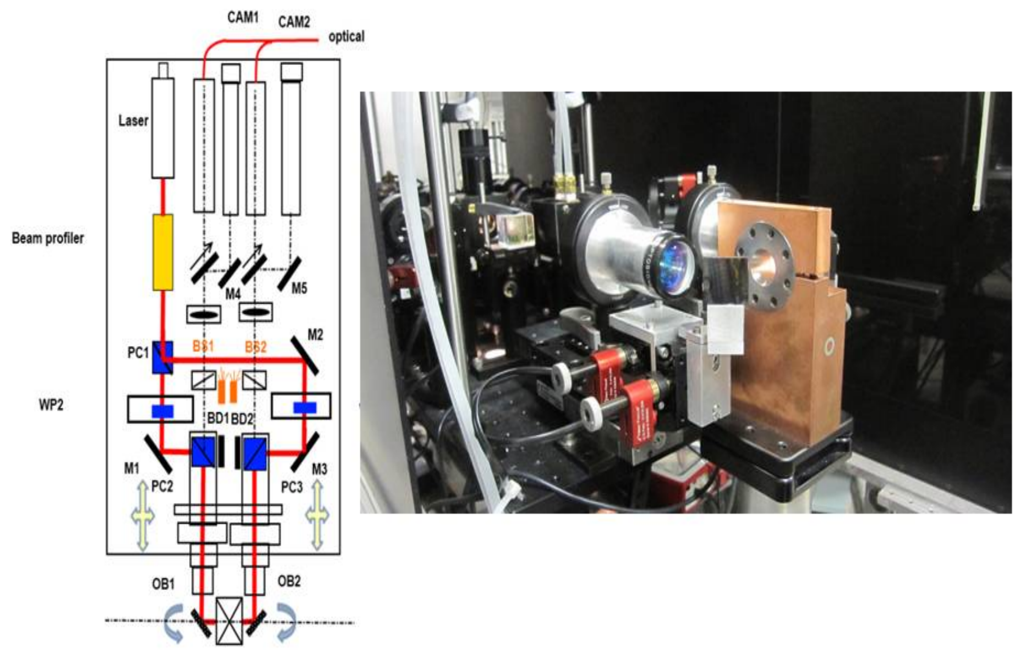


Figure 5. Double sided laser heating system at X17B3, NSLS. A schematic of the beampath is shown at left. The focusing objectives, carbon mirror, and diamond anvil cell are shown at right.

X17C and X17B3

At X17C, users conduct angle and energy dispersive X-ray diffraction experiments on polycrystalline samples in either axial or radial geometry. A Kirkpatrick-Baez mirror system enables double focusing of the beam to ~15-20 μm beam size. Energy dispersive single-crystal diffraction for phase identification, orientation determination, and unit cell refinement is also available. Experiments can be carried out at room temperature or at high temperatures (up to 800°C) using various external heating techniques such as user-supplied hydrothermal diamond anvil cells. A new advanced CCD detector (Rayonix SX-165) has been in operation since 2009.

Station X17B3 supports experiments at two X-ray energies: ~30 keV and ~80 keV. In the lower energy range, angle and energy dispersive X-ray diffraction experiments are carried out, similar to the capabilities at X17C. A Kirkpatrick-Baez mirror system enables double focusing of the beam to a ~10-15 μm beam size. In addition to external heating, a double-side laser heating system was commissioned in 2011 and is available to users (Fig. 5). The laser heating system consists of a 100 W fiber laser, optics to enable double-sided heating, and a spectrometer and CCD detector for temperature measurement.

At 80 keV, total scattering pair distribution function (PDF) measurements are performed. This is a new developing technique that involves measuring both Bragg and diffuse scattering for structural analysis of complex materials, allowing determination of local atomic structure for both crystalline and amorphous materials. A recent paper by Ehm et al. (2010) demonstrates the capability of the technique. This method has considerable potential to study the structural properties of liquids, glasses, melts, nanomaterials and disordered crystals. Geophysical applications include the study of the structural evolution of melts and glasses with pressure and order-disorder phenomena under mantle conditions.

High-Pressure Diamond Cell Laboratory

A high-pressure sample preparation laboratory houses equipment for DAC sample preparation and includes a micro electric discharge machine (EDM) system, mechanical micro-drill, and high-resolution optical microscopes. We have completely revamped this laboratory and all major equipment is now updated. We have a wide selection of diamond anvil cells available for beamline staff and users including symmetric and panoramic cells as well as an Almax plate DAC. The ruby fluorescence spectrometer received a new laser, spectrometer, and CCD detector in 2010. Our sample preparation lab and ruby spectroscopy system are used annually by more than 100 users from six or more beamlines (X17C, X17B3, U2A, X14A, X27A and X7A).

Fig. 6: The new 1000-ton press at beamline X17B2

X-Ray Large Volume Press Facility (X17-LVP, Beamlines X17B2)

The X17B2 beamline has pioneered high-pressure, high-temperature acoustic velocity measurements on mineral systems and high-pressure, high-temperature rheology experiments (Karato and Weidner, 2008; Karato, 2011). The beamline saw the first synchrotron measurements of melt acoustic velocity and density (by X-ray absorption) in the US involving synchrotron radiation. This is the first beamline in the world to measure Q of elastic deformation at seismic frequencies at pressures of several GPa (Li and Weidner, 2008). This beamline continues to contribute to high-pressure crystallography, phase equilibrium, and equations of state.

The X17B2 station consists of a main line and a side station. The main branch primarily uses X-ray diffraction in energy dispersive mode, a technique well suited for large-volume press experiments. The pressure generating system in current use is a primarily 200-ton press with a DDIA installed in it.

A fully functional monochromatic side-station, developed in part with funds from the COMPRES Infrastructure Development program, runs simultaneously with the main energy-dispersive station. Pressure cells in use at this station include the Paris-Edinburgh cell. Under development is the D-Tcup (deformation Tcup) cell that promises to extend the range of deformation experiments to 30 GPa and 2000 K. The development of this side station during COMPRES II effectively doubled the amount of beamtime available for high-pressure experiments at X17B2.

Ultrasonics

Ultrasonic interferometry is used to measure sound velocities and elastic properties. Simultaneous X-ray diffraction and X-ray imaging measurements give length and density changes. High pressure and high temperature techniques developed at X17B2/NSLS continue to be used as a model for similar facilities that have been implemented at other synchrotron facilities around the world. In addition to measurements of velocities and elasticity of minerals at extreme P-T conditions, these techniques can also be applied to (1) determine the density equation of state for amorphous materials through measurements of ultrasonic velocities with sample length measurements (e.g., Antao et al., 2008), (2) establish absolute pressure scales, and (3) conduct in-situ investigations of time-dependent processes such as phase transformations and melting. The newest developments allow us to conduct measurements up to P=20 GPa and T=1773 K, close to the P-T conditions in Earths transition zone.

Rheology

The rheology experiments associated with the X17B2 beamline have set an entirely new range of conditions for these measurements. We can now conduct uniaxial stress deformation experiments at 10 GPa and 2000K with near the precision of experiments limited to 0.3 GPa a decade ago. Our goal for the immediate future is to extend these measurements to 25 GPa with the equipment now being installed at the NSLS. Through these developments, not only can we infer pressure dependence of mineral properties, but also we can examine the properties of high-pressure mineral phases that were impossible before.

In situ measurement of stress in polycrystalline samples forms the basis for studies of the mechanical properties of materials with very broad Earth science and materials science applications. Synchrotron X-rays have been used to define the local elastic strain in these samples, which in turn define stress. We have developed a new energy dispersive detection system for white radiation, which has been installed at the National Synchrotron Light Source (Weidner et al., 2010). The new system provides differential strain measurements with a precision of 3×10-5 for volumes that are 50×50×500 microns. This gives a stress precision of about 10 MPa for silicate minerals. This system enables accurate steady-state, high-pressure and high-temperature rheological studies of Earth minerals at mantle conditions.

Large shear strains can be applied to a torus shaped sample by rotating the top relative to the bottom. S. Karato and colleagues have designed and employed a high-pressure system that takes advantage of this process (Yamazaki and Karato, 2001; Nichihara et al., 2008; Kawazoe et al., 2010). The Rotational Drickamer Apparatus (RDA) has been developed and used at X17B2 to study the rheological properties of many mantle materials under high-pressure and temperature conditions. The experimental studies involve three components: (1) development of a new type of deformation apparatus, (2) applications of X-ray facilities at X17B2 at the NSLS, and (3) the development of a theoretical model to interpret X-ray diffraction data. The maximum pressure and temperature range explored so far is P to ~23 GPa and T to ~2200 K. Using this technique, we have determined (1) the pressure dependence of creep strength of water-free olivine to P~10 GPa and T~1900 K (Kawazoe et al., 2009), (2) obtained the creep strength data for wadsleyite and ringwoodite to P~23 GPa, T~2200 K (Nishihara et al., 2008). These results have been used, for example, to understand the stability of deep continental roots and the energy dissipation associated with deep slab deformation (Karato, 2010).

The new pressure cells and measurement tools also allow a wide array of new characterizations that are still being explored, including measurements of phase transition kinetics through stress oscillations with frequencies in the seismic zone, Q measurements at high P and T, and thermal diffusivity at high P and T. New science will emerge as these tools are used to study polycrystalline samples, partially molten samples, and single crystal samples. The next five years promises to be a time of great discoveries, taking the tools at hand and pushing our understanding of relevant materials.

Thermal Diffusivity

A new method was devised by David Dobson and his research team to measure thermal diffusivity of samples at elevated pressure and temperature. X-radiographic images of a sample are analyzed to define the distance between two wires as a function of a time varying temperature. The phase lag of the line separation is determined as a function of radius. This phenomenon represents the thermal pulse moving into the sample from the furnace. Thermal diffusivity is determined from the motion of the pulse. This is an entirely new technique that will be used to measure the thermal diffusivity for many materials relevant to the Earth's interior. It will be possible to refine models of the thermal structure and heat flow in regions characterized by high thermal gradients (e.g., the lithosphere, subducting slabs).

New Development: 1000-Ton Press

The current 200-ton press is being replaced with a new press with 5 times greater load capacity. The new system will allow interchange of high-pressure tooling. The 1000-ton press will allow higher pressure and can work with a Kawai type two-stage high-pressure system. This system, complete with motorized positioning table, has been constructed and is presently being commissioned.

In the new press we will soon install a newly designed modified Kawai system (DT25 guide-block) that will have the capability of providing a differential load to the sample while it is at high pressure and temperature. The anvil cube is 25 mm on this system and so will be very similar to the standard laboratory Kawai pressure system. The main difference is that the upper and lower anvils are pushed by an independent hydraulic jack, thereby applying a differential (uniaxial) stress. This system follows the philosophy of the D-DIA but with the Kawai geometry. Our side station system is a small-scale prototype of this new guideblock. The Kawai geometry has a long proven track record of providing higher pressure than the DIA on samples with the same volume.

New Scientific Opportunities at Low Pressure

The next frontier in high-pressure studies is to utilize all of the new capabilities to address problems at lower pressures. The Earth's 'critical zone' is the region that interacts with humans. It contains energy sources, ground water, is home to most of the devastating earthquakes, and the mechanical and chemical behavior of materials in this zone is vital to mankind. The pressure in this zone is less than 1 GPa, but the types of information desired from experiments are quite varied. Carbon sequestration goals require us to know the reactivity of supercritical carbon dioxide. Interactions with water and rock will define the ability of any geologic structure to sequester the carbon. We plan to develop and build a system that can address these types of problems. It will include the ability to control pore pressure, to inject fluids into the system, to control deviatoric stress. The synchrotron will be used to define 3-D distribution of stress, chemistry, and porosity as a function of time.

Development of New Techniques for High-Pressure: Diffraction Tomography

The Three-Dimensional X-ray Diffraction Microscopy (3DXRD) technique can provide complete microstructural information within a volume containing up to thousands of individual grains (e.g., Wert et al., 2007; Oddershede et al., 2010). A full-field beam illuminates the sample and 2D transmission diffraction images are taken using the rotation method. Using a large-area far-field detector and reconstruction software, the full orientation, elastic strain tensor, volume, center of mass (5-10 microns), and unit cell refinement can be determined for every grain within the illuminated volume. In addition, by placing a high-resolution semi-transparent 2D or 3D near-field area detector close to the sample (~10mm) the 3D grain boundary morphology can be reconstructed using a back projection method. In this way the spatial and angular information are decoupled and more difficult samples (e.g., high mosaicity) can be reconstructed in extreme cases. For low mosaicity polycrystalline materials, however, the use of just a far-field detector with the appropriate analysis software allows for time resolved studies of 100's – 1,000's of grains simultaneously following changes in orientation, strain, stoichiometry, and size as a function of applied forces (P/T). Although detailed local grain boundary information cannot be achieved without the use of a high-resolution detector, centers of mass can be determined along with volumes allowing for a tessellation process to determine the most likely grain neighbors. In this way, correlations between kinetics and local microstructural heterogeneities can be probed. The ability to collect grain-by-grain kinetics on a statistically significant number of grains rather than just measuring a powder-averaged value, will allow more realistic models to be developed that incorporate the true kinetic distributions of behavior due to the inhomogeneous nature of all polycrystalline materials.

Infrared Diamond Anvil Cell Facility (IR-DAC, Beamline U2A, NSLS)

Infrared (IR) spectroscopy provides a key and often unique experimental approach, with exceptional sensitivity to O-H bonds that makes it an invaluable tool for evaluating the behavior of hydrous and nominally anhydrous minerals under extreme conditions. The diamond anvil cell IR beamline at the National Synchrotron Light Source (NSLS-U2A) is an integrated and dedicated facility for the measurement of far- to near-infrared spectra of materials from ambient to ultrahigh pressures at variable temperatures by coupling synchrotron IR microspectroscopy, Raman scattering, and visible spectroscopy with diamond-cell methods. Complementary and often unique information on the properties of Earth and planetary materials from near-surface conditions to those of the deepest interiors such as the bonding properties of crystals, glass, and melts can be obtained with these spectroscopic techniques. The presence of an IR beamline together with X-ray facilities for high-pressure experiments is one of the unique features of the COMPRES program at NSLS.

Beamline Upgrades: The major beamline upgrades during the period of 2007-2011 have significantly improved the beamline performance and made the beamline operations more user-friendly. It also ensures that this unique facility is supplied with cutting-edge instrumentation.

New Raman/IR spectrometer

A new Raman/IR system has significantly improved the beamline performance. The micro-Raman system at the U2A beamline is not only an important complementary probe to synchrotron FTIR spectroscopy but also crucial for *in situ* pressure calibration at extreme conditions (e.g., a diamond cell in a cryostat or a resistive heating cell). A user-friendly IR/Raman microscope system with the capacity of far-IR reflection with diffraction-limited spatial resolution has been built with support from COMPRES and the Carnegie/DOE Alliance Center (CDAC).

U2A Side Station

With funds in part supplied by COMPRES, a new side station at NSLS-U2A has been constructed, commissioned, and has been in operation since January 2010. The side station includes a Bruker Vertex 80v FTIR spectrometer and a Bruker Hyperion 2000 IR microscope ideally for the mapping of natural samples (*e.g.,* solid and fluid inclusions in thin section), heterogeneous charges from high-pressure experiments, as well as laser heated samples *in situ* at very high pressure in diamond anvil cells.

The high flux and high brightness of synchrotron IR radiation is required for high-pressure experiments using a DAC. An important performance parameter of an IR beamline is the distance a beam travels from the source spot to the end station. This limitation poses problems for experiments that require the highest spatial resolution (*e.g.,* IR mapping of samples below 5 μm). The distance from the synchrotron source to the new side station is only ~3 meters, which effectively eliminates the problems of beam divergence and image distortion.

Ongoing development at the side station is focused on building additional custom IR microscopes dedicated to far-IR experiments at high pressure or low-T, and high-P experiments from far- to near-IR. The side station project will be completed by the end of 2011, with a compact ruby system and enclosure surrounding all instruments on the optical table.

The combined high-pressure and low-temperature techniques are important to address a broad range of problems in planetary sciences. Such capabilities should be attractive to many users. A new cryostat from Cryoindustries with a compact design for accommodating standard symmetric DACs was purchased with COMPRES supplemental equipment funds and was delivered in February 2010. The first user experiment took place on March 10, 2010. These experiments demonstrated that the cryostat performance is well above specifications and user friendly. We can now routinely and reliably perform *in situ* high-pressure/low-temperature IR studies at NSLS-U2A. This new low-temperature capability is being used to investigate the nature of lakes and dark features on Titan, the largest moon of Saturn, and to study nominally anhydrous minerals (for better peak resolution) (Jacobsen, Northwestern U., unpublished).

CO_2 laser heating

The ability to generate simultaneous high pressure and high temperature is crucial for simulating conditions in the Earth's interior. A CO_2 laser heating system is under development at U2A for experiments at extreme P-T conditions with the diamond anvil cell. One of the initial prime scientific targets is to study water solubility in lower mantle minerals. The system includes a 100 W laser and a spectrometer with an OMA-InGaAs detector (Princeton Instruments). The system is initially being developed off-line, including designing enclosures and interlocks to satisfy the formidable safety requirements at all synchrotron facilities. Subsequent development of *in situ* laser heating capability combined with synchrotron IR spectroscopy will then be pursued as a main project under the next phase of COMPRES.

New Opportunities at the NSLS-II

The NSLS-II is a state-of-the-art storage ring under construction at Brookhaven National Laboratory. The spectral coverage of the 3 GeV ring ranges from the far IR to hard X-rays and has up to ~10^4 times higher brightness than NSLS (up to 20 keV). It will be the premier source in the country for performing experiments below X-ray energies of 25 keV and above 50 keV, depending on the insertion device. Advanced X-ray optics will enable high spatial resolution (to 1 nm) and high energy resolution (0.1 meV) at specialized beamlines. Improved capabilities will result for diffraction, imaging, X-ray Raman scattering, X-ray emission spectroscopy, and nuclear resonant scattering.

The facility will accommodate 58 total beamlines including a large number (~27) with advanced insertion devices. The project is on schedule and within budget and the 50% construction milestone was passed in March 2011. Operations are scheduled to start in 2014 and it will be ready for scientific experiments in 2015. The NSLS is scheduled to end operations in October 2014.

COMPRES at NSLS II

In 2010, three proposals for beamlines in high-pressure research – "4DE" (4-D Studies in Extreme Environments), "TEC" (Time-resolved X-ray Diffraction and Spectroscopy Under Extreme Conditions) and "FIS" (Frontier Synchrotron Infrared Spectroscopy Beamline Under Extreme Conditions) - were endorsed by COMPRES and approved by NSLS-II for further development. The proposal 4DE, headed by Donald J. Weidner of Stony Brook University, represents continued development of the program currently running at X17B2, B3, and C with several innovations. Additionally, the COMPRES community is involved in the TEC and FIS initiatives, which would provide distinct but complementary experimental capabilities to the proposed 4DE beamline.

The project beamlines XPD (X-ray Powder Diffraction), HXN (Hard X-ray Nanoprobe), IXS (Inelastic X-ray Scattering), and SRX (Submicron Resolution X-ray Spectroscopy), are likely to provide exceptional additional experimental capabilities to the geosciences high-pressure community for specific scientific questions. While all three high-pressure proposals (4DE, FIS, TEC) were awarded Type I status for further development, construction of these beamlines is currently not scheduled for completion over the course of this proposal period (2012-2017).

Fig 7. The NSLS-II is currently under construction at Brookhaven National Laboratory. Commissioning is scheduled to begin in 2014 and user operations in 2014. Circumference of the ring is 792 meters.

II

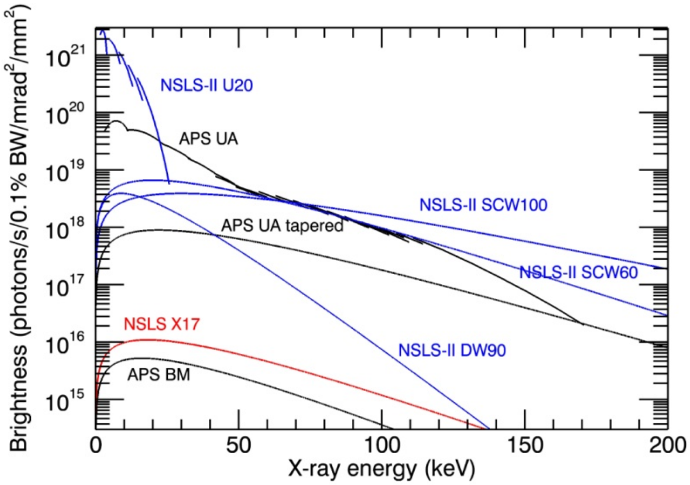


Figure 8. Figures of merit comparing NSLS-II to other synchrotron sources. The synchrotron sources shown include the NSLS-II 20 mm period undulator tuning curve; NSLS-II superconducting wiggler 100 mm period, 6T field; NSLS superconducting wiggler 60mm period, 4T field; NSLS-II damping wiggler, 90 mm period; NSLS X17 superconducting wiggler; APS 33 mm period undulator tuning curve; same APS undulator with gap tapered from 10.5 to 12.5 mm, modeled as a wiggler source; APS bending magnet. From: M. Rivers, APS.

In late 2014, the X17 multi-anvil and diamond-cell programs will transition to the NSLS-II. Our vision for NSLS-II involves a dual approach: 1) establishment of a dedicated high-pressure (both LVP and DAC) X-ray diffraction station at XPD, one of the six flagship project beamlines that are part of the NSLS-II construction project. 2) Build a state-of-the-art high-pressure DAC support laboratory and support scientific staff that will enable forefront DAC research projects to be carried out at many beamlines around the ring through partner user proposals (PUPs) and other activities. This plan has the considerable advantage of allowing experiments to be carried out at the most appropriate beamline (e.g. highest energy resolution or smallest spatial resolution) rather than restricted to a dedicated beamline for which various compromises and tradeoffs in beamline capabilities must be made. Ultimately, we envision one or more fully dedicated high-pressure beamlines in addition to the above. The program outlined here will establish high-pressure as an important component of research at the NSLS-II from its inception and extend the forefront high-pressure geoscience research program active at NSLS for the past ~20 years. We will take advantage of the NSLS-II ring's outstanding spatial and energy resolution for new and improved experiments in high-pressure geoscience research. Our key scientific goals are to constrain sound velocities, elastic properties, and structural variations under Earth interior conditions using X-ray diffraction and inelastic scattering techniques. NSLS-II also offers a unique opportunity to understand texture development, deformation mechanisms, phase relationships in complex systems, and element partitioning across the entire P-T range of Earth's mantle by exploiting the high spatial (sub-micron to 10's of nm) and energy resolution (<1 meV) offered by the NSLS-II beam.

High-Pressure Diamond-Anvil Cell and Multi-Anvil Program at the XPD Beamline

XPD is a powder diffraction beamline that is one of the 6 project beamlines of the NSLS-II. The insertion device is a damping wiggler and will provide tunable energy in the range of 30-80 keV. The beamline will have unique features including fast readout rates and high angular resolution. It is designed to emphasize measurements in various environmental cells including diamond anvil cells.

At the mature stage of the project, there will be both a main branch and a side branch, each of which would be capable of supporting high-pressure experiments. The main branch has 3 in-line endstations: station A houses beamline optics; station C has a diffractometer that can accommodate various sample environments (including diamond anvil cells); station D can house various custom sample environments. Station B is a side station optimized to a fixed high energy (~70 keV) for total scattering experiments (including those at high pressure). Station B can operate concurrently with the C and D stations which share beam. The beamline location and associated lab and office space for XPD are already assigned and the preliminary design report has been completed and approved. The project is on-track for commissioning to begin in 2014.

Through an agreement with NSLS-II, COMPRES will join the XPD beamline and establish dedicated LVP and DAC programs in station D. The large size of this station (~10 m) will enable MAP and DAC set-ups simultaneously. Secondary focusing optics will be used to provide a small beam size (~10 um) for DAC experiments. All user beamtime for XPD will be allocated by the general user proposal review system with science impact as the main criterion for acceptance. COMPRES will support technical and scientific staff with expertise in high-pressure research at XPD. COMPRES will have representatives on the beamline advisory team (BAT), which represents the user community and works with the facility to define the scientific mission and technical scope of the beamline.

At XPD, COMPRES will install the 1000-ton press with interchangeable guide-blocks that will allow continuation of all existing MAP programs. We will furthermore work to develop cells for 'critical zone' studies and 3DXRD capabilities described above. In addition, we will install the hardware and support facilities for a diamond anvil X-ray diffraction station with on-line double-sided laser heating capabilities and *in situ* temperature measurements. This will include a diffractometer optimized for DAC samples and appropriate detectors (CCD, flat panel). We will establish an off-line high-pressure laboratory that will be available to all XPD users and include a range of diamond cell designs and specialized anvils, all necessary sample preparation equipment, capabilities for high-pressure and cryogenic gas loading, laser milling, and fluorescence and Raman spectroscopy.

As part of XPD, high-pressure DAC experiments will be possible in stations B, C, and D. Station D will provide the capabilities of X-ray diffraction with the laser heating that are in strong demand by the user community. High-energy experiments in station B will enable us to enhance our program for high-resolution structural analysis of complex samples including silicate melts and glasses at high pressures using the X-ray total scattering and pair distribution analysis. As part of the XPD beamline, high-pressure capabilities will be immediately available to users on opening of the NSLS-II. There is overlap in scientific and technical agendas between the COMPRES community and that of XPD, which foster collaborations and developments that would not arise otherwise. COMPRES participation in XPD will initially be for three years beginning in October 2014, covering the period of this proposal. After that time, a thorough review will define further directions.

Infra-Red Beamline at the NSLS-II

The National Synchrotron Light Source II (NSLS-II) will provide an ideal infrared source to couple high *P-T* DAC techniques with FTIR spectroscopic measurements. This will make it possible to address a broader range of scientific questions and challenges related to the Earth and Planetary Sciences. A proposal titled "Frontier Synchrotron Infrared Spectroscopy Beamline under Extreme Conditions (FIS)" has been approved by the NSLS-II Scientific Advisory Committee, and the conceptual design is currently underway. The proposed high-pressure IR facility has a large-gap (90 mm) dipole infrared source and extraction port providing the full IR spectral range (including the far-infrared) to two experimental endstations. One of the endstations will be for the DAC, and the other will be for a dynamic compression (such as a gas-gun) apparatus. All equipment and techniques currently available or under development at NSLS U2A will be transitioned to the new FIS facility at NSLS-II. The experimental capabilities of the two IR endstations are complementary to other high-pressure X-ray diffraction beamlines proposed for the NSLS-II.

Overall, the proposed high-pressure IR beamline should produce spectral brightness equal to the world class performance of the NSLS in the far-IR region, and up to an order of magnitude greater in the mid-IR range which is crucial for the *in-situ* high *P-T* IR studies on hydrous and nominally anhydrous minerals. In addition, the ring is designed for an extremely stable beam, which is an important characteristic for the standard rapid-scan interferometric techniques for infrared time-resolved applications. Typically, the RMS pulse length will be in the range of 15-30 picoseconds and the time between bunches will be 2 nanoseconds.

Station A – Diamond Anvil Cell Station

Station A will be an integrated and dedicated IR beamline for experiments at simultaneous high pressure and variable temperature. The experimental setup will include the Bruker Vertex-80v FTIR spectrometer attached to a Hyperion-2000 IR microscope and other custom IR microscopes, a permanent CO_2 and fiber laser heating system, a compact cryostat with CVD diamond windows, and micro-Raman. The station will be optimized for the following high-demand experimental techniques:

Infrared spectroscopy at high-pressure and ambient temperature: Measurements of phonon vibrations, phase transformation, band structures, and optical properties at high pressure.

In-situ laser heating infrared spectroscopy at high P-T conditions: Studies of hydrous and nominally anhydrous minerals under lower mantle conditions to determine the incorporation of water (as hydroxyl) in minerals; synthesis and characterization of new materials under high *P-T* conditions.

In-situ spectroscopy at high pressure and low temperature: Measurements of phonon vibrations, phase transformations, band structure, and optical properties at high pressure and low temperature using synchrotron IR, Raman scattering, and visible-UV spectroscopy.

Station B – Dynamic Measurement Station

Station B will be a multi-purpose station for dynamic shock wave measurements led by a team from Sandia National Laboratories. Impact experiments, using gas or powder launchers, will be possible. Pulsed power systems, which utilize electromagnetic compression, will be considered for the future. Infrared/visible reflectance and/or transmission will be the primary diagnostics in the dynamic compression experiments. Secondary diagnostics, such as laser interferometry, will be used to monitor the performance of the drivers. High-speed diagnostic development and testing may be performed at Station B when dynamic compression experiments are not underway. This station will be also made available for other dynamic measurements, such as transient laser heating.

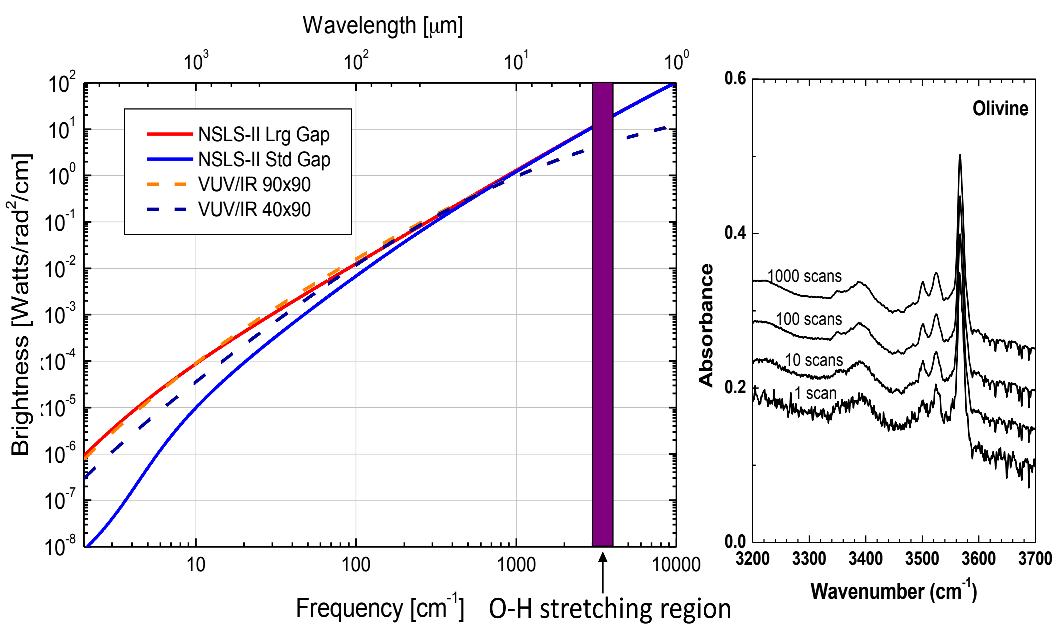


Figure 9. Brightness of NSLS-II Large Gap Source compared with current VUV/IR source at U2A (left). In addition to increased brightness, the stability is expected to be 1000x better, which is crucial for weak samples requiring multiple, scans (right).

Continued support through COMPRES will be essential to ensure a smooth transition of the high-pressure IR program from NSLS to NSLS-II. In return, an advanced IR facility for the entire COMPRES community will be available as early as 2015 at NSLS-II.

DAC Program at Other NSLS-II Beamlines and BNL facilities

NSLS-II will provide new and exciting experimental capabilities for the COMPRES community. Additional beamlines with specialized capabilities for which novel and forefront DAC experiments can be carried out are described below: Together with XPD, a total of 4 of the 6 project beamlines present opportunities for forefront high-pressure research.

Other NSLS II Project Beamlines

Inelastic X-ray scattering beamline (IXS): Inelastic X-ray scattering provides a powerful, high-resolution (~meV) technique for studying vibrational dynamics and electronic excitations at high pressures. For geophysics, the key capability is to measure the anisotropic elastic wave velocities as well as characterizing the detailed lattice vibrational spectrum. IXS experiments complement and extend more standard techniques such as Raman and Brillouin scattering at high pressure, overcoming limitations of optical experiments while providing unique information on phonon dispersion. Both single-crystal and powder experiments at high pressures are possible. Applications such as X-ray Raman will also be feasible. X-ray Raman scattering is a medium-resolution (~1 meV) element-specific technique that provides similar information as XAS and EXAFS with the key advantage of not requiring very soft X-rays, which do not penetrate the DAC. The IXS beamline is designed to take advantage of the brightness and flux of the NSLS source by operating at ~10 keV and provide both medium (1 meV) and high (0.1 meV) resolution IXS capabilities, achieving an order of magnitude improvement in resolution over existing beamlines around the world. Capability to accommodate DAC experiments has been built into the projects since inception (i.e., focusing to achieve ~1-10 um beam sizes).

Hard X-ray nanoprobe beamline (HXN). This beamline is dedicated to providing high spatial resolution capability. Spatial resolution as low as 1 nm at 6-25 keV energy is the long-term goal. For high-pressure experiments, 10-100 nm beam sizes with adequate working distances for diamond anvil cell will be attained. Submicron beam size and nano-diffraction capability is a frontier research direction for the high-pressure geosciences. Phases synthesized using the laser-heated DAC often have sub-micron dimensions. The beamline provides capabilities for analyzing very small single crystals, for selecting individual grains for study in a complex multi-component sample, and for miniaturization of the DAC to achieve much higher peak pressures.

Sub-micron X-ray spectroscopy beamline (SRX). This beamline is designed for characterization of heterogeneous materials and structures on micron to nanometer scales. Planned capabilities with potentially novel DAC applications include: micro- X-ray absorption spectroscopy; X-ray emission spectroscopy; micro diffraction, and tomography with sub-micron resolution. Focusing capabilities operating up to 25 keV will provide a 100 nm-sized beam with high flux compared to APS.

DAC Fabrication and Characterization Capabilities

Our high-pressure technology center and team at NSLS-II (described below) will also develop a micro/nano fabrication facility and an advanced analytical facility to develop DAC technology and analysis, taking advantage of the Center for Functional Nanomaterials (CFN) at BNL. The CFN is a user facility providing access to state-of-the-art capabilities including nanofabrication, lithography, dual beam SEM/FIB, deposition and etching, advanced electron microscopy, combined AFM/Raman instrumentation as well as synthesis and spectroscopy instrumentation. These resources offer important new capabilities for advanced sample preparation through specially designed and modified anvils and sample geometries as well as detailed chemical analysis of samples through extraction of recovered samples using the FIB technique together with high-resolution TEM analysis of composition and structure at the sub-micron level. The synthesis of high-resolution beamline capabilities, advanced analytical instrumentation, and staff with the expertise to advance the forefront of high-pressure DAC technology and synchrotron techniques for geoscience applications is a unique combination that promises to make the COMPRES/NSLS-II program a worldwide leader in high-pressure Earth science and deep Earth geophysics research.

COMPRES Technology Team: COMPTECH at NSLS-II

COMPRES resources will be used to establish a team of scientists and technicians at Brookhaven National Laboratory, who will develop and promote synchrotron based geosciences research. The objectives for the team would be:

- Assure successful experiments for COMPRES community members.
- Develop new experimental capabilities for beamlines at NSLS-II (e.g. next generation pressure tools, data evaluation tools etc.).
- Conduct research at the forefront of geosciences utilizing NSLS-II and Center for Functional Nanomaterials (CFN) experimental capabilities.
- Operation of an outreach program, which will provide training and education to researchers in the geosciences community and develops new user communities in the field of Earths Sciences.

In addition to beamline support, the COMPRES technology team will assist COMPRES users in pioneering methods for DAC sample preparation and post-run quantitative analysis using facilities at the CFN. Micromachining gaskets, insets and samples, will increase the success rate for experiments that are pushing the envelope of what is technologically possible. Samples recovered from high-pressure DAC experiments could be further characterized at the state-of-the-art electron microscopy facilities at the CFN or, after the transition of the X17 high-pressure program, at the nanoprobe beamlines (HXN and SRX).

The benefit for NSLS-II is an independent on-site center of expertise in high-pressure geosciences. Furthermore, the envisioned technique and tool development of the team will add new and complementary capabilities to the existing experimental infrastructure at NSLS-II. The outreach and training effort will lead to (i) a broader user community for NSLS-II beamlines, (ii) a higher success rate for cutting-edge geosciences experiments due to well trained users, and (iii) contribute to development of the next generation of users and facility scientists.

We request funds in Years 3-5 for an experienced Research Scientist to establish the COMPRES Technology Office at NSLS-II. The activities of this person will be coordinated with those of a COMPTECH office at the APS (see program description below) and will be managed by the COMPTECH management team, the Technology Advisory Board (see below).

Equipment Upgrades and Support Laboratory

Our current high-pressure equipment base has been significantly upgraded with COMPRES support and will allow us to establish a first-rate high-pressure program at NSLS-II immediately. This will be augmented with a number of equipment updates in the 2014-2017 period. The main equipment upgrades proposed for this period will be:

--Table-top Kirkpatrick-Baez mirrors for XPD beamline providing ~10 μm focal spot

--Gas loading system at NSLS-II. This system is essential for providing quasi-hydrostatic media and thermal insulation for laser heating.

-- On-line ruby spectroscopy system. In combination with diaphragm membrane pressure system, the time used for realignment and pressure changes will be drastically reduced

-- Portable laser heating system. We have already developed a compact design for laser heating, and we will modify to develop a modular, portable system that can be used at different beamlines.

-- We will be well positioned to tackle time resolved experiments at high pressure, opening a currently rather unexplored field of in situ studies of phase transition kinetics, reactions, and crystallization.

COMPTECH: COMPRES Technology Center at Argonne

Summary: Advanced synchrotron X-ray techniques that have been developed at highly specialized beamlines offer unique opportunities to understand the properties of matter under extreme pressure-temperature conditions. These techniques are not readily accessible to the non-expert user, nor are they necessarily easily adapted for high pressure-temperature experimentation of interest to the COMPRES community. The COMPRES Technology Center is a new initiative that will partner with beamlines to develop high-pressure capabilities, and will develop software data analysis tools that make these beamlines accessible to the broader COMPRES community. COMPTECH will enable new ways to measure sound velocities and elastic properties on a wider range of samples under extreme conditions, capabilities for nanodiffraction on sub-micron crystals retrieved from static or dynamic compression experiments, and will allow determination of strain states and texture evolution studies in polycrystalline rock samples in diamond anvil cell.

The mission of COMPRES is driven by its scientific goals, but it is the experimental technology available at central facilities such as synchrotron beamlines, that enables this science. Argonne National Laboratory's synchrotron source, the Advanced Photon Source (APS) is currently the leading central facility for synchrotron science in the United States. APS beamlines are heavily utilized by members of the COMPRES community to carry out their research. A major midterm upgrade of the APS will significantly boost the current capabilities and increase the amount of beam time available to users. Since its inception, COMPRES has maintained a presence at the APS by funding Infrastructure Development projects located at high-pressure beamlines. The success of these projects has had a significant impact on the COMPRES community and their research output, as well as on the APS itself. Thus far COMPRES has not operated a permanent facility at APS. This proposal requests funds to create a new facility - COMPRES Technology Center (COMPTECH) at Argonne - with the main mission to initiate, facilitate and coordinate new Partner User Proposals that will create new capabilities and improve the ease of use of state-of-the art facilities at existing beamlines at APS for the COMPRES community. Partnerships with existing beamlines will enhance novel experimental technology and instrumentation suitable for high-pressure Earth science research at these facilities. A letter in support of the COMPTECH initiative is provided by G. Brian Stephenson, Interim Director of the APS, as supplementary information to this proposal.

At APS regular beam time proposals allow users to carry out individual synchrotron experiments. A special category of proposal, called a Partner User Proposal (PUP) has broader scope. In addition to science goals, PUPs also usually address development of new capabilities or methodologies that are in demand by broad community of users at existing beamlines. PUPs span a longer time period (typically 3 years), require the user to contribute to the project in a substantial way (personnel, instrumentation, or responsibility for part of the development (e.g. software)), and in return include guaranteed access to some portion (typically up to 15%) of the beam time available at the facility for the duration of the project. The PUP model of supporting new beamline facilities will bring the advantage of assured access to a specified fraction of beam time to COMPRES researchers at a cost incomparably lower than funding and operating a beamline. This will allow COMPRES influence on the direction of instrumentation and methodology development at participating beamlines. The PUPs will also allow for flexibility in addressing the most important current needs of the community (typical PUP projects last 2-3 years, and can be renewed though a new proposal if both sides are interested). Carrying out several separate PUP projects independently would still be moderately costly at the scale of COMPRES' budget, as each project would require a separate independent investment in personnel and/or instrumentation. The main idea behind COMPTECH is to streamline and coordinate these independent projects though centralized technology-oriented resources that can be utilized and shared to support several PUP projects at once. With the COMPTECH located at Argonne and expected to eventually include several staff scientists, assigning personnel to PUP projects will be much easier than having to fund a new position and finding a skilled candidate each time. A very significant advantage of having long-term staff, as opposed to typical

2-year term postdoctoral researchers working on PUP projects will be accumulated experience and expertise which will make the contributions of these scientists to new projects much more significant.

In order to effectively operate Partner User programs involving several synchrotron beamlines COMPRES will need dedicated and experienced technology-oriented staff. This proposal requests funds to hire an experienced research scientist, above the postdoctoral level, to serve as the COMPRES Technology Officer (CTO) and co-PI of the COMPTECH Center at Argonne. This person would have a strong technical background (synchrotron technology, scientific instrumentation, software development, high-pressure techniques). The CTO will have four main goals during the five years of this project duration: (i) Establish a successful technical development program (involving instrumentation, method and/or software development) focused on issues relevant to the COMPRES community and emphasizing transferability/portability of the solutions so they can be applied at many beamlines, (ii) Establish a successful research program in mineral physics based on the high-pressure facilities available at the APS; (iii) Prepare and submit Partner User Proposals to beamlines at APS that are identified by the COMPRES Executive Committee as important for community progress (currently Sectors 3, 30 and 34 have been identified as potential Partner User Proposal facilities, and have expressed interest in a PUP relation with COMPRES) and (iv) Through writing and submitting grant proposals spearhead efforts to raise additional funds needed to carry on effective PUP projects. Additionally, the CTO would serve as a liaison and point of contact with the APS administration regarding current or future needs or initiatives that the COMPRES community might identify.

The beamlines identified as possible locations of the first three COMPTECH PUP projects already have, to varying degrees, been involved in research with the mineral physics community or, as in the case of the COMPRES relationship with Sector 3, are part of a successful Earth science high-pressure program. All of these facilities offer unique experimental capabilities that are of potential very high impact on the field of mineral physics, but have not yet been heavily utilized due to limited access and technical challenges. All of these facilities struggle with limited staff and lack of easy-to-use and intuitive instrument control and/or data collection software. These shortcomings are a huge impediment when trying to build a broad community-wide user base for the mineral physics community. COMPTECH staff will focus on making these techniques easily accessible and optimized for the needs of the COMPRES community, with significant benefit for the experimental capabilities, efficiency of beamtime utilization, and scientific output.

COMPRES will appoint a Technology Advisory Board (TAB) to oversee and guide the activities of COMPTECH. TAB will be comprised of synchrotron technology experts, members of the central high-pressure facilities (e.g. HPCAT, GSECARS), managers of the other COMPRES facilities (ALS, NSLS) and mineral physics researchers. The initial members will be Przemyslaw K. Dera (chair), Guoyin Shen, Quentin Williams, Lars Ehm, Yanbin Wang, Robert T. Downs, and Daniel L. Farber. The President of COMPRES as well as chairs of the two standing committees will serve as *ex officio* members of the TAB. The TAB will oversee and coordinate all other COMPRES efforts at non-COMPRES beamlines, such as the IXS and Mossbauer project at Sector 3, and the COMPTECH efforts at the NSLS-II.

In the process of developing new, unconventional techniques with novel capabilities, an effort to build a wide community of users requires outreach and education. The community will be informed about new capabilities and trained in general aspects of experiments through workshops at the APS and at the COMPRES annual meeting. COMPRES has an excellent track record in implementing new capabilities at beamlines and in building broad user bases. Examples are the IR beamline U2A at the NSLS, the Brillouin scattering system at GSECARS, and the IXS project at Sector 3 of the APS. We plan similar efforts to attract a large community of new Earth science users to the facilities that are developed by COMPTECH. The software developed at COMPTECH and information about new experimental capabilities at participating beamlines will be distributed through a COMPTECH website. Through its association with Argonne National Lab COMPTECH will also participate in the Argonne-wide summer internship for undergraduates program (funded by DOE).

There are currently several organizations at APS that focus on and promote high-pressure science, including GSECARS, HPCAT. Another organization focused on high pressure, HPSynC, has a primary emphasis on materials sciences. COMPTECH will be distinct from these organizations in that it will be: (i) 100% focused on geoscience and mineral physics (ii) Actively engaged in collaboration with new synchrotron beamline facilities through Partner User Projects (iii) Priorities, research, and development goals will be set by the COMPRES community through the Technology Advisory Board. Free from regular user support and facility maintenance duties, the COMPTECH personnel would be able to devote a more significant portion of their time to developments identified as COMPRES priorities (iv) Significant effort (50%) will be devoted to development of transferable, shared instrumentation, methodology and software solutions for high-pressure geosciences. The majority of this will be done in collaboration with the existing expert base at GSECARS, HPCAT and HPSynC.

COMPTECH will enable a new suite of sophisticated synchrotron tools to address a broad range of important scientific questions in studies of the Earth's deep interior. Specific capabilities that will result from COMPTECH and the science that will be addressed include:

Studying acoustic phonons with non-resonant momentum-resolved inelastic X-ray scattering (Sectors 30 and 3): In the last decade, synchrotron-based momentum-resolved inelastic X-ray scattering (IXS) has been developed, allowing measurements of sound velocities and elasticity. Measurements on single crystals give velocity anisotropy. These experiments require 3rd generation synchrotrons and high energy resolution (1 meV range). Samples for IXS do not need to be transparent, which is an advantage over light scattering techniques such as Brillouin scattering. This opens up the possibility to measure the velocities and anisotropy of possible core-forming materials at high pressures and temperatures. Extracting information on elastic anisotropy is a promising area for the future, but will take significant developments in software and data analysis tools. To fully exploit this technique for the geosciences we plan to develop: 1) A basic set of symmetry-based crystallographic software for the prediction of phonon intensities and scanning directions given a sample orientation matrix; 2) Integration of *ab initio* tools into the experimental development program to predict the position and behavior of phonon modes as a function of intensive parameters; 3) Standardized software for the extraction of the phonon density of states from powder samples; 4) Software for the extraction of full phonon dispersions from measurements on polycrystalline samples. Individual users (especially new ones) cannot be expected to develop these complex capabilities on their own. Such a set of tools would not only facilitate a new class of experiments but would have an especially large impact on the types of properties we could extract from earth materials at extreme conditions.

*Development of data analysis software for in-situ and ex-situ characterization of crystal structure, chemical composition and morphology and strain/stress state of sub-micrometer crystallites***:**

The leading nanodiffraction beamlines, including Sector 34 at APS, offer nanofocusing capabilities reaching 200 nm. This progress opens new opportunities in high-pressure science, making possible experiments at much higher-pressure conditions (above 2 megabars) and reducing thermal gradients in laser heating experiments. Even with polycrystalline and chemically complex samples, nanobeam techniques offer possibilities to obtain information about the structure and composition of the individual grains without the complications of overlapping signals. While the progress in this field has been impressive, the data analysis solutions available today do not yet offer full functionality for identification and structure determination of unknown phases (e.g. produced as a result of a phase transition, high-temperature chemical reaction, or incongruent melting). We plan a formal collaboration with APS Sector 34 to further development the experimental methodology and data analysis method of nanodiffraction, including *ab-initio* structure determinations of unknown phases from sub-micrometer sized grains, and strain/stress mapping in polycrystalline aggregates. The latter application is identified as a new technology of interest to the proposed 4DE high-pressure beamline at the NSLS-II.

Develop capabilities to study atomic structure and properties of highly disordered and non-crystalline Earth materials:

Knowledge of the structure and properties of highly disordered and non-crystalline Earth material at pressure and temperature conditions of Earth's interior are at a comparatively primitive stage. The lack of experimental data on these important classes of Earth materials limits our understanding of important topics in Earth structure and evolution such as the formation and ascent of magma, the origin of large igneous provinces, the role of magmatic liquids in mass and heat transfer in Earth's interior, and the influence of disorder on the elasticity of minerals.

Recent developments in X-ray total scattering now allow the study of atomic arrangements in highly disordered and non-crystalline Earth materials (Ehm et al., 2007; Michael 2007). However, some challenges on the experimental and data evaluation side remain, such as: (i) reliable inert containment of liquids in pressure vessels, (ii) improvement of angular access in pressure cells, and (iii) development and/or adaptation of data evaluation methods based on large atom assemblies (e.g. Reverse Monte-Carlo approaches).

The CTO in this project will engage researchers at APS Sectors 1 (High-Energy X-ray Scattering beamline) and Sector 11 (Dedicated Pair Distribution Function and High-energy Diffraction beamlines) to further develop in situ X-ray total scattering technique. We will coordinate with the program at X17B3 at the National Synchrotron Light Source (NSLS) on optimization of pressure cells, data evaluation, and data based modeling. This project will bundle efforts currently progressing independently at APS and COMPRES supported beamline X17B3at NSLS. The instrumentation and methodology development will benefit the scientific program at the proposed high-pressure beamline 4DE at NSLS-II.

5.2 COMPRES Infrastructure Development

An Infrastructure Development program has been an integral part of the COMPRES structure from the beginning, with one of the COMPRES standing committees dedicated to overseeing this program. A number of highly successful, even transformative projects have come out of this program. For example, building a gas loading system at GSECARS significantly raised the level of all high-pressure diamond cell research in the US at a very modest cost (~$85K). Performing very nearly hydrostatic DAC experiments above 15 GPa is now the norm, not the exception, resulting in higher-quality data from most DAC experiments. Single-crystal X-ray diffraction at pressures above 10-15GPa would probably not be feasible without gas loading in Ne or He, because of peak broadening from non-hydrostatic stresses. Another example is the Mössbauer spectroscopy lab at APS. We now know that the Fe^{2+}/Fe^{3+} ratio can dramatically influence physical properties and phase transitions (e.g. high-spin low-spin transitions), making the characterization of the valence state of Fe crucial for many experiments. The best method of measuring valence states of Fe is Mössbauer, but Mössbauer labs are not common, and no central facility existed. Until one year ago, US researchers with appropriate foreign connections were sending samples overseas for characterization; those without a connection were out of luck. The COMPRES Mössbauer project makes a high-quality facility available to the entire community and, equally important, provides technical support for using it. COMPRES issues a CFP every October for Infrastructure projects. Typically we receive 5-8 proposals, and typically 1-2 new projects are started each year. We have recently made an effort to encourage the submission of proposals on education and outreach. The Infrastructure Development program made it possible to fund two recent COMPRES efforts in E&O by (P. Burnley, UNLV).

We describe below the Infrastructure Development projects that have been recommended thus far by the Infrastructure Development and Executive Committees for the next five years of COMPRES.

Multi-anvil Cell Development Project

PIs: Kurt Leinenweber, James Tyburczy, and Thomas Sharpe, Arizona State University

The multi-anvil cell assembly development project has existed as an infrastructure development project since the inception of COMPRES. The purpose of the project is to develop multi-anvil cell assemblies and to make them readily available to any laboratory with a multi-anvil press. A series of cell assemblies of different sizes and pressure/temperature capabilities has been developed, using both preexisting and new materials and techniques. These cell assemblies involve many components with complex shapes and compositions that must fit together and function as a successful working high-pressure cell. All components – the pressure medium, gaskets, thermocouple, thermal insulation, furnace, and sample container – are specially made and are not generally available "off the shelf." This requires a significant amount of development to achieve "first pressure" in a new laboratory starting from scratch. This project has made it possible for many laboratories, both new and established, to achieve predefined pressure/temperature conditions readily, and to more quickly pursue the research that their laboratories were created for. This has been a major cost and timesaving for many multi-anvil labs worldwide. In 2010-2011, the project supplied 930 cell assemblies to 42 high-pressure labs.

Since the beginning, a parallel purpose of the project has been to provide a way for users to readily obtain large-volume high-pressure data on a synchrotron beam line. A series of cell assemblies that are based standard designs but are modified to allow the passage of X-ray beams, have been simultaneously developed and used for *in-situ* studies by groups who have received synchrotron beam time. The familiarity of the assemblies to those who use them offline makes these modified assemblies easy to use, allowing the researchers to focus on data collection and interpretation of their experiments, rather than having to learn to use entirely new cells.

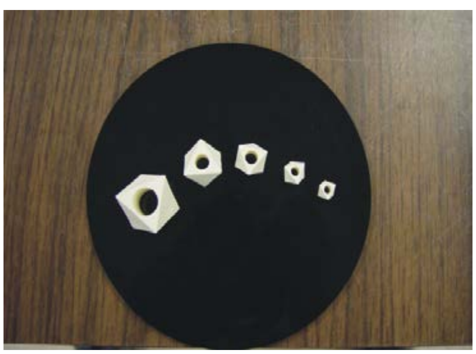



Figure 10. (Left) Five injection-molded octahedra, used in five sizes of multi-anvil cell assemblies in the COMPRES project, ranging from 8 mm to 25 mm. Larger assemblies are used for lower pressures and larger sample volumes, while the smaller assemblies are for higher pressures, up to 27 GPa for the 8 mm assembly. (Right) 3 mm "Fei-style" cell assembly used to make $MgSiO_3$ perovskite. Carbide cubes (grey), ceramic octahedron (brown), rhenium metal furnace, and two type-C thermocouple wires extending from the octahedron are all visible.

The next stage of this project will feature the following:

1. Standard assemblies that are currently in production will continue to be provided to the community. These assemblies are in widespread use many laboratories around the world. Cost recovery from these assemblies makes this part of the project self sustaining.

2. We currently lack higher temperature capabilities at lower pressures (pressures below 15 GPa and temperatures above 1200°-1500°C). We will develop and supply cell assemblies specifically to reach 2000°C and above in the low-pressure range. This cell will enhance studies of melting and phase equilibria at upper mantle and transition zone conditions.

3. We will develop and optimize larger-volume assemblies that will enhance the synthesis of larger samples. Initial designs have been developed during this project but are not yet routine to fabricate and some further work on the cell assembly is needed. This assembly will be useful for growing large single crystal samples and larger quantities of materials for recovery (e.g. superhard solids).

4. Some of our standard assemblies are not performing as well as expected. We will devote effort to diagnosing and solving these problems.

5. There is growing demand for cell assemblies that can be used for *in situ* experiments at X-ray beamlines such as X17B2 of the NSLS (Leinenweber 2006; 2011). We plan to develop a new set of assemblies optimized for synchrotron X-ray experiments. The key development needed is to optimize the accessible pressure and temperature range while drastically reducing absorption of the X-ray beam. X-ray absorption due to containing materials is a key limitation in large-volume press experiments due to attenuation of X-rays and extraneous signals, which can interfere with desired measurements. This will be achieved by having virtually the entire X-ray beam path composed of low atomic number materials. Other areas of development for synchrotron use will be in ultrasonics, deformation, and electrical conductivity experiments,

6. Several other initiatives will be initiated, including work on pressure standards and improved sample encapsulation techniques.

Applications of FIB/SEM CrossBeam Technology for High-pressure Research

PI: Yingwei Fei, Carnegie Institution of Washington

Very small sample sizes (micron to sub-micron dimensions) are characteristic of ultrahigh pressure experiments that simulate conditions of deep Earth. There has been significant development in probe techniques associated with intense synchrotron radiation sources. What have been lagging in high-pressure research are probes of the chemistry of materials under extreme *P-T* conditions. This was clearly voiced by the COMPRES community at a Town Hall meeting held at the 2010 Fall AGU meeting. An additional need that was identified as urgent by a broad cross section of our community was the ability to micro-machine samples, diamond-anvil sample chambers, and anvils themselves for the next generation of ultra-high pressure experiments. The Infrastructure project by Fei addresses these needs, which were identified through community input as one of the highest priorities for the coming five years.

A state-of-the-art Carl Zeiss AURIGA CrossBeam FIB/SEM (focused ion beam/scanning electron microscope) system has recently been installed at the Geophysical Laboratory. The system is dedicated for high-pressure research and has been used for characterization of high-pressure samples, micro/nano-fabrication, and sample preparation for various analytical tools. The CrossBeam FIB/SEM Workstation integrates a FIB system and a field-emission scanning electron microscope (FE-SEM) in one powerful instrument.

The use of FIB techniques has revolutionized the preparation of samples for micro- and nano-analysis in material sciences. The new generation of CrossBeam FIB/SEM systems combine precision milling and ultra-high resolution; it is a versatile instrument. The principal emphasis of our FIB applications is to advance high-pressure research. We have identified several applications of FIB technology for deep-earth study, including precise sample recovery from diamond cell and other high-pressure experiments for composition and texture analyses, 3D reconstruction of quenched high-pressure samples to study melt migration, and micro/nano-fabrication of smart anvils for transport property measurements and enabling new design of high-P-T experiments.

Many COMPRES users may have access to a FIB facility in their own institutions. The challenge for the high-pressure community is to access expertise to deal with delicate high-pressure samples and applications specific to high-pressure research. As a user of a materials science orientated FIB facility, the high-pressure user commonly does not have enough time to develop FIB tools specific for high-pressure experiments, or cannot get the type of help needed to deal with high-pressure samples from a traditionally trained FIB technician. This infrastructural development program will provide training for COMPRES users to acquire skills in FIB technology for high-pressure research. The program will develop basic FIB tools specific for high-pressure research that can be applied at any FIB facility after training. Specific tools needed for the research of participants will be developed. COMPRES will support a ½-time research associate who will be available to consult with users to develop needed FIB training and tools for high-pressure research.

The key aspect of this ID project is to empower COMPRES users to effectively use FIB technology to solve deep-Earth problems. It will open doors for new research opportunities and greatly improve our scientific productivity. The involvement of COMPRES community will lead to novel uses of FIB technology and advance a number of scientific research fields.

Mineral Physics on the World Wide Web – A Comprehensive Approach

Pamela Burnley and Sylvia-Monique Thomas, Department of Geoscience, University of Nevada, Las Vegas

Both students and the general public increasingly rely on internet sources of information in all aspects of their lives. However, the web presents a bewildering amount of information that is ranked by search engines in terms of popularity rather than veracity. To maximize our efficiency in reaching the public we propose to use a two pronged internet based approach; improving the education and outreach section of the COMPRES web site and populating Wikipedia with articles about mineral physics topics.

COMPRES Wikipedia project

Wikipedia is a free multilingual web-based encyclopedia written collaboratively by volunteers. According to Wikipedia, it has become the largest and most popular general reference work on the Internet, with approximately 365 million readers. Despite the fact that it is a general reference work, fairly esoteric topics, for example "Martensitic transformation", "Burgers vector", "von Mises yield criterion " receive comprehensive and accurate coverage. In contrast COMPRES-related topics enjoy spotty coverage, are not interlinked to related pages or do not mention mineral physics. For example "Diamond Anvil Cell" has a good entry but entry does not mention geophysics as a possible use of the DAC. The entry for the Earth's interior covers seismology but does not mention mineral physics. With 365 million readers, Wikipedia is not a bad place to put mineral physics information for people to find.

The COMPRES Wikipedia project will encourage graduate students and postdocs to generate articles for Wikipedia and to link existing articles to their article so that their article can be more easily found. The articles will also be loaded on the COMPRES web site. COMPRES will facilitate this activity by providing editorial guidance including feedback on writing for the general public and a small stipend for each completed work. To kick off the project, Burnley and Thomas will generate new articles and modify or correct existing articles. In addition to building a permanent mineral physics presence on Wikipedia, the project will also help graduate students and postdocs improve their communication skills and encourage them to continue making contributions to education and outreach.

Undergraduate Portal to Mineral Physics

COMPRES will expand the outreach portion to its website with a goal of engaging undergraduates. The website will include information on how to pick a graduate program and connect with an advisor, profiles of mineral physics jobs including first person articles by beamline scientists, faculty, and national lab researchers, list of mineral physics faculty currently searching for graduate students, introductory overviews of COMPRES community facilities and other mineral physics topics. Burnley and Thomas will provide the content for the website and coordinate posting the materials with the central office.

Inelastic X-ray scattering and nuclear resonant scattering under extreme conditions

(Sectors ID-3 and ID-30 at the Advanced Photon Source)

PI: Ercan Alp, Argonne National Laboratory

High-resolution inelastic X-ray scattering (IXS) techniques provide the Earth and Planetary science community with unique opportunities for new and exciting results on the properties of materials at high pressure and temperature conditions. Our infrastructure development project is aimed at outreach to the COMPRES community on the capabilities and use of these techniques and at creating state of the art inelastic X-ray scattering techniques for characterizing the properties of materials under the high-PT conditions of planetary interiors, as well as geophysics and geochemistry of rocks, minerals, and meteorites. We intend to provide three different advanced techniques

1) Synchrotron Mössbauer Spectroscopy, **SMS** and imaging (Sector-3)
2) Nuclear Resonant Inelastic Scattering, **NRIXS**, and imaging (Sector -3)
3) Momentum resolved inelastic X-ray scattering, **IXS** (Sector 3 and Sector 30)

This project requests partial support (at the 2/3 level) for a post-doctoral researcher to work at Sector 3 of the APS. The responsibilities of the post-doc will be: 1) working with the COMPRES community in developing competitive proposals for beamtime; 2) assisting COMPRES users of Sector 3 during their beamtime, and on analysis of their results (which is formidable); performing education and outreach by organizing workshops; 4) assisting all users of the conventional Mössbauer spectrometer at the APS (see below); 5) writing instructional manuals for the complex software used in analyzing results. This post-doc will be a primary point of contact for the COMPRES community with Sector 3.

The IXS technique, which measures phonon dispersion relations from single crystals, powders, glasses and liquids, is also maturing for geophysical purposes as a result of advances in X-ray focusing optics, and development of two advanced spectrometers at the APS: HERIX-3 and HERIX-30. Geophysical applications include investigations of spin transitions (Lin et al., 2008; Catalli et al., 2010) and the properties of core materials at high pressures and temperatures (e.g., Mao et al., 2008; Murphy et al., 2011)

Both of these methods are in many ways ideally or even uniquely suited for addressing a number of important geophysical questions. While Nuclear Resonant Scattering, **NRS** provides information on electronic, vibrational, and elastic properties, such as the density of states and sound velocities, momentum-resolved IXS directly gives the dispersion relation of low-energy collective excitations to provide directional information on vibrational and elastic properties, such as the elastic tensor and sound velocities.

During the last 5 years we have initiated high-pressure experiments at the new IXS beam line (sector 30-ID) of the Advanced Photon Source and improved the experimental capabilities of the NRS and IXS beam line (sector 3-ID) to enhance its performance for high-pressure research. We will continue to offer special capabilities for SMS, NRIXS, IXS (HERIX-3) and X-ray diffraction in 3-ID-B and 3-ID-C stations, combined with laser heating or external heating. We are adding the HERIX-30 spectrometer as a new tool available for the COMPRES community, located at Sector 30.

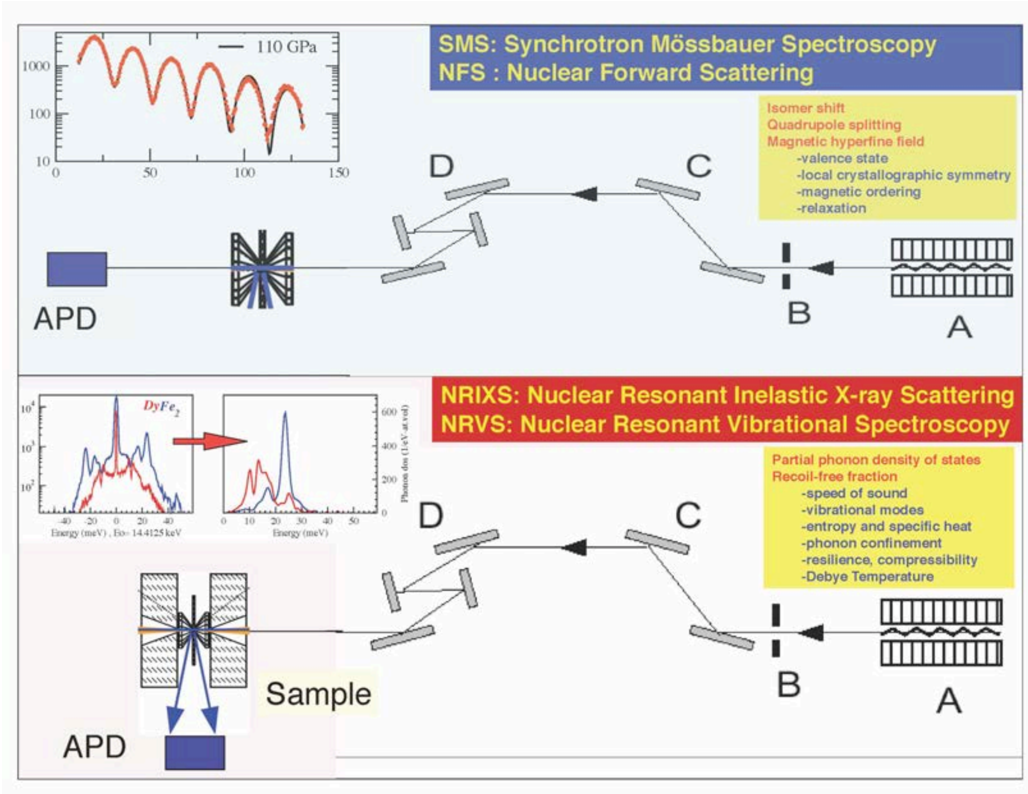


Fig. 11. Schematic experimental set-ups for Synchrotron Mossbauer Spectroscopy (valence states, magnetism, local symmetry) and Nuclear Resonant Inelastic X-ray Scattering (Sound velocity, entropy and specific heat) at Sector 3 of the APS.

Over the next few years we will be able to increase the number of users at Sector 3 by reducing the beamtime needed for experiments. This will increase the number of COMPRES users that can be accommodated. For SMS, this will be possible with the introduction of a mechanical chopper. We will develop an upgraded HERIX instruments with increased number of analyzers, combined with in-situ X-ray diffraction and pressure-readout, and improve laser-heating capability for high P-T experiments.

We will offer the use of a laboratory-based (conventional) Mössbauer spectrometer, suitable for high-pressure work, and data analysis support. This facility is especially useful in developing strategies for data analysis obtained at the beamline by characterizing the samples ahead of time, as well as providing starting parameters for the data analysis of the time domain SMS. Sample purity and valence state are issues that beset every experiment, and the availability of this laboratory year round is an enormous asset for the COMPRES community. A micron-resolution Mössbauer microscope facility for mineralogy will also be available. These instruments are not generally available in university laboratories, but are much needed for any studies on samples containing Fe.

In the next phase of this infrastructure development project, there will be continued emphasis on the outreach to the COMPRES community by assisting interested groups in design, preparation, execution, and evaluation of their high-resolution IXS experiments. In this context, we make the CONUSS data analysis package available for nuclear forward scattering (NFS) data evaluation, and the PHOENIX package for nuclear resonant inelastic scattering measurements (NRIXS), as well as FitEoS for equation of state.

We are also installing web-based cameras for remote-access and classroom access. This will allow COMPRES PI's to observe experiments from their labs, as well as demonstrate the experiment to students who are not part of an experiment team for that particular run period.

COMPRES/GSECARS Gas Loading System (Sector 13, Advanced Photon Source)

PI: Mark Rivers, GSECARS, The University of Chicago

The importance of achieving quasi-hydrostatic conditions in diamond anvil cell experiments cannot be overstated. Non-hydrostatic stress leads to systematic errors in determination of many types of physical and thermodynamic properties. Systematic error in bulk modulus and/or its pressure derivatives determination from X-ray equation of state measurements are one notorious example (Duffy et al 99). Rare gas solids (Ne and He), being non-reactive and of low strength, are among the best quasi-hydrostatic media but must be loaded into the DAC at high pressures (~0.2 GPa). They are also optimal for use as insulating media in laser heating experiments – critical for achieving a uniform temperature distribution.

The development of a robust, easy-to-use gas loading system by GSECARS and COMPRES (Rivers et al) has vastly improved the quality of high-pressure science that the COMPRES community can perform on a routine basis. The system is heavily used by APS users at many beamlines, and is widely used by the COMPRES community for experiments at APS and elsewhere. The high demand for the system requires substantial user support. COMPRES has provided partial support for a staff member to assist non-GSECARS users including mail-in and take-out service for COMPRES users. This effort has been successful and the community favors continued support.

Fig. 12. COMPRES/GSECARS gas loading system at Sector 13 of APS.

On-going Community Capabilities Resulting From Completed COMPRES Initiatives

Many projects initiated and sponsored by COMPRES under the Infrastructure Development program are in operation and, although no longer supported financially by COMPRES, are now available to the community. A list of such projects is given below. As the following list shows, COMPRES has established strong partnerships with beamlines at APS to develop high-pressure infrastructure.

- **Brillouin Scattering + Synchrotron X-ray diffraction system** (13-BM-D, GSECARS, APS)
- **Offline CO_2 laser heating system** (GSECARS, APS)
- Gas loading of Diamond Anvil Cells (GSECARS, APS) (postdoc support continues)
- **Portable Paris-Edinburgh cell for melt and liquid property determination at high pressures** (GSECARS, APS)
- **DDIA-30: A new high-pressure apparatus for the COMPRES community** (GSECARS, APS).
- **Heating Externally to Extreme Temperatures in the Diamond Anvil Cell (HEETDAC)**

6. COMPRES Management and Administration

The COMPRES management structure is designed to achieve the following:

1. Provide a continually renewed vision of the scientific and educational goals.
2. Utilize the entrepreneurial resources in the community to initiate and manage specific programs (such as beamlines).

3. Oversee ongoing programs to assure that they are serving the needs of the community and to intervene when they are not.
4. Reach into the community for new ideas and needs.
5. Leverage NSF funds by involving university faculty in key operational positions.

Overview of Management Structure

COMPRES is governed by a set of by-laws that define the process of management. Membership in COMPRES is granted to institutions (e.g., universities) through an application process. Applications are reviewed for consistency with COMPRES goals. Each institutional member of COMPRES is given one vote in all issues that require a vote. Non-US members are given all privileges of membership except for voting. An annual election is held for membership in three committees and their chairs: the Executive Committee, the Facilities Committee, and the Infrastructure Development committee. Membership on a committee is generally three years and is renewable except for the chair of the Executive Committee who cannot serve successive terms. The CEO of COMPRES is the President who is employed by COMPRES and selected by the executive committee.

COMPRES President and Central Office

The President of COMPRES acts as the Principal Investigator of the Cooperative Agreement and the Chief Administrative Officer of the consortium. He/she is appointed by the Executive Committee, in consultation with the cognizant NSF Program Director. From August 2003 to January 2010, Robert Liebermann of Stony Brook University served as the President of COMPRES. When Prof. Liebermann announced his plans to step down, the Executive Committee appointed a Search Committee to lead the effort to find a new President. The Search Committee was originally chaired by David Walker (Columbia) and he was succeeded by Abby Kavner (UCLA) after he recused himself from the search. Other Search Committee members included Harry Green (U.C. Riverside), Guy Masters (Scripps), Russell Hemley (CIW), and John Parise (Stony Brook). Professor Jay Bass of the University of Illinois at Urbana-Champaign was offered the position of President of COMPRES and he accepted. Professor Bass assumed the role of President on January 1, 2010. The Central Office of COMPRES and the Cooperative Agreement moved to the University of Illinois on June 1, 2010. The Central Office staff includes Dr. Bass and Chong-Hwey Fee, Coordinator of Research Programs, both of whom are supported by the COMPRES Cooperative Agreement with the NSF. The Geology Department of UIUC is providing in-kind support of the COMPRES Central Office that is necessary for COMPRES operations. UIUC provides adjoining newly renovated office space for the President and an administrative assistant to form a coherent COMPRES Central Office. Dr. Steven Hurst of the Geology Department, School of Earth Society and the Environment will be performing IT support year-round, website maintenance, administrative support as necessary, and will handle IT/computer requirements at the COMPRES Annual Meeting. Scott Morris is available to provide in-house assistance on handling financial and proposal-related aspects of operating COMPRES.

Committees

In accordance with the bylaws, COMPRES is administered by an Executive Committee, and Committees for Facilities and Infrastructure Development. The Executive Committee is comprised of the Chair and four members, each elected by the Electorate. The responsibilities of the Executive Committee include oversight of research activities, meetings, workshops, and educational and outreach programs. At all meetings of the Executive Committee, the presence of a majority of its members constitutes a quorum. The elected chairs of the Standing Committees on Facilities and Infrastructure Development serve as non-voting advisors to the Executive Committee. The President attends all meetings of the Executive Committee as a nonvoting member. A statement of the Policies and Procedures for the COMPRES Executive Committee and Standing Committees can be found at: http://www.compres.us/index

The management of COMPRES community facilities and infrastructure development projects is monitored by Standing Committees elected by the representatives of the member institutions of

COMPRES under policies and procedures established by the committees and endorsed by the Executive Committee, to which the Standing Committees report. All Facilities and Infrastructure Development projects submit an annual report that is evaluated by the standing committees. Site visits and comprehensive reviews of all Facilities are performed every 3-4 years, and a report is prepared. The most recent Facility site visits were in 2009 to the ALS, and in 2011 to the three NSLS Facilities. The 2009 ALS site visit led to a recommendation for a change in management of that facility, which was enacted in 2010.

An Advisory Council of Earth scientists from other disciplines provides independent advice and oversight to COMPRES on its performance in all of its roles and functions. The current membership of the Advisory Council is Drs. Peter Heaney, Andrew Jephcoat, Peter van Keken, Louise Kellogg, Thorne Lay, and Barbara Romanowicz. Each member serves for a three-year term. The Advisory Council attends the COMPRES Annual Meeting each year and is informed on the operations of COMPRES. After each Annual Meeting, the Advisory Council prepares a report for the COMPRES Executive Committee on its observations and findings.

A list of the current and past members of all COMPRES committees is provided in an Appendix.

Communication

COMPRES provides an important conduit for communication within the mineral physics community. The COMPRES list server is widely used for announcements of meetings, workshops, job opportunities, and other matters of community interest. Other avenues of communication include the COMPRES annual meeting, newsletters, and a recently redesigned website (http://www.compres.us).

Community Input and Planning for this Proposal

The process of community preparation for this proposal began in March 2009 with an NSF-funded workshop entitled "Long-Range Planning Workshop For High Pressure Earth Sciences" organized by J. Tyburczy (ASU), M. Brown (UW) and J. van Orman (CWRU) and held in Tempe Arizona. This workshop considered promising research directions in this field over the next decade. This two-day workshop featured nine plenary talks and breakout discussion sessions on four themes:

- The Deeper Reaches of the Planet: Properties of Iron and its Alloys and the Novel Materials of the Deepest Mantle
- The Dynamic Ceramic Mantle
- Mineral Physics and Society
- Enabling Cutting-Edge Science: Tools and the Accomplishments They Will Drive in the Next Decade of Discovery.

Participants of the workshop reviewed how the field of high-pressure geosciences has impacted other subdisciplines of the Earth sciences, including seismology, geodynamics and petrology. They also discussed the future of high-pressure geosciences: what are the next likely major breakthroughs of our community, and what infrastructure will be necessary to achieve them? The March 2009 workshop led directly to the new 2010 Report on "Understanding the Building Blocks of the Planet: The Materials Science of Earth Processes, edited by Q. Williams.

The next step in the community planning process was an open discussion of opportunities and long-range planning needs that was held at the June 2010 COMPRES meeting. A long-range planning group headed by Donald Weidner (SBU) and including Harry Green (Riverside), Thomas Duffy (Princeton), and Guy Masters (Scripps) was organized. The long-range planning team established working groups who continued community discussions on various topics through a Wiki website. The categories for discussion on the Website consisted of: 1) Education and Outreach, 2) NSLS II programs, 3) Beamline coordination, 4) New Tools: X-ray Raman, nano XRD, nano TXM, and time-resolved SAS, 5) Computational, 6) Imaging, nanofabrication, 7) Rock mechanics, 8) Multi-anvil cell assembly, 9)

5000-ton press system, 10) Shock wave studies, 11) Spallation Neutron Source programs, 12) Free-electron laser programs, 13) Advanced Photon Source programs, 14) Advanced Light Source program

The blog/Wiki was active for several months, after which the leader of each discussion group composed a final report. Some areas gained more traction than others, and this was taken as an indication of community interest and enthusiasm. A COMPRES Town Hall meeting was held during the Fall 2010 AGU meeting and more than 100 people attended. Reports on many of these topics were presented to the community. Some reports formed the basis for Infrastructure and Facility proposals for the current COMPRES proposal. Others may nucleate into separate proposals either as Grand Challenges to NSF EAR or as proposals to other funding agencies or other programs in NSF.

In early 2011, COMPRES issued a call for Facility and Infrastructure Development Proposals for inclusion in this proposal. The proposals received were evaluated by the Infrastructure and Facilities Committees who made recommendations to the Executive Committee. Final decisions on which projects to include in the renewal and budget levels were made by the Executive Committee in consultation with the President. A community-wide discussion of the status and plans for the renewal proposal was then held at the 2011 COMPRES Annual Meeting in Williamsburg, VA, where the community provided additional input to the Executive Committee and the President on the emerging shape and structure of this proposal.

7. Broader Impacts

Annual Meeting

The COMPRES annual meeting, held in June of each year, features keynote talks, many from prominent scientists in allied geoscience disciplines (seismology, geodynamics, geochemistry, planetary science), graduate student/postdoc presentations, facility and infrastructure reports, a poster session and a business meeting for election of standing committee membership. In recent years the meeting has regularly included technical tutorials for students on topics including “Software for High-Pressure Crystallography” and “Basics of Neutron Scattering.” Student-initiated panel discussions have also been well received and are becoming a regular feature of the meeting. These have covered such areas as: “International Experiences”, “Jobs in Academic Research”, and “Fund Your Science”, a grant-writing tutorial led by Barbara Ransom of NSF.

The 2011 COMPRES meeting in Williamsburg, VA attracted 132 participants, the largest COMPRES meeting thus far. We attracted nearly 100 posters and the meeting featured 15 talks and 37 posters by students and postdoctoral fellows. Because it is now difficult for students to give talks at major meetings like the Fall AGU, the COMPRES Annual Meeting is commonly the place where student deliver their first professional oral presentation. The annual meeting attracts diverse population (39% of attendees in 2011 were women) and is well attended by graduate students and postdocs (54% of total attendees in 2011). COMPRES offers travel grants to the annual meeting to encourage participation by young scientists and new investigators.

Distinguished Lecturer Program

In 2008-09, COMPRES established a Distinguished Lecture series in the field of mineral physics. The goal is to (1) inform students and colleagues in geosciences and related fields about how high-pressure research is contributing to the understanding of Earth processes, (2) inform interested undergraduates about research opportunities within the COMPRES community, and (3) to promote visibility for mineral physics and a better understanding of scientific problems in studies of the deep Earth. The target audience for this lecture series is 4-year undergraduate colleges and non-PhD granting institutions that do not have a mineral physicist on the faculty. Lecturers tailor their talks to be accessible to a broad audience at the upper-level undergraduate level.

Each year since 2008 we have selected two outstanding lecturers and scheduled them for visits to 6-8 schools. In the first couple of years of the program, most requests came from larger PhD-granting universities. Starting in 2010 we no longer asked hosts to pay local lodging and meals, with COMPRES paying 100% of the cost for each visit. At a relatively small price, this change in format had a dramatic effect on the number and types of schools that applied for a lecturer. We are now able to fill the schedule predominantly with schools from our target audience. We learned that most of the smaller schools we want to hear from have *zero* budgets for invited speakers. For the 2010-2011 year, COMPRES received 28 requests (a record number), with majority of those requests coming from undergraduate institutions with no mineral physicist on the faculty.

The impact of the lecture series goes beyond a one-hour colloquium. We ask lecturers to set up meals and an open discussion session with undergraduates. Our lecturers have found students very receptive to these meetings, and eager for knowledge. During these meetings, students often ask questions about how to apply to graduate school, financial aid, which schools best match their interests, and what courses to take if one is interested in grad school. Our lecturers have even been contacted after their visits for advice and long-distance mentoring.

The speakers selected for the COMPRES lecture program in past years are:
2008-2009 Dave Walker (Columbia), Wendy Mao (Stanford)
2009-2010 Jackie Li (Illinois), Harry Green (UC-Riverside)
2010-2011 Wendy Panero (Ohio State), James van Orman (Case Western)

The lecturers for the upcoming year will be:
2011-2012 Abby Kavner (UCLA), Andrew Campbell (Chicago)

The list of schools visited in 2010-2011 is: College of Wooster, Illinois State Univ., Indiana Univ. South Bend, Miami Univ. (Ohio), Louisiana State Univ., Univ. of Houston, Vanderbilt (all by Jim van Orman); James Madison Univ., Lafayette College, West Chester Univ. (PA), Carleton College, Univ. of Minnesota Duluth, Chapman Univ., Harvey Mudd College (all by Wendy Panero)

Workshops

Workshops serve as a major outreach mechanism for COMPRES. The consortium supports workshops each year that cover a variety of topics relating to the consortium's science and methodologies are targeted towards specific audiences. For graduate students and potential new users of facilities, COMPRES offers intensive hands-on workshops designed to bring attendees up to speed in specific techniques. A list of workshops held in 2010-2011 is given below (a full list of all workshops held since 2007 is given as a supplement). These workshops were well attended, and have been successful in bringing in new users for specific techniques and capabilities. Some of these workshops are offered in coordination with other organizations (e.g. NSLS). Travel and workshop expenses are supported for students, post docs and young investigators based on both merit and financial need.

COMPRES-sponsored Workshops (2010-2011):

- *Workshop on Computational Infrastructure For Mineral Physics: A Community Consultation Workshop*: August 29-31 2010 University of Minnesota Supercomputer Center
- *4-Dimensional Studies in Extreme Environments (4DE): A High- Pressure Beamline Workshop for the National Synchrotron Light Source II*: April 29-30, 2010 National Synchrotron Light Source, Brookhaven National Laboratory

- *Time-Resolved X-ray Diffraction and Spectroscopy at Extreme Conditions (TEC): A High-Pressure Beamline Workshop for the National Synchrotron Light Source II (NSLS-II)*: June 15-16 2010 National Synchrotron Light Source, Brookhaven National Laboratory
- *Lujan Workshop: Applications of Neutron Scattering to Materials and Earth Sciences*: December 11, 2010, University of California at Berkeley
- *Dynamic Phenomena under Extremes*: January 24 – 28 2011, University of Texas at Austin
- *Applications of FIB/SEM CrossBeam Technology for High-Pressure Research Workshop* June 20-21, 2011 Carnegie Institution of Washington

Forthcoming workshops in 2011:

- *Single Crystal Diffraction Techniques*: October 4, 2011, Advanced Light Source, LBNL
- *Evolutionary Crystal Structure Prediction using the USPEX code: Discovery of new materials and mineral phases*: TBA, Stony Brook University

Education

COMPRES recognizes that maintaining a robust student population trained in high-pressure techniques is critical for future scientific progress and contributes to the scientific infrastructure of the U.S. Our recent success at moving students into the professoriate has been excellent: the high-pressure geosciences has placed over 30 of our Ph.D. students into new faculty positions in the last decade. COMPRES has a longstanding track record of reaching out to students through education and outreach efforts, including workshops, meetings, and collaborating with existing curricular initiatives in Earth Science (such as the "Teaching Mineral Physics across the Curriculum" project described below).

During the past five years, COMPRES has worked with other organizations to promote inquiry-based education and outreach as nationwide collaborations between scientists, educators, materials developers, government agencies and other stakeholders. These efforts include collaborations with the DLESE (the Digital Library for Earth Systems Education) projects, and the Science Education Resource Center at Carleton College (SERC).

The COMPRES community has also promoted opportunities for undergraduate students to become involved in high-pressure research. Members of the high-pressure Earth sciences community have been involved with the Research Experiences for Undergraduate Program of NSF, with some of the students doing research at COMPRES supported facilities. In addition, many high-pressure researchers actively engage undergraduate students in their research by supporting them with their regular research grants (see http://www.compres.us/index.php?option=com_content&task=view&id=138&Itemid=173 for a partial list). Many of these students present papers at the AGU meeting, co-author publications, and some go on to research careers in science. Several undergraduates have attended the COMPRES Annual Meeting, this often being their first experience at a professional conference and their introduction to the mineral physics community. Through these efforts, the community has exposed large numbers of undergraduate students and in some cases high school students to high-pressure geoscience.

Mineral Physics Educational Modules for Advanced Undergraduates and Graduate Students

A COMPRES project begun in January 2010 is working to assemble a group of web-based educational modules for a course entitled "Introduction to Mineral Physics". The modules are being designed to function as part of a full semester course, although each module is also able to serve as a stand-alone resource on a topic. The modules are targeted at entry-level graduate students and advanced undergraduate students. Learning outcomes for the course have been developed in consultation with educators throughout the COMPRES community. The materials are being designed to be compatible with common distance learning platforms. Potential users include COMPRES members teaching "bricks and mortar" classes at their own institutions, COMPRES members teaching in a distance education setting, mineralogy teachers interested in supplementary material for their mineralogy class, undergraduates doing independent study projects and graduate students and colleagues in other sub disciplines who wish to brush up on a mineral physics topic. The modules will reside on the SERC "On the Cutting Edge" web site (see below) in the Teaching Mineralogy collection and there will be direct links to the materials from the COMPRES web site. The existence of the modules will facilitate the creation of graduate distance education courses in mineral physics that could serve mineral physics graduate students nationwide. The creation of such courses would address current problems faced by faculty in state universities where rising minimum enrollments are making it difficult to teach a suitable graduate course to incoming students. Dr. Pamela Burnley of UNLV is leading this project and coordinating the effort with faculty in other COMPRES institutions.

The above project will contribute to a growing partnership between COMPRES and the *On the Cutting Edge* project supervised by David Mogk of Montana State University as part of the Science Education Research Center (SERC) of Carleton University (see: http://serc.carleton.edu/NAGTWorkshops/mineralogy/mineral_physics.html). Dave Mogk gave a presentation at the 2009 Annual Meeting of COMPRES and interacted with many of the attendees. A number of members of our community including Glenn Richard (SBU), Bob Liebermann (SBU) Mike Brown (Washington), Pamela Burnley (UNLV), Abby Kavner (UCLA), Wendy Panero (Ohio State), Alex Navrotsky (Davis), Ann Chopelas (UCLA) and Artem Oganov (SBU) have made mineral physics-related contributions of educational modules and tools to the SERC website. As another example of our collaboration with the *On the Cutting Edge* professional development program, Wendy Panero (Ohio State), was a co-convener for an August 2011 workshop on *Teaching Mineralogy, Petrology, and Geochemistry in the 21st Century* held at the University of Minnesota. Several members of the COMPRES community participated in a 2010 online workshop on *Understanding the Deep Earth*.

Other COMPRES-Related Initiatives

COMPRES actively seeks to increase the representation of minorities and women in our community. New efforts in minority recruitment include participation by COMPRES members in the National Synchrotron Light Source (NSLS) collaboration with the HBCU (Historically Black Colleges and Universities) Interdisciplinary Consortium for Research and Education Access in Science and Engineering (INCREASE); Gabriel Gwanmesia of Delaware State is a founding member of INCREASE. The goal of INCREASE is to engage faculty from HBCUs in research using synchrotron facilities and to train students from these institutions in synchrotron research. COMPRES members, R. Liebermann (SBU), G. Gwanmesia (Delaware State) and L. Ehm (BNL) have been funded in this area for 3 years beginning in August 2011 through the NSF Geosciences Directorate Program for Opportunities for Enhancement of Diversity in Geosciences (OEDG). This will provide funding, when combined with matching money from NSLS-BNL and the Graduate School Dean at Stony Brook University, for up to three graduate students per year to be enrolled in a MS program in Geosciences with an instrumentation focus. Internship research will be done at BNL on COMPRES beamlines.

Cooperative Institute for Deep Earth Research (CIDER)

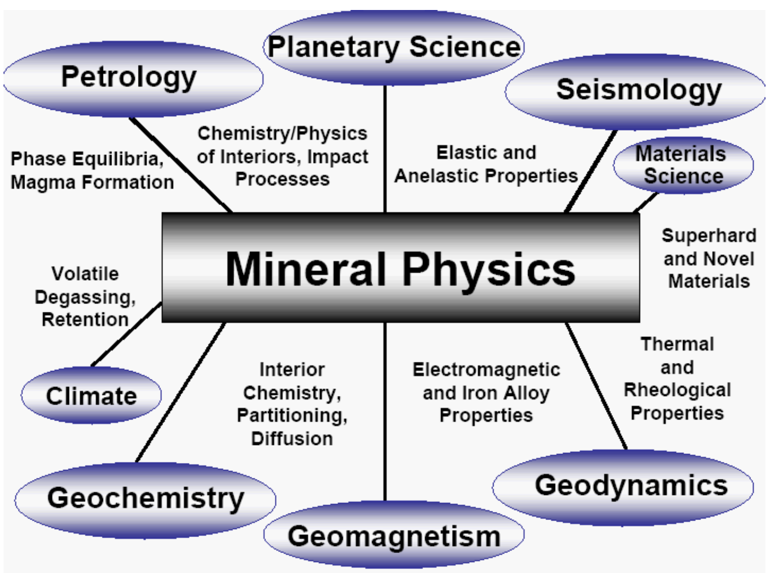
CIDER is an interdisciplinary approach to solving complex problems in Earth sciences. Its goals are to provide an optimal environment for transformative studies with efforts by leading researchers from different areas of Earth Sciences: high-pressure material science, geodynamics, seismology, geochemistry and geomagnetism. A second goal is to educate a new generation of Earth scientists with breadth of competence across disciplines, contributing to a better understanding of the deep Earth. Since its inception, COMPRES members have been involved in CIDER including members of the steering committee (Duffy, Stixrude, Weidner, Jeanloz) and active participants and instructors in summer workshops (e.g. Duffy, Liebermann, Kavner, Stixrude, Li, and Panero).

Mineral Physics Database Development

There is also a broad-based need in the high-pressure geosciences to construct reliable, readily accessible state-of-the-art databases on the properties of mineral, melt and fluid assemblages at the extreme conditions of Earth's interior. One of the values of such an infrastructure is that it would supply our neighboring disciplines - geodynamics which relies on thermal buoyancy forces, petrology with its dependence on rock chemistries, seismology which hinges on the elastic properties of minerals, geomagnetism which depends on core properties and the conductivity properties of the planet - with ready access to information that the high-pressure geosciences can provide. This need was reinforced by the report of the COMPRES Advisory Council in 2010. The challenge of constructing such a database (or databases) lies in the chemical complexity and extreme thermodynamic conditions of the planet's interior. The most viable means of constructing such a database involves combining the best information from both the experimental and theoretical domains to construct a consistent and comprehensive database for use by the entire geophysics community. The ambition is to create a web-based and interactive database that would also fulfill a pedagogical function in offering hands-on experience in thermodynamics or elasticity of minerals to both beginners in the high-pressure geosciences community, and users in other disciplines. A start on constructing such a database is being made by the Central Office with graduate student involvement. An up-to-date compilation of elastic and thermodynamic data has been started. This work will later be a shared role of the COMPRES Technology Office at APS.

Contributions to Other Scientific Disciplines

Earth and Planetary Sciences



Our collective focus on Earth and planetary materials leads to a broadly interactive character of our field within the Earth sciences. For example, seismology depends upon our studies of the mechanics of failure, and the elastic properties of materials; geodynamics hinges on our characterizations of the viscous flow of materials; geomagnetism depends on our determinations of the electromagnetic properties of materials; petrology relies on characterizations of mineral/melt equilibria; planetary science incorporates the equations of state and dynamic behavior that we determine in modeling the interiors and impact-history of planets; and, ultimately, the planet's climate is controlled by outgassing from the planet's interior that, modulated by the surface environment, have generated our atmosphere. Our overall view is that we provide a framework for how the materials of the planet behave; a framework that supports all of our adjoining disciplines within the Earth sciences (Fig. 13, at left).

Materials Science

The field of high-pressure geosciences is naturally concerned with Earth materials but another goal of our discipline is to explore the societal, technological or industrial utility of these or related materials. Indeed, the application of pressure often results in materials adopting new crystal structures, or allows compounds to form that cannot be produced at low-pressure conditions. High pressures have been used to synthesize materials that are extremely hard (e.g., diamond, cBN), or have novel electronic or chemical properties. In some cases, such new materials can be quenched to ambient pressures. Examples of the types of materials for which high-pressures have found considerable applications include not only ultra-hard materials (Chung et al., 2007; Chen et al., 2008; Weinberger et al. 2009; Dong et al., 2009), but also materials used for radioactive waste disposal (Lange et al., 2010; Scott et al., 2011) and possible hydrogen storage materials (George et al., 2009; Strobel et al., 2011). While our core research focus is high-pressure geosciences, the COMPRES community and COMPRES facilities have fostered advances in materials science, chemistry, and condensed matter physics (See Vol. II Accomplishments: "Physics and Chemistry of Materials").

8. Budget

For the period June 2012 to May 2017 funding is requested for the activities described above. The table below gives a budget breakdown in terms of the main categories of COMPRES activities: Facilities, Infrastructure Development, Community Activities, and Central Office.

All in units of $1K

TOTAL BUDGET

	Year 1	Year 2	Year 3	Year 4	Year 5	Total
Facilities	1506.1	1529.2	1689.0	1715.0	1719.5	8158.8
Infrastructure Dev.	404.3	377.2	318.0	321.0	324.0	1744.5
Community Activities	220.0	245.0	250.0	277.0	177.0	1269.0
Central Office	519.4	539.8	551.0	562.4	574.2	2746.8
Total	2649.8	2691.2	2808.0	2875.5	2894.7	13919.1

Facilities includes: The Advanced Light Source beamline 12.2.2, NSLS XRD DAC beamlines X17B3 & C, NSLS Multi-Anvil beamline X17B2, NSLS-II XPD beamline for MAP/DAC, Infra-red beamlines at NSLS (U2A) and NSLS-II, COMPTECH, beamline housing support, and subaward indirect costs.

Infrastructure Development includes: Gas Loading at the APS, inelastic X-ray scattering at Sector 3 APS, Multi-Anvil Cell development, FIB/SEM training, Mineral Physics on the Internet education/outreach, infrastructure projects to be assigned through annual calls for proposals (years 2-5), and subawards IDC.

Community Activities include: The Annual Meeting, travel for committees, the Distinguished Lecturer series, workshops, workshop/meeting supplies. All activities in this category are considered participant support, and are not assessed indirect cost.

Central Office includes: Salaries for the President and an administrative assistant (Chong-Hwey Fee), benefits for the Central Office staff, materials and supplies, telephone, postage, travel, web services, and indirect costs.

Budget Notes

Leveraging of NSF-EAR Funding: COMPRES derives significant fiscal benefits from leveraging of various types to support its diverse range of activities. Other organizations contribute significantly to COMPRES facilities and projects. Notable examples are contributions of the Mineral Physics Institute (MPI) at Stony Brook and the Advanced Light Source to the operations of X-ray beamlines X17B2, X17B3/C, and 12.2.2. The ALS contributes 2.33 FTE's of staff to the operation of beamline 12.2.2, funds for supplies, materials, optics, and has made large commitments for equipment (a gas loading apparatus, detectors, etc.). MPI contributes a full FTE in Dr. Michael Vaughan, 2/3 FTE of electronics and computer control support (Ken Baldwin), and subsidizes other necessary machine and electronic shop time. Beamline U2A benefits from contributions from Dr. R. Hemley's programs at Carnegie (e.g., CDAC). Research grants such as the Rheology Grand Challenge (Karato, Weidner, Durham) contribute equipment, technical expertise, and some operational funds. A sizeable in-kind contribution comes from the time commitment of COMPRES PI's and project managers. Q. Williams, D.J. Weidner, T. Duffy, and R. Hemley do not receive salary compensation for the considerable time they put into managing COMPRES-supported facilities. The same is true for most PI's of Infrastructure Development projects.

Infrastructure Development Projects: We request unassigned funds for new Infrastructure Development projects at the level of $75K (Year 2) and $150K (Years 3-5) to seed the development of new ideas from the community for novel infrastructure, methodologies, and education/outreach projects. The program is fully subscribed for Year 1. Funds in our proposed budget will allow us to support 1-2 projects per year in Years 2-5.

Funding Level: The 2011-2012 COMPRES budget for 2011-2012 (see appendix on Funding History of COMPRES) was $2,400K. Our proposed budget for Year 1 represents an 11.04% increase over the current 2011-2012 funding level. Without the unavoidable one-time indirect costs for setting up new subawards (see below), our requested Year 1 budget is 10.68% larger than our current budget. This increase will allow us to accommodate institutionally-mandated salary increases for staff, rapidly increasing indirect cost and benefit rates at all institutions (especially public universities), and to initiate COMPTECH, which is the first new facility for COMPRES since its inception. We consider COMPTECH to be a logical and necessary new direction for COMPRES. Rapid progress in synchrotron X-ray science is making new classes of experiments possible. These new capabilities are beyond what is available at current COMPRES facilities or GSECARS, but offer exciting opportunities for new ways to address fundamental questions about the Earth's interior. COMPTECH will make it possible to develop these capabilities for the entire mineral physics community.

Indirect Costs on Subawards: It should be noted that the Year 1 budget is impacted by one-time ICR charges for a new Cooperative Agreement (CAGR). At the beginning of a new CAGR, there is a one-time IDC charge on the first $25,000 of each subaward. For COMPRES, 6 subawards would need to be set up for Stony Brook (NSLS and NSLS-II MAP and DAC operations), Carnegie Institution of Washington (U2A IR beamline and FIB/SEM training), Univ. Nevada Las Vegas, Arizona State Univ., Univ. Chicago, and Univ. Cal. Santa Cruz.

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COMPRES Data Management Plan

Data Policy

COMPRES facilities provide five major types of data for samples that are brought to the facility by the user.

1. X-ray diffraction data.
2. X-ray imaging data.
3. Infra-red spectral data
4. Support data such as Raman spectra or ultrasonic data.
5. Meta data in the form of log books or log files that describe the experiment

The COMPRES policy for managing these data include the following:

1. All data are archived by the beamline where they are collected.
2. The archived data are available exclusively to the Principal Investigator or their designee of the specific project for two years after the experiment.
3. The archived data are available to anyone who requests it after the two-year period.

Exceptions to this may be available through special arrangements with the DOE facility that operates the beamlines (some of the facilities have provisions for proprietary users)

Data Format

The data will be stored in a format that can be accessed by commercially available data analysis programs or by programs that are available through the beamline.

Software Access

Software produced at COMPRES facilities will be available to the public, usually upon request to staff of beamlines that developed and use an application of interest.

Mentoring Plan for COMPRES Post-Doctoral Researchers

Some COMPRES post-docs are jointly funded by a COMPRES sub-award and a separate science grant or matching institutional funds. In either case, mentoring activities will be carried out by one of the PI's of the principal grant or COMPRES subaward on which a post-doc is funded, with the goal of providing guidance in career development in addition to a stimulating, productive scientific experience.

Post-docs will receive thorough education and training in the roles for which they were hired. Where appropriate this education will be augmented by beamline scientists and staff. Post-docs will acquire a wide range of scientific knowledge and technical skills that should advance their career goals.

Post-docs will receive career counseling, meeting at least quarterly with his/her mentor to evaluate career goals and pathways to achieve these goals.

To train post-docs in writing grant proposals, the post-doctoral researcher will work with the mentor in the preparation of a grant proposal at least once during the postdoctoral appointment. In addition they will be involved in administration of grants to familiarize them with those processes.

Post-docs will meet regularly with the mentor to discuss publication of their research, defining the scope and timing of the publication. Post-docs will be given the opportunity to present their research findings at a national meeting. Toward this end, COMPRES normally includes travel for post-docs in awards, so that a post-doc can attend the COMPRES Annual Meeting and an international conference in their field (such as the AGU meeting). The COMPRES Annual Meeting is an ideal venue for the post-doc to present and discuss their work with a large cross-section of the mineral physics community.

Where appropriate, post-docs will be given the opportunity to participate as an instructor/lecturer in courses. The mentor will provide feedback on goals and performance.

It is expected that the mentor will meet with the researcher at least every other week for at least one hour. Discussions will include all of topics mentioned above, as appropriate, but will involve each of them at least once every three months