Letter of Interest

For a

High Pressure Superconducting Wiggler Beamline

at the NSLS-II

Contents:

Introduction

Members of the High Pressure community met during the breakout session “Materials at High Pressure” during the joint workshop for “The NSLS-II Powder Diffraction Project Beamline” and “Materials Science Engineering Strategic Planning for NSLS and NSLS-II”, held on January 17-18, 2008. The outcome of that meeting was that this community would propose three beamlines for NSLS-II: a high-energy beamline using a superconducting wiggler as a source, with four end stations; an infrared beamline with two endstations, and a modest energy beamline using an undulator. This is a category A Letter of Interest for the superconducting wiggler beamline.

1. Title: High Pressure High Energy X-ray Beamline

Acronym: HiPHEX

2. Beamline Advisory Team (BAT) Members:

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3. Scientific Case

Introduction

Pressure is one of the fundamental thermodynamic variables, which can be varied over a range of more than sixty orders of magnitude, from the vacuum of outer space to pressures in the interior of neutron stars. The exploration of matter at extreme conditions is a central theme in a broad range of scientific disciplines (e.g. material science chemistry, physics, and Earth and planetary science). The application of pressure can induce both continuous and discontinuous changes in atomic and electronic structure. Learning how atomic and electronic arrangements change under extreme conditions provide insight into the nature of phase transformations, chemical reaction, and also evolution in micro- and nanostructural components, such as crystallite size, dislocations, voids, and grain boundaries. Once these processes are understood, it will be possible to predict responses of materials under thermomechanical extremes using advanced computational tools. Further, this fundamental knowledge will open new avenues for designing and synthesizing materials with unique properties. Using these thermomechanical extremes will allow tuning the atomic structure and the very nature of chemical bonds to produce revolutionary new materials.

Scientific Challenges

The scientific challenges in high-pressure research are manifold and involve overlapping scientific disciplines. In the past decade, advances in synchrotron x-ray based analytical techniques fostered remarkable breakthroughs in high pressure sciences, including discovery of the post-perovskite phase of $MgSiO_3$ stable at more than 100 GPa (2, 3), the unusually low melting temperatures of sodium, reaching 300 K at 118 GPa (4), complex structures of alkali metals at high pressure (5-8), observation of a spin state transition in iron under conditions in Earth's lower mantle (9), the changes in the bond characteristic of compressed graphite (10), and the measurement of the spin and charge order in chromium at high pressure (11).

Earth and Planetary Science

Study of the structure, composition, and history of the Earth and planetary interiors is an extremely challenging task because the deep interior is inaccessible. Seismological investigations are the primary source about the interior structure of the Earth and other planets. Advances in seismology provide detailed 3D tomographic images that show heterogeneities, anisotropy, attenuation and discontinuities from the surface to the center of the core. Seismic models of the variation of compressional and shear wave velocities and densities presumably reflect radial and lateral variations of chemical composition, mineralogy, pressure and temperature. Experimentally derived information of the density and elastic properties of Earth and planetary materials under geologically relevant pressure and temperature conditions are needed for successful interpretation of the seismic models.

Examples of Grand Challenges for Earth Science

Mission to the Earth's core and beyond

The Lehmann discontinuity at 5150 km marks the boundary of the liquid outer core and the solid inner core. The structure and properties of a planetary core promise to provide a wealth of information about the evolution and dynamic processes within the planet. However, limitations in pressure generation and related properties measurements at such extremely high pressures and temperatures hinder the mission to the Earth's core (21). As analytical techniques set restrictions on the minimum sizes of high pressure samples and higher pressures normally require smaller samples, the sub-micrometer spatial resolution of the NSLS II X-ray beams will enable new ground breaking work to challenge accessibility to the pressure at the center of the Earth's core (3.5 million atmospheres) and beyond. The high spatial resolution X-ray beam will also significantly enhance the capability to recognize heterogeneities of pressure, temperature, chemistry, structure and phase within small samples and to improve reliability of experimental data obtain at such high pressures. With such advances in experimental capabilities, we expect to address the long-standing issue of core composition and to understand the new observations of inner core seismic anisotropy, super-rotation and magnetism.

Rheology

The plastic properties of ceramics – rocks – at high pressure and temperature control the evolution of the Earth and planets (22). The pressure envelope for quantitative rheological experiments has limited us to properties of the upper layers of the Earth until very recently when synchrotron methods have extended the pressure range by about two orders of magnitude. This has come with synchrotron X-ray imaging techniques and stress metrics. The current experimental capability limits the strain precision to 10_{-4} (resolving 100nm length change over 1 mm long sample) in multi-anvil apparatus. The high spatial resolution of less than 10 nm will improve by one to two orders of magnitude strain precision to about 10^{-6} and strain rate precision to 10^{-9}-10^{-10} s^{-1} and will significantly reduce the gap of strain rates between laboratory experiments and geological flow (10^{-12}-10^{-16} s^{-1}). On the other hand, seismic studies use millihertz acoustic waves to probe the Earth, while laboratory studies often use megahertz acoustic waves. Differences in these time scales are expressed in the attenuation, or the Q (quality factor), of stress-strain relationships. To measure Q, we need to measure stress relaxation times and strain retardation times as a function of frequency. With the advances of synchrotron tools, unprecedented flexibility in controlling the stress and strain during the deformation process at high pressure and temperature is feasible. The strain precision to be achieved at the NSLS II will allow us to describe seismic wave attenuation and related transient creep with a requirement of strain resolution (10^{-6}) relevant to seismic attenuation in the mantle. Finally, the nanometer spatial resolution could enable quantitative flow measurements in a diamond anvil cell. This will be a new era of rheology research, promising to extend the pressure envelope for rheological studies nearly one order of magnitude, from the pressure limit in multi-anvil apparatus to that of diamond anvil cell at the same strain precision of 10^{-4} (resolving less than 5 nm length change over 10 µm long sample). Knowledge gained thereby will place important constraints on the thermal, velocity, and density structure of Earth's interior.

Material Science and Chemistry

Super hard materials

Compounds can be defined as super hard materials, when their micro-hardness exceeds 40 GPa. In addition to high hardness, they usually possess other unique properties such as compression strength, shear resistance, large bulk moduli, high melting temperatures, chemical inertness, high thermal conductivity, etc., which makes them materials highly desirable for a number of industrial applications. One prominent goal is to synthesize new phases in systems such as B-C-N-O or Si-B-C-N that are thermally and chemically more stable than diamond, and harder than cubic BN, and thus would be excellent materials for high-speed cutting and polishing of ferrous alloys. The most common conditions employed to synthesize super hard materials involve extreme pressures or extreme pressures in combination with temperatures. Fundamental research to better understand the atomic structure and the bonding characteristics are badly needed. Knowledge of these fundamentals will help materials scientists understanding how and why a material becomes super-hard.

The source characteristics of NSLS-II and the unique experimental capabilities at the proposed high-pressure stations will open new possibilities in synthesis and characterization of super hard materials.

Synthesis of Novel Materials

Research at elevated pressure and temperature provide a new insight into synthesis of materials with properties important for industrial, technical and scientific applications (34). These include super hard materials, high-temperature superconductors, ferroelectrics, multiferroics, high energy density materials, hydrogen storage materials, materials for computers and communications, and nano-materials. High-pressure studies provide otherwise unattainable information about the phase diagrams, thermodynamic properties, and electronic structure which can predict directions for search of materials with desirable properties. Moreover, high-pressure synthesis remains unique in many cases.

Physics

Highly Correlated Electron Systems

Systems with strongly correlated electrons have fascinated materials scientists time and again, by revealing such intriguing phenomena as high temperature superconductivity, the colossal magneto resistance, and heavy fermion behavior and unusual dynamic ground states. There is growing evidence that in many of these systems, as for example the transition metal oxides, the unusual physical properties result from a competition between different electronic phases, of which some show instability towards a nanoscopically inhomogeneous electronic ground state (39). Understanding the phenomenon of “competing-order” and the inherent electronic inhomogeneities is considered to be key to identify the microscopic mechanism of many of these exotic ground states. In principle, pressure provides a formidable tool to study these phases, as it allows manipulating the band structure as well as the lattice parameters and symmetry. However, the challenge has been to detect the ultra weak lattice modulations associated with the electronic in homogeneities in a high pressure environment, and only recently groups have succeeded (11). The NSLS-II will enable such diffraction experiments with an unprecedented degree of resolution, and provide a direct probe of electron-lattice interactions in some of the most unconventional states of condensed matter at high pressure.

The ability to combine high pressure with other extreme environments such as high magnetic or electric fields is vital for studies of complex interactions in strongly correlated electron systems, such as questions concerning the competition or coexistence of magnetism and superconductivity, or the interplay between electronic order and Fermi surface instabilities. The combination of high pressure with other extreme environments (in addition to temperature) is world wide still in its infancy. The NSLS-II offers a unique chance to develop a world-leading program.

High Pressure Program at NSLS-II

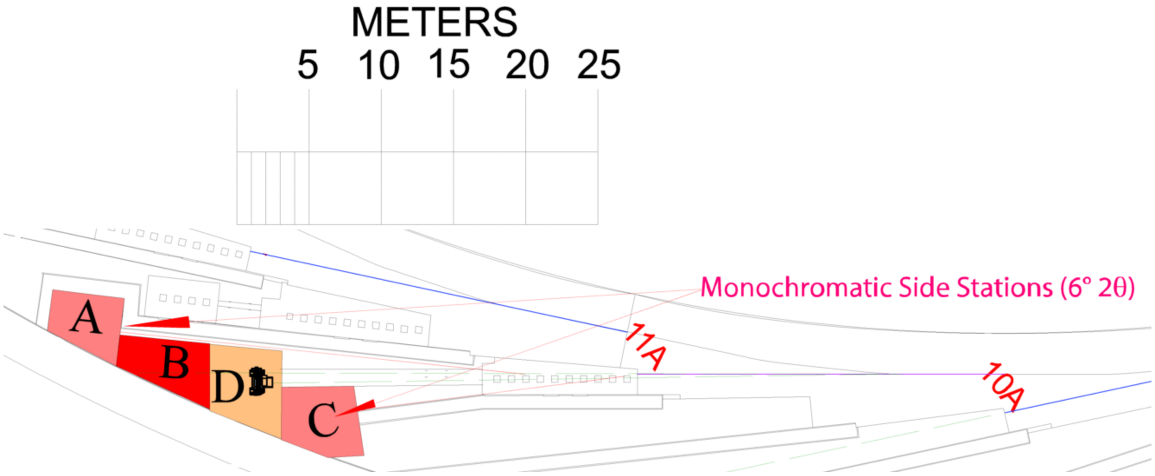
The future scientific challenges in high pressure research involve sophisticated experiments on increasingly complex systems at ever higher pressures and temperatures. Most of the modern scientific questions in research at extreme conditions require integration of multiple experimental techniques. The sample environment for experiments at extreme conditions poses a rigorous restriction to sample size and volume and often contaminates the collected data. Therefore, the requirements on focal size, collimation and beam stability are very high. The small source size and the high brilliance over a large range of X-ray energies of NSLS-II will greatly benefit experiments at extreme conditions and stimulate new directions in research of materials at extreme conditions.

4. Technical Requirements

We are requesting the six Tesla superconducting wiggler with four experimental endstations (see diagram below). Two of the endstations will be for the Diamond Anvil Cell (DAC) or other small high-pressure cell, and two of them will be for the Large Volume Press (LVP). Most of the points listed below are covered in greater detail in the white paper, which is included as Appendix E.

Diamond Anvil Cell Stations

The high pressure community identified the need for two extreme conditions diffraction stations utilizing small pressure generating devices like diamond anvil cells (DAC) or small Paris-Edinburgh (PE) cells, located at the superconducting wiggler port. The experimental capabilities of the two diffraction beamlines are complementary to each other and to other diffraction beamlines proposed for NSLS-II.



Station A – fixed energy side station

Station A will be a diffraction beamline for experiments at simultaneous high pressure and temperature. An experimental hutch of sufficient size (4×5 m) to accommodate the experimental setup including a permanent laser heating system and possibly other spectroscopic (Raman, Brillouin) systems is necessary. The station will operate at a fixed energy in the range of 35-40 keV and will be optimized for the following high-demand experimental techniques:

- **Powder diffraction:** Measurements of PVT equations of state, compressibility, structural evolution, phase transformation, element partitioning, melting, strength, rheology, etc of simple to moderately complex structures at pressure and temperature.
- **Single crystal diffraction:** Determination of complex crystal structures and the investigation of their compression behavior.
- **Quasi single-crystal diffraction:** The micro-beam capabilities will make a new class of experiments at high pressure and temperature possible.

The following components for the beamline and the experimental station are proposed:

- The monochromator will be a side scattering asymmetric bent Laue crystal.

- Microfocusing optics.
- Sample stages with degrees of freedom in x, y, z, ω, φ.
- An area detector.
- A double-sided laser heating system.
- A micro-Raman spectrometer for simultaneous X-ray diffraction and Raman spectroscopy.

Station B - variable energy

Station B will be a diffraction beamline for experiments at simultaneous high pressure and high/low temperatures. An experimental hutch of sufficient size (3×5 m) to accommodate the experimental setup including the laser heating systems and a cryostat is necessary. The station will operate in the energy range from 20-120 keV. The wide energy range will allow large variety of scattering experiments at extreme conditions, currently not possible at other dedicated high-pressure beamlines in the world. In addition to conventional powder and single crystal diffraction at extreme conditions, Station B will allow the following experimental techniques.

- **X-ray total scattering:** Total elastic X-ray scattering, including the Bragg and diffuse contributions, in conjunction with pair distribution function analysis allows determining the short-, intermediate- and long-range atomic arrangement.
- **Resonant scattering:** The energy range of the proposed experimental station will allow resonant diffraction experiments on absorption edges of elements with $Z > 43$.

The following components for the beamline and the experimental station are proposed:

- A tunable monochromator to cover a wide energy.
- Mirrors in Kirkpatrick-Baez geometry.
- Sample stages with degrees of freedom in $x, y, z, \omega, \chi, \varphi$, and 2θ.
- An area detector
- A double-sided laser heating system.
- A closed cycle He-cryostat.
- A micro-Raman spectrometer for simultaneous X-ray diffraction and Raman spectroscopy.

. Large Volume Press Stations

The high pressure community identified the need for two extreme conditions diffraction stations with large hydraulic presses to generate sample environments at extreme pressure and temperature in situations where large samples (1 mm) are required or uniform pressure and temperature are important. These systems will generally work at pressures up to about 60 GPa.

Station C – fixed energy side station

Station C will be a diffraction beamline for experiments at simultaneous high pressure and temperature. An experimental hutch of sufficient size (4×5 m) to accommodate the experimental setup and space for several large Paris-Edinburgh type pressure cells is necessary. The station will operate at a fixed energy in the range of 35-40 keV and will be used to explore samples at extreme conditions using X-ray diffraction and imaging. Interchangeable high pressure systems will be used here. The different systems will be optimized for a variety of experimental goals.

- **Slow dynamic processes:** This hutch will allow a high pressure experiment to continue over several days/weeks but not continually be in the X-ray beam.
- **Sample imaging:** Cells with a large angular access will be used for tomographic imaging of the sample.
- **Powder diffraction**.

The following components for the beamline and the experimental station are proposed:

- The monochromator will be a side scattering sagittal-focusing asymmetric bent Laue crystal.
- Detector: an area detector will be primarily used in this hutch.
- Paris-Edinburgh type high pressure cells with variable pressure modules designs.
- Soller slit system

Station D – white or variable energy monochromatic

Station D will house a 2000-ton hydraulic press with interchangeable high pressure toolings. These toolings will be specialized to serve several different experiments where a high pressure – high temperature environment is important. This provides a versatile experimental environment that can continually expand as new needs arise by the design and implementation of new tooling sets. The station will operate in the energy range from 20-120 keV. Both monochromatic and white x-rays will be available for the experiments as some high pressure configurations have very limited angular access for the detection. The wide energy range will allow large variety of scattering experiments at extreme conditions, currently not possible at other dedicated high pressure beamlines in the world.

- **Rheology:** The strength of material at high pressure and temperature – and the viscosity of solids can be studied using deformation tooling.
- **Ultrasonic elastic properties:** Elastic properties are fundamental properties of materials that map into the equation of state and further define the response to stress.

Tomographic imaging: Phenomena from fluid flow to faulting are possible to study with 3-d mapping of the sample with time**,** and density and viscosity of liquids.

Beamline with monochromatic and white beam capabilities

- 2000 t hydraulic jack and frame
  - Kawai style system: routine c**apabl**e of 30 GPa and 3000K
  - Deformation K**a**wai style, pressure of Kawai device with uniaxial stress capability.
  - Rock mechanics imaging system for fluid flow studies using tomographic imaging.
  - Rotational Drickamer device: 50 GPa, 3000K with shearing stress.
- A focusing monochromator which covers a wide energy range.
- Imaging requires a parallel incident beam.
- Diffraction. High d-spacing resolution in multiple azimuthal directions is required for stress measurements.
- A multielement energy-dispersive detector, coupled with a large diameter conical slit.

5. Community Outreach Efforts

The High Pressure community has held three workshops at Brookhaven National Laboratory in anticipation of NSLS-II: on February 25-26. 2006. COMPRES and MPI sponsored “NSLS X-Ray High Pressure Research Workshop: Current operation and vision into NSLS II” (http://www.mpi.stonybrook.edu/NSLS/XHP/Main.html); on July 17, 2007, there was a High Pressure discussion as part of an NSLS-II workshop, and on January 17-18, 2008, there was a breakout session during the joint workshop for “The NSLS-II Powder Diffraction Project Beamline” and “Materials Science Engineering Strategic Planning for NSLS and NSLS-II”. The first of these workshops produced a white paper, Appendix D; the final workshop produced Appendix E. The attendees at all three workshops are listed as Appendix A. We will continue the dialogue with the community through additional future workshops. The first one will be held in May 2008 during the NSLS/CFN joint user meeting at Brookhaven National Laboratory.

6. High Pressure Working Group

During the scientific planning workshops for NSLS and NSLS-II and the technique-based workshops, many scientific communities expressed interest in high pressure sample environments. High pressure research was a topic in many of the technique based workshops and the desire to incorporate high pressure capabilities in many of the six project beamlines was shown. A large variety of high pressure cells are portable and can be installed at beamlines not dedicated to high pressure. However, certain choices in the design of a beamline, which would prohibit the use of high pressure sample environments, need to be avoided. Ideally, a representative of the high pressure community would be a member on the Beamline Advisory Team (BAT), for each beamline interested in allowing high pressure research. However, currently just the Inelastic X-ray Scattering Beamline and the Powder Instrument New Generation have members with a background in high pressure research on their BAT. Therefore, the high pressure community formed the “High Pressure Working Group” for NSLS-II.

The two main functions for the members of the working group are:

1. The “High Pressure Working Group” will serve as point of contact for BATs, providing in depth knowledge of high pressure instrumentation. The members can advice on how to best integrate high pressure equipment in beamline designs in order to optimize the research capability
2. Creating a synergy effect with other BNL institutions. Several BNL institutions (e.g. CFN, CMPMSD) possess experimental capabilities and instruments that would be useful for a sample characterization after a high pressure experiment. The “High Pressure Working Group” can initiate contact with these institutions and develop a plan to integrate these experimental capabilities in the high pressure program at NSLS-II.

The members of this high-pressure working group are included as Appendix D:

Qualifications of BAT members.

Donald Weidner, Distinguished Professor of Geophysics at Stony Brook is currently spokesperson for the multi-anvil high pressure station at the NSLS (X17B2). He has been involved with this beamline since its beginning and he was chair of the multi-anvil design team for the GSECARS multi-anvil installation. His research interests are in the properties of the deep Earth. **Tom Duffy,** Professor of Geophysics at Princeton University has experience with laser heating, diamond anvil cell techniques, beamline management, synchrotron powder diffraction, optical spectroscopy. He is currently spokesperson for the diamond anvil high pressure beamlines X17B3 and X17C at the NSLS. **Andrew Campbell**, assistant Professor at the University of Maryland, has 20 years experience in high pressure, high temperature mineral physics, using a variety of high-P,T experimental methods. His expertise in laser heated diamond anvil cell applications will be particularly useful to the high pressure BAT for NSLS-II. He has previously designed and built laser heating systems for synchrotron x-ray diffraction experiments, and is actively developing new laser heating technologies in his laboratory at the University of Maryland. **Alex Goncharov** has extensive experience in optical systems for high-pressure research. He will be intimately involved in the design, testing, construction, and operation of laser-heating, Raman and ruby fluorescence systems at NSLS-II. He also will serve as a liaison between the x-ray and infrared facilities at NSLS-II. **Jiuhua Chen**, associate Professor at Florida International University, is one of the pioneers in developing multi-anvil monochromatic synchrotron x-ray diffraction. He has been working on high pressure synchrotron beamtime development for nearly two decades since his PhD thesis, in which developed the first multi-anvil two-dimensional x-ray diffraction at Photon Factory. Not only he brings the multi-anvil expertise to the BAT, he also represents the user community of mechanical and materials engineering. His research interest features a multidisciplinary nature, including mechanical properties at high pressure, crystal structures, and phase transitions in the fields of nanomaterials, geomaterials, noncrystalline materials and energy materials. His recent research has extended to diamond anvil cell as well. He served as the first High Pressure Special Interest Group Representative at the NSLS in 2006. **Michael Vaughan**, Research Professor of Stony Brook University, is a pioneer in the development of multi-anvil beamlines. He oversees the continually varying design of the X17B2 beamline at the NSLS. He was a member of the GSECARS design team for high pressure.

Appendices:

Appendix A: Workshop Attendees

List of Participants of the February 25-26, 2006 workshop (see Appendix D:)

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List of Participants of the January 17-18, 2008 workshop (see Appendix E:)

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Appendix B: High Pressure Working Group

The “High Pressure Working Group” is comprised of the following members:

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Appendix C:

List of people who have expressed interest by email since January 2008 workshop:

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2	David Walker	Columbia University
3	Michael Kruger	University of Missouri
4	Andrew Campbell	University of Maryland
5	Surendra Saxena	Florida International University
6	Shun-ichiro Karato	Yale University
7	Kanani Lee	Yale University
8	Justin Hustoft	Yale University
9	Takaaki Kawazoe	Yale University
10	Mainak Mookherjee	Yale University
11	Tomohiro Ohuchi	Yale University
12	Kazuhiko Ostuka	Yale University
13	Zhicheng Jing	Yale University
14	Sang-Heon Dan Shim	Massachusetts Institute of Technology
15	John Tse	University of Saskatchewan
16	Alexandra Navrotsky	University of California at Davis
17	Isaac Silvera	Harvard University
18	Yanbin Wang	University of Chicago
19	Lars Ehm	Stony Brook University
20	Michael Vaughan	Stony Brook University
21	Donald Weidner	Stony Brook University
22	William Durham	Massachusetts Institute of Technology
23	Baosheng Li	Stony Brook University
24	Li Li	Stony Brook University
25	Jiuhua Chen	Florida International University
26	Thomas Duffy	Princeton University
27	Yanzhang Ma	Texas Tech University
28	Hyunchae Cynn	Lawrence Livermore National Laboratory
29	James A Tyburczy	Arizona State University
30	Jung-Fu Lin	The University of Texas at Austin

31	Chris Tulk	Oak Ridge National Laboratory
32	Pamela C. Burnley	University of Nevada, Las Vegas
33	Murli H. Manghnani	University of Hawaii
34	Larissa Dobrzhinetskaya	University California at Riverside
35	Oliver Tschauner	University of Nevada, Las Vegas
36	Markus Hücker	Brookhaven National Laboratory
37	Viktor Struzhkin	Carnegie Institution of Washington
38	Mark Rivers	University of Chicago
39	Yanbin Wang	University of Chicago
40	Lili Gao	University of Illinois, Urbana-Champaign
41	William J Evans	Lawrence Livermore National Laboratory
42	Li Chung Ming	University of Hawaii
43	Quentin Williams	University of California, Santa Cruz
44	Sean Shieh	University of Western Ontario
45	Liping Wang	Stony Brook University

Appendix D: White Paper from February, 2006 workshop

NSLS X-Ray High Pressure Research Workshop: Current operation and vision into NSLS II

High pressure X-ray studies at NSLS

The National Synchrotron Light Source offers the COMPRES community a considerable opportunity for x-ray studies using the superconducting wiggler at X17. This beamline has a steep history of high pressure innovations including diamond anvil studies and large volume studies. The superconducting wiggler continues to provide an x-ray source that is competitive with third generation sources for x-ray diffraction studies. In addition, the current plans to build the next x-ray synchrotron at Brookhaven (NSLSII) provides a significant future at the NSLS that requires the presence of COMPRES research to assure access to the NSLSII.

With this vision of the NSLS, we held a workshop on February 25 – 26 to assess the community needs and hopes for the next five years. Forty five attendees discussed the strengths and weaknesses, the science goals and technical limitations. We enumerated the needs for support staff and the needs for new equipment to enable initiatives. We set priorities and estimated budgets. Here we present the results of the workshop and provide a budget plan for the next five years. We include a list of participants and the agenda for the workshop as appendices Here we address some of the conclusions of the workshop followed by the detailed proposal for the next five years.

Phase transitions

Experimental and theoretical investigations of phase transitions in Earth and planetary materials under pressure and temperature conditions of their interiors are of fundamental importance to our understanding of the nature and dynamics of planetary bodies in the solar system. A number of recent findings have led to major paradigm shifts in Earth's interior models. The discovery of the perovskite to post-perovskite transition in the predominant phase of the Earth's mantle may be considered "the discovery of the decade" in mineral physics, with multidisciplinary impact on the study of the core-mantle boundary (Murakami et al. 2004; Lay et al. 2005, Hernlund et al. 2005). The recent controversies regarding the post-spinel transition has challenged the established view of the transition zone and stimulated extensive research on pressure calibration at high temperatures, which is the basis for comparing field observations with laboratory measurements (Irifune et al. 1998; Shim et al.; Fei et al. 2004). With the unsettled claims of the beta-phase by experimentalists and the bcc phase by theoreticians, the issue of the structure of iron under core conditions also remains uncertain (e.g. Saxena et al. 1996; Alfè et al. 2002 ; Andrault et al. 2000; Ma et al. 2004).

In the next five years, new data on phase transitions in the following areas have been identified as of primary interest to the study of the Earth and planetary interiors. For crustal and upper mantle materials, new experimental data on the phase transitions in ultra-high-pressure metamorphic rocks are needed to assist the study of deep focus earthquakes. A thorough investigation of the post-spinel transition will help interpret detailed seismic observations on the transition zone, including the magnitude, sharpness, lateral heterogeneity, and topography of the 410 and 660-km discontinuities. Further studies of the post-perovskite transition including the determination of the Clapeyron slope are necessary for unraveling the mysteries concerning the D” zone and ultra-low-velocity-zone at the core-mantle boundary. A new class of phase transition in planetary materials such as CAIs, chondules, and basaltic glasses from the Moon promise to shed light on the origin and evolution of the early Earth.

Phase transition is sensitive to stress conditions. A poorly understood factor is the effect of non-hydrostatic stress on the conditions of phase equilibrium. From the technical point of view, holding pressure constant while monitoring phase transformation is an overlooked issue that deserve more attention. In most experiments with static compression, pressure is not directly measured. It may be more meaningful to determine phase transitions at a given strain state instead of pressure.

It has been recognized that the presence of the second phase may affect the transition conditions of the phase of interest (Stixrude 1997). Phase boundary may also be sensitive to the amount of minor or trace elements in the sample. Although many current research have focused on single phase systems, natural geological systems contain multiple components, among which chemical reaction may take place upon changes in pressure, temperature and composition. Studying chemical reactions in multi-component systems under high pressures and high temperatures that are prevalent in the Earth’s deep interior is a frontier in the phase transition study.

As pressure increases, the experimental sample size becomes smaller. To ensure that the experimental data collected at micron or sub-micron scale are applicable to the Earth, we must understand the effect of grain size, surface effect and the presence of nanometer-sized inclusions on phase transitions.

Before equilibrium is reached, phase transition proceeds as a function of time. Investigating the kinetics of phase transition is important for assessing the fate of the subducted slabs and understanding the dynamics of the core-mantle boundary.

A variety of experimental techniques are available to detect a phase transition, including x-ray diffraction, various spectroscopic methods, imaging (also known as x-ray radiography), and resistivity measurements. Special techniques such as magic angle diffraction may be useful in eliminating the effect of non-hydrostatic stress on phase transition.

In addition to structural phase transition, there is a resurgence of interest in electronic spin crossover in the lower mantle minerals (Badro et al. 2003, Li et al. 2004; Badro et al. 2004; Jackson et al. 2005; Li et al. 2005). This is an example of non-quenchable transition that must be studied using in-situ experimental techniques. Another novel type of phase transition is liquid-liquid transition, which may be important for understanding high-pressure melt including silicate magma in the crust and mantle and metallic magma in the core.

Specific topics were defined that help define the technological challenges:

Topic: An accurate petrogenetic grid. An accurate petrogenetic grid to 30 GPa with good coverage would allow an accurate mapping of the P-T plane, giving access to more detailed pressure and temperature knowledge in high-pressure devices that do not allow in-situ P-T measurements. The grid could be used for detailed P,T measurements in offline high-pressure devices, and samples of a particular composition could be used as internal standards in measurements of phase equilibria in any system. The location of some invariant points as anchor points or standard reference points for the P-T plane would also be very useful (similar to the use of the triple point of H2O as a standard reference point for temperature, for example). The creation of such a grid will require:

A. In-situ x-ray diffraction measurements of univariant boundaries.
B. A set of independent primary standards valid at the relevant P-T conditions. Some workers have mentioned the possibility of a set of "internally compared" standards based on one primary standard. However, this introduces unnecessary propagation of random or systematic errors from the primary data set. A better method will be to measure many standards (using elasticity and volume measurements, for example) and treat each one as a primary standard, with inter-comparisons as a cross-check. Elasticity and volume measurements of these standards (such as NaCl, MgO, CsCl, Au, Pt, W, etc.) will need to be performed at all the P, T conditions and an equation of state agreed upon for each in order to create this series of standards.
C. The determination of the pressure effect of thermocouple emf needs to be pursued. The Johnson Noise equipment created by Ivan Getting, and relocated to a beam line or other appropriate facility, will be a good mode of action for this (Sector 13 at GSECARS may already be doing this).
D. High-pressure, large-volume assemblies with lower thermal gradients will be needed to increase the accuracy of these measurements. Cell assembly development will thus need to continue.
E. High d-spacing accuracy and resolution will be needed for the phase equilibrium measurements at the beam line. This should be negotiated with the experts at the beam line.
F. Long duration runs may be necessary to reach a state of equilibrium in many cases. This will benefit from the existence of side stations and multiple experimental apparati.

Topic: Lower mantle phase equilibria. The complexity of phase behavior in the lower mantle is just being uncovered. The phase transition in CaSiO3 perovskite, expected in the mid-lower mantle, and the post-perovskite phase transition in (Mg,Si)O3, are very recent discoveries and it is assured that detailed studies of the phase equilibria and properties will be necessary to apply these findings to the mantle in appropriate detail. Transition pressures will need to be more accurately determined, including the effects of secondary elements on the pressures of the transitions. The partitioning of secondary and minor elements will be important in understanding the chemical evolution of the Earth. The property changes caused by the phase transitions are now an issue. Stress effects, kinetics will need to be known. These studies will benefit from improvements in x-ray resolution, temperature measurement in the diamond-anvil cell, creation of isothermal temperatures in the laser-heated diamond-anvil cell, and the performance of associated experiments such as spectroscopy and elasticity measurements (for example to more precisely locate and characterize the symmetry transition in CaSiO3, since the x-ray effects very close to the transition may be too subtle to see).

Topic: Melting. In a field dominated by x-ray diffraction measurements, the determination of the onset of melting is a difficult problem. However, the onset of melting, and the phase equilibria of melting including solidus and liquidus locations, element partitioning, as well as the mechanics and geometry of melting, are all important in Earth's evolution and structure. The high temperatures and chemical reactivity of melts also lead to problems in containment and pressure measurement that need to be continually solved as they arise. High-resolution imaging of samples in the LVP, combined with marking of the melts with heavy incompatible elements, could help in locating onset and geometry of melts (though the effect of the dopants on the melting needs to be considered). A combined energy- and angle-dispersive facility for the laser-heated DAC could be used to switch between accurate d-spacing measurements (angle-dispersive) and the easier identification of melting (energy-dispersive) (suggested by Tom Duffy). Associated optical and spectroscopic measurements would also be very useful.

Equation of state of melts are important in defining the thermodynamics of melting and motivate new studies. For example, the notion of phase transitions within melts is important to define. Certainly coordination changes occur for elements such as silicon or magnesium with increasing pressure. Whether these changes are sudden or gradual affects our understanding of melts. X-ray absorption studies can define density. X-ray diffraction can yield the pair distribution function. The first of these studies is currently in progress at X-17B2 using an imbedded reference sphere in a melt. The PDF studies require a wide range in Q and very low background. We propose below to purchase a solar slit system, such as the one in use at the ESFR. This system can yield the required low background for these ;measurements.

Topic: Effect of stress on phase transitions. The pressure/temperature conditions and kinetics of phase transitions are affected by stress, and in the low-stress limit this is applicable to phase transitions in subducting slabs and other deforming environments in the mantle. The understanding of this will require the accurate control and measurement of stress and strain. *In-situ* stress/strain measurements are active parts of the D-DIA, R-Drickamer and R-DAC programs at present, and the application to phase transitions is in the formative stages. Problems such as the effect of stress on the forsterite to wadsleyite phase transition in subducting slabs would be of keen interest in mineral physics, for phenomena such as deep earthquakes. Technical developments include high resolution stress detection, high dynamic range for the initial detection of phase transitions in a strained solid, magic angle diffraction for isolating the "stress-free" state, high-resolution radiography and tomography for imaging of phases and cracks (using metal markers, for example), and ultrasonic measurements of events in the sample coupled with imaging. Such studies of stress will be of interest in materials science as well as mineral physics. One distinction to make is the presence of stress as a "problem" in phase transitions when the equilibrium behavior at isostatic pressure is desired, as opposed to the use of stress as an imposed variable whose effects on phase transitions are of primary interest (Harry Green).

Topic: Effect of grain size/surfaces on phase transitions. This is an active part of the study of nanomaterials. Grain size and surface energy have significant effects on phase transitions, allowing metastable phases to be accessed and changing phase diagrams. Materials scientists are interested in the phase behavior of compounds with well-characterized grain sizes in the nanoscale range. This can also apply to nanophases or nano-inclusions (nuclei) in natural minerals, in which metastable behavior has been observed (TiO_2 inclusions in natural minerals was mentioned by Harry Green).

Topic: Second-order phase transitions. In order to better see the small lattice splittings near second-order phase transitions, good control of hydrostaticity and high-resolution x-ray measurements are needed. The detection of second-order or nearly second-order transitions is also aided greatly by the use of complimentary methods, such as Raman, IR and other lattice dynamic measurements.

Topic: Non-conventional phase transitions. Spin transitions (high-spin to low spin) in transition metals and polyamorphous phase transitions (glass to glass or liquid to liquid transitions) are unusual types of phase transitions requiring special measurements. High-q radial distribution function measurements (both x-ray and neutron) are useful for polyamorphous transitions, while nuclear forward scattering (NFS) and other specialized techniques are needed to study HS-LS transitions. For Earth compositions such as $(Mg,Fe)\ SiO_3$ with smaller amounts of the transition metal, higher-resolution x-ray diffraction would be useful for discriminating the small lattice parameter differences between HS and LS states.

Topic: Thermodynamic measurements. The accessible properties of phase transitions that can reveal the thermodynamics of systems are the P-T slopes of univariant phase transitions, molar volumes of crystalline solids available by x-ray measurements, melt volumes by falling sphere, radiography, or tomography measurements. These can be combined with other data, such as heats of solution, vibrational measurements, and calculations, to obtain the full thermodynamic characterization of complex systems.

Topic: Binary (and higher multicomponent) phase equilibria. As the detailed studies of mantle systems continue, it is becoming more and more important to be able to interpret the phase equilibria of systems with more components from in-situ measurements. For example, in the study of the effects of Fe, Ca, Al, and other elements on the post-perovskite phase transition in $MgSiO_3$, it is necessary to interpret the phase behavior of a multi-component system using x-ray diffraction at ultrahigh pressures. This and other multi-component systems require good discrimination of d-spacings, accurate simultaneous measurement of P and T, and low thermal gradients to map out binary and higher phase diagrams. This is in its infancy and will rely on technical developments in both large-volume and diamond cell research.

Topic: High-pressure boiling and critical points. This will require the identification of liquids and gases in situ, which can be done with imaging and with liquid structural measurements. Very high temperature furnaces will also be required.

Topic: Kinetic studies. For slow kinetics, turrets of diamond cells and multi-anvil side stations would be very useful for taking occasional measurements without occupying the beam unecessarily. For very fast kinetics, techniques of more rapid data collection would be highly desireable.

Topic: Incommensurate structures. The study of incommensurate structures, such as are found in the post-close-packed structures of alkali metals, for example, requires the detection of small superlattice reflections, which in turn will rely on high dynamic range and x-ray sensitivity. The needs are similar to those for second-order phase transitions.

Topic: UHP metamorphism. The creation of more detailed phase diagrams for crustal rocks will be needed to unravel the new metamorphic grades that have been found in ultrahigh-pressure terranes.

Melt and glass structure

High resolution x-ray diffraction for crystallographic studies and high energy x-ray scattering for pair distribution function (PDF) studies of non-crystalline materials (melts and glasses) at high pressure pressure/temperature has drawn great attention among the participants at the workshop. While properties of crystalline minerals have been extensively studied from the crystallographic point of view, melts and glasses increasingly become of geophysical interest because melts and partial melting play an important role in mantle dynamics

Structure determination of glasses and melts at high-pressure(P) and –temperature(T) require high quality data. These data must be free from parasitic scattering from cell components, such as: anvils, gaskets, and furnace materials. Several methods are used to eliminate or reduce background scattering and are applied either in the data processing stages or during data collection. These include: background measurement and subsequent subtraction from high PT data or the use of slit systems to completely eliminate parasitic scattering from reaching the detector. In practice, it is generally not enough to simply collect backgrounds or blanks at ambient conditions and apply these to high PT data because backgrounds change with P and T, and may not be easily determined at high PT. On the other hand, Soller slit systems, such as the one illustrated in Figure 1, can be used to completely eliminate parasitic scattering from reaching the detector and are functional at any PT conditions. Soller slits, when properly installed and aligned, can provide high quality data.

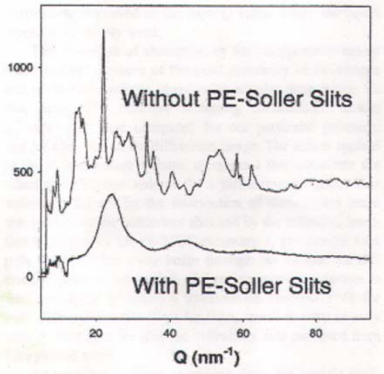

Figure 1. Diffraction pattern of liquid tin with and without Soller slits. Figure from Mezouar et al., 2002 [2].

Soller slits are currently being used with multi-anvil [1] and Paris-Edinburgh [2] pressure systems. An example of liquid diffraction data collected using a Paris-Edinburgh press, with and without Soller slits, is displayed in Figure 2. This figure illustrates a very important point about liquid(melt) and glass scattering. Namely, melts and glasses are very weak scatters and their signals can be “washed out” by parasitic scattering. However, it is immediately clear that Soller slits are remarkable at removing parasitic scattering and allow the collection of high quality diffraction data necessary for structure determination of glasses and melts at high PT conditions.

Elasticity

The most robust fingerprint of chemical and thermal state of the Earth’s interior are the elastic properties of the materials. Recovered by seismology, the radial variations in seismic velocity points to phase transitions, melting, and general pressure increase. Painted as blue and red, lateral variations in seismic velocity lead to dynamic modeling as the colors transform to temperature or composition, and further to buoyancy. These transitions require the input of a comprehensive understanding of the elastic properties of earth materials as a function of all of the relevant variables. These last few years has seen tremendous growth in our data base as well as our experimental tools for defining this information. Here we outline some of this excitement with a focus on the next phase of development.

Recent Highlights – Equations of State P-V-T Equations of state of mantle and core minerals are essential to interpreting the observed seismic structure of the Earth in terms of its mineralogy. Recently numerous important advances in measuring equations of state (EOS) have been made using synchrotron x-ray diffraction at high pressure. Measurements of room temperature EOS of minerals remain important. Recent examples include the compression curves for the newly discovered post-perovskite phase of (Mg,Fe)SiO3, which may be an important constituent of the lowermost mantle D" region (Mao et al., Princeton group).

High-P,T EOS of minerals (e.g., MgSiO3 perovskite (ESRF); CaSiO3 (Shim et al.; hcp-Fe (Dubrovinsky et al.)) have been measured using laser heating in diamond anvil cells. These advances illustrate the tremendous potential of this technique. The precision and accuracy of this powerful tool will benefit further from continued development.

Evaluations of high-temperature pressure standards are of critical concern to further development in high pressure science. A recent comprehensive study by Fei et al. (2004) examined the high-P,T equations of state of numerous candidate pressure calibration standards (e.g., MgO, Au, Pt, W, Mo, Pd), and documented inconsistencies between previously determined EOSs of these materials. This study was carried out using a multi-anvil press with synchrotron x-ray diffraction to determine cell volumes, and reached pressures up to 20 GPa and temperatures of 2000 ºC. The inconsistencies highlighted in this study allowed a critical assessment of the earlier equations of state, and made recommendations regarding the most reliable pressure calibrations at high T. A related study focussed on the widely used ruby fluorescence scale in relation to the compression of a number of metals at room temperature (Dewaele et al.).

Recent Highlights – Elasticity A variety of techniques are now being used to determine acoustic velocities of materials at high pressure. These include Brillouin spectroscopy, NRIXS, inelastic x-ray scattering, and ultrasonic interferometry.

Brillouin spectroscopy in the diamond anvil cell continues to provide novel and important results. A recent example is the measurement of acoustic velocities in polycrystalline, Al-bearing silicate perovskite to 45 GPa (Jackson et al., 2005). These data point to Al content as a plausible explanation for lateral shear wave velocity variations in the lower mantle. Additionally, a Brillouin spectroscopy system has recently been installed at the GSECARS sector of APS. The combination of Brillouin spectroscopy and simultaneous x-ray diffraction can provide an absolute pressure scale, which will be welcomed by the high pressure community.

Inelastic x-ray scattering methods have recently been developed for high-pressure applications, and used to study the elastic properties hcp-Fe, the principal component of the Earth's inner core (e.g., Fiquet et al., 2001; Lin et al., 2004). This tool may well be an important component of the NSLSII program.

Simultaneous ultrasonics + XRD investigations in the multi-anvil press permit the equation of state and acoustic properties of minerals to be evaluated under high-P,T conditions. An example is the recent study of MgSiO3 perovskite to 9 GPa and 873 K by Li and Zhang (2005). In principle this technique can be extended to 20 GPa and high temperatures. Gigahertz ultrasonic techniques are also being carried out at very high pressures in the diamond anvil cell.

Finally, it should be noted that with synchrotron XRD techniques, characterizing stress and strain is now done routinely in a variety of high-P,T experiments. This is an important advance over past experimental methods, in which the stress/strain state of samples were commonly uncertain or unknown.

Scientific challenges – Equations of state Equations of state of deep Earth materials are essential in the interpretation of seismological properties and geodynamics of the planet's interior. The emergence of synchrotron radiation sources has allowed tremendous advances in the development of technologies that can soon be used to precisely measure these pressure-volume-temperature relationships under extreme conditions of P and T. In addition, synchrotron XRD of an internal calibrant is commonly used to determine pressure in studies of phase equilibria, crystallography, acoustic properties, and other measurements at high-P,T conditions. Now that these methods are being employed, it is imperative that their accuracy and precision be validated.

In the last few years a number of studies have revealed significant inconsistencies between several high-P,T pressure standards that are widely used. The efforts to correct this situation have focussed on the pressure range below ~20 GPa, normally accessible using the multi-anvil press. It is apparent that a similar, and probably worse, situation exists among pressure standards that are now being used in laser heated diamond anvil cell studies. A key challenge to the high pressure community is to develop standards that can be used as internal pressure calibrants for x-ray diffraction experiments in the laser heated diamond anvil cell. This should also include the cross calibration of multiple standards, because no single standard is appropriate for use in all experiments. A comparison of these calibrations across different beamlines will be helpful to strengthen the standardization of the adopted equations of state, and also to identify any difficulties in making inter-facility comparisons of data.

A related concern is the lack of pressure calibrants for use in high temperature experiments that take place at users' home institutions, where x-ray diffraction is not an available method. The development of a tool, similar to the ruby fluorescence scale, that can be used to determine pressure at high temperatures without XRD would be of tremendous benefit to the high pressure community.

The determination of P-V-T equations of state of liquids, by synchrotron x-ray radiography, is recognized as a promising direction for future studies. The properties and dynamics of melts are critical to understanding many geophysical processes..

Scientific Challenges – Elasticity The interpretation of seismological profiles of the Earth's interior has long been the principal motivation for measuring the acoustic velocities and the elastic tensors of minerals, both at ambient and high P or T conditions. As the resolution of seismological studies continues to improve, the need for more and better elasticity data, under simultaneous high pressures and high temperatures, increases.

Two specific challenges that can be highlighted include: the interpretation of seismic anisotropy throughout the planet, from uppermost mantle to inner core conditions; and understanding lateral variations of compressional and shear wave velocities (∂Vp and ∂Vs) in terms of composition and/or temperature variations. These goals require the mineral physics community to provide complete characterization of elastic anisotropy, as well as aggregate acoustic velocities, in minerals, and also the variation of these properties with pressure, temperature, and composition.

As mentioned above, there are several technologies that hold promise in this regard. These include Brillouin spectroscopy, inelastic x-ray scattering, and ultrasonic interferometry,, all of which have been demonstrated to be useful at high pressures and/or high temperatures. Each of these techniques has its own unique advantages, and all are expected to provide important contributions toward these goals.

In order to further develop the ultrasonic studies at X17B2, a 2000-ton press with exchangeable modules is immediately needed to expand pressure ranges of a variety of experiments, including equation of state, phase transformation, and ultrasonics. Sintered diamond cubes are needed for expanding the pressure to the top of the lower mantle pressures to narrow gap/expand the overlap in pressure range between diamond anvil and large volume apparatus to ensure consistency from different techniques. These new acquisitions will benefit the experiments for equation of state, ultrasonics, lattice strain studies.

Rheology

The quantitative relationship between stress, strain, and time in minerals forms the basis for our view of the evolving Earth. Plate tectonics, earthquakes, volcanic eruptions all respond to these intrinsic properties of Earth materials. Laboratory studies have recently made a significant breakthrough in capability for defining these properties at mantle pressures and temperatures using x-rays generated by synchrotrons at national laboratories. This progress has set the stage for new and exciting research efforts.

Significance of deviatoric stress measurements at high pressure. Thermal convection in Earth's deep interior cools the planet and in the process generates earthquakes and volcanoes, moves tectonic plates, and disturbs the uniform chemical layering of a differentiated Earth. Laboratory measurements of the relationship between deviatoric stress and deviatoric strain rate of rocks and minerals at high pressure are driven by the need to understand this circulation at depth. Characterizing the state of deviatoric stress during experiments under high confining pressure is also critical in a number of other mineral physics studies that have important bearing on the frontiers of solid Earth science (e.g., accurate characterization of seismic velocities of high-pressure phases). Current research on global geodynamics strongly suggests that the dynamics and evolution of this planet are controlled largely by materials properties under deep Earth conditions, including rheological properties, phase relationships, elastic properties and chemical properties such as the diffusivity and solubility of certain elements [e.g., [*Bercovici and Karato*, 2003; *Kellogg, et al.*, 1999; *Schubert, et al.*, 2001; *Tackley*, 2000; *van Keken, et al.*, 2002]. For instance, the lateral and radial variation of viscosity have an important influence on the convection pattern and generation of deep earthquakes [e.g., [*Bunge, et al.*, 1996; *Christensen*, 1984; *Green and Houston*, 1995; *Green and Marone*, 2002; *Karato, et al.*, 2001; *van Keken and Ballantine*, 1998], whereas the solubility and diffusivity of elements in various phases control the chemical evolution associated with mantle convection [e.g., [*Hart*, 1988; *Hofmann*, 1997; *Van Orman, et al.*, 2002]. Also, the way in which materials are distributed or the flow pattern in Earth can, in principle, be inferred from seismological observations, but the interpretation of seismological data relies entirely on our understanding of elastic and anelastic properties of minerals under deep Earth conditions [e.g., [*Jackson*, 2000; *Karato and Karki*, 2001; *Karki, et al.*, 2001; *Liebermann*, 2000].

In the experimental study of these physical properties, characterization of stress plays an important role in one way or another. For example, in the study of rheological properties, the relation between (deviatoric) stress and strain rate is most appropriately determined under the conditions equivalent to those in Earth's interior. Consequently, precise measurements of stress and strain at high pressure have direct influence on the quality of the experimental results. In particular, the demand for high-resolution stress measurements is critical for the study of rheological properties in order to obtain results that can be extrapolated to Earth's interior (see more details later). In addition, some transport properties, such as diffusion, should be measured under low deviatoric stress because dislocations generated by deviatoric stress are known to have a strong influence on diffusion coefficients [e.g., [*Flynn*, 1972; *Shewmon*, 1989]. Defects such as dislocations and grain-boundaries may also have an important effect on element partitioning [e.g., [*Hiraga, et al.*, 2004].

Recent progress. During the last few years, there has been important progress in measuring the state of stress of samples during high-pressure experiments. Firstly, there have been significant advances in high-pressure, high-temperature deformation apparatuses, in particular, the successful development of two instruments: the Deformation DIA (D-DIA) [*Wang, et al.*, 2003], and the Rotational Drickamer apparatus (RDA) [*Xu, et al.*, 2004; *Yamazaki and Karato*, 2001], by which quantitative rheological experiments have become feasible well beyond a pressure of ~4 GPa. Insights provided by these new instruments will be key to better understanding of the evolution and dynamics of terrestrial planets. An important new dimension currently in its early stages is development of ways to use the diamond anvil cell (DAC) to extend such deformation studies to much higher pressures.

Secondly, there is an increased appreciation of the importance of stress in the experimental studies of equations of state (EOS) and elasticity [*Wang, et al.*, 1998; *Weidner, et al.*, 1992] Some discrepancy in reported EOS is likely due to the influence of deviatoric stress that causes systematic differences in the positions of x-ray diffraction peaks. For an anisotropic material such as brucite, values of bulk modulus reported from synchrotron studies in the 1990s varied by a factor of two owing to the uncorrected effect of deviatoric stress at high pressure [*Xia, et al.*, 1998]. Improved stress measurements are also critical to multianvil studies of elasticity. For example, acoustic measurements of EOS in a multianvil apparatus are hindered by the lack of knowledge of sample dimensions at high pressure. It is now possible to use the D-DIA to hold sample length constant during acoustic measurement [*Li, et al.*, 2005a]. At this point direct imaging is used as feedback. As we are able to resolve differential stress levels below the elastic limit and achieve higher resolution of sample dimensions, we will be able to bring even finer control to acoustic measurements and, by intentionally imposing a differential stress, begin to define third order elastic moduli.

Thirdly, it is often critical to measure many phenomena such as phase equilibria or diffusion coefficients in a purely hydrostatic environment. Yet, cell assemblies are often elastically anisotropic, so that when compressed "hydrostatically" in a multianvil apparatus, a non-zero state of deviatoric stress is unavoidable. If, however, deviatoric stress can be determined, then steps can be taken (e.g., operation of D-DIA anvils) to reduce the stress state to hydrostatic.

We have recently developed a method for measuring stress in a sample under high-pressure and temperature conditions in a multianvil apparatus using x-ray diffraction from a synchrotron source *[Li et al, 2004]*. The spacings of the lattice planes are measured both parallel and perpendicular to the principal stress axes. The stress is then derived from this measured elastic strain using the elastic moduli [*Singh, et al.*, 1998]. We have used both white x-ray and monochromatic techniques. For the white beam studies, we have used a multi-element solid-state detector that was designed for EXAFS studies. With it we use four elements that are positioned at 90^o from each other. A conical slit system was designed and built to fit the detector. Because of the small diameter of detector, we could not build a slit system that optimized the optics such as the acceptance angle and spatial resolution. Nevertheless, we obtain precision of 100 MPa. The number of detectors in our current system precludes defining the orientation of the principal stress axes projected on the plane of the detectors (so they must be known *a priori*), and the dimensions of the slits limits the x-ray resolution. The monochromatic system yields about the same precision, with a greater ability to define the axis of the stress field because a 2-D detector is used. However, the monochromatic system cannot readily collimate the diffracted x-ray beam, so the background due to diffraction from the pressure medium and parts of the sample assembly can easily hide diffraction from the sample, which limits our choices of building materials.

At the workshop the following issues were expressed:

- In order to characterize the flow properties of many important earth phases, we need higher pressure. Although the DAC can provide much wider pressure range than LVP, there are still concerns about whether the DAC is an appropriate tool for the characterization of flow laws.

- Although some concern was expressed about trying to characterize the behavior of too many phases, we need to cognizant that crustal phases are returned to the mantle and subducted to great depth.

For rheology studies: Quantify effect of H_2O on rheology

- Progress has been made but there is more work to be done especially at high pressure.
- We do not fully understand where water resides – in crystals? Along grain boundaries? Does water stay in the same place upon quench? Do we need to look for in-situ techniques that will allow us to probe the structural sites for water at high pressure and temperature? Or are quenched samples representative?
- Making good measurements at low stress levels will be important for properly characterizing activation volumes
- making sure that we measure the flow mechanisms appropriate to the mantle
- We need to better understand the effect of other volatiles and impurities on rheology.
- We need to better understand the character of grain boundaries at high pressure and temperature as they are likely to become more like defects (or grain boundaries in metals). If atoms on the grain boundary behave as if they are in the liquid state then we can anticipate a larger pressure effect on their behavior than we might otherwise anticipate.
- Grain boundary characteristics will be important for grain boundary sliding.
- The small probe size of NSLS II opens up the possibility of nano-imaging or tomography techniques that will allow us to observe defects in-situ during deformation.
- Techniques that allow us to create high strains will be important for studying the development and effects of lattice preferred orientation and the development and effect of rock textures (e.g. two phase mixtures, foliated or textured rocks etc.)

Challenges:

- **Strain measurement** of 10^{-6} would allow us to do anelasticity measurements with small source size. At NSLS II this would be possible.
- Need to build optics to enlarge the image before we convert it to light (x-ray microscope)
- This higher resolution would also improve deformation measurements in the DAC (their sample size is small which limits their ability to measure strain.)
- Possibly single crystal Q experiments combined with polycrystalline Q experiments would allow us to examine “micro-creep” vs “macro-creep” and therefore shed light on the interpretation of post glacial rebound data.
- Perhaps we can establish equations that relate micro-creep and macro-creep.
- Rotational diamond cell? (future potential tool that could be useful)
- Strength increases with pressure therefore, we need to go to much **higher temperature** to get low stress to compensate. Therefore, we need to develop cells that can go to higher temperatures than we currently achieve.
- Software **data processing** issues: need to get high precision stress/strain results in real time.

Current status at X17B2. We now have an MRI proposal pending at the NSF requesting funds to upgrade the conical slit system with a new detector that is optimized for stress resolution. We expect that we can achieve 10 MPa precision with the new system if funded. We have also recently purchased (with a grant from the Air Force) a MAR345 imaging plate detector which will be used with monochromatic x-rays. We will be able to refine stress measurements with this system. We are nearing the final design of a D-Tcup which is a deformation system similar to the DDIA, but using the T-cup tooling. We expect that this system will allow us to carry out deformation experiments at high temperature and pressures exceeding 20 GPa. We currently have funds for the purchase of this system.

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Appendix E: White Paper from January 2008 workshop

Materials at High Pressure

Future directions in high pressure science and instrumentation at NSLS & NSLS-II

From the breakout session
"Materials at High Pressure"

during the joint workshop for: "The NSLS-II Powder Diffraction Project Beamline" and "Materials Science Engineering Strategic Planning for NSLS and NSLS-II"

January 17-18, 2008

Prepared by
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This report is prepared from the results of the breakout session and by using the white papers: ***"High Pressure Needs at the NSLS II Synchrotron"*** from the NSLS II workshop July 17 – 18, 2007 by *Donald Weidner* and *"**Earth Science Research***

***Perspective (Material Properties at Extreme Conditions) at the NSLS II" by** Jiuhua Chen, Malcolm Nicol, Donald Weidner, David Mao.*

Introduction

Pressure is one of the fundamental thermodynamic variables, which can be varied over a range of more than sixty orders of magnitude, from the vacuum of outer space to pressures in the interior of neutron stars. The exploration of matter at extreme conditions is a central theme in a broad range of scientific disciplines (e.g. material science chemistry, physics, and Earth and planetary science). The application of pressure can induce both continuous and discontinuous changes in atomic and electronic structure. Learning how atomic and electronic arrangements change under extreme conditions provide insight into the nature of phase transformations, chemical reaction, and also evolution in micro- and nanostructural components, such as crystallite size, dislocations, voids, and grain boundaries. Once these processes are understood, it will be possible to predict responses of materials under thermomechanical extremes using advanced computational tools. Further, this fundamental knowledge will open new avenues for designing and synthesizing materials with unique properties. Using these thermomechanical extremes will allow tuning the atomic structure and the very nature of chemical bonds to produce revolutionary new materials.

Powder and single-crystal diffraction and infrared spectroscopy have been on the forefront of synchrotron-based techniques used to study materials at high pressure. Many scientific breakthroughs have been made during the last 30 years that advanced our knowledge of materials at high pressure and the structure of Earth's interior. The introduction of 3^{rd} generation synchrotron sources about a decade ago has lead to a major step forward in high-pressure science. New applications of synchrotron spectroscopy methods at high pressures in a diamond anvil cell (DAC) have been developed at the third-generation synchrotron sources: spin-sensitive x-ray emission, nuclear resonant scattering methods, inelastic scattering from electron and phonon excitations, resonant inelastic scattering techniques (RIXS). The rapid development of inelastic scattering techniques provides a multitude of probes of elementary excitations in condensed matter in a broad energy and momentum parameter space. As a result of synergetic developments in synchrotron and pressure cell design a broad range of x-ray studies of the physical and chemical properties of solids can be now conducted *in situ* at high pressures to several hundred gigapascals.

Addressing forefront scientific questions in high-pressure research is only achievable through combination of the results from experiments obtained from complementary high-pressure techniques. Furthermore, current scientific challenges in high pressure involve multiple extreme conditions in addition to the static or dynamic high pressure environment, e.g. high and low temperature, magnetic fields. The combination of state-of-the-art diffraction with optical and X-ray spectroscopy, imaging and computational methods open new frontiers in the study of the high pressure behavior of a material.

Scientific Challenges

The scientific challenges in high-pressure research are manifold and involve overlapping scientific disciplines. In the past decade, advances in synchrotron x-ray based analytical techniques fostered remarkable breakthroughs in high pressure sciences, including discovery of the post-perovskite phase of $MgSiO_3$ stable at more than 100 GPa (2, 3), the unusually low melting temperatures of sodium, reaching 300 K at 118 GPa (4), complex structures of alkali metals at high pressure (5-8), observation of a spin state transition in iron under conditions in Earth's lower mantle (9), the changes in the bond characteristic of compressed graphite (10), and the measurement of the spin and charge order in chromium at high pressure (11).

The following chapter describes the current and future scientific challenges defined by the high-pressure community at workshops and conferences held during the period of 2005-2008. The scientific case covers challenges from several fields, such as material science, chemistry, physics, and earth sciences. Some classifications for these scientific challenges are arbitrary, since they would fit in any of the scientific fields mentioned above.

Earth and Planetary Science

Study of the structure, composition, and history of the Earth and planetary interiors is an extremely challenging task because the deep interior is inaccessible. Seismological investigations are the primary source about the interior structure of the Earth and other planets. Advances in seismology provide detailed 3D tomographic images that show heterogeneities, anisotropy, attenuation and discontinuities from the surface to the center of the core. Seismic models of the variation of compressional and shear wave velocities and densities presumably reflect radial and lateral variations of chemical composition, mineralogy, pressure and temperature. Experimentally derived information of the density and elastic properties of Earth and planetary materials under geologically relevant pressure and temperature conditions are needed for successful interpretation of the seismic models.

Refinement of the Earth's interior structure

Subduction Zones

Subduction zones (Figure 1) are the geologically most active areas on Earth, greatly impacting life on Earth's surface (12-15). Subduction zones exist at convergent plate boundaries where oceanic lithosphere converges with another plate and plunges into Earth's interior. Thereby, crustal and upper mantle materials get recycled into the mantle.

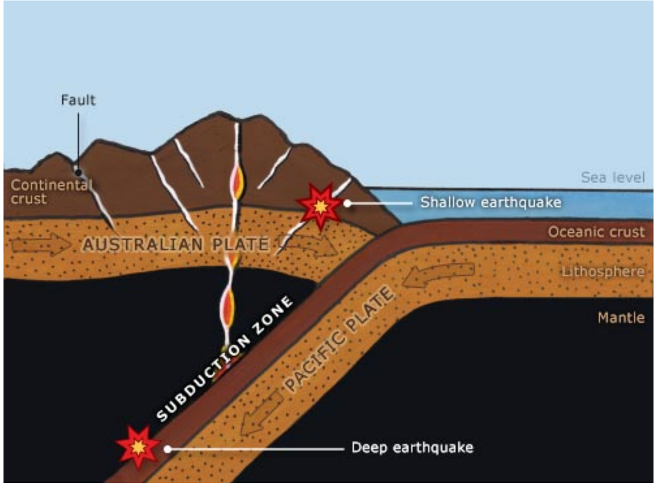

Figure 1 Structure of a subduction zone. The descending plate presses against the overlying continental plate, causing the overlying plate to fracture and producing shallow earthquakes. Deep earthquakes occur in the oceanic crust that is being bent downward into the subsurface. As the Plate descends into the hot interior of the earth, rock near the plate boundary starts to melt, feeding volcanoes above.

Increased volcanic and earthquake activity can be found at plate boundaries, where subduction is active. The general mechanism of subduction is well understood through the concept of plate tectonics. However, the processes in the subduction zone, that lead to volcanism and earthquakes are poorly understood. The technical capabilities to study the complex processes in subduction zones *in situ*, has recently emerged with the availability of 3rd generation synchrotron sources. With the current experimental facilities at hand and the unique experimental capabilities that NSLS-II will provide on the horizon, experiments that simulate the complex conditions (pressure, temperature, composition, stress etc.) in the subduction zone are in reach.

One of the key issues related to subduction zones is the influence of volatiles, in particular water and carbon dioxide, on mineral and rock properties and stabilities at high pressure and temperature. The determination of the efficiency of the recycling of volatiles in the mantle and the identification of possible mineral reservoirs for volatiles at Earth's mantle conditions will allow us to gain a deeper understanding of Earth's water and carbon dioxide budget and Earth-Atmosphere interactions. Synchrotron IR spectroscopy at extreme conditions is the only technique that allows *in situ* investigations of the volatile content of minerals and provides information on the speciation of hydrous components. In the lower mantle, where silicate perovskite (PV) and magnesiowüstite (MW) are the stable assemblage, the water storage capacity remains uncertain, with current estimates ranging by three orders of magnitude, from ~1 ppm (16) to over 2000 ppm wt. H_2O (17) in silicate perovskite. The major question now is whether or not hydrogen observed in synthetic samples occurs as structurally bound hydroxyl in the perovskite, or is present as hydrous mineral inclusions or melt quench.

Earthquakes are among the most destructive natural events happening in subduction zones and are almost impossible to predict. The earthquake process involves the interaction of stress fields with minerals and volatiles from the macro scale to the micro scale. Deep earthquakes happening along subduction slabs offer a nature probe for Earth's interior. However, the mechanisms of these earthquakes have remained uncertain for decades. Improved understanding of these dynamic phenomena requires *in situ*, time-resolved studies of surface physics and chemistry during stress and strain episodes. High-resolution strain mapping, chemical mapping, and interface phenomena at controlled environmental conditions of pressure, temperature, and stress holds the hope of new insights into the phenomena of earthquake processes.

Core-Mantle Boundary

The Core-Mantle-Boundary (CMB) at depth of 2900 km separates the liquid outer core from the silicate lower mantle (Figure 2). The change in physical properties across this boundary is as great as that between the solid Earth and the atmosphere at Earth's surface. The CMB region is highly anomalous, and holds the key to a number of fundamental geophysical questions including: thermal structure of the deep Earth, origin of geochemical heterogeneity, ultimate repository of subduction slab material, and chemical interactions between mantle and core. Just above the CMB at 2700 km a discontinuity in seismic wave velocities is observed commonly referred to as D”. Recent advances in high-pressure science make it now possible to routinely generate pressure and temperature conditions of the CMB in the laboratory.

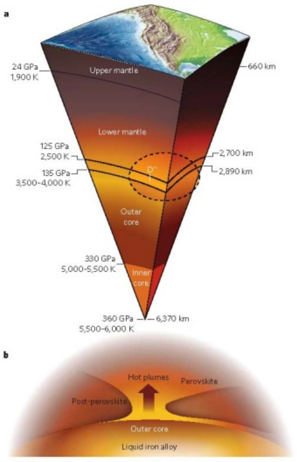

Figure 2 Cross section of Earth's interior B. Close up showing possible complex structures near the core mantel boundary (from (1)).

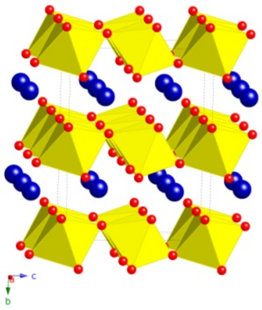

Figure 3 Crystal structure of $CaIrO_3$-type (post-perovskite) phase of (Mg,Fe)SiO3 (from (1)).

The discovery of the structural phase transition from perovskite to $CaIrO_3$-type phase (post-perovskite) () at pressure and temperature conditions of the D” discontinuity has revolutionized our understanding of the CMB (2, 3) (Figure 3). But many fundamental questions regarding D” and the CMB remain (18). The interaction of the molten outer core with the silicate mantle is largely unknown (19, 20). Knowledge of exchange reactions at high pressures and high temperatures between a metal from one side and refractory oxides and silicates from another side is important for understanding the early Earth differentiation. The temperature of the liquid outer core and the temperature profile over the CMB are still unknown(21). Measurements of the melting temperature, elastic properties and crystal structures of iron alloys, metal oxides and lower mantle silicates (e.g.

perovskite and post-perovskite) at high pressure and temperature will allow us a further insight into the composition, temperature, and structure of the CMB.

Mission to the Earth's core and beyond

The Lehmann discontinuity at 5150 km marks the boundary of the liquid outer core and the solid inner core. The structure and properties of a planetary core promise to provide a wealth of information about the evolution and dynamic processes within the planet. However, limitations in pressure generation and related properties measurements at such extremely high pressures and temperatures hinder the mission to the Earth's core (21). As analytical techniques set restrictions on the minimum sizes of high pressure samples and higher pressures normally require smaller samples, the sub-micrometer spatial resolution of the NSLS II X-ray beams will enable new ground breaking work to challenge accessibility to the pressure at the center of the Earth's core (3.5 million atmospheres) and beyond. The high spatial resolution X-ray beam will also significantly enhance the capability to recognize heterogeneities of pressure, temperature, chemistry, structure and phase within small samples and to improve reliability of experimental data obtain at such high pressures. With such advances in experimental capabilities, we expect to address the long-standing issue of core composition and to understand the new observations of inner core seismic anisotropy, super-rotation and magnetism.

Rheology

The plastic properties of ceramics – rocks – at high pressure and temperature control the evolution of the Earth and planets (22). The pressure envelope for quantitative rheological experiments has limited us to properties of the upper layers of the Earth until very recently when synchrotron methods have extended the pressure range by about two orders of magnitude. This has come with synchrotron X-ray imaging techniques and stress metrics. The current experimental capability limits the strain precision to 10^{-4} (resolving 100nm length change over 1 mm long sample) in multi-anvil apparatus. The high spatial resolution of less than 10 nm will improve by one to two orders of magnitude strain precision to about 10^{-6} and strain rate precision to 10^{-9}-10^{-10} s^{-1} and will significantly reduce the gap of strain rates between laboratory experiments and geological flow (10^{-12}-10^{-16} s^{-1}). On the other hand, seismic studies use millihertz acoustic waves to probe the Earth, while laboratory studies often use megahertz acoustic waves. Differences in these time scales are expressed in the attenuation, or the Q (quality factor), of stress-strain relationships. To measure Q, we need to measure stress relaxation times and strain retardation times as a function of frequency. With the advances of synchrotron tools, unprecedented flexibility in controlling the stress and strain during the deformation process at high pressure and temperature is feasible. The strain precision to be achieved at the NSLS II will allow us to describe seismic wave attenuation and related transient creep with a requirement of strain resolution (10^{-6}) relevant to seismic attenuation in the mantle. Finally, the nanometer spatial resolution could enable quantitative flow measurements in a diamond anvil cell. This will be a new era of rheology research, promising to extend the pressure envelope for rheological studies nearly one order of magnitude, from the pressure limit in multi-anvil apparatus to that of diamond anvil cell at the same strain precision of 10^{-4} (resolving less than 5 nm length change over 10 μm long sample). Knowledge gained thereby will place important constraints on the thermal, velocity, and density structure of Earth's interior.

Planets

The discovery of 273 extra solar planets, since 1995, demonstrated that planetary systems are very common in the universe. Understanding the formation, evolution and current structure and dynamics of planets is a paramount challenge for planetary scientists. High pressure and temperature experiments can help interpret the data gained from satellites and exploration missions on the current structure and dynamics of planets and provide insight into planetary evolution. The scientific challenges differ from the ones in Earth sciences, since the range of compositions and thermodynamic conditions in the solar system is much greater than for Earth. The 8 planets and the planetary bodies in our solar system can be divided in four categories: Gas giants (Jupiter, Saturn), Ice giants (Neptune, Uranus), ice/rock bodies (Europa, Ganymede, Callisto, Titan, Triton, Pluto), and terrestrial bodies (Mercury, Earth, Mars, Venus, Moon, Io).

The investigations of hydrogen and hydrogen-helium mixtures at high pressure and temperature are key to understand the structure of gas giants and will contribute to understand their formation. Precise measurements of the equation of state of hydrogen and hydrogen-helium mixtures in the relevant pressure and temperature range will help to determine, if Jupiter has a rocky core. Furthermore, the detection of continuous or discontinuous transitions in the high pressure and temperature behavior of H_2 and He-H_2 mixtures will provide important information about the interior structure of gas giant planets (23).

High pressure and temperature investigation of water, water mixtures with ammonia, methane, and water-rock interaction will provide further insight into the interior structure of ice giants and solid ice/rock bodies (24, 25). The determination of the properties of aqueous fluids at moderate pressure and temperature, e.g. reactivity, although technically very challenging, is crucial to understand the internal evolution of many solid ice/rock bodies in our solar system.

Further insight into the formation, structure and evolution of terrestrial planets can be gained by determining the phase diagrams of chemical compositions relevant to these planets experimentally and correlate these data with results from exploratory and satellite missions. Extra solar terrestrial planets which encompass up to 10 Earth masses are expected to have central pressures and temperatures up to 3500 GPa and 8000 K, much greater than found in terrestrial planets in our own solar system (26) and constraining their interior structure will consequently require experiments to extend to much more extreme conditions.

Material Science and Chemistry

Super hard materials

Compounds can be defined as super hard materials, when their micro-hardness exceeds 40 GPa. In addition to high hardness, they usually possess other unique properties such as compression strength, shear resistance, large bulk moduli, high melting temperatures, chemical inertness, high thermal conductivity, etc., which makes them materials highly desirable for a number of industrial applications. One prominent goal is to synthesize new phases in systems such as B-C-N-O or Si-B-C-N that are thermally and chemically more stable than diamond, and harder than cubic BN, and thus would be excellent materials for high-speed cutting and polishing of ferrous alloys. The most common conditions employed to synthesize super hard materials involve extreme pressures or extreme pressures in combination with temperatures. Fundamental research to better understand the atomic structure and the bonding characteristics are badly needed. Knowledge of these fundamentals will help materials scientists understanding how and why a material becomes super-hard.

The source characteristics of NSLS-II and the unique experimental capabilities at the proposed high-pressure stations will open new possibilities in synthesis and characterization of super hard materials.

Nano-crystalline Materials

The field of nano-crystalline materials is in rapid development (27). Materials consisting of nanometer-sized crystallites are characterized by a large fraction of surface or inter-surface atoms. Correspondingly, these materials have novel physical and chemical properties compared to their bulk counterparts, which could lead to new functional materials. One of the main goals of high pressure research in this area would be a thorough investigation of crystallite size effects on the equation of state (bulk modulus and other elastic constants), strength (28) and possible solid-solid phase transformations. As for nano-materials, the common rule seems to be that the smaller the particle size, the higher the transition pressure. However, a few systems with the opposite trend have been reported in the literature. Competing processes are determining the high-pressure behavior, and there is a need for systematic studies of the influence of crystallite size on the transition pressures and other physical parameters.

Recent developments in high-energy X-ray total scattering techniques at high pressure combined with pair distribution function analysis allow now extracting information of the atomic structure of nano-particles from diffraction data. This new technique will mature over the next years and will provide fundamental insight in structure-property relationships of nano-crystalline materials at extreme conditions.

Porous Materials form Micro- to Nano-Pores

Porous materials play an important role in many technological processing applications (29). These materials are widely used as catalysts, catalyst supports and membranes, and form the basis of new technologies, involving energy storage, novel reactions, waste sequestration etc. Any process that takes place within the pores of a solid is strongly influenced by the geometry and topology of the host's pore matrix. Therefore, the determination of the structural or physicochemical parameters that are related to the mechanism of these processes is the key for the characterization of porous materials. In order to understand the processes in the pores, the bonding and dynamic of guest ions and molecules in the porous compounds need to be determined (30, 31).

The application of pressure to porous materials often leads to unexpected structural response, e.g. amorphization (32), penetration of liquid media into the pore volume (30). Understanding the mechanism of geometric deformation of the structure with pressure and temperature is important to evaluate its stability at non-ambient conditions. Compressibility and thermal expansion data are necessary for thermodynamic calculations and to yield thermo-chemical parameters with internal consistency. Possible interactions with penetrating pressure transmitting media will give new insight on the nanoscopic poroelasticity of the materials (30). The thermal behavior of many porous materials has been extensively studied and interesting effects, for example negative thermal expansion behavior have been discovered (33). However, the literature on the effect of pressure is limited, and until recently little quantitative information on pressure-induced structural modifications and phase transformations has been reported. The combination of structural data of the host and guest structure and data on the dynamic and mobility of the guest yields the information necessary to clarify the mechanism of structural deformation and to understand technological relevant processes.

Chemical Reactions and Reaction Kinetics

Chemical reactions are ubiquitous in nature. Their comprehensive studies are necessary for defense, industry, and academic science. Better understanding of the chemical reactions in the condensed phase at elevated pressure and temperature is currently required. Almost all industrial and synthetic chemistry occurs in the condensed phase. Chemistry in the condensed phase is the basis of life. Condensed phase chemistry is essential to planetary processes on the Earth as well as other terrestrial bodies. The knowledge of the reaction chemistry of energetic materials at high pressure and temperature is necessary to understand their behavior under impact and in detonation conditions. Understanding of a nature of chemical reactions in simple molecular materials (e.g., hydrogen and nitrogen) will provide a basis for designing and synthesizing of fuel for the future.

Following chemical reactions using the unique time structure of synchrotron sources will allow deep insight into reaction kinetics and reaction mechanisms previously inaccessible. The high brilliance of NSLS-II will facilitate these *in situ* studies of reactions at extreme conditions.

Synthesis of Novel Materials

Research at elevated pressure and temperature provide a new insight into synthesis of materials with properties important for industrial, technical and scientific applications (34). These include super hard materials, high-temperature superconductors, ferroelectrics, multiferroics, high energy density materials, hydrogen storage materials, materials for computers and communications, and nano-materials. High-pressure studies provide otherwise unattainable information about the phase diagrams, thermodynamic properties, and electronic structure which can predict directions for search of materials with desirable properties. Moreover, high-pressure synthesis remains unique in many cases.

Physics

Element Structure and Complex Alloys

The exploration of high-pressure modifications of elements has revealed a surprising complexity of their properties and crystal structures. Recently, a rich polymorphism under high pressure in elementary materials has been observed and reported. In addition, theoretical studies predict highly unusual properties of materials containing light elements, e.g. superionicity, metallization and superconducting superfluids.

Light elements like hydrogen, sodium and lithium are a long-standing subject of scientific interest. For hydrogen, predicted of metallization motivated a large scientific effort over many decades. For lithium, the recent discovery of low-symmetry high-pressure allotropes in combination with theoretical findings concerning the compression-induced transition of the valence electron from s- to p-like behavior has stimulated a number of investigations concerning their physical properties (35-37). Measurements of the melting curve of sodium revealed an unexpected and unpredicted behavior at high pressures. The melting temperature of sodium reaches a maximum at about 31 GPa and shows a decrease in the melting temperature to 300 K at 118 GPa (4). The experimental exploration of light elements at high pressures requires the brilliance of 3rd generation synchrotron radiation sources, due to their weak scattering power.

A large number of elements show unexpected electronic transformations e.g. metal-insulator transitions, or transition to superconducting state (Figure 4).

Figure 4 Periodic table of the elements. The purple color highlights the elements for which superconductivity was observed at high pressure (Figure from Ashcroft (37)).

It was shown that several elements, e.g., the heavy alkaline metals undergo pressure-induced s-d transitions. In the regime of the electronic change the occurrence of low symmetry atomic arrangements has been observed. Some of the structural patterns correspond to partial structures of intermetallic compounds, e.g., that of Rb-IV (38) (Figure 5) to that of W_5Si_3.

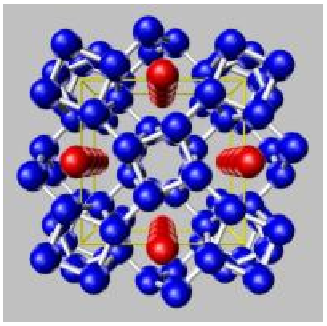

Figure 5 The host-guest structure of Rb-IV showing host (blue) and guest (red) atoms. (Figure from McMahon *et al* (38))

Similar framework structures have been found for the allotropes Bi-III and Sb-II, which are additionally characterized by incommensurate modulations of host and guest lattice. In the light of these investigations, phase stability and crystal structures of a number of as-yet undetermined high-pressure modifications of elements like silicon and germanium have been characterized. The studies of metallic elements and the findings concerning their electronic and structural organization have motivated a number of projects investigating the pressure dependence of the electronic configuration in intermetallic phases. It was shown that in a number of ytterbium containing intermetallic compounds compression induces changes of the oxidation state of the rare-earth metal. The observations of these valence transitions have become a focal point of ongoing theoretical and experimental investigations.

Highly Correlated Electron Systems

Systems with strongly correlated electrons have fascinated materials scientists time and again, by revealing such intriguing phenomena as high temperature superconductivity, the colossal magneto resistance, and heavy fermion behavior and unusual dynamic ground states. There is growing evidence that in many of these systems, as for example the transition metal oxides, the unusual physical properties result from a competition between different electronic phases, of which some show instability towards a nanoscopically inhomogeneous electronic ground state (39). Understanding the phenomenon of “competing-order” and the inherent electronic inhomogeneities is considered to be key to identify the microscopic mechanism of many of these exotic ground states. In principle, pressure provides a formidable tool to study these phases, as it allows manipulating the band structure as well as the lattice parameters and symmetry. However, the challenge has been to detect the ultra weak lattice modulations associated with the electronic in homogeneities in a high pressure environment, and only recently groups have succeeded (11). The NSLS-II will enable such diffraction experiments with an unprecedented degree of resolution, and provide a direct probe of electron-lattice interactions in some of the most unconventional states of condensed matter at high pressure.

The ability to combine high pressure with other extreme environments such as high magnetic or electric fields is vital for studies of complex interactions in strongly correlated electron systems, such as questions concerning the competition or coexistence of magnetism and superconductivity, or the interplay between electronic order and Fermi surface instabilities. The combination of high pressure with other extreme environments (in addition to temperature) is world wide still in its infancy. The NSLS-II offers a unique chance to develop a world-leading program.

High Pressure Program at NSLS

High-pressure research has a strong presence at NSLS. Currently, four experimental end stations are dedicated to high-pressure research using diamond anvil cells and large volume presses. The experiments are located at the superconducting wiggler X17 at the X-ray ring and the bending magnet U2 at the UV ring. X17B2 provides the high-pressure community with state of the art capabilities for experiments in large volume presses. Diffraction experiments at high pressure and temperature in a diamond anvil cell can be performed at X17B3 and X17C. The bending magnet beamline U2A offers the unique capability of conducting infrared spectroscopy measurements at high pressure and moderate temperatures using a diamond anvil cell.

The experimental capabilities provided by the high-pressure program at NSLS serves each year a user community of about 200 users from 50 national and international institutions. The topics of the conducted experiments originate in a range of scientific disciplines, such as material sciences, physics, Earth sciences and chemistry.

During the past six years, the high-pressure program a NSLS has been mainly supported by NSF, through COMPRES (COnsortium for Materials Properties Research in Earth Sciences). Additional funds for the IR spectroscopy beamline U2A have been provided by DOE CDAC (Carnegie/DOE Alliance Center) and by NSF-EAR and DOD for large volume program at X17B2.

The high-pressure program at NSLS is currently improving the capabilities of the experimental stations by addition of new hardware and by development and implementation of new experimental techniques. Some of the new additions are already made with the unique beam characteristic of NSLS-II in mind.

The following additions will be made to the beamlines during 2008 and 2009:

- **X17B2**

    - Development of a monochromatic X-ray diffraction side station. The side station will allow experiments in a Paris-Edinburgh type pressure cell at pressures up to 30 GPa and about 2000 K. Experiments in side station can be conducted simultaneously with experiments in the large volume press resulting in more effective use of beamtime.
    - Implementation of a new ten element solid state detector for precise stress measurements.

- **X17B3**

    - Development of a compact laser heating system based on a Yb:fiber laser. This will add simultaneous high pressure and temperature capabilities to the beamline. Furthermore, this is the first step towards the development of a potentially portable laser heating system for NSLS-II.
    - Development of micro beam capabilities (beam size ~ 1µm) by focusing with kinoform refractive lenses in collaboration with K. Evans-Lutterodt (NSLS). This development is the first step towards sub micron beams at the high pressure stations at NSLS-II (e.g. proposed Station A)
    - Further development of the total X-ray scattering technique at high pressures and temperatures for the investigation of disordered, amorphous and liquid materials in diamond anvil cells.

- **X17C**
    - Implementation of angle dispersive and energy dispersive single crystal diffraction, in collaboration with P. Dera (GSECARS).

- **U2A**

    - Development of in-situ high pressure and temperature synchrotron IR spectroscopy and applications to Earth sciences and material sciences under extreme condition (up to 300 GPa and 5000 K). The first step is to build an offline laser heating system based on a CO_2 laser, allowing the investigations of samples quenched from high temperatures.
    - Coupling dynamic-compression with pulsed synchrotron radiation for time resolved measurements. A feasibility study by a team led by Daniel Dolan from Sandia National Laboratories in October 2006 achieved an important milestone when they were able to couple a broadband synchrotron IR radiation from U2A beamline to characterize the emissivity of a copper film under shock compression.
    - Development of an experimental side station. The new facility will allow measurements on high-pressure samples with the highest spatial resolution possible at a synchrotron source while also having the highest broadband IR brightness. With a new microscope coupling a newly developed IR focal plane array detector and FTIR instrument, the facility will be ideal for mapping of natural samples (e.g., solid and fluid inclusions in thin section), heterogeneous charges from high-pressure experiments, as well as samples *in situ* at very high pressure in diamond or moissanite anvil cells.

Due to the continual development of the experimental stations, we expect a significant growth of the user community over the next years.

A large portion of the high-pressure research at NSLS takes place in experimental stations at the superconducting wiggler X17 and therefore depends on greatly on the reliability of this insertion device. The high-pressure community follows with great interest the solutions to the problem with the cryogenic cooling system of the wiggler X17. From the currently discussed solutions, the high pressure community is largely in favor of the replacement of the wiggler X17 with a new superconducting wiggler, which can be operated at reduced capabilities (limited field and/or periods) at NSLS and be transferred to NSLS-II. The advantages of this solution for the high pressure program at NSLS as follows: (i) the high pressure experiments would be served by a new and reliable insertion device; (ii) the reduced capabilities of the new superconducting wiggler would be equal or superior to the current wiggler; and (iii) a superconducting wiggler, suitable for high pressure research and taking full advantage of the unique source characteristics of NSLS-II would be present at the new ring on day one.

The high-pressure community applauds the decision of the NSLS to build a new beamline, X17A, at the superconducting wiggler port. The unique capability of this beamline will be ideal for investigation of disordered, nano-crystalline and amorphous materials at high pressure, using X-ray total scattering in conjunction with pair distribution function analysis. The condensed matter physics department at BNL has submitted an energy-related Laboratory Directed Research and Development proposal (Tranquada, Huecker, Bozovic, Davis). As part of this proposal it is planned to develop the capability to perform high-pressure single-crystal X-ray diffraction at low temperatures at X17A. This is in addition to the upgrade of this beamline for powder diffraction. The decision on this proposal is still pending. These additional high-pressure capabilities will further strengthen the high pressure research program at NSLS and could be transferred to a high-pressure or high-energy beamline at the NSLS-II.

The development of a new generation of X-ray detectors, lead by D.P. Siddons at NSLS, is of great interest to the high-pressure researchers. The current generation of area detectors was developed mostly for protein crystallography and therefore has the highest sensitivity at X-ray energies of 8-12 keV. Diffraction experiments at high pressure are usually conducted at energies of 30-40 keV, where these detectors have a remaining efficiency of less than 40 %. The proposed microstrip and a hybrid pixel-array detector using germanium sensors will be an ideal detector for diffraction experiments at high energies. High pressure diffraction experiments will mainly benefit form the superior signal-to-noise ratio, the fast read-out time and the large dynamic range. We envision the germanium hybrid pixel-array detector as the standard detector at the dedicated high pressure diffraction stations proposed for NSLS-II.

High Pressure Program at NSLS-II

The future scientific challenges in high pressure research involve sophisticated experiments on increasingly complex systems at ever higher pressures and temperatures. Most of the modern scientific questions in research at extreme conditions require integration of multiple experimental techniques. The sample environment for experiments at extreme conditions poses a rigorous restriction to sample size and volume and often contaminates the collected data. Therefore, the requirements on focal size, collimation and beam stability are very high. The small source size and the high brilliance over a large range of X-ray energies of NSLS-II will greatly benefit experiments at extreme conditions and stimulate new directions in research of materials at extreme conditions.

The high-pressure program at NSLS-II should have two components: dedicated high pressure beam lines and support for high-pressure research at a variety of other beamlines around the ring. Many high pressure cells are compact and portable and thus there is a prime opportunity to integrate high-pressure techniques into other beamlines built at NSLS-II from the beginning. We envision the development of portable and compact laser heating systems that will allow simultaneous high-pressure and temperature experiments to be performed using diamond anvil cells at nearly any beamline. Our experience at other synchrotron sources is that new X-ray techniques are commonly adaptable to high-pressure application, but this often requires restructuring of the sample stage and/or X-ray optics. However, the special needs of high-pressure equipment need to be considered now, in the design phase of the experimental stations for NSLS-II. This will be of great benefit, enable a greater array of groundbreaking scientific research, and ultimately reduced cost.

The NSLS-II x-ray sources offer great improvements over the existing NSLS beamlines for experiments at extreme conditions. These improvements arise from the following four factors:

1. The storage ring emittance is much smaller, meaning that the source size is smaller. The source divergence is also less, which is a significant factor for undulator beamlines, although not for bending magnet or wiggler beamlines, where the natural opening angle of the synchrotron radiation dominates the divergence.
2. The maximum length of insertion devices is increased from 4.5 to 7 meters.
3. The ring current is increased from 300 to 500 mA.
4. The ring energy is increased from 2.8 GeV to 3.0 GeV.

There are three figures of merit that are commonly used when comparing synchrotron sources:

1. Flux: This is the number of photons per 0.1% energy bandwidth, integrated over the full vertical opening angle, per 1 mrad of horizontal angle. Flux is the appropriate figure of merit for a beamline with optics that can collect a large fraction of the output of a wiggler or bending magnet source. It is not very useful for high-pressure beamlines, because the high energies and small beam sizes required preclude collecting a large solid angle.
2. Intensity. This is the flux density in the center of a synchrotron beam, i.e. the number of photons per 0.1% energy bandwidth, per mrad^2 of solid angle. It is the appropriate figure of merit for a beamline with optics consisting of a small slit to define the beam, and that does not use focusing optics. An example would be white beam in the multi-anvil press. Figure 6 shows the intensity of a number of synchrotron sources, including NSLS-II undulators and wigglers, NSLS X17, APS undulator A, and the APS bending magnet.
3. Brightness. This is the intensity per unit source size. It is the appropriate figure of merit for a beamline that has focusing optics. Figure 7 shows the brightness of the same synchrotron sources plotted in Figure 6. Note that because NSLS-II has a very small source size, it has a very large brightness. In order to take deliver

this brightness to the experiment, it will be necessary to have x-ray optics of extremely high quality.

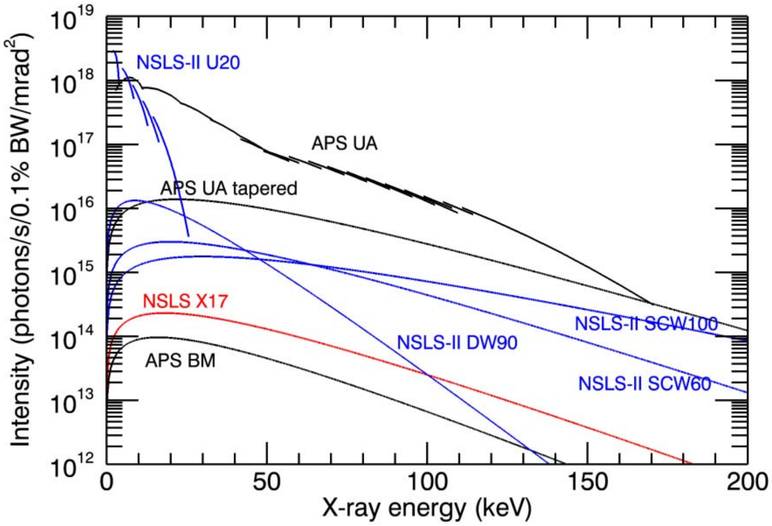

Figure 6 Intensity of synchrotron x-ray sources. These include NSLS-II 20 mm period undulator tuning curve; NSLS-II superconducting wiggler 100 mm period, 6T field; NSLS II superconducting wiggler 60mm period, 4T field; NSLS-II damping wiggler, 90 mm period; NSLS X17 superconducting wiggler; APS 33 mm 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.

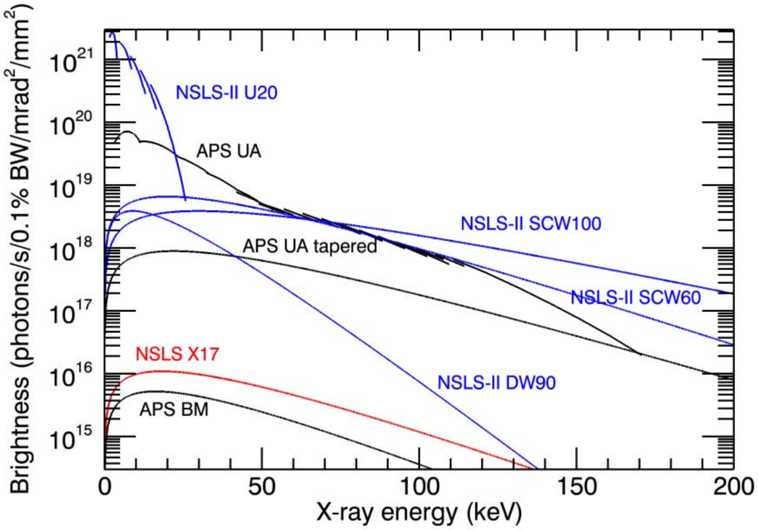

Figure 7 : Brightness of the same synchrotron x-ray sources plotted in Figure 6.

Table 1. Parameters of synchrotron sources plotted in Figures 1 and 2

Source	E (GeV)	Current (mA)	Magnetic field (T)	Period (mm)	# poles	Source size (σ_x, σ_y, μm)
NSLS-II undulator (U20)	3.0	500		20	300	28, 2.6
NSLS-II damping wiggler (DW90)	3.0	500	1.8	90	150	99, 5.5
NSLS-II superconducting wiggler (SCW100)	3.0	500	6.0	100	20	28, 2.6
NSLS-II superconducting wiggler (SCW60)	3.0	500	4.0	60	34	28, 2.6
NSLS X-17 superconducting wiggler	2.8	300	4.2	174	5	307, 11
APS bending magnet	7.0	100	6		1	109, 27
APS undulator A	7.0	100		33	144	275, 9
APS undulator A (tapered)	7.0	100	0.81	33	144	275, 9

Multi-anvil press experiments:

There are two superconducting wigglers that could be considered for the multi-anvil press high pressure beamline at NSLS-II. The first is a 6 T device with a 100 mm period, and the second is a 4 T device with a 60 mm period. The lower field device can have more periods (at a fixed 1 m length), and thus higher intensity up to about 65 keV. The lower field device also has many fewer photons at very high energy (e.g. 300 keV), which could greatly simply the shielding in the hutch when using white beam. These wigglers provide an intensity that is 10-20 times greater than X17 up to 100 keV. Given that the experiments at NSLS-II will be about twice the distance from the source as those at NSLS, the gain in photons on the sample through a slit will be about 2.5 to 5 over the existing setup at X17B2. The fact that the source size is much smaller at NSLS-II will not have a significant impact on these experiments, since they do not use focusing optics. Relative to the APS undulator operated in tapered mode, the NSLS-II will be a factor of 2 to 10 lower in intensity, depending on the energy and which wiggler is selected.

Diamond anvil cell experiments:

The diamond cell experiments at NSLS-II will use focusing optics, and so brightness is the appropriate figure of merit (Figure 7). It can be seen that NSLS-II superconducting wigglers offer increases of more than 300 relative to X17. Even more impressive are the gains from the U20 undulator at NSLS. This has a brightness up to 5 orders of magnitude greater than X17, and the brightness exceeds that of the NSLS-II superconducting wigglers up to about 30 keV. Indeed the U20 undulator has a higher brightness than the APS undulator up to about 25 keV. The U20 undulator will be an excellent source for spectroscopy, inelastic scattering, and diffraction below about 25 keV. It will offer a tremendous increase in capabilities relative to X17. The large gap (90 mm) bending magnet is the ideal source for the proposed far-infrared beamlines. It will provide better flux and brightness over the entire IR region and a 10-1000 times better stability. This will enhance the experimental capabilities for IR spectroscopy at extreme conditions.

A major challenge will be the development of optics that can take advantage of the very small source sizes at NSLS-II. For example, in order to preserve the brightness of the source an optic such as a Kirkpatrick-Baez mirror must have slope errors that are less than about 25% of the angular size of the source as viewed from the optic. At NSLS-II the vertical source size for the undulator is 2.6 microns, and the optic will be about 50 m from the source. The slope error requirement is thus $0.25\times2.6\times10^{-6}/50 = 1.3\times10^{-8}$. This is a slope error of 0.013 μrad. The best mirrors we are currently able to purchase have slope errors of about 0.50 μrad, so factors of 40 improvements in quality are required.

In summary, the above discussion illustrates that the three proposed extreme conditions beamlines for extreme conditions will provide unique capabilities currently not available in the portfolio of DOE beamlines at synchrotron radiation facilities.

Superconducting Wiggler

Diamond Anvil Cell Stations

The high pressure community identified the need for two extreme conditions diffraction stations utilizing small pressure generating devices like diamond anvil cells (DAC) or small Paris-Edinburgh (PE) cells, located at the superconducting wiggler port. The experimental capabilities of the two diffraction beamlines are complementary to each other and to other diffraction beamlines proposed for NSLS-II.

Station A

Station A will be a diffraction beamline for experiments at simultaneous high pressure and temperature. An experimental hutch of sufficient size (4×5 m) to accommodate the experimental setup including a permanent laser heating system and possibly other spectroscopic (Raman, Brillouin) systems is necessary. The station will operate at a fixed energy in the range of 35-40 keV and will be optimized for the following high-demand experimental techniques:

- **Powder diffraction:** Measurements of PVT equations of state, compressibility, structural evolution, phase transformation, element partitioning, melting, strength, rheology, etc of simple to moderately complex structures at pressure and temperature. Time resolved measurements of phase transformations and reactions to determine kinetic parameters.

- **Single crystal diffraction:** Determination of complex crystal structures and the investigation of their compression behavior.

- **Quasi single-crystal diffraction:** The micro-beam capabilities will make a new class of experiments at high pressure and temperature possible. Experiments at high pressure and temperature lead often to transitions of a single phased compound to a multi phase assemblage. The micro-beam will allow to probe desired grains in the polycrystalline and multiphase sample and perform single crystal diffraction on these grains with sizes < 1μm.

The following components for the beamline and the experimental station are proposed:

- The monochromator will be a side scattering asymmetric bent Laue crystal utilizing the (111) or (311) reflection of silicon. To gain a high stability the monochromator needs to be liquid N_2 cooled. The energy resolution of the monochromator should be aimed for $\Delta E/E$ of 1×10^{-3} to 1×10^{-4}.

- Microfocusing optic, including silicon kinoform Fresnel lenses, Kirkpatrick-Baez mirrors, or zone plates will be used to focus the beam in the horizontal and vertical directions. The beam size for Station A should be adjustable between 5μm and 100 nm.

- The sample stages need degrees of freedom in x, y, z, ω, φ in order to perform the above-mentioned experiments. The mechanical stability of the optical table and the translation and rotation stages needs to be high, due to the small beam size in combination with the laser heating setup. Furthermore, the sphere of confusion of the translation and rotation stages needs to very small, to meet the extraordinary demands of micro diffraction.

- An area detector will be used to detect the diffraction patterns. The use of the germanium pixel-array detector, currently under developed by D.P. Siddons at NSLS, is anticipated to be one of the detector options for Station A.

- A double-sided laser heating system suited for CO_2 and Yb:fiber laser will add high temperature capabilities to the beamline. Extrapolating the current advancements in laser technology, a very compact, but mechanically stable, design for the laser heating system might be possible.

- A micro-Raman spectrometer for simultaneous X-ray diffraction and Raman spectroscopy studies will be installed at the beamline. This system will be used for online pressure measurements by fluorescence methods as well.

- Additional the following beamline components will be needed: Slit systems, cleanup slits and pinholes, motorized beam-stop, cameras, and ionization chambers.

Station B

Station B will be a diffraction beamline for experiments at simultaneous high pressure and high/low temperatures. An experimental hutch of sufficient size (3×5 m) to accommodate the experimental setup including the laser heating systems and a cryostat is necessary. The station will operate in the energy range from 20-120 keV. The wide energy range will allow large variety of scattering experiments at extreme conditions, currently not possible at other dedicated high-pressure beamlines in the world. In addition to conventional powder and single crystal diffraction at extreme conditions, Station B will allow the following experimental techniques.

- **X-ray total scattering:** Standard X-ray diffraction techniques that are only take the Bragg component of the elastic scattering into account for structure determination fail on whole classes of materials (e.g. nanocrystalline, amorphous materials and liquids) because of their limited structural coherence. Total elastic X-ray scattering, including the Bragg and diffuse contributions, in conjunction with pair distribution function analysis allows determining the short-, intermediate- and long-range atomic arrangement. A high-energy incident X-ray beam with large detector coverage is necessary to measure high wave vector transfers in order to obtain a real space resolution of better than 1 Å.

- **Resonant scattering:** The high brilliance of NSLS-II will allow measurements of the anomalous dispersion of the structure factor close to the *K*- and *L*- absorption edges at extreme conditions. Gaining additional information of the crystal structure of complex crystalline and non-crystalline materials at extreme conditions. The energy range of the proposed experimental station will allow resonant scattering experiments on absorption edges of elements with $Z > 43$.

The following components for the beamline and the experimental station are proposed:

- The monochromator needs to cover a wide energy range and the energy needs to be tunable. Two monochromators are needed to fulfill these requirements. A silicon (111) double crystal monochromator (Bragg geometry) for the energy range of 20-50 keV and a silicon (311) sagitally bent Laue double crystal monochromator for the energy range above 50 keV.

- Mirrors in Kirkpatrick-Baez geometry will achieve horizontal and vertical focusing. The beam size for Station B should be between 1-5 μm.

- The sample stages need degrees of freedom in $x, y, z, \omega, \chi, \varphi, 2\theta$ in order to perform the above-mentioned experiments. The mechanical stability of the optical table and the translation and rotation stages needs to be high, due to the small beam size in combination with the laser heating or cryostat setup.

- An area detector will be used to detect the diffraction patterns. The use of the germanium pixel-array detector, currently under developed by D.P. Siddons at NSLS, is anticipated to be one of the detector options for Station A. Single crystal diffraction measurements and resonant scattering experiments will benefit from the availability of a point detector, usable with and without analyzer crystal.

- A double-sided laser heating system suited for CO_2 and Yb:fiber laser will add high temperature capabilities to the beamline. Extrapolating the current advancements in laser technology, a very compact, but mechanically stable, design for the laser heating system might be possible.

- A closed cycle He-cryostat capable of reaching temperatures of < 1 K will add low temperature capabilities to the beamline.

- A micro-Raman spectrometer for simultaneous X-ray diffraction and Raman spectroscopy studies will be installed at the beamline. This system will be used for online pressure measurements by fluorescence methods as well.

- Additional the following beamline components will be needed: Slit systems, cleanup slits and pinholes, motorized beam-stop, small crane for moving heavy equipment (e.g. cryostat), cameras, and ionization chambers.

Large Volume Press Stations

The high pressure community identified the need for two extreme conditions diffraction stations with large hydraulic presses to generate sample environments at extreme pressure and temperature in situations where large samples (1 mm) are required or uniform pressure and temperature are important. These systems will generally work at pressures up to about 60 GPa.

Station C

Station C will be a diffraction beamline for experiments at simultaneous high pressure and temperature. An experimental hutch of sufficient size (4×5 m) to accommodate the experimental setup and space for several large Paris-Edinburgh type pressure cells is necessary. The station will operate at a fixed energy in the range of 35-40 keV and will be used to explore samples at extreme conditions using X-ray diffraction and imaging. Interchangeable high pressure systems will be used here. The different systems will be optimized for a variety of experimental goals.

- **Slow dynamic processes:** Materials respond to pressure, temperature and stress on various time scales. Several time-resolved experiments require long periods of time to define kinetics or rheology at slow strain rates. This hutch will allow a high pressure experiment to continue over several days/weeks but not continually be in the X-ray beam. The experiment can be started, be characterized with X-rays and then continue at high pressure and temperature off-line while other experiments take the beam time. In certain time intervals, the pressure cell will be moved onto the experiment and characterized with X-ray techniques.

- **Sample imaging:** Cells with a large angular access will be used for tomographic imaging of the sample. This will allow studies of fluid flow through the sample at elevated pressure and temperature. Melting phenomena can also be studied with this technique.

- **Powder diffraction:** Equation of state measurements, phase transformations, kinetics can be studied with diffraction measurements.

The following components for the beamline and the experimental station are proposed:

- The monochromator will be a side scattering sagittal-focusing asymmetric bent Laue crystal utilizing the (111) or (311) reflection of silicon. To gain a high stability the monochromator needs to be liquid N_2 cooled. The energy resolution of the monochromator should be aimed for $\Delta E/E$ of 1×10^{-4}, since we expect a major advancement in the spatial resolution of area detectors. The focusing capacity of the monochromator will be sufficient for a beam size of about 100 μm.

- Detector: an area detector will be primarily used in this hutch. Also available will be a high-resolution detector system with two detectors, one about a two theta axis that is vertical, the other horizontal. This will enable high accuracy stress measurements.

- Paris-Edinburgh type high pressure cells with variable pressure modules designs. Opposed Anvil, T-Cup, DT-Cup. Clamp cells with cryostat.

- Additionally, the following beamline components will be needed: Slit systems, cleanup slits and pinholes, motorized beam-stop, small crane for moving heavy equipment (e.g. PE cell), cameras, and ionization chambers.

Station D

Station D will house a 2000-ton hydraulic press with interchangeable high pressure toolings. These toolings will be specialized to serve several different experiments where a high pressure – high temperature environment is important. This provides a versatile experimental environment that can continually expand as new needs arise by the design and implementation of new tooling sets. The station will operate in the energy range from 20-120 keV. Both monochromatic and white x-rays will be available for the experiments as some high pressure configurations have very limited angular access for the detection. The wide energy range will allow large variety of scattering experiments at extreme conditions, currently not possible at other dedicated high pressure beamlines in the world.

- **Rheology:** The strength of material at high pressure and temperature – and the viscosity of solids can be studied using deformation tooling. A combination of diffraction and imaging provide the needed data for this information.

- **Ultrasonic elastic properties:** Elastic properties are fundamental properties of materials that map into the equation of state and further define the response to stress. Acoustic waves sample this information, but require mm sized samples.

- **Tomographic imaging:** Phenomena from fluid flow to faulting are possible to study with 3-d mapping of the sample with time. By doping the sample with materials that have x-ray contrast allows these techniques to be applied at high pressure and temperature.

Beamline with monochromatic and white beam capabilities

- 2000 t hydraulic jack and frame
  - Kawai style system: routine capable of 30 GPa and 3000K, but may reach 60 GPa and 3000K, for 1×1×1 mm^3 dimension samples.
  - DDIA Deformation system. Capable of 10 GPA and 3000K with uniaxial stress capability, for 1×1×1 mm^3 samples

  - Deformation Kawai style, pressure of Kawai device with uniaxial stress capability. Currently under development.

  - Rock mechanics imaging system: 1 GPa pressure, 1000K 10x10x10 cm samples for fluid flow studies using tomographic imaging.

  - Rotational Drickamer device: 50 GPa, 3000K with shearing stress, 3×1×1 mm^3 sample. Also useful for tomographic imaging at high pressure.

- The monochromator needs to cover a wide energy range and the energy needs to be tunable. Two monochromators are needed to fulfill these requirements. A silicon (111) double crystal monochromator for the energy range of 20-50 keV and a silicon (311) sagitally bent Laue double crystal monochromator for the energy range above 50 keV.

- Focusing should be available for both white and monochromatic beams. Spot sizes from 0.5 mm to 0.005 mm are required. The small size will be used to investigate lateral variations within the large sample.

- Imaging requires a parallel incident beam and an expansion of the transmitted beam. The optics for this need to be developed.

- Diffraction. High d-spacing resolution in multiple azimuthal directions is required for stress measurements. Goals of 10^{-6} are required for d-spacing resolution.

Undulator U20

The rapid development of inelastic scattering techniques provides a multitude of probes of elementary excitations in condensed matter in a broad energy and momentum parameter space. High resolution techniques usually require tight focusing of X-rays, which is ideally matched to the experimental conditions in DAC to very high pressures in excess of 300 GPa The experimental station proposed here is specialized on a suite of techniques, which matches ideally the future NSLS-II coherent sub-meV resolution x-ray sources. The brightness of the X-rays at NSLS-II is an order of magnitude greater than at the APS (few keV to 20 keV range), are ideally matched to the multitude of high pressure spectroscopic techniques thriving at 3rd generation synchrotron sources.

The high pressure community proposes one experimental station at the undulator U20 port which will be specialized on X-ray spectroscopy at extreme conditions. Although the energy range provided by the undulator is not ideally suited for diffraction experiments at extreme conditions, some diffraction capabilities should be available at this beamlines to allow characterization of the same sample by spectroscopic and diffraction methods.

Station A

Station A specializes on X-ray spectroscopy experiments at simultaneous high pressure and high/low temperatures. An experimental hutch of sufficient size (4×6 m) to accommodate a large goniometer and equipment to generate high and low temperatures is necessary. The station will operate in the energy range from 5-25 keV and will be optimized for the following techniques.

- **X-ray absorption spectroscopy:** X-ray absorption spectroscopy can be divided into near edge spectroscopy (XANES) and extended X-ray absorption fine structure (EXAFS). In the EXAFS region, the excited electron has significant kinetic energy and EXAFS spectrum contains information on the local geometry around the absorbing atom. The XANES structure can be described be the multiple scattering, or alternatively, one can use electronic structure models such as density-functional theory to calculate the unoccupied density of states (DOS). X-ray magnetic circular dichroism (XMCD) is an important phenomenon in both X-ray absorption and X-ray emission. The magnetic structure of a system is studied by making use of circular polarized X-rays. XMCD can be observed in both XANES and EXAFS. XMCD in XANES can measure spin-resolved conduction band densities of states, whereas XMCD in EXAFS provides local magnetic structural information. The unique advantage of NSLS-II for the suite of high-pressure EXAFS, XANES, and XMCD is in tightly focused x-ray beams, which will allow detailed analysis of the samples in the high-pressure environment by mapping of local structure, valence states, magnetic structure, and spin-dependent density of states with high spatial resolution at ultra-high pressures.

- **X-ray near-edge spectroscopy:** Near core-electron absorption edge features measured by soft x-ray absorption (XANES) or electron energy loss spectroscopy (EELS) reveal information on chemical bonding. Such information is particularly pronounced and important for light elements, but has been inaccessible for high-pressure studies as the pressure vessel completely blocks the soft x-ray and electron beams. With x-ray inelastic near-edge spectroscopy (XINES), the high-energy incident x-ray penetrates the pressure vessel and reaches the sample. The scattered photon loses a portion of energy corresponding to the *K*-edge of the low-Z sample, but can still exit the vessel to be registered on the analyzer-detector system. Inelastic *K*-edge scattering spectra of second-row elements from Li (56 eV) to O (543 eV) at high pressures opened a wide new field of near *K*-edge spectroscopy of the second row elements.

- **X-ray emission spectroscopy:** In the x-ray emission (XES) technique, deep-core electrons in the sample are excited by x-rays. The core-holes then decay through either radiative or non-radiative processes. For deep-core holes, the dominant decay channels are radiative processes, producing fluorescence, which is analyzed to provide information on the filled electronic states of the sample. The information provided by XES is complementary to that provided by x-ray absorption spectroscopy. The final state of the fluorescent process is a one-hole state, similar to the final state of a photoemission process. Thus, the important information provided by photoelectron spectroscopy, namely large chemical shifts in the core-level binding energies and the valence band density of states, is available in XES.

- **Nuclear resonant inelastic X-ray scattering:** The inelastic method provides specific information about materials vibrational states, e.g., the phonon density of states. The Mössbauer method is a technique of choice to measure hyperfine interactions. All nuclear resonance techniques take full advantage of the unique properties of synchrotron radiation: intensity, collimation, time structure, and polarization. As a result both methods have led to novel applications for materials under extreme conditions. Nuclear resonant scattering yields information on the phonon density of states (DOS) through an inelastic scattering. In principle, the DOS provides constraints on dynamic, thermodynamic, and elastic information of a material, including vibrational kinetic energy, zero-point vibrational energy, vibrational entropy, vibrational heat capacity, Debye temperature, Grüneisen parameter, thermal expansivity, longitudinal velocity, shear velocities, bulk modulus, and shear modulus.

- **Nuclear forward scattering:** Mössbauer spectroscopy has been used extensively in high-pressure mineralogy in laboratory studies with a radioactive parent source. High-pressure studies using a conventional Mössbauer source suffer from limited intensity for measurements on small samples, absorption by anvils, and background scattering. The nuclear forward scattering can be used to measure magnetic transitions and hyperfine fields at high and low temperatures, and to probe valence changes under pressure and temperature.

The following components for the beamline and the experimental station are proposed:

- A cryogenically cooled monolithic silicon (111) monochromator will be used at the beamline, giving an energy resolution of 1eV. An additional cryogenically cooled double channel-cut silicon monochromator will be employed for experiments, which need a higher energy resolution (2meV).

- Large mirrors in Kirkpatrick-Baez geometry will allow to collect nearly the entire fan emitted by the undulator. The beam can be focused to a size of about 10 μm with this set of mirrors. For experiments that need a smaller focal size, a set of small mirrors in Kirkpatrick-Baez geometry will be available, allowing a beam size of 1 μm.

- A variety of detectors and analyzers should be available for the different inelastic X-ray scattering techniques depending on the needed energy resolution. We anticipate the need for a silicon pixel-array detector, a multi-element silicon drift diode for fluorescence measurements and a multi-crystal analyzer. Furthermore, a CCD or germanium pixel-array will serve as detector for diffraction experiments.

- A large 6-circle Kappa-geometry diffractometer, which can accommodate heavy equipment on the detector arm (e.g. detector and multi-crystal analyzer) and on the sample position (e.g. cryostat), will be installed.

- A double-sided laser heating system suited for Yb:fiber laser will add high temperature capabilities to the beamline. Extrapolating the current advancements in laser technology, a very compact, but mechanically stable, design for the laser heating system might be possible.

- A closed cycle He-cryostat capable of reaching temperatures of < 1 K will add low temperature capabilities to the beamline.

- Additional the following beamline components will be needed: Slit systems, cleanup slits and pinholes, motorized beam-stop, small crane for moving heavy equipment (e.g. cryostat), cameras, and ionization chambers.

Bending Magnet

The beamline for infrared spectroscopy at extreme conditions should be located on a bending magnet port with a wide gap (90 mm) dipole. The energy range should cover the far infrared to visible spectrum. An experimental hutch of 4×6 m is needed to accommodate the experimental setup. The interlock system should allow for simultaneous operation of IR spectroscopy station, an ion Argon and a high power CO_2 lasers for the laser heating system. The hutch should be located nearby the high-pressure undulator X-ray beamlines to create the opportunity to connect the IR beam through an extension pipe into the undulator hutches in order to perform *in si*tu X-ray and IR studies for same samples under extreme conditions. Beside standard IR spectroscopy at extreme conditions, a large growth potential lies in the following two experiments that will be facilitated by the unique beam characteristic of NSLS-II.

- **IR spectroscopy at simultaneous high pressure and high temperature:** Currently, IR spectroscopy measurements at high pressure are limited to temperatures of 1000K or investigations of samples quenched after offline laser heating. The high flux and the high spatial resolution of NSLS-II will allow performing IR spectroscopy measurement on samples heated simultaneously by a CO_2 laser. This unique capability will open exiting new research directions in Earth and material sciences.

- **IR spectroscopy coupled with dynamic compression:** Material emissivity measurements at extreme conditions can provide fundamentally important data that allow the measurement of temperature on short time scales, which is crucial for the complete characterization of dynamic compression events. For opaque materials such as metals, reflectivity measurements are necessary and must be conducted under dynamic compression in order to provide the necessary information. Although synchrotron radiation has been extensively adapted to different static high-pressure techniques for many years, the time-resolved capability from a pulsed synchrotron source has never been utilized to study the optical properties for materials under dynamic compression.

It is anticipated that the current IR spectroscopy end station U2A will be further upgraded and finally be moved to NSLS-II after the shutdown of NSLS. The move of the complete infrared end station can be accomplished in 4-6 weeks; therefore, the high pressure IR beamline will serve the extreme conditions community at NSLS until the last photons are emitted.

Ancillary Laboratories and Office Space

The support laboratories are almost as important as state of the art synchrotron radiation beamlines for a successful high pressure program at NSLS and NSLS-II. The sample and cell preparation for diamond anvil cell and large volume press experiments is space intensive and needs various specialized equipment. The high pressure laboratory will not only be supporting the dedicated high pressure beamlines, but function as a home for the high pressure research around the NSLS-II ring. Beside the laboratory facilities, lined out in detail below, sufficient office space for the beamline personnel is needed. Furthermore, since the current ring design is lacking space for beamline control and data collection areas at the beamlines, beamline control rooms are needed in the Laboratory and Office Building.

- Sample preparation laboratory (50 m^2)
    - 4 Stereo zoom microscopes with cameras and monitors
    - Workbench with granite surface
    - Fume hood
    - Glove box
    - 3 Furnaces (regular and vacuum)
    - Refrigerator
    - Microwave
    - 2 Ultrasonic baths
    - Small hydraulic press
    - Buffing & polishing machine
    - Diamond saw and cutting equipment
    - Balance
    - Heating plates
    - Micro drilling machines (spark erosion, mechanical, laser)

- Pressure medium loading laboratory (25 m^2)
    - Cryogenic loading equipment
    - Gas loading apparatus

- Laser laboratory (25 m^2)
    - Raman spectrometer (Ruby fluorescence and standard Raman measurements)
    - Offline laser heating station (Yb:fiber laser, CO_2 laser)

- User machine shop (25m^2)
    - Lathe
    - Polishing and buffing machine
    - Drilling machine
    - Thermocouple welder

- Staging and storage area (50m^2)

In the next decade, micro-engineering of the diamond anvil cell sample environment promises to undergo major development. Also, advanced methods for chemical analysis of recovered samples also offer great promise that complement structural probes. These are areas with potential synergistic interactions with the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory. We propose that a Diamond anvil cell micro-preparation and nano-analysis facility be established at CFN and NSLS-II. This may include such capabilities as CVD growth of designer anvils, ion implantation, micro- and nano-scale fabrication of sample assemblages, as well as material synthesis and characterization capability. For chemical analysis of recovered samples, focused ion beam milling systems combined with TEM or nano-SIMS devices will be increasingly required in the coming decade for a complete characterization of the chemical and structural states of materials achieved under extreme conditions.

High Pressure Working Group

During the scientific planning workshops for NSLS and NSLS-II and the technique-based workshops, many scientific communities expressed interest in high pressure sample environments. High pressure research was a topic in many of the technique based workshops and the desire to incorporate high pressure capabilities in many of the six project beamlines was shown. A large variety of high pressure cells are portable and can be installed at beamlines not dedicated to high pressure. However, certain choices in the design of a beamline, which would prohibit the use of high pressure sample environments, need to be avoided. Ideally, a representative of the high pressure community would be a member on the Beamline Advisory Team (BAT), for each beamline interested in allowing high pressure research. However, currently just the Inelastic X-ray Scattering Beamline and the Powder Instrument New Generation have members with a background in high pressure research on their BAT. Therefore, the high pressure community formed the “High Pressure Working Group” for NSLS-II.

The two main functions for the members of the working group are:

3. The “High Pressure Working Group” will serve as point of contact for BATs, providing in depth knowledge of high pressure instrumentation. The members can advice on how to best integrate high pressure equipment in beamline designs in order to optimize the research capability

4. Creating a synergy effect with other BNL institutions. Several BNL institutions (e.g. CFN, CMPMSD) possess experimental capabilities and instruments that would be useful for a sample characterization after a high pressure experiment. The “High Pressure Working Group” can initiate contact with these institutions and develop a plan to integrate these experimental capabilities in the high pressure program at NSLS-II.

The “High Pressure Working Group” is comprised of the following members:

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Appendix A

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Appendix B

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7	Kanani Lee	Yale University
8	Justin Hustoft	Yale University
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1967-1972 Massachusetts Institute of Technology, Ph.D, Geophysics

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1977-1982 Associate Professor, State University of New York at Stony Brook
1982- Professor of Geophysics, State University of New York at Stony Brook
1988- Director, Mineral Physics Institute, State University of New York at Stony Brook
1991- 2002 Director, Center for High Pressure Research
2001-2004 Chairman of the Executive Committee for COMPRES
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1998- Distinguished Professor of the State University of New York.

Honors:

James B. Macelwane Award, American Geophysical Union, 1981.
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SELECTED PUBLICATIONS

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2007-	
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2000-2008	Mineral and Rock Physics Focus Group, American Geophysical Union, Chair, 2002-2004
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Selected Publications

Mao, Z., S. D. Jacobsen, F. Jiang, J.R. Smyth, C. Holl, D. J. Frost, and T. S. Duffy, Single-crystal elasticity of wadsleyites, β-Mg_2SiO_4 containing 0.37-1.66 wt % H_2O, *Earth and Planetary Science Letters*, 266, 78-89, 2008.

Duffy, T. S., Strength of materials under static loading in the diamond anvil cell, in *Shock Compression of Condensed Matter – 2007*, edited by M. D. Furnish et al., AIP, New York, 639-644, 2007.

Shim, S.-H., A. Kubo, and T. S. Duffy, Raman spectroscopy of perovskite and post-perovskite phases of $MgGeO_3$ to 123 GPa, *Earth and Planetary Science Letters*, 260, 166-178, 2007.

Merkel, S., A. K. McNamara, A. Kubo, S. Speziale, L. Miyagi, Y. Meng, T. S. Duffy, and H.-R. Wenk, Deformation of (Mg,Fe)SiO_3 post-perovskite and modeling of D" anisotropy, *Science*, *316*, 1729-1732, 2007.

Kubo, A., B. Kiefer, G. Shen, V. Prakapenka, R. J. Cava, and T. S. Duffy, Stability and equation of state of the post-perovskite phase in $MgGeO_3$ to 2 Mbar, *Geophysical Research Letters, 33,* L12S12, 2006.

Shieh, S. R., T. S. Duffy, A. Kubo, G. Shen, V. B. Prakapenka, N. Sata, K. Hirose, and Y. Ohishi, Equation of state of the post-perovskite phase synthesized from a natural $(Mg,Fe)SiO_3$ orthopyroxene, *Proceedings of the National Academy of Sciences,* 103, 3039-3043, 2006.

Merkel, S., A. Kubo, L. Miyagi, S. Speziale, H.-k. Mao, T. S. Duffy, and H.-R. Wenk, Plastic deformation of $MgGeO_3$ post-perovskite at lower mantle pressures, *Science*, 311, 644-646, 2006.

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Education

Ph.D., Geophysics, University of Chicago, 1993
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Professional Positions and Affiliations

2005-present	Assistant Professor, Department of Geology, University of Maryland
2005	Research Associate, Department of Geology, Field Museum
2004-2005	Sr. Research Associate, Dept. of Geophysical Sciences, Univ. of Chicago
2004-2005	Chicago Center for Cosmochemistry
2001-2004	Research Scientist, Dept. of Geophysical Sciences, Univ. of Chicago
1999-2004	NASA Genesis Mission Science Team
1998-2001	Research Associate, Dept. of Geophysical Sciences, Univ. of Chicago
1995-1997	Senior Development Engineer, GE Superabrasives, General Electric Co.
1993-1995	Postdoctoral Research Fellow, Geophysical Laboratory, Carnegie Institution of Washington

Selected Publications (complete list and reprints available at http://www.geol.umd.edu/~ajc)

Campbell A. J. (2008) Measurement of temperature distributions across laser-heated spots by multispectral imaging radiometry. *Rev. Sci. Instrum., 79*, 015108.

Mao W. L., Campbell A. J., Prakapenka V. B., Hemley R. J. and Mao H.-K. (2007) Effect of iron on the properties of post-perovskite silicate. In *Post-perovskite: The Last Mantle Phase Transition*, eds. K. Hirose, J. Brodholt, T. Lay, D. Yuen. American Geophysical Union Monograph Series, Volume 174. pp. 37-46.

Seagle C. S., Heinz D. L., Campbell A. J., Prakapenka V. B., and Wanless S. T. (2007) Melting and thermal expansion in the Fe – FeO system at high pressure. *Earth Planet. Sci. Lett., 265*, 655-665.

Campbell A. J., Seagle C. S., Heinz D. L., Shen G., and Prakapenka V. B. (2007) Partial melting in the iron-sulfur system at high pressure: A synchrotron x-ray diffraction study. *Phys. Earth Planet. Int., 162*, 119-128.

Seagle C. T., Campbell A. J., Heinz D. L., Shen G., and Prakapenka V. (2006) Thermal equation of state of Fe_3S and implications for sulfur in the Earth's core. *J. Geophys. Res., 111*, B06209, doi:10.1029/2005JB004091.

Mao W. L., Campbell A. J., Shen G., and Heinz D. L. (2006) Phase relations of Fe-Ni alloys at high pressure and temperature. *Phys. Earth Planet. Int., 155*, 146-150.

Campbell A. J., Zanda B., Perron C., Meibom A., and Petaev M. I. (2005) Origin and thermal history of Fe-Ni metal in primitive chondrites. In *Chondrites and the Protoplanetary Disk*, eds. A. N. Krot, E. R. D. Scott, and B. Reipurth. Astronomical Society of the Pacific Conference Series, Volume 341. pp. 407-431.

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Educations/Career Preparations:

Department of Geosciences State University of New York at Stony Brook	Mineral Physics	Post-doc.	1994-1996
Japan Graduate University for Advanced Studies Institute of Materials Structure Science	Physics	Ph.D.	1994
Jilin University	Condensed Matter Physics	M.S.	1987
Jilin University	Physics	B.S.	1984

Appointments:

Associate Professor Mechanical and Materials Engineering Department	2007-present
Associate Director Center for Study of Matters under Extreme Conditions	
Florida International University	
Adjunct Professor	2007-present
Adjunct Associate Professor	2004-2007
Geoscience Department, Stony Brook University	
Adjunct Research Professor	2007-present
Assistant, Associate Research Professor	1996-2007
Mineral Physics Institute, Stony Brook University	
Assistant, Associate Dean of Admissions	2005-2007
Associate Director, Mineral Physics Institute	2002-2007
State University of New York at Stony Brook	
Research Associate, Changchun Institute of Applied Chemistry	1987-1990

Publications:

Paul Raterron, Jiuhua Chen, Li Li, Donald Weidner and Patrick Cordier, Pressure-induced slip-system transition in forsterite: Single-crystal rheological properties at mantle pressure and temperature, *American Mineralogist* 92, 1436-1445, (2007)

Chen, Jiuhua, Li Li, Tony Yu, Hongbo Long, Donald Weidner, Liping Wang and Michael Vaughan, Do Reuss and Voigt bounds really bound in high-pressure rheology experiments? Journal of Physics: Condensed Matter 18, S1049-S1059 (2006)

Chen, Jiuhua, Haozhe Liu, C. David Martin, John Parise, Donald Weidner, Crystal chemistry of $NaMgF_3$ perovskite at high pressure and temperature, *Am. Min.*, 90 (10), 1534-1539 (2005).

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Chen, J., D. J. Weidner, and M. T. Vaughan, Strength of $Mg_{0.9}Fe_{0.1}SiO_3$ Perovskite at High Pressure and Temperature, *Nature,* 419, 824-826 (2002).

Chen, J., D. J. Weidner, J. B. Parise, M. T. Vaughan, and Paul Raterron, Observation Of Cation Ordering During Olivine-Spinel Phase Transition In Fayalite by Time-Resolved In-Situ Synchrotron X-Ray Diffraction, *Physical Review Letters,* 86, 4072-4075 (2001).

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Professional Preparation

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Appointments

2005- present Staff Scientist, Geophysical Laboratory, Carnegie Inst. of Washington
2002- 2005 Staff Scientist, Lawrence Livermore National Laboratory
1999-09/2002 Research Scientist, Geophysical Laboratory, Carnegie Inst. of Washington
1995-1999: Senior Research Associate, Geophysical Laboratory
1993-1995 Carnegie Fellow, Geophysical Laboratory
1992-1993 A. von Humboldt Fellow, Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany
1989-1991 Senior Research Scientist, Institute of Crystallography, Russian Academy of Sciences, Moscow, Russia
1982-1989 Research Fellow, Institute of Crystallography, Academy of Sciences, Moscow, Russia

Recent publications (out of 140 total)

J. C. Crowhurst, J. M. Brown, A. F. Goncharov, S. D. Jacobsen (2008). “Elasticity of (Mg,Fe)O Through the Spin Transition of Iron in the Lower Mantle”. *Science,* **319**, 451-453.

A. F. Goncharov, J. C. Crowhurst, J. K. Dewhurst, S. Sharma, C. Sanloup, E. Gregoryanz, M. Mezouar, N. Guignot (2007). “Thermal equation of state of cubic boron nitride. Implication for the high-pressure scale at high temperature”. *Phys. Rev. B*, **75**, 224114-(1-6).

A. F. Goncharov, V. V. Struzhkin, and S. D. Jacobsen (2006). Reduced radiative conductivity of low-spin (Mg,Fe)O in the lower mantle. *Science,* **288**, 1626-1629.

J. C. Crowhurst., A. F. Goncharov, B. Sadigh, C. L. Evans, P. G. Morrall, J. L. Ferreira, and A. J. Nelson. “Synthesis and Characterization of the Nitrides of Platinum and Iridium”. *Science* **311**: 1275-1278 (2006).

A. F. Goncharov, N. Goldman, L. E. Fried, J. C. Crowhurst, I-F. W. Kuo, C. J. Mundy, and J. M. Zaug. Dynamic ionization of water under extreme conditions, *Phys. Rev. Lett.,* 94, 125508 (2005).

Other significant publications:

W. L. Mao, H.-K. Mao, A. F. Goncharov, V. V. Struzhkin, Q. Guo, J. Hu, Jinfu Shu, R. J. Hemley, M. Somayazulu, and Y. Zhao. Hydrogen Clusters in Clathrate Hydrate. *Science* **297**, 2247 (2002).

A. F. Goncharov, E. Gregoryanz, H.-K. Mao, Z. Liu, and R. J. Hemley. Optical evidence for nonmolecular phase in nitrogen above 150 GPa. *Phys. Rev. Lett.*, **85,** 1262-1265 (2000).

S. Merkel, A. F. Goncharov, H-K. Mao, Ph. Gillet, and R. J. Hemley. Raman Spectroscopy of iron to 152 Gigapascals: Implications for Earth's Inner Core. *Science,* **288**, 1626-1629 (2000).

A. F. Goncharov, R. J. Hemley, H.-K. Mao, and J. F. Shu. New High-Pressure Excitations in para-Hydrogen. *Phys. Rev. Lett.*, **80,** 101-104 (1998).

A. F. Goncharov, V. V. Struzhkin, M. S. Somayazulu, R. J. Hemley, H. K. Mao, Compression of Ice to 210 Gigapascals: Infrared Evidence for a Symmetric Hydrogen-Bonded Phase. *Science,* **273**, 218-220 (1996).

Synergistic Activities

COMPRES Workshop Organizer "Current vision and prospects for establishing of the high-pressure scale at high temperature", Washington D.C., January 26-28. 2007.

Symposium Organizer, MRS 2006 Fall Meeting.

Session chair, APS March Meeting 2007.

Reviewer for Nature Materials, Physical Review Letters, Physical Review B, Journal of Physical Chemistry, Journal *Fizika Nizkikh Temperatur* (Physics of Low Temperatures), Journal of Applied Physics, High-pressure Research, and Proceedings of the National Academy of Sciences.

Honors:

Lawrence Livermore National Laboratory Associate Director (CMS) Award, 2005.
Research Fellowship of the *Alexander von Humboldt Foundation*, 1992-1993.
Annual *European High Pressure Research Group* Award, 1991.

Recent collaborators:

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EDUCATION

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M.S. 1965, University of Cincinnati, solid state physics.
M.S. 1976, Stony Brook University, geology
PhD 1979, Stony Brook University, geophysics

EXPERIENCE

1989-present: Research Associate or Associate Professor, Mineral Physics Institute, Stony Brook University

1988-1989: Research Associate, Department of Geophysical Sciences, University of Chicago

1981-1988: Assistant Professor, Department of Geological Sciences, University of Illinois at Chicago

Relevant Publications

Wang, Y., D. J. Weidner, R. C. Liebermann, X. Liu, J. Ko, M. T. Vaughan, Y. Zhao, A. Yeganeh-Haeri, and R. E. G. Pacalo, Phase transition and thermal expansion of $MgSiO_3$ perovskite, Science, 251, 410-413. MPI Pub. No. 31 1991

Vaughan, M. T. In situ x-ray diffraction using synchrotron radiation at high P & T using a multi-anvil device. Short Course Handbook on Experiments at High Pressure and Applications to the Earth's Mantle, ed. R. W. Luth. (Edmonton, Alberta: Mineralogical Association of Canada). MPI Pub. No. 101 1993

Weidner, D. J., Y. Wang, and M. T. Vaughan, Yield strength at high pressure and temperature, Geophys. Res. Lett., 21, 753-756. MPI Pub. No. 97 1994

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