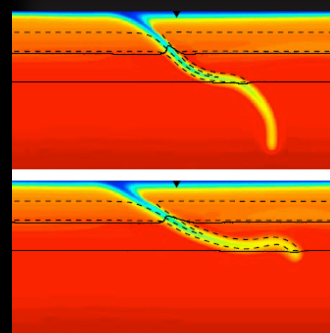
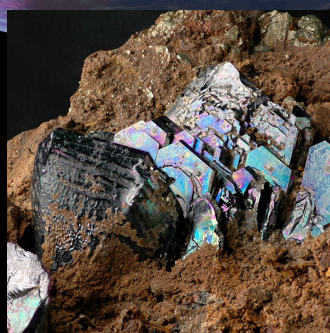
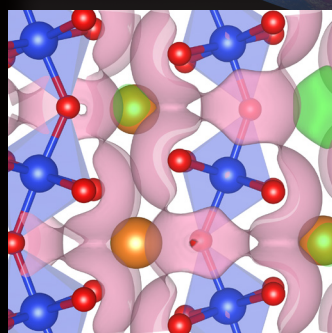


Mineral Physics

**Harnessing the Extremes: From Atoms and Bonds
to Earthquakes and Plate Tectonics**



2016 LONG-RANGE PLANNING REPORT

EDITORS

Przemyslaw Dera and
Donald Weidner

CO-CHAIRS

Abby Kavner, Jennifer M. Jackson,
Mark L. Rivers, and Guoyin Shen

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FRONT COVER. (left) Electron isosurfaces of hydrous postperovskite from Density Functional Theory calculations. *Courtesy of J. Townsend (Northwestern University)* (center) Photomicrograph of moissanite (SiC) mineral crystals. *Courtesy of R. Downs (University of Arizona) and the RRUFF project* (right) Subduction dynamics affected by meta-stable preservation of pyroxene minerals. *From Agrusta et al. (2014)*

BACK COVER. (left) Experimental sample chamber at the Matter in Extreme Conditions beamline of the Linear Coherent Light Source. *From https://portal.slac.stanford.edu/sites/lcls_public/instruments/mec/Pages/default.aspx* (center) Earth's magnetic field depends on the composition and physical properties of the molten iron-rich alloy in the core. *Figure courtesy of B. Buffett (University of California, Berkeley)* (right) Photomicrograph of perovskite (CaTiO₃) mineral crystals. *Courtesy of R. Downs (University of Arizona) and the RRUFF project*

1. Executive Summary

Mineral physics is the materials science of geological and geo-inspired synthetic materials, with emphasis on variations of structure, properties, and behavior of minerals, melts, and fluids as a function of pressure and temperature. Our field is transitioning from assembling an immense dossier of information about these Earth materials to elucidating the dynamic response of Earth to planetary-scale driving forces. Answers to many outstanding post-plate tectonics revolution geoscience questions hinge on knowledge of the equilibrium and dynamic properties of rocks, minerals, and melts; for example: How were Earth and the solar system formed? What is Earth's current state in the context of our planetary-scale evolutionary trajectory? What combination of factors has resulted in Earth's distinct geology and habitability?

The field of mineral physics provides ever-improving measurements of and constraints on material behavior that refine interpretation of growing suites of geophysical and geochemical observations. Groundbreaking discoveries driven by technological advances in materials synthesis, experiments, and analysis stimulate development of new hypotheses about the inner workings of Earth and other planets. As a result, mineral physics has grown hand in hand with the geosciences, responsive to the needs of the broader scientific community while simultaneously catalyzing transformative advances.

The same suite of tools used to study Earth materials also successfully addresses some of society's needs for new and improved materials to drive economic development and technological innovation that serve the planet, while striving for energy sustainability. Examples include discovery of new superhard ceramics and improvements to high-temperature superconductors, multiferroics, selective gas absorbers, and photovoltaics.

The goal of the planning workshop held in Argonne, Illinois, on October 10–12, 2014, and this report is to scope the array of promising technological developments and connect them with some of the most compelling questions in the geosciences. Compared to five years ago, we can now reach considerably higher pressures and higher temperatures with larger sample volumes, study more complex and more realistic samples, reliably constrain the compressional behavior of melts and liquids, and access the domain of dynamic effects and strain/stress rates. Many of these innovations have become available only recently or are still in development, thus, their full technological potential has yet to be realized. Making the most of new technologies

requires concerted and coordinated planning of research and development efforts, partnered with a crystal-clear focus on framing the most compelling Earth and planetary science questions and providing the sharpest answers.

Breakthroughs in experimental technology and cyberinfrastructure stimulate new research directions and open doors to experiments and computations that we could only dream about a decade ago. Mineral physics has proven very adaptable to technological advances and has been able to quickly and creatively take advantage of these new capabilities. Based on the workshop discussions, several very promising directions were identified as priority areas for technological development: (1) superfast detectors and innovations in pressure-generating devices that enable remote, digital pressure control and modulation according to specific shape functions for use in time-resolved studies of dynamic phenomena; (2) a high-performance, large-volume, multi-anvil press to explore aspects of multicomponent phase equilibria, melt properties, mineral elasticity, trace element partitioning, volatiles, and oxygen fugacity in Earth's lower mantle; (3) microfabrication techniques that offer exceptional opportunities for designing the next generation of experiments with microscale control; and (4) cyberinfrastructure solutions designed for extreme-conditions science and mineral physics. To implement these technological developments requires additional resources and enhanced efforts over the next five years.

The mineral physics community needs continued access to state-of-the-art facilities, instruments, and cyberinfrastructure in order to effectively work the magic of extreme conditions for the betterment of society and to remain internationally competitive in this discipline. Workshop participants emphasized that beyond stewardship of existing shared instruments, we have to seize opportunities of emerging new programs and major upcoming facility upgrades, a number of which are on the horizon in the next five years. Taking advantage of these opportunities requires strategic and proactive planning and community coordination. Such activities focused on several new projects are already underway, but will also require major investments on the part of the funding agencies beyond the operating costs of high-pressure research organizations such as the Consortium for Materials Properties Research in Earth Sciences (COMPRES), GeoSoilEnviro Center for Advanced Radiation Sources (GSECARS), and High Pressure Collaborative Access Team (HPCAT).

2. Planning Workshop

As new and exciting opportunities and breakthroughs, particularly in experimental technology and cyberinfrastructure continue to emerge, the mineral physics community convened a planning workshop to identify the most important challenges and opportunities in our discipline for the next decade (Figure 1). The workshop was held in Argonne, Illinois, on October 10–12, 2014, and followed in the footsteps of the two previous planning workshops, in Miami, Florida, in 2003 and in Tempe, Arizona, in 2009, as well as the EarthCube Domain End-user Workshop on Rock Deformation and Mineral Physics, held in Alexandria, Virginia, in November 2013.

Fifty-six people attended the 2014 workshop, which featured plenary talks by Bruce Buffett, Mark Rivers, William McDonough, Kerstin Lehnert, George Sroyer, and Craig Manning. Workshop participants were divided into eight groups to discuss the most exciting accomplishments and future opportunities from different perspectives. Four of the groups focused on scientific concepts: (1) equation of state, (2) extreme petrology, (3) transport properties: thermal, electrical, magnetic, and (4) rheology/grain boundary/diffusion. The remaining four groups emphasized capabilities and facilities, including (1) synchrotron X-ray diffraction, (2) X-ray/neutron inelastic scattering and spectroscopy, (3) cyberinfrastructure and data management, and (4) advances in fabrication/characterization.

Similar to the two previous long-range planning workshops, the goal of the Chicago workshop was to produce a written long-range vision report, following the examples of the 2003 Bass Report and 2009 Williams Report. This document is the result of these efforts. An editorial team coordinated the writing effort, and included co-editors Donald Weidner and Przemek Dera, as well as co-chairs of the workshop committee, Jennifer Jackson, Abby Kavner, Mark Rivers, and Guoyien Shen. Contributions to this document from many community members, including Pamela Burnley, Bin Chen, Thomas Duffy, Lars Ehm, Robert Hazen, Raymond Jeanloz, Shun-Ichiro Karato, Bill McDonough, Wendy Panero, Jeff Pigott, Nancy Ross, Anat Shahar, Joseph Smyth, Oliver Tschauner, and Jin Zhang are greatly appreciated.

Both the Planning Workshop as well as production of this document were supported by a special supplement to National Science Foundation grant EAR 1606856. We would like to express our sincere thanks to Ellen Kappel and Johanna Adams at Geo Prose and Sylvia Monique Thomas at the University of Nevada, Las Vegas, for their truly outstanding editorial help and tireless efforts to bring this document into its current form.



FIGURE 1. Participants of the Long-Range Planning Workshop held in Argonne, Illinois, on October 10–12, 2014.

3. Introduction

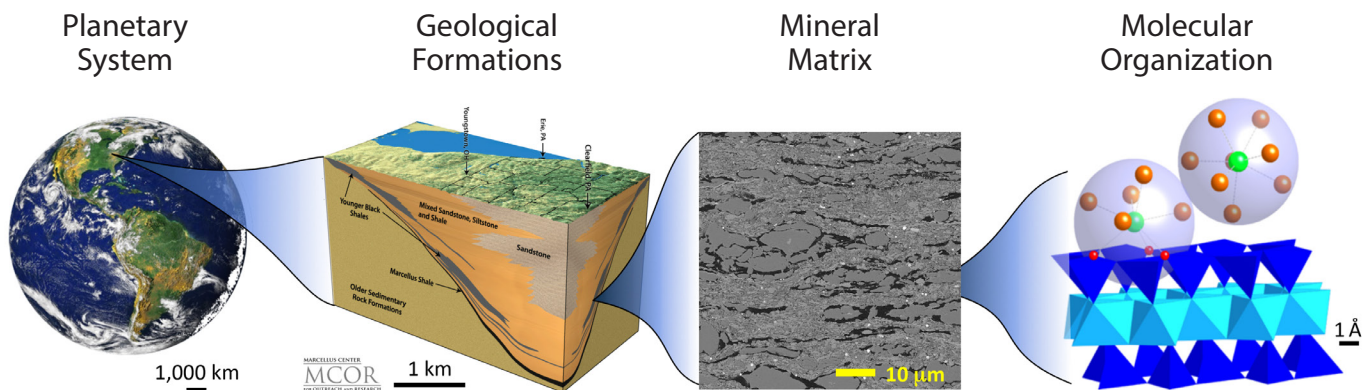


FIGURE 2. The challenge of understanding complex geosystems involves their inherent heterogeneity, ranging from molecular to planetary length scales and beyond (e.g., solar dust). Graphics courtesy of P. Fenter (Argonne National Lab)

Earth is a very complex and dynamic system in which global as well as local chemical fluxes and physical and mechanical processes act on the environment on multiple temporal and spatial scales (**Figure 2**). Some processes require millennia to have noticeable effects, but they are responsible for moving continents and raising and eroding mountain ranges. Other Earth processes such as volcanic eruptions, earthquakes, and tsunamis manifest themselves as abrupt and violent events that are more localized but can affect life in radical ways.

Life on Earth is constrained to the immediate vicinity of the planet's surface, however, processes taking place in Earth's interior control and affect surface habitability and the availability of natural resources on which humankind relies. Civilization has grown to the point that industrial activities and natural resource exploitation are having significant and potentially permanent effects on the planet. From this perspective, it is critical to better understand how relevant chemical cycles and fluxes involving the whole Earth system impact life on Earth so that our planet remains habitable for future generations.

One of the major goals of the solid Earth sciences is to advance understanding of the inner workings of our planet to enable development of models that have sufficient predictive power and reliability to warn us about imminent major natural disasters and to inform policymakers who regulate natural resource exploration and industrial emissions. Such understanding requires knowledge of the structure, composition, properties, heterogeneities, and dynamic processes taking place in Earth's interior. The main challenge in developing this body of knowledge is

that the vast majority of our planet is inaccessible to direct sampling. We have a good idea about the physics and chemistry of minerals that constitute the ~10–50 km thick crustal layer of our planet, but we have only been able to directly access Earth's subsurface down to about 12 km in the crust through drilling (1960s Soviet drilling project on the Kola Peninsula). Even the current International Ocean Discovery Program, which hopes to drill 6 km into the seafloor where the oceanic crust is the thinnest (but to date has only reached <2 km into oceanic crust), barely scratches the surface, as the complex mantle, hidden beneath the relatively familiar crust, is 3000 km thick.

Without the ability to deploy analytical probes into the deep interior, we are like the blind men examining an elephant—it is very easy to come to the wrong conclusion based on interpretation of limited and mostly indirect facts. Mineral physics has a central place among solid Earth science disciplines because the well-defined, quantitative information and constraints it generates allow expression of complex, large-scale geological processes and interpretation of indirect seismic observations by means of simple chemical and physical models. Despite a century of active research, mineral physics remains a dynamic field and continues to produce many exciting discoveries, some of which change the generally accepted picture of Earth's interior.

Recent significant improvements in global seismographic station coverage and advances in seismic modeling techniques reveal important new complexities in Earth's interior. One example is the discovery of two large, coherent structures in the lower mantle, now known as large low-shear velocity provinces (LLSVPs). Located

beneath Africa and the Pacific Ocean, they contain 1.5–2.4% by volume and ~2% by mass of the mantle and occupy almost 20% of the surface area at the core-mantle boundary. Yet, the nature of LLSVPs is uncertain: they may be passive piles, plume clusters, purely thermal anomalies, or metastable superdomes. Each of these possibilities has different implications for their origin, evolution, and effect on surface geological and geochemical expressions. Plate reconstructions suggest that LLSVPs play a fundamental role in the timing and spatial occurrence of the most voluminous plume volcanism over the last several hundred million years. When combined with geodynamic models, reconstructions suggest an intimate connection between LLSVPs and the supercontinent cycle. These unresolved questions fuel a strong need to supply new reliable mineral physics constraints that could help to resolve the underlying nature of LLSVPs.

Because of the extreme range of variations in pressure and temperature in Earth's interior, a great challenge for mineral physics is recreating these conditions in a laboratory setting in a well-constrained and reproducible manner. Researchers typically must work with extremely minuscule samples enclosed in high-pressure devices and conduct in situ experiments through access windows. Thus, progress in our discipline has been closely tied to technological developments and breakthroughs in spectroscopic and X-ray beam technologies, detectors, precision motion control devices, microfabrication techniques, and other laboratory methods. Department of Energy national user facilities, where the majority of modern mineral physics research is conducted, lead the way in implementing these advances in experimental instrumentation for basic and applied research. A strong presence of mineral physics research at these facilities, and the availability of dedicated beamlines that either entirely focus on research at extreme conditions or emphasize it as one of the main programmatic areas, has had a profound positive effect on progress in our field.

Very beneficial symbiotic by-products of development of methods and instrumentation for mineral physics are growth and advancement of extreme conditions research in materials science, condensed matter physics, and solid-state chemistry. The same experimental and computational tools being used to study compression effects on mantle minerals are successfully applied to discover new materials with unique, often exotic, properties and potential technological applications, including superhard ceramics, high-temperature superconductors, multiferroics, and selective gas absorbers.

Within the last five years, a number of important improvements in experimental technologies relevant to mineral physics have been introduced. Examples include

innovative superfast detectors for X-ray experiments that enable time-resolved sampling and studies of time-dependent phenomena such as chemical reaction rates or physical transformations with unprecedented reliability and level of detail. Innovations in pressure-generating devices enable researchers to change pressure with controllable rates and modulate pressure according to specific shape functions. Advances in microfabrication techniques offer exciting opportunities for designing more complex and more controlled experiments. For example, novel focused ion beam (FIB) instrumentation allows samples to be engineered with controlled geometry and diamond anvils to be micromachined to custom shapes, deposited with insulating layers or with electrical leads of atomic thickness. Significant progress has also been made in quantitative studies of liquids and melts. Density, viscosity, average short-range structure, and even acoustic wave velocities can be reliably measured with the newly commissioned methods utilizing large-volume, high-pressure devices.

The arena of national user facilities is also not static. The Department of Energy continuously reevaluates priorities and identifies opportunities for upgrading and constructing new major facilities to stay abreast of international competition. Within the last five years, one of the leading synchrotron labs, the National Synchrotron Light Source (NSLS) in Brookhaven, New York, which hosted a number of high-pressure beamline instruments used by the mineral physics community, has been decommissioned and replaced by the new NSLS-II, with dramatically improved beam characteristics. Thanks to our community's efforts, the experimental programs from NSLS have either been successfully relocated to the new ring in Brookhaven or moved to the sister facility, the Advanced Photon Source (APS) in Argonne, Illinois. More major changes of this type are on the horizon, with the APS preparing for an upgrade in 2020. Once again, it will be up to our community to provide the scientific justification and a forward-looking vision to compete for access to new instruments and capabilities that this upgrade will enable.

A new considerable challenge, closely related to rapid improvements in experimental techniques, that has emerged with increasing urgency over the last few years and has been recognized by the mineral physics community, is efficient analysis of massive amounts of experimental data. With brighter synchrotron beams and faster detectors, we can collect experimental data at unprecedented rates. The experiments are often decision-driven and require at least partial real-time data interpretation to provide the experimenter with the necessary guidance on how to proceed (e.g., monitoring the progress of sample transformation or detecting a subtle discontinuity that

may require more careful investigation). For such time-constrained synchrotron experiments, software tools must provide fast, and preferably automated, data evaluation capabilities. The majority of conventional software tools that perform satisfactorily with individual small data sets are inadequate when faced with massive serial data. There is a clear need for more efforts focused on development of reusable, well-documented, open source software tools that emphasize automation, computational efficiency, and user friendliness.

Beyond experiments, a very important part of mineral physics is running hydrodynamic to quantum mechanics level computer simulations. Because of the experimental challenges and limitations, all relevant physical properties of Earth minerals cannot be reliably measured in situ. There also remain the practical limits of pressure and temperature that can be achieved with individual in situ probes. In these cases, computational methods such as density functional theory or molecular dynamics enable insights into structural, thermodynamic, and electronic properties. Computational methods evolve as well, becoming more robust and able to address elusive questions such as phonon properties or spin states at high pressure and temperature. With ongoing efforts toward automation and increased user friendliness, these computational tools are becoming more accessible to researchers who do not have an extensive computational background.

Mineral physics is a prominent generator of both quantitative and qualitative thermodynamic information used by researchers in geodynamics, seismology, petrology, and geochemistry. There already exists a range of excellent

software tools that can carry out thermodynamic phase equilibria calculations and produce petrologic/mineralogic models predicting the dominant rock types as a function of depth, as well as provide information about density variations and acoustic wave velocity profiles that can be correlated with seismic observations. This software relies on the availability of comprehensive databases of thermochemical and elastic properties of relevant mineral phases. Such databases currently exist only as static compilations. What has been missing thus far, however, is a well-coordinated and focused effort at creating an easily accessible, reliable, and critically evaluated “live” online database of thermodynamic information that would be available to the mineral physics community, but much more importantly, to other Earth science communities that are the major data consumers. Such a database would provide easy mechanisms for depositing new data sets and conducting automated self-consistency assessments, and enable derivation, evaluation, and publication of custom data compilations as well as integration of experimental and computational results. The database would be cross connected with other existing major databases from other fields. New emphasis on data-driven science and data sharing, including broad and multidisciplinary programs such as EarthCube, opens possibilities for addressing this urgent need without having to reinvent the wheel. Professional data facilities such as the Interdisciplinary Earth Data Alliance (IEDA) at Columbia University, as well as some ongoing EarthCube projects, offer opportunities for adopting well-designed and tested data sharing framework solutions to create a modern mineral physics data repository (Figure 3).

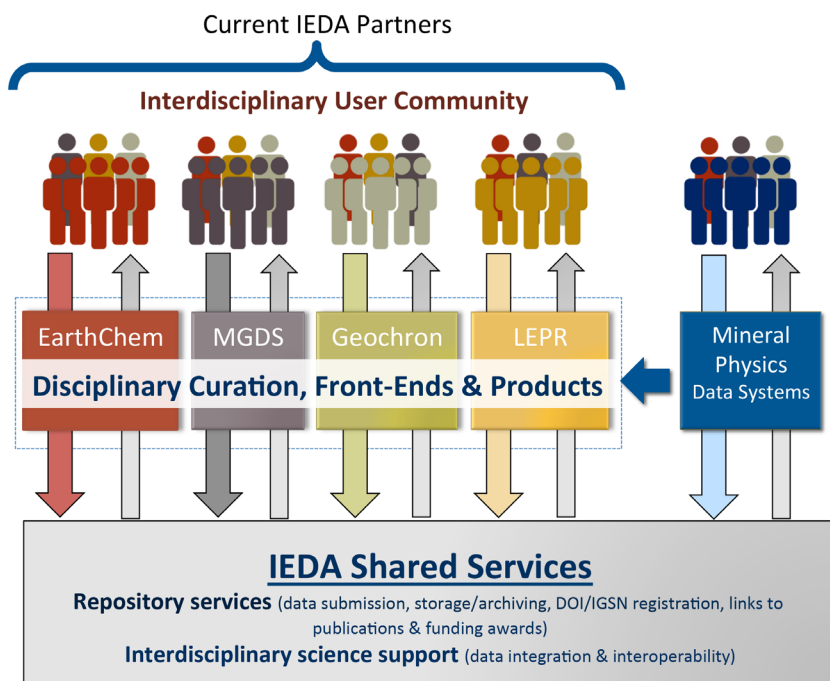


FIGURE 3. The Interdisciplinary Earth Data Alliance's (IEDA's) service structure is composed of (a) discipline-specific services (data curation, user interfaces, data products) that are provided by a suite of different data systems, and (b) shared services that are used by all systems and support scientific data management across domains, for example, data registration with digital object identifiers (DOIs), long-term archiving, links to publications and funding awards, and tools for discovery and access of data across systems in support of interdisciplinary science. With support from the National Science Foundation's EarthCube program, the mineral physics community is currently exploring possibilities to work with IEDA to develop and maintain data system(s) that would serve the needs of broader science community, taking advantage of IEDA's infrastructure and resources, including the IEDA Shared Services. Figure courtesy of K. Lehnert (Columbia University)

Compared to five years ago, we can now reach considerably higher pressures in many types of experiments, study much more complex and more realistic samples, reliably constrain the compressional behavior of melts and liquids, and access the domain of dynamic effects and strain/stress rates. While significant progress has unquestionably been made, the work certainly does not stop here. Many of these innovations have just recently been made widely available, thus, full realization of their potential for the mineral physics field will take concerted and coordinated planning, research and development, and time. High-pressure research organizations, such as the Consortium for Materials Properties Research in Earth Sciences (COMPRES), the GeoSoilEnviro Center for Advanced Radiation Sources (GSECARS), and the High Pressure Collaborative Access Team (HPCAT), continue to play pivotal roles in driving these improvements and innovations, but require help and input from the community to define priorities and keep track of evolving primary science drivers.

4. Extreme Earth Science

4.1. ELASTICITY

Sound velocity, as measured by seismic waves, is the most precisely defined Earth property at any point within the planet's interior. Furthermore, sound velocity is a property that can be scaled to small samples and short time scales. This attribute makes elastic properties, the defining factor of sound velocities, a vital focus of study. Quantitative knowledge of the elastic properties of minerals and rocks at a range of temperatures and pressures provides critical linkages between mineralogical and petrologic models of deep rocks and geophysical observations. Examples of how this information is used include interpretation of the mineral and rock properties that are expressed in the deep Earth as major seismic discontinuities; determination of the relative contributions of temperature, composition, spin state, and other factors to seismic velocities; descriptions of how seismic anisotropy is connected to the core and mantle flow field; and identification of locations of hot mantle upwellings or cold downwellings.

Both experimental and computational tools are used to conduct such studies (Figure 4). They yield determinations of density, unit cell parameters, and sound velocities of constituent minerals as a function of pressure and temperature, which constrain equations of state (EoS) and pressure-temperature dependencies of elastic tensors, enabling modeling of elastic behavior of mineral

assemblages in various Earth environments. EoS studies encompass not only continuous behavior, but they also reveal discontinuities associated with isochemical phase changes (e.g., structural, electronic, order-disorder) that may contribute to observed seismic discontinuities and affect, for example, mantle convection by changing buoyancy relations. For example, the isochemical polymorphic phase changes in olivine, $(\text{Mg,Fe})_2\text{SiO}_4$, have long been recognized as the likely contributor to the 410 km and 660 km seismic discontinuities.

After more than 60 years of concentrated efforts in mineral elasticity studies, acoustic velocities of most relevant deep-Earth phases have been determined to first order under high pressure and temperature. The main objective of further elasticity studies for the coming decade is to define acoustic velocities and anisotropies for real rocks at Earth pressures and temperatures and for seismic frequencies.

Key challenges include:

- Characterizing the thermal-elastic EoS for all principal deep-Earth minerals as a function of major element chemistry over the relevant pressure, temperature, and composition range
- Understanding the influence of trace elements such as hydrogen that may significantly affect the EoS
- Extending the pressure-temperature range for high-accuracy determinations of the EoS of lower mantle

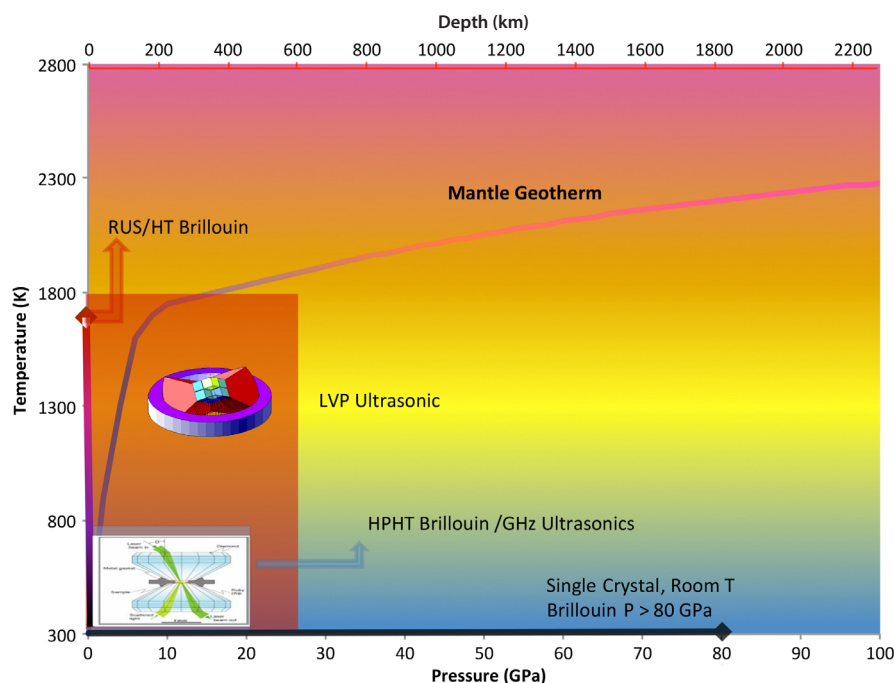


FIGURE 4. Current capabilities of experimental methods for laboratory acoustic measurements. Courtesy of B. Li (Stony Brook University) and S. Sinogeikin (HPCAT)

- and core constituents
- Understanding the effect of order–disorder phenomena on the EoS that may be active inside Earth and characterize the equilibrium state
- Better understanding the influence of phase changes on acoustic velocities and attenuation in the region where transitions are occurring
- Understanding dynamic time- and stress-rate-dependent effects
- Better constraining the elastic properties of melts and partial melts

Over this last decade, knowledge of elastic properties of relevant minerals has increased significantly. In the laboratory, this growth has come through the expansion of ultrasonic acoustic velocity measurements and laser spectroscopy such as Brillouin scattering or impulsive stimulated scattering. It also can be attributed to quantum mechanical calculations using density functional theory, a tool that has proven capable of accurate predictions. Methods using shock waves, static compression, and nuclear resonant scattering have also contributed to the database, but each with a more limited capacity. Contributions using ultrasonic techniques have increased. Multi-anvil cells can now reach 30 GPa and 1500 K with megahertz interferometric measurements, while with diamond anvil cells, even gigahertz frequencies are becoming accessible.

The combination of all of these techniques has led to major increases in the quality of information gathered through experiments conducted at synchrotron facilities. Calibration of pressure and temperature has been greatly enhanced. Indeed, the combination of P and S velocity measurements with sample density through X-ray

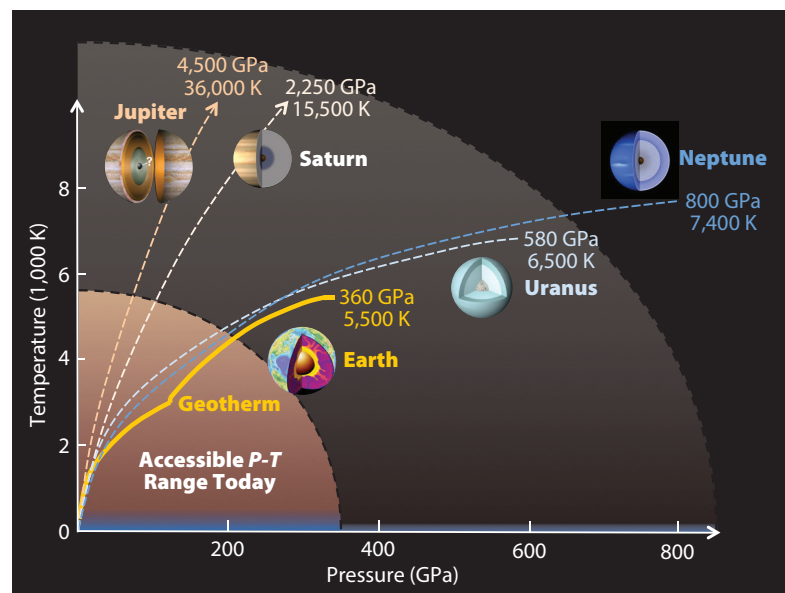
diffraction provides an absolute pressure calibration that is independent of standards.

Quantum mechanical tools have matured with the sound knowledge of the role temperature plays in the elastic properties of rocks and minerals. Both quasi-harmonic calculations and molecular dynamics have succeeded in overcoming the thermal limitations of this technique. Molecular dynamics, while much more computationally intensive, provides insights when the vibrations are anharmonic. The more precise and computationally simple use of quasi-harmonic models proves adequate for the majority of minerals in most of the relevant P-T ranges. Theoretical models become extremely important, as they are not bound by laboratory restrictions of pressure and temperature, chemical composition, or stable phase.

For iron-rich materials, nuclear resonant scattering offers a strong basis for exploring some elastic properties. The “Debye” acoustic velocity can be obtained from the phonon density of states. This velocity is most sensitive to the material’s shear velocity. Thus, with knowledge of the bulk modulus, it is possible to estimate acoustic velocities. As these experiments can be done in a laser-heated diamond anvil cell, conditions in Earth’s and other planets’ cores are potentially accessible (**Figure 5**).

The time dependence of the stress–strain relation is important on many scales. Stress relaxation that occurs faster than the period of a seismic wave will reduce acoustic velocity and introduce attenuation. Phase transitions, partial melting, grain boundary sliding, and dislocation motion are all mechanisms that introduce time dependence into the stress–strain curve. Furthermore, rates of stress change that Earth-forming materials experience in their natural environments due to convection, tectonics,

FIGURE 5. Pressure and temperature paths relevant for modeling of various planetary bodies in the universe. *Courtesy of G. Shen (Carnegie Institution)*



or volcanism vary over many orders of magnitude, from a slow tectonic process such as glacial isostatic adjustment to rapid and violent stress releases during major earthquakes. Shock events such as meteorite or asteroid impacts are another class of phenomena with very unique stress rate domain. Stress change rates have been demonstrated to have significant effects on the behavior and transformations of minerals that constitute the rocks. They can control deformation mechanism and slip systems, suppress equilibrium phase changes, and in some cases induce changes that are unique to a given stress rate regime. Our ability to reproduce naturally occurring stress rates in the laboratory is significantly limited (some of the processes would require thousands or millions of years of lab observation), but any capabilities for quantifying the dynamic effects are extremely valuable. Beyond stress rate control, the kinetic aspects of high-pressure phenomena like diffusion, solid-state chemical reactions, and structural phase transition rates are important to understand for realistic and reliable modeling of Earth evolution and dynamics.

Over the last five years, mineral physics has made some significant advances in time- and stress-rate-resolved studies. New types of devices, including piezo-driven and electronically controlled gas-membrane-driven diamond anvil cells that allow remote and digital pressure changes, have been introduced. In large-volume press experiments, new capabilities permit us to vary stress according to a well-defined shape function and monitor sample stress and strain as a function of time. These novel tools present new opportunities for mineral physics exploration in the time domain.

Looking toward the next decade, we see expansion of experimental techniques that will enable higher pressure and temperature environments for many of these experiments. Multi-anvil ultrasonic experiments that have been limited to 30 GPa and 1500 K have the potential of operating to the full limit of the multi-anvil system, which is now about 100 GPa and 2000 K. With a laser-heated diamond anvil cell (CO₂ laser or Nd-YAG [neodymium-doped yttrium aluminum garnet] lasers), the pressure and temperature ranges are now expanded to more than 300 GPa and over 5000 K. Such experiments have been successfully performed in combination with synchrotron powder X-ray diffraction and Brillouin spectroscopy (Figure 4). However, temperature gradients and uncertainty are relatively large for laser heating experiments. Double-sided laser heating and special thermal insulation solutions, particularly those taking advantage of new microfabrication capabilities, help to reduce these effects and greatly improve reliability of thermoelastic measurements. Another recently introduced approach to minimize temperature uncertainty

during laser heating is to reduce the data collection time. With novel super-fast X-ray detectors, the data collection time for regular X-ray diffraction experiments can be reduced to milliseconds, and at such a small time scale, temperature fluctuations are greatly minimized. The accuracy of pressure measurements is related to the accuracy of different pressure standards and the availability of reliable cross-calibrations. It is known that the discrepancies introduced by different pressure standards could be as large as 5% at elevated pressure and temperature conditions. Focused efforts in developing reliable and robust cross-calibrations of a set of internally consistent pressure standards to high-pressure and high-temperature conditions simultaneously have been initiated, and will undoubtedly continue through the next decade.

Reaching pressures higher than 250 GPa has been very challenging using the traditional single-stage diamond anvil cell. The historical highest-pressure record of 416 GPa stood unbroken for over two decades. Experiments aimed at recreating inner core conditions to study metal alloys expected to be present in this mysterious region require pressures up to 360 GPa. In contrast, pressures over 500 GPa are required for studying elements and compounds, such as metallic hydrogen, relevant to the interiors of giant planets (e.g., Saturn). A recently developed revolutionary double-stage anvil cell technique with hemispherical nano-polycrystalline second-stage diamond anvils has now expanded the static pressure range to over 600 GPa under room temperature. However, realizing the full potential of this new capability and developing analytical probes that can provide reliable in situ characterization of the sample properties at the associated size scale requires significant further efforts (Figure 6).

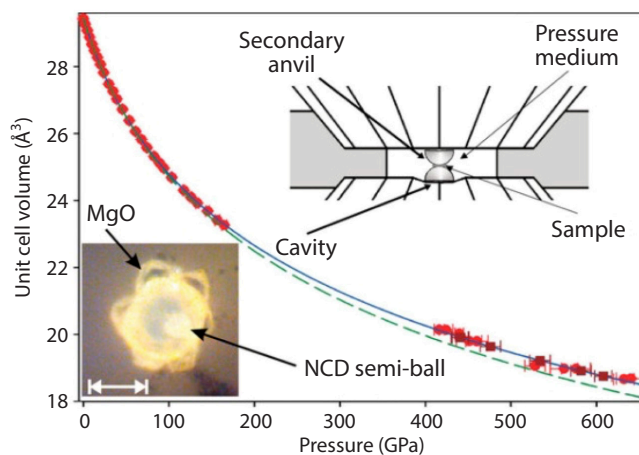


FIGURE 6. Innovative double-stage diamond anvil cell design enables access to pressures over twice as high as at the center of Earth's core. From Dubrovinsky et al. (2012), reproduced with publisher's permission

The new generation of synchrotrons at national facilities offers great promise for the coming decade. At Brookhaven National Laboratory, the new NSLS-II features a highly coherent X-ray beam that provides improved spatial and energy resolution. At the same time, plans are underway to upgrade the synchrotron at Argonne National Laboratory to be fully coherent. These new machines will encourage novel areas of research to be explored. X-ray imaging has been used to define stress and strain in cyclically deformed samples. The improved imaging tools offer more precise measurement of velocity and attenuation at seismic frequencies. The high coherence enables better energy resolution for studying inelastic scattering. The X-ray beam can be focused to a smaller spot, enabling diffraction from samples in two-stage diamond anvil cells.

With few exceptions, the equilibrium phase transitions of major rock-forming minerals are now reasonably well understood and the structures and properties of equilibrium high-pressure phases have been satisfactorily characterized, at least at ambient temperature. However, equilibrium transformations usually require very high

temperatures in order to overcome kinetic barriers. There are abundant and geologically relevant environments in Earth's interior such as subduction zones where the temperature conditions are much lower than the average geotherm and where metastability effects play a significant role. The last few years witnessed a marked advance in our ability to detect and characterize subtle displacive phase transitions that occur in major mineral phases metastably overpressurized beyond their equilibrium stability limits, such as at convergent margins within the coldest part of the subducting slab. For example, previously unknown metastable polymorphs of the major upper mantle phases olivine, orthoenstatite, diopside, and coesite have recently been reported (**Figure 7**). Understanding these new polymorphs often reveals previously unknown pieces of information about processes such as the structural mechanism of silica densification (change of coordination number of silicon from four to six at high pressure) in silicate minerals and offers marked improvements in our ability to interpret the complex seismic observation from convergent margin regions and model buoyancy dynamics (**Figure 7**).

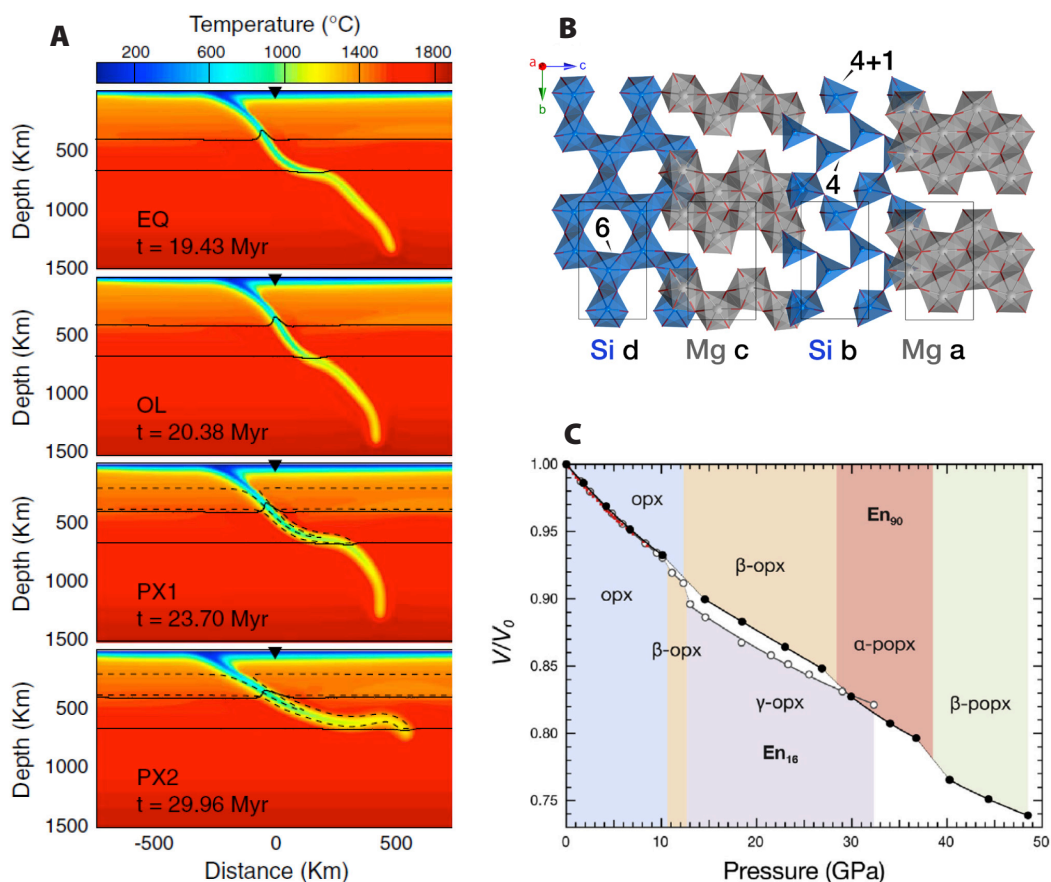


FIGURE 7. (A) Geodynamic consequences of metastable preservation of lower mantle mineral phases olivine and pyroxene in cold subduction zones. From Agrusta et al. (2014) (B) Crystal structure of newly discovered metastable post-pyroxene phase of enstatite En_{90} , which may be present in cold slabs that penetrate the lower mantle. (C) Discontinuities in the compressional behavior of density of enstatite En_{90} and ferrosilite En_{16} pyroxenes at ambient temperature due to metastable phase transitions. (B) and (C) from Finkelstein et al. (2015), reproduced with publisher's permission

4.2. CRYSTALLOGRAPHY

Most rock constituents possess well-defined crystal structures and symmetries that control their physical properties. X-ray diffraction experiments reveal details of the atomic arrangement and chemical bonding in these materials, and when carried out in situ at high pressure and high temperature, offer insights into atomic-scale response of the crystal to external forces that act on rocks in Earth's interior.

Experimental crystallography and computational mineral physics are closely coupled. Experimental elucidation of crystal structures of high-pressure phases opens doors for first principles calculations to predict properties (e.g., transport) too difficult or impossible to measure experimentally, and to extend beyond pressure and temperature limits accessible to experiments. While there has been considerable progress in the power of computational methods to predict high-pressure phases, experimental data are always required to help make tractable the extreme multidimensional configurational space of all possible atomic arrangements of polymorphic varieties.

Key questions include:

- What are the stable and metastable structural arrangements of all major mantle and core minerals at relevant pressure and temperature conditions?
- How do structural modifications of these minerals translate into changes in physical and chemical properties?

Pioneering developments in high-pressure crystallography go hand in hand with advances in X-ray accessible pressure-generating devices. Rapid advances in extreme crystallography began with home lab-based instruments in the early 1970s, shortly after development of the first gasketed diamond anvil cells. Within a few decades, this progress led to the charting of phase diagrams of the most important Earth-forming minerals up to pressures of about 10 GPa, corresponding to a depth of approximately 300 km in the upper mantle. The field dramatically transformed and moved forward in the late 1980s when synchrotron instruments compatible with high-pressure devices became available and limits imposed by sample sizes required by the home lab instruments were no longer a restriction. However, the methodology of synchrotron experiments took a fairly long time to mature to its current stage, and the detectors, X-ray focusing optics, accessibility of devices such as the GSECARS-COMPRES gas-loading system, and innovations in data collection and analysis were the enabling factors.

New opportunities include routine crystallographic structure determination at pressures well beyond 10 GPa,

with a number of recent reports successfully resolving crystallographic details of samples in the megabar range. Single crystal-like analysis of multigrain data collected on coarse powder samples composed of hundreds of individual crystallites offers new ways to quantitatively characterize development of lattice preferred orientation (LPO) during sample deformation, thus linking crystallographic studies to geophysical-scale flow in Earth. The ability to include time-resolved measurements of crystal structure at high pressures and temperatures will further allow mineral physics to solve mysteries about Earth rheology.

Many of the phases formed as a result of pressure-induced polymorphic phase transitions are not quenchable, which means that they revert to the common ambient pressure forms upon decompression. The only way to reveal the secrets of these enigmatic high-pressure structures is to conduct in situ high-pressure crystallographic experiments. In this regard, the history of extreme crystallography has been dotted with both buried mysteries as well as doors that simply have not been opened yet. A significant number of unresolved important discontinuous transformations and new unquenchable phases were reported, but the corresponding structures have not been determined due to technique limitations.

One example of a buried extreme crystallography challenge that was left uncovered for several decades, but has finally been revealed, is the crystal structure of phases III and IV of CaCO_3 calcite. Calcite is one of the principal carbonate minerals, and its behavior and transformations at high pressures and temperatures have an impact on Earth's global carbon cycle. First identified by spectroscopy studies, and tentatively assigned monoclinic symmetry in the early days of high-pressure single crystal diffraction, the structure CaCO_3 -III had taunted mineral physicists until 2012. Twinning that develops during the phase transition and coexistence of two closely related structural modifications make the data analysis and interpretation very challenging, particularly when an older style point detector is used for data collection. Taking advantage of synchrotron instrument equipped with area detector and modern analysis software, scientists at the European Synchrotron Radiation Facility were finally able to resolve the structure and describe the exact atomic arrangement, which for CaCO_3 -III turned out to be triclinic. This has opened a new research area to examine the high-pressure structural behavior of carbonates, including high-pressure phases that confirm theoretical predictions of a pressure-induced switchover in carbon-oxygen coordination from trigonal planar to tetrahedral. Depending on the details of the structural energetics, this could have important implications for carbon's solubility within mantle silicate phases.

Another example of a classical mineral system in which new unanticipated crystallographic discoveries have been reported is the iron-oxygen binary. Oxygen and iron are two of Earth's most abundant elements, and they drive the redox equilibria of Earth's interior. Iron oxides such as hematite and magnetite are common crustal minerals and carry evidence of the magnetic field. Fe-bearing MgO is believed to be an important component of Earth's lower mantle and core-mantle boundary (CMB). For the last few centuries, until 2011, only three stoichiometries of iron oxide were assumed to exist, Fe_{1-x}O , Fe_3O_4 , and Fe_2O_3 . High-pressure, high-temperature crystallographic studies of the last five years demonstrated that this family is in fact much larger, and the redox equilibria dependence on pressure and temperature in this system is quite complex. A series of iron-oxygen binaries has been expanded to include Fe_4O_5 , Fe_5O_6 , and $\text{Fe}_{13}\text{O}_{19}$ (Figure 8). These exotic iron oxides were synthesized at different P-T-oxygen fugacity conditions inside diamond anvil cells, and their existence inside Earth might serve as a potential oxybarometer to determine the redox state of Earth's interior.

Some of the opportunities and challenges for the near future include high-pressure experiments at temperatures

exceeding 1000°C, with detailed structural determination and time-resolved studies capable of capturing transient states and transformation kinetics. New types of synchrotron instruments specifically designed for advanced extreme crystallography applications are being immediately adopted. Thanks to funding from COMPRES, an advanced six-circle diffractometer has been commissioned at the GSECARS facility at APS as part of the Partnership for eXtreme Xtallography (PX²) project. The PX² diffractometer will soon enable single crystal laser heating experiments (Figure 9). Single crystal facilities have also been developed at the COMPRES-funded high-pressure beamline at APS.

In the last five years, modern extreme crystallography ventured beyond simply unraveling atomic arrangements and symmetries of crystalline solids. Another active research direction is the development of methods for quantitative characterization of defects and lattice dynamics, based on analysis of X-ray diffuse scattering at high pressure, but it will require continued efforts over the next several years to mature.

4.3. TRANSPORT PROPERTIES

Geodynamic Perspective

The dynamic behavior of Earth and planets is controlled by the ability of constituent materials to transport mass and heat. Transport properties such as electrical and thermal conductivity in planetary interiors determine whether a dynamo-based magnetic field is present and how it behaves. They greatly influence Earth's geodynamics and evolution, from deep processes such as mantle

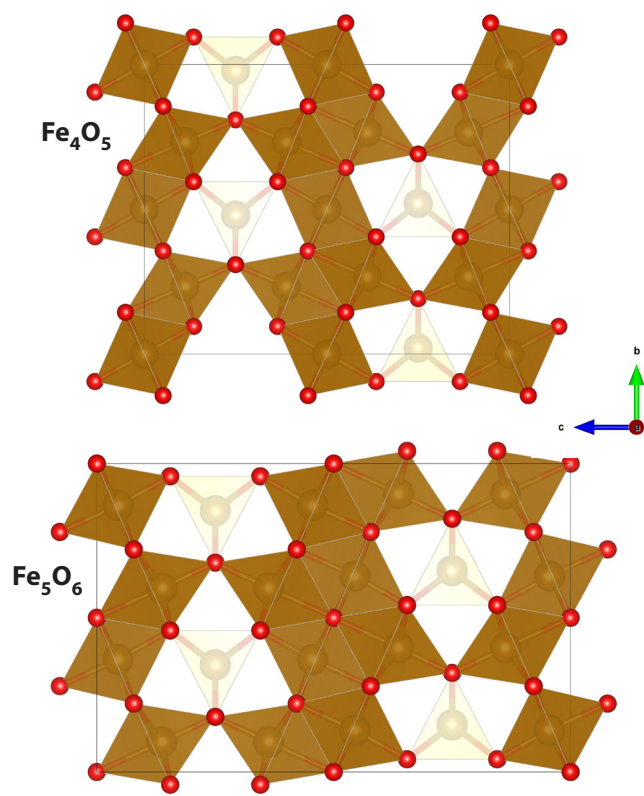


FIGURE 8. Recently discovered high-pressure iron oxides Fe_4O_5 and Fe_5O_6 . Structure drawings were prepared based on atomic coordinates reported by Lavina et al. (2011) and Lavina and Meng (2015). Figure courtesy of D. Zhang (University of Hawaii)

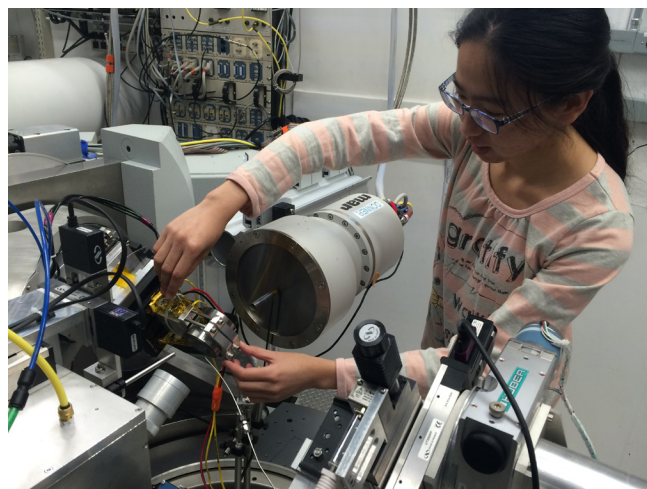


FIGURE 9. A graduate student uses a resistively heated diamond anvil cell with a membrane pressure controller at the GSECARS 13BM-C experimental station (PX² project) for advanced extreme crystallography research as part of her PhD thesis. Figure courtesy of D. Zhang (University of Hawaii)

convection and core-mantle interactions, to shallower processes such as volcanic eruptions, ore formation, and surface heat flow, which are directly relevant to societal interests. Convection in highly conductive planetary cores generates planets' magnetic fields (**Figure 10**). On Earth, the magnetic field acts as a shield for radiation and modulates the atmosphere, thus helping to support life. The composition of the core records the history of early Earth formation, including volatile elements (e.g., H and C). Due to their different density, light elements contribute substantially to the operation of core convection and, hence, the geodynamo. However, the amount of light elements and their speciation are poorly constrained. Also, the processes (driving forces) that transport light elements are poorly understood.

Heat flow in the mantle—by a combination of convective (mostly) and radiative and conductive transport—governs the three-dimensional patterns and the vigor of mantle convection. Under cool conditions and large stresses and strain rates, rocks are brittle and deform via faulting, creating earthquakes. Under hotter conditions and geological-scale strain rates, rocks flow plastically. The nature of this ductile-brittle transition in Earth rocks provides the mechanical boundary conditions for plate tectonics, and is ultimately responsible for its surface expression via volcanoes and earthquakes. Mantle convection controls heat flux from the core and, thereby, geodynamo activity. It also circulates volatiles and, hence, controls the evolution of the atmosphere and hydrosphere. A big question relevant for development of a model of volatile circulation (evolution of the atmosphere/hydrosphere) is whether the core is the source or sink for these elements.

Key questions include:

- What are the full-Earth depth-dependent profiles of the properties governing dynamic behavior, such as thermal conductivity, electrical conductivity, and viscosity?
- How do these transport properties vary as a function of temperature and composition throughout Earth?

Techniques for measuring thermal and electric conductivities using a large-volume apparatus at relatively lower pressures (<30 GPa) are mature. To adopt these techniques for higher pressures, we need to develop better anvil materials. Sintered nanodiamond composites (NDC) are a promising route. Making such anvils for a large-volume press requires a hydraulic press of 5000 tons or more, which could be designated as a user facility and also serve the mineral physics community for growing large single crystals. Pressures and temperatures close to those at Earth's core can be achieved using a diamond anvil cell (DAC). However, direct measurement of transport properties is a difficult task due to small sample sizes, and mature techniques are lacking. Ultrafast detectors, submicron synchrotron beam (X-ray or infrared), and nano-level sample fabrication will greatly facilitate implementation of various direct or indirect techniques.

Over the last decade, significant progress has been made in some areas of deep Earth transport properties research. The thermal conductivity of pure iron has been determined with much improved accuracy through indirect experiments and calculations, yielding values substantially higher than previous estimates. This finding has had a big impact on our understanding of the core dynamo and core-mantle thermal history. Thermal diffusivity of several key mantle minerals has been constrained to approximately 140 GPa,

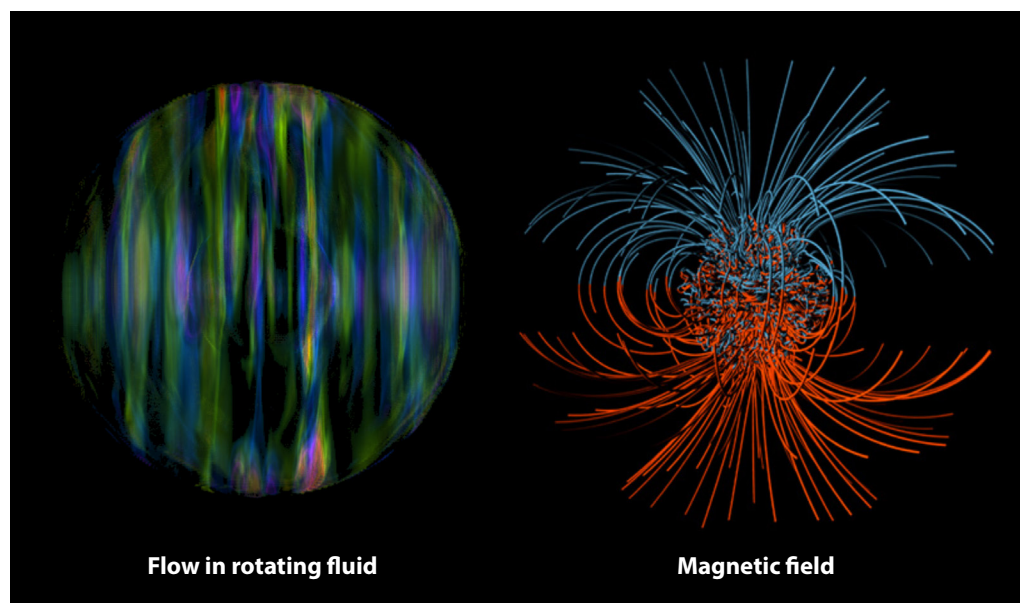


FIGURE 10. Flow and rotation in the outer core control Earth's magnetic field, and depend strongly on the composition and physical properties of the molten iron-rich alloy. *Figure courtesy of B. Buffett (University of California, Berkeley)*

helping to better estimate the heat flux at the CMB. In the mantle, electrical conductivity of silicates and oxides at high pressures and temperatures determines how the magnetic signature generated in the core is filtered through Earth's mantle, and ultimately observed at the surface. Full determination of a one-dimensional electrical conductivity profile is on the horizon, including variations as a function of temperature, major element chemistry, water, oxygen fugacity, and iron spin state.

Among the most important future directions over the next decade are obtaining accurate measurements of the thermal conductivity of molten iron alloyed with light elements as well as of mantle minerals. This information is needed to constrain the Rayleigh number, which controls convection. Changes in thermal diffusivity with compression tend to be very large, comparable to changes in viscosity, and thermal diffusivity also changes with phase transformations, including radiative conductivity, which may potentially be important in the hot, deep mantle.

It is also important to better constrain the electrical conductivity of lower mantle minerals. As discussed in more detail in the following sections, water distribution in the lower mantle is poorly understood, but it potentially strongly affects electrical conductivity. Incorporation of hydrogen into nominally anhydrous minerals leads to structural defects that in turn affect conductivity. Geophysical studies have made much progress in recent years, and conductivity models down to ~1500 km have been established, except for few special cases, where laboratory data on the role hydrogen plays in the electrical conductivity of lower mantle minerals are missing.

Melting, melt density, and melt-solid separation are among the most important process controlling planetary-scale evolution. Volatiles assist melting in the deep Earth. The density contrast between melt and solid depends critically on melt composition, which in turn depends on the temperature at which the melt is formed. The influence of partial melting on physical properties and the processes of melt transport depend strongly on the geometry of melt pockets in a material that is largely made of solid minerals. In order to obtain quantitative information about solid-melt interactions at extreme conditions, major improvements in high-resolution X-ray tomography are necessary, and are already on the horizon. This experimental technique will also be key in understanding non-diffusive mass transfer (morphological instabilities), which is relevant for the materials transport at the CMB and the nature of material exchange between the core and the mantle. Currently, only preliminary data on (Mg,Fe)O are available. Future studies of other relevant CMB materials, including bridgmanite and post-perovskite, are needed.

4.4. RHEOLOGY

The dynamic nature of the solid Earth is expressed in earthquakes, mountain building, volcanic eruptions, and plate tectonics, and plays a pivotal role in all aspects of Earth evolution, from the development of the atmosphere and ocean to the production of continents and dry land. The motions of Earth's crust, mantle, and core are governed by the brittle and plastic material properties at the conditions in Earth's interior. Because many of these phenomena occur on a time scale far greater than those available to scientists, laboratory model studies are needed to validate mechanisms that control the deformation behavior of Earth materials.

Key questions include:

- How do we use observations of seismic wave anisotropy in Earth's mantle, coupled with laboratory measurements on lattice-preferred orientation, to inform our understanding of mantle flow?
- How do chemical composition, volatiles, temperature, and trace elements affect convection inside Earth? How does convection affect the distribution of water inside Earth and help control the evolution of the atmosphere and hydrosphere?
- What is the three-dimensional nature of the strain-rate dependent viscosity of Earth, and how does that help control plate tectonics on the surface, mantle convection, and core dynamo and inner core behavior? How does this four-dimensional viscosity state vary as a function of temperature, composition, and history?

While elastic properties are related to the equilibrium thermodynamics of materials, material plasticity—flow—is the minerals' response to disequilibrium and is governed by defects in the crystal structure. This plastic mechanical response is therefore strongly dependent on the dominant defect-based mechanism, which changes with state variables such as stress state, temperature, and composition, and point defect populations, as well as variables that are time- and history-dependent, such as strain rate, and grain boundary and dislocation populations. Thus, the challenge of the mineral physics of rheology is two-fold: measuring and understanding the deformation mechanisms operating in the laboratory, and extrapolating laboratory-determined flow behavior to Earth and planetary scales.

Experimental deformation studies have a long and rich history in the Earth sciences. They tackle one of the most complex types of problems: defining a set of properties that constrain an inherently non-equilibrium process. The flow strength of rocks depends not only on mineralogy, but

also on crystal defects within grains; on grain size, shape, and orientation; and on the presence of trace materials, including water. Rock strength is strongly sensitive to environmental conditions such as temperature, pressure, and time scale. Environmental conditions profoundly affect deformation mechanisms, but also affect strength indirectly through phase changes and trace element solubility changes. Experimental tools and techniques for testing these various dependencies in rocks have been developed over decades and have met with great success, with the exception of pressure, where development has lagged because of extreme demands on mechanical equipment and sensing methods. Fifteen years ago, the introduction of apparatus for controlled deformation at high pressure that utilizes synchrotron X-rays to measure stress and strain in samples has opened a wide range of pressure-temperature conditions to deformation studies. In addition, the use of diffraction to probe the internal stress state of samples has provided researchers with an entirely new source of information about deformation processes.

It is now possible to make accurate rheological experiments at pressures more than an order of magnitude higher than we could access 15 years ago. With the advent of new, sophisticated X-ray imaging tools, we anticipate that the next 15 years will present even more exciting advances in this research area.

Interfaces: Improved understanding of the nature of grain boundaries and other types of interfaces at pressure and temperature. What is the impact of interfaces on Earth's interior? What is the grain size distribution in the deep Earth? Does it vary from region to region? Has it changed over time?

Defects: Improved understanding of the nature of crystalline defects at pressure and temperature. What is the impact of defects on the rheology of Earth's interior?

Rock geochemistry: Improved understanding of the physical and chemical properties of rocks and minerals with natural chemical compositions. How does the rheology (coupled with melting behavior and phase equilibria) of mantle rocks with natural compositions differ from those of well-characterized end-member chemical systems typically worked on? How do realistic compositions impact the rheology of grain boundaries?

Mineral aggregates: Improved understanding of the physical and chemical properties of polyphase aggregates. How do the elasticity, rheology, and melting behavior of polymineralic mantle rocks differ from well-characterized

mono- and two-phase aggregates that have been typically worked on? Can polyphase properties be determined from characterization of monophase materials?

Fluids and solids: Improved understanding of the interaction between fluids and solids in the mantle (e.g., precipitation and dissolution, crystallization and melting at high pressure and temperature).

Extrapolation: Improved understanding of how to extrapolate from laboratory to Earth conditions. How do we extrapolate from mineral physics experimental time scales to geologic time scales? How do we extrapolate from experimental spatial scales to planetary dimensions? Extrapolation from laboratory conditions to Earth conditions has traditionally been accomplished through empirical flow laws that quantify the relationship between the state of deviatoric stress and the resultant rate of permanent change of shape or strain rate. Our best constraints on rock strength have been developed through experimental deformation of rock samples and analogs and the application of flow laws.

In contrast to simple elastic deformation, plastic deformation is effected by a number of mechanisms, each dependent on environmental conditions in its own way. Thus, to the extent that the same mechanisms are operating in both the lab and in Earth, the lab-determined flow law can be extrapolated to geological strain rates. However, if different deformation mechanisms are operating in the lab, then the extrapolation is potentially very inaccurate. Therefore, an important goal in designing an experimental study is to choose conditions such that the relevant mechanisms are operating. Deformation mechanisms that likely operate in Earth's deep interior include diffusion creep, power-law dislocation creep, and the Peierls mechanism. Existing extensive data sets on olivine and new data on wadsleyite and ringwoodite suggest that at typical lab conditions for grain sizes of a few microns, these three mechanisms compete closely. Plastic deformation in most regions of the deep Earth occurs at high homologous temperatures and slow strain rate and, consequently, the stress level is expected to be low (~1–100 MPa). Under these conditions, likely deformation mechanisms are power-law dislocation creep and diffusion creep. In order to infer the deformation mechanisms operating in an experiment, the stress exponent, activation energy, and grain-size dependence of strain rate need to be determined. With a typical stress level of experimental studies of deformation (~100 MPa), the necessary precision of stress measurements is ~10 MPa. Also, specimens with a range of grain sizes (submicron to several microns) need to be used.

Flow Laws

The flow laws of olivine and other upper mantle minerals have been well studied. Particularly critical are the flow laws of deep mantle minerals (Figure 11). Only semi-quantitative data on flow laws exist for the transition zone minerals wadsleyite and ringwoodite, and virtually no flow law data exist for perovskite and post-perovskite. In order to determine the flow laws of these minerals (and also their polyphase aggregates), new technical developments are needed.

An important advantage of in situ synchrotron X-ray stress measurements is that information about plastic anisotropy, the strength difference among different slip systems, can be inferred. It is also possible to determine the strength differences among coexisting phases. With high spatial resolution, it may also be possible to determine stress distribution in a deforming material, which will provide highly useful information on the processes of shear localization and resultant shear instability.

Synchrotron X-ray diffraction presents an unprecedented opportunity to investigate the inner workings of polycrystals. We now see directly what we should know intuitively—that a single-valued state of stress does not exist in a polycrystal. Grains have directional strength properties, and crystallographic orientations vary from grain to grain. We now have access to a spectacular amount of information about the states of stress inside a polycrystal, expressed not only in the centroid position of a diffraction peak but also by the peak shape, which informs us about the spatial distribution of stress. This window into grain-scale stress distribution in a deforming material may advance understanding of the link between broad-scale applied stress and the deformation physics operating at the grain and subgrain scale, which is necessary for extrapolation.

While experiments form the backbone of understanding the plastic properties of Earth's interior, it is essential to develop models that link Earth with lab data. To make this linkage requires several levels of development. Plastic processes by nature are related to atom-level processes, whether they are driven by diffusion or dislocation. To date, atom-level interactions, particularly those involving large displacements of atoms, require a quantum mechanical basis, such as density functional theory. While some theoretical studies have begun in this area, many more are necessary to find the proper path to generating first-principle models of plastic properties.

A rock's plastic behavior is not a simple consequence of average mechanical properties of individual single-phase crystallites, as grain interactions through boundaries play a significant role in the process. In this area, numerical simulations, for example, those based on mean field theory, have been successful in identifying deformation mechanisms consistent with experimental data. These models solve the mechanical problem for a large number of grains, but are subject to the mean stress/strain field of the sample. Real deformation behavior of a rock, however, is not completely described by such mean field models, as these models do not account for multiple grain (many-body) interactions.

In response to these shortcomings of elastic-plastic self-consistent theory, stress percolation models have been helpful in understanding the modulation of boundary conditions at the grain scale. Stress percolation shows great promise for linking broad-scale applied stress to microscopic stresses. However, as with all models, there are assumptions and simplifications regarding polycrystal physics that need to be examined critically. Synchrotron diffraction can provide the kind of data needed to test and

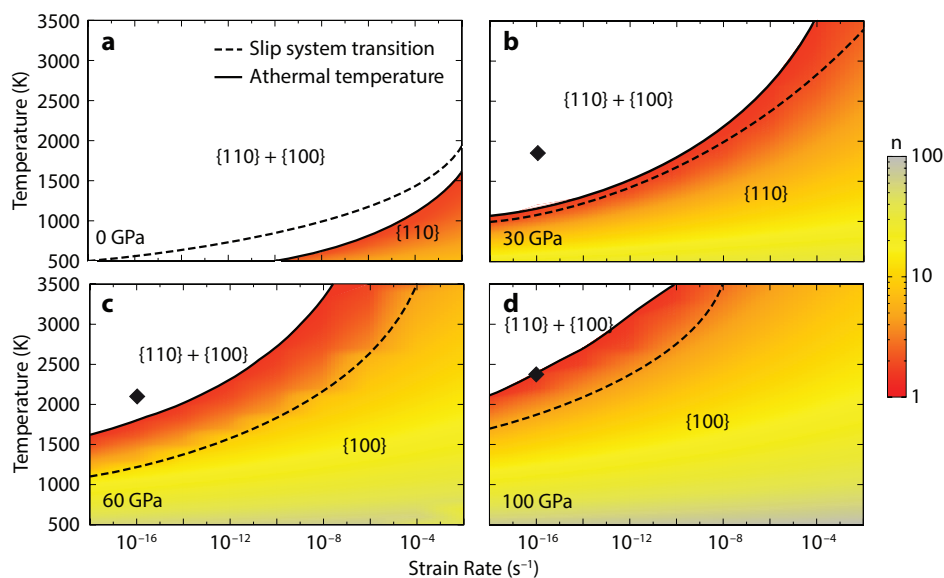


FIGURE 11. Pressure affects the way in which strain rate and temperature control the deformation mechanism and dominant slip system in MgO periclase. From Cordier et al. (2012), reproduced with publisher's permission

refine stress percolation and other polycrystalline models. Since polycrystal physics has wide application for Earth materials at low pressure and also for materials science, we anticipate this work will have extensive broader impacts.

Deformation Fabrics

Deformation of a polycrystal in some cases may lead to lattice-preferred orientation and may generate observable anisotropy in the timing of seismic wave propagation through Earth's interior. Therefore, if the relationship between LPO and flow geometry is known, then measured seismic anisotropy can be used to infer patterns of mantle flow. Rich experimental data exist for upper mantle materials, and there has been some success in connecting observed seismic anisotropy signatures to mantle flow. However laboratory-generated LPOs are sensitive to sample history, and also the presence or absence of water in the rock structure can significantly alter the sense of the preferred orientation. While this complicates interpretation of seismic information in some areas, it also suggests that seismic signatures may be used as a chemical probe—especially for the presence of volatiles. Interpreting observed seismic anisotropy in terms of mantle flow below the transition zone is difficult because experimental data on LPO and even the dominant slip systems are limited. LPO study requires examination of significant sample strain over a broad range of physical and chemical conditions because, like the flow law, preferred orientation development is likely sensitive to these conditions. We anticipate that continued development of instruments designed to produce high strain, like the rotational Drickamer apparatus (RDA), will allow major advances in this area in the future.

Earthquake Process

The field of rheology is dedicated to understanding the flow processes of material at a variety of physical and chemical conditions. In some regions, the material flows via a mechanism that releases stress such that the stress drop is spatially and temporally localized, resulting in earthquakes. Although earthquakes are mostly limited to the shallow crust, they can occur as deep as the top of the lower mantle in the coldest parts of Earth's interior. Many questions remain about the similarity between deep and shallow earthquakes and the processes that are responsible for the events. We know that brittle fracture causes earthquakes at the shallowest depths, and there has been extensive laboratory work on brittle fracture at low pressures. However, due to past experimental limitations, there has been no work on brittle fracture at the high pressure and high strain rates required for rocks to stay in the brittle field. Other failure mechanisms such as phase-transformation-induced

faulting or faulting caused by the formation of nano-materials have been observed but are poorly understood, and the relationship or interaction between brittle failure and these mechanisms is speculative. With recent advances in X-ray diffraction and three-dimensional imaging techniques, we can expect significant progress in our understanding of these phenomena.

4.5. PETROLOGY

Understanding whole-Earth dynamic processes requires measuring the phase diagrams of rocks—not just minerals—across immense ranges of pressure and temperature. Knowledge of the thermodynamics of multi-component systems, especially parameters and functions controlling melting behavior, phase changes, and distribution of elements among various mineral phases, constrains boundary conditions for the large-scale chemical and physical evolution of the whole Earth (**Figure 12**). Until recently, small sample volumes combined with extreme temperature gradients precluded all but the most rudimentary petrology experiments at lower Earth mantle and core/mantle boundary conditions. Advances in microscopic sample fabrication and sophisticated high-resolution characterization techniques are enabling new extremes in metamorphic petrology experiments.

Key questions include:

- In multicomponent silicates, oxides, and metals relevant to planetary interiors, what are the partition coefficients of major and minor elements across the phase boundaries, especially the melting boundaries?
- How does the relative buoyancy of partial melts compared with their coexisting solids change across ranges of pressure, temperature, and composition?
- What is the distribution of radiogenic heat-producing elements on a global scale?
- How can trace element and isotopic geochemical information provide insight into whole-Earth evolutionary processes?
- As planets are formed, what determines which suites of elements will ultimately form the core, and which will be retained in the oxidized mantle?
- Is the core-mantle boundary a chemically reactive boundary? If so, is the core growing at the expense of the mantle? Or, is the mantle growing at the expense of the core?

Melting is an especially important process for interpreting global-scale differentiation in Earth's interior. In the mantle, even small amounts of melt can generate large changes in physical properties such as lowering viscosity or

increasing electrical conductivity. Large volumes of buoyant melt can result in global chemical differentiation. Thus, the history of melting, and the density difference between melt and solid, help govern Earth's large-scale evolution. The last 10 years have seen advances in using X-ray techniques to measure the melting point of single-component systems. The next target is measuring melting relations—solidus, liquidus, and temperature-, pressure-, and compositional-dependent melt production.

Earth's core-mantle boundary is a zone of extreme heterogeneity in physical, chemical, and thermal properties. In addition, it is the dividing point between reduced metal and oxidized mantle. Chemical reactions across this interface are therefore redox reactions. How do the energetics of these redox reactions vary across the large pressure ranges of the deep mantle? Recent sets of experiments have suggested a crossover in the $\text{Fe}^{+2} - \text{Fe}^{+3}$ and $\text{Fe} - \text{Fe}^{+2}$ redox systems, which predict a disproportionation of Fe^{+2} to Fe^{+3} and Fe metal in the mantle. This redox state change suggests that significant differences in physical properties might exist within the lower mantle. Other redox crossovers might also exist, signaling pressure-dependent changes in the thermodynamic preference of components to partition into metal or an oxide phase, thus providing depth-dependent readjustment of the composition of a percolating core.

Correlated sets of geochemical evidence are powerful tools for testing hypotheses concerning the evolution of Earth's interior. Minor and trace elements are relevant to our understanding of Earth. K is a minor element in Earth's mantle, yet it also serves as one of the most important heat sources. Other minor elements such as Cr and Ti provide information about partial melt extraction from the mantle.

Th and U, though traces in the bulk Earth, are important as heat sources in the mantle and also through their daughter isotopes, which provide information about time scales of geologic processes and the origin of reservoirs in Earth. Thus, we are not only interested in the major element distribution between mineral assemblages but also in minor and trace element distributions and their mobility in the presence of melts and fluids.

Consequently, the study of rock-forming minerals alone provides an incomplete picture. For example, platinum group elements are incompatible with rock-forming minerals and occur only in rare, minuscule inclusions of alloys and chalcogenides in the mantle. Other incompatible elements may reside at interfaces between rock-forming minerals or remain enriched in fluid phases. Novel techniques such as X-ray tomography can reveal the interaction of fluids and melts with minerals in situ and provide insight into chemical enrichment processes at interfaces between mineral grains.

Defects in minerals play an important role in rock deformation, but they are also expected to be the major hosts for noble gases in Earth's interior. Important progress has been made in the past few years in noble gas and isotope geochemistry. Although complementary geochemical experiments could provide essential information on the geological settings of noble gas reservoirs in the mantle, they remain difficult to conduct. In situ probes such as X-ray diffraction, X-ray spectroscopy, and optical spectroscopy, and novel techniques such as X-ray tomography, are complemented by microchemical analysis of recovered samples. Previously, chemical analysis of samples recovered from extreme pressures was compromised by the small grain size of phases and mixed analyses. Recent progress

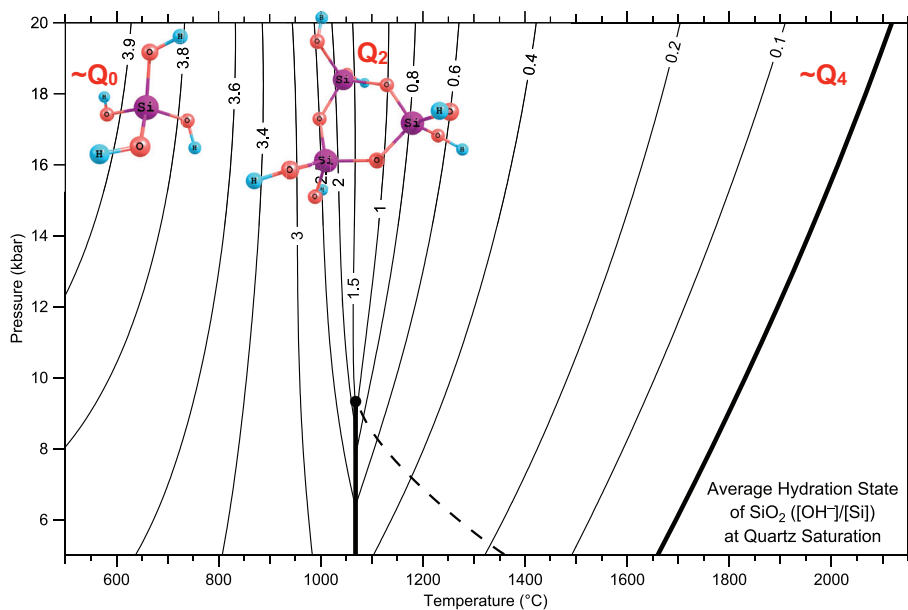


FIGURE 12. In $\text{SiO}_2\text{-H}_2\text{O}$ fluids, the average hydration state and degree of polymerization of SiO_4 units change at different pressures and temperatures. Figure courtesy of C. Manning (University of California)

in sample preparation by FIB as well as in the analytical instrumentation itself has led to much improved quantitative chemical analysis of samples recovered from lower mantle pressures. This set of novel and improved tools requires accordingly well-controlled experiments where observed chemical reactions, phase formation, and diffusion reflect evolution toward thermodynamic equilibrium at defined pressure and temperature rather than steady-state temperature gradients or slowly evolving patterns of anisotropic stress fields and temperature changes.

Much progress in extreme petrology is expected from microfabricated sample assemblies. Strategies for reversed diffusion experiments and for reversal of phase boundaries that are standard in ambient and low-pressure experimental petrology need to be adapted to experiments at extreme pressures where diffusion rates are commonly low. Modeling and monitoring of temperature and stress gradients in actual sample assemblages during experiments provide an important corrective for data analysis and interpretation of chemical gradients in recovered samples.

Another promising path is the development of pressure-temperature generating devices that combine the advantages of large sample chambers in large volume presses, such as low or vanishing temperature gradients, with the advantages of diamond anvil cells, such as direct temperature measurement from incandescent light and large apertures for probing the sample by diffraction and spectroscopy. Design and construction of such hybrid high-pressure devices are now becoming feasible thanks to the development of nano-diamond and nano-stishovite anvils and pistons.

4.6. UNDERSTANDING THE COMPLEXITIES OF EARTH'S MANTLE

Mg, Si, Fe, and O account for 94% of Earth's mantle elemental composition, with an additional 5% attributed to Ca and Al. Thus, lower mantle mineralogy can be described as a mixture of MgSiO_3 -perovskite (bridgmanite), Ca-perovskite, and ferropericlase ((Mg,Fe)O). The factor that determines the proportions of Mg-perovskite (bridgmanite) to ferropericlase is the Mg/Si value of the lower mantle. Bulk silicate Earth (BSE) compositional models that invoke enstatite chondrites or CI carbonaceous chondrites (primitive, undifferentiated meteorites) as planetary building blocks predict differences in upper and lower mantle composition and have limited amounts of, or no, ferropericlase in the lower mantle. In contrast, models that predict an upper and lower mantle of similar composition imply that the amount of ferropericlase in the lower mantle is at the level of 15% by mode. One of the big outstanding challenges regarding

lower mantle mineralogy is narrowing the uncertainty of the amount of ferropericlase that is consistent with the Preliminary Reference Earth Model (PREM).

Another enigmatic but very important mineral component of the lower mantle is CaSiO_3 perovskite. Ca-perovskite is expected to be the primary host of calcium in the lower mantle. Therefore, a significant research target is to precisely and accurately measure the mode proportion of Ca-perovskite in the lower mantle, as this would constrain the absolute amount of refractory elements Earth contains. Observations suggest that all chondrite groups inherited similar relative abundances of refractory elements, which are those with 50% condensation temperatures above 1350 K for a nebular gas of $\sim 10^1$ Pascals of hydrogen. Given that the refractory elements (e.g., Al, Ca, Ti, rare earth elements, Th, and U) are in *chondritic proportions*, if we know the absolute abundance of one of these elements, we can then determine the abundance of the rest of them assuming chondritic ratios (e.g., Al/Ca, Al/Ti, Al/Th, Al/U). Therefore, by defining the amount of Ca in the lower mantle, we can constrain the amount of Th and U inside Earth, which accounts for 80% of the total radiogenic heat production.

Water Cycle in Earth's Deep Interior

Key questions include:

- Why is Earth able to support life?
- What is the deep Earth's contribution to the water cycle?

Hydrogen is the most poorly constrained major element compositional variable in Earth's interior. The mantle is composed of oxygen minerals, thus "water" is equated to hydrogen distribution. Hydrogen is present in all mineral phases within Earth to a greater or lesser extent. Just as water controls surface processes, it also affects all interior processes, including melting, rheology, anisotropy, seismic velocity, P-T conditions of phase boundaries, and electrical conductivity (**Figure 13**). Because the ocean accounts for only 0.023% of Earth's total mass, small amounts of H incorporated in the silicate phases are likely to constitute the planet's largest water reservoir. This interior reservoir is likely to maintain some dynamic equilibrium with the surface ocean through internal convective overturn.

Hydrogen storage is determined by synthesis, usually in a multi-anvil press, and by measurement of H contents through Fourier transform infrared (FTIR) spectroscopy, Raman spectroscopy, Elastic Recoil Detection Analysis (ERDA), and secondary ion mass spectrometry (SIMS). H is incorporated into many nominally anhydrous mantle minerals in sufficient quantities to affect elastic properties,

density, and deformation mechanisms. Mineral physics elasticity results on hydrated minerals are used to interpret seismic studies of travel time, reflections, and anisotropy in order to understand the role water plays in Earth's interior.

The storage of H in the major mineral phases of the upper mantle and transition zone (TZ) is fairly well measured, as are the effects of H on the elasticity of olivine, wadsleyite, and ringwoodite. Protonation of lower mantle phases is less well understood, and there is no consensus on the possible role H plays in this region. Recent observation of a natural terrestrial ringwoodite inclusion with 14,000 wt ppm H_2O in a diamond is direct evidence of significant hydration of the transition zone (Figure 14). This major discovery was made possible by prior synthesis and characterization of hydrous ringwoodite. Observation of low-velocity regions above 410 km and below 660 km have been interpreted as dehydration melting of minerals passing from a region of high water content to one of lower concentration.

In addition to these recent discoveries, measurements

of the elastic properties of synthetic hydrous ringwoodite and wadsleyite have made it possible to compare expected S- and P-wave velocities in the transition zone with observed seismic velocity profiles. It is possible to match velocity models with a transition zone that is hydrous (5000–10,000 wt ppm H_2O), but not with a dry pyrolite composition. It is now fairly well established that significant hydration in the TZ is possible; however, firm conclusions about the hydration state of the lower mantle are not yet feasible. The lower mantle is thought to be composed of bridgmanite (60–80%), ferropericlase (10–20%), and a Ca-perovskite phase (5–15%). The H_2O storage capacity of bridgmanite and ferropericlase is much less than that of the TZ phases with estimates ranging from 20 wt ppm up to as much as 4000 wt ppm. Al substitution appears to be critical in the bridgmanite phase, as the dominant hydration mechanism is Al + H substituting for Si in the octahedral site, while only minimal Al gets incorporated into the Mg site. There is also a nominally hydrous Phase D ($MgSi_2H_2O_6$)

FIGURE 13. A cross section of Earth shows the location of ringwoodite, which makes up approximately 60% by volume of the lower transition zone. The diagram also shows how water gets transported down to those depths and how diamonds and water move back to the surface. Figure from <http://www.cbc.ca/news/technology/deep-earth-has-oceans-worth-of-water-10-diamond-reveals-1.2569564> by Kathy Mather

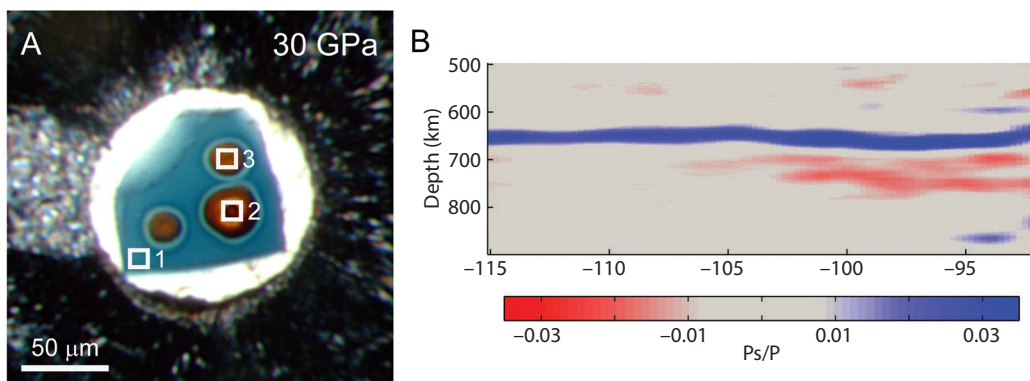
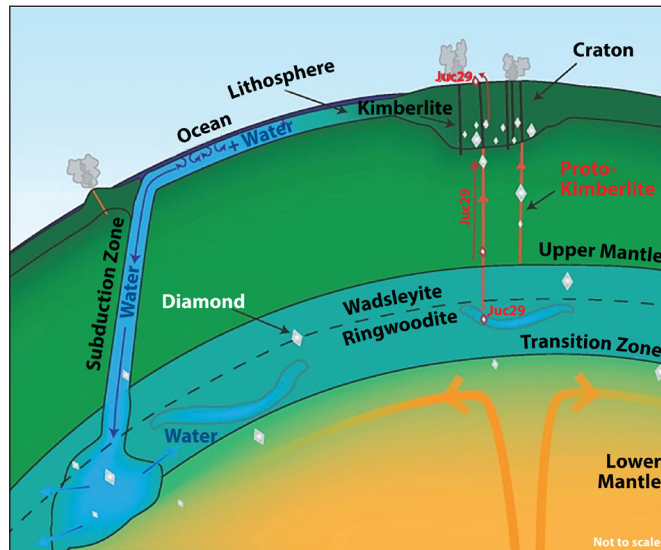


FIGURE 14. (A) Blue hydrous ringwoodite crystal in a diamond anvil cell laser-heated to induce transformation to high-pressure $MgSiO_3$ -perovskite (brown circles). (B) Seismic data corresponding to positive (blue) and negative (red) velocity gradients beneath North America showing possible evidence of regional-scale dehydration melt beneath 660 km, corresponding to the same transformation observed in experiments. From Schmandt et al. (2014), reproduced with publisher's permission

that is stable at depths of 660 km to about 1500 km but may not be stable at geotherm temperatures. Phase D contains both Mg and Si in octahedral coordination and appears to be stabilized to higher temperatures by Al substitution in both sites. A very significant quantity of water can be contained in a small amount of Phase D because it incorporates so much H, which may not be detectable by seismic methods unless its breakdown induces melting.

Over the coming decade, it may be possible to constrain the amount of water in the lower mantle by mineral physics using methods of synthesis and full characterization of water contents and elastic properties. Large volume press synthesis is possible to ~28 GPa and 2200°C. The sample size required for these studies is limited by the size/tonnage of the large-volume press devices, but sufficiently large crystals can be successfully synthesized in a 5000-ton press, making it possible to fully characterize the elasticity.

H concentration in the liquid metal outer core is very high. The core's potential to store vast amounts of H may control its total abundance on the planet. It is possible that this reduced H could escape and reduce Fe or Si at the CMB. H content is expected to be higher in the post-perovskite phase (ppv) at the CMB than in bridgmanite, which may stabilize ppv in this region.

Multiscale Heterogeneities in the Deep Mantle

Recent advances in inelastic X-ray scattering techniques with high energy resolution permit unique atomic-scale vibrational measurements of Earth materials under extreme conditions. For example, nuclear resonant inelastic X-ray scattering of iron-bearing phases allows determination of sound velocities under extreme conditions that test hypotheses concerning the chemistry of small-scale ultra-low velocity zones (ULVZs; Figure 15). With constraints from equations of state, geodynamic models of the steady-state relief of iron-rich (Mg,Fe)O-bearing structures at the core-mantle boundary show a certain range of density contrasts that produce shapes matching many preferred seismic small-scale, low-velocity structures at the CMB (Figure 16).

Larger coherent structures such as large low shear velocity provinces are often associated with smaller-scale ULVZs. Located beneath Africa and the Pacific Ocean, LLSVPs contain 1.5–2.4% by volume and ~2% by mass of the mantle and occupy almost 20% of the surface area at the CMB. However, the nature of these multiscale structures is uncertain. The development of inelastic scattering techniques paired with X-ray diffraction allows constraints

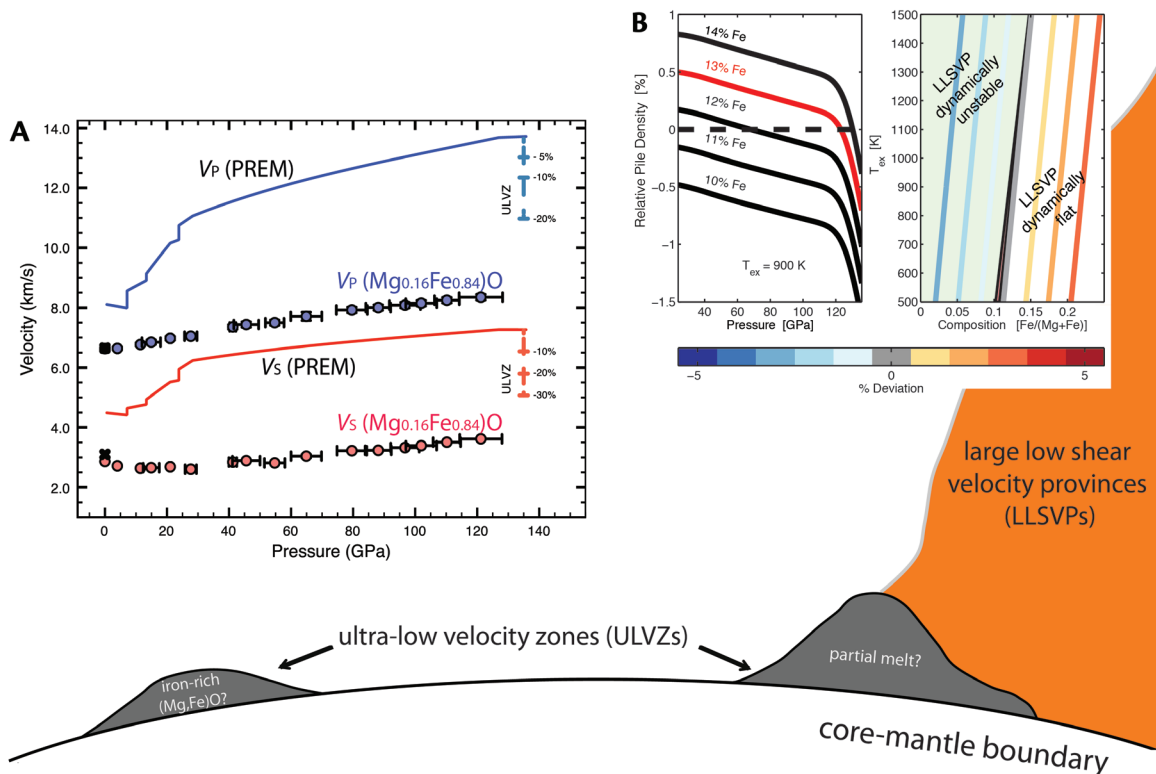


FIGURE 15. Multiscale heterogeneities in Earth's deep mantle. (A) Experimental determination of the wave velocities of solid $(Mg_{0.16}Fe_{0.84})O$ to pressures approaching Earth's core-mantle boundary reveal significant velocity reductions compared to the one-dimensional PREM (solid lines). Modified from Wicks et al. (2010) (B) Equation of state determinations of iron-bearing bridgmanite help constrain the relative buoyancy of speculated bridgmanite-rich LLSVPs. Part (B) modified from Wolf et al. (2015). Figure compiled by J.M. Jackson, J.K. Wicks, and A.S. Wolf (Caltech)

on wave velocities and density of candidate assemblages to be realized. As such, processes that generate and control multiscale structures in Earth's deep mantle will become clear (Figure 15).

Spin and Valence of Iron Under High Pressure

Iron is the most abundant transition metal element in the mantle and therefore plays a key role in Earth's geochemistry and geodynamics. Pressure is known to induce an electronic transition in iron, which changes its spin (electron spin pairing within individual orbitals) from a high to a low state, and also a discontinuous reduction of the effective

ionic radius. Spin transitions are usually isosymmetric (there is no change of the symmetry). Spin transitions in iron occur, for example, in magnesiowüstite, silicate perovskite, and post-perovskite and have noticeable effects on elasticity, causing abnormal compressional behavior.

A number of new experiments involving understanding the oxidation and spin states of iron in pyrolytic and basaltic glass samples at high pressure has led to a better understanding of the role the spin state of iron plays in melts at high pressures. It is claimed that high-spin to low-spin changes of iron in Mg-silicate melt are potential sources of iron partitioning changes between silicate melt and minerals at deep mantle conditions (Figure 17).

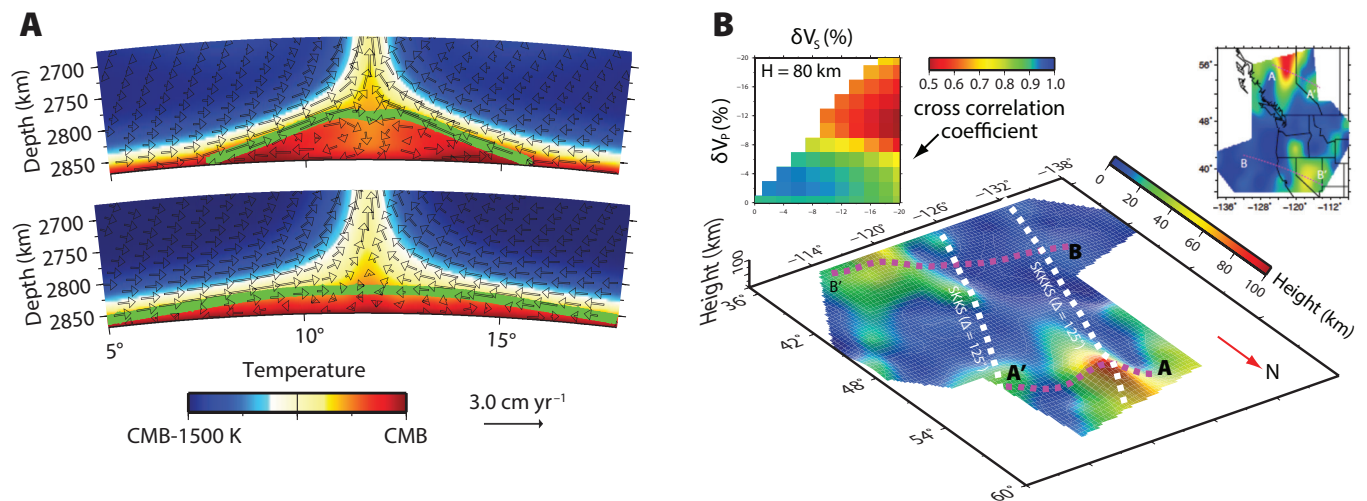


FIGURE 16. Mineral physics informs geodynamic modeling and interpretations of seismic observations. (A) Geodynamic modeling of the steady-state relief of $(\text{Mg}_{0.16}\text{Fe}_{0.84})\text{O}$ -bearing structures at the core-mantle boundary shows a certain range of density contrasts that produce shapes matching many preferred seismic low-velocity, small-scale structures at this boundary. Modified from Bower et al. (2011) (B) Seismic observations constrain a three-dimensional laterally varying structure on the core-mantle boundary with average $\delta V_S = -8\%$ and $\delta V_P = -5\%$ compared to PREM, which can be explained by the presence of about 5 vol.% $(\text{Mg}_{0.16}\text{Fe}_{0.84})\text{O}$. Modified from Sun et al. (2013), Figures courtesy of J.M. Jackson (Caltech)

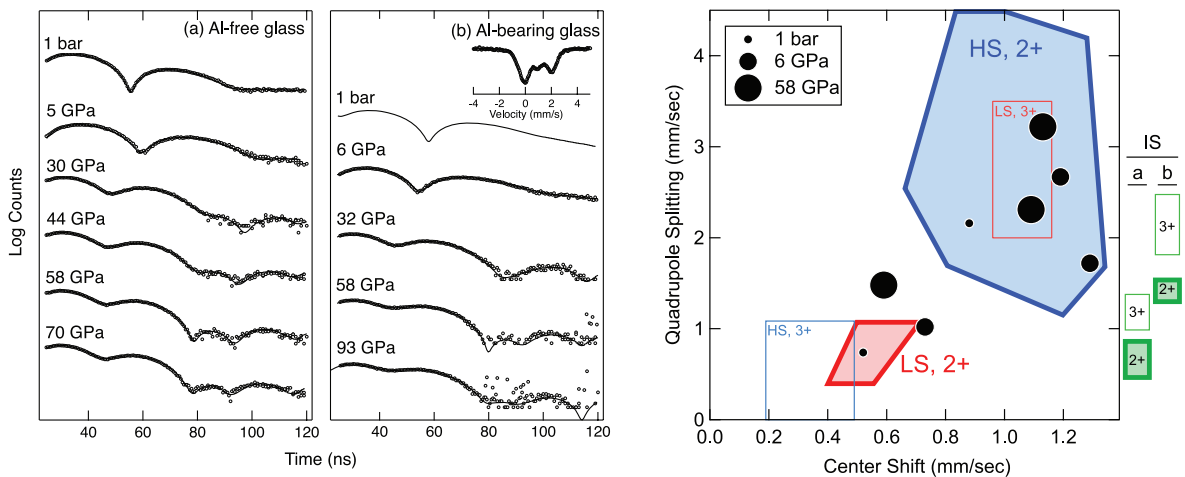


FIGURE 17. The synchrotron Mössbauer spectroscopy technique can be used to determine hyperfine interactions (effects leading to small shifts and splitting in the energy levels of atoms) in mineral samples at high pressure and allows measurement of nuclear parameters such as center shift (CS) and quadrupole splitting (QS) through Mössbauer spectral fitting (left panels). CS and QS values for intermediate-spin iron in silicates are plotted on the right side. From Gu et al. (2012), reproduced with publisher's permission

4.7. UNDERSTANDING EARTH'S CORE

Core Density Deficit

Our knowledge of Earth's core is derived from geophysical, geochemical, geomagnetic, and orbital studies. Earth's core, consisting of a liquid outer core (OC) and a solid inner core (IC), is known to be predominately iron diluted with ~8–10% nickel and a considerable amount of lighter elements, suggested by the density deficit and sound velocity discrepancies between pure Fe and seismic reference Earth models such as PREM (Figure 18). Most recent estimates of the core density deficit fall between 8% and 12% for the liquid OC, and between 3% and 5% for the solid IC. With respect to sound velocity discrepancies, the P-wave velocity (V_p) of liquid Fe measured by shock-wave experiments is lower than that of the OC, and both V_p and S-wave velocity (V_s) of solid Fe are significantly higher than those of the IC,

even after correcting for the anticipated velocity depression from high temperatures (see Figure 19). Therefore, it is widely accepted that the incorporation of light elements in the core mitigates the density deficit and sound velocity discrepancies. The leading candidates for alloying light elements include S, Si, C, O, and H. However, the identity and abundance of the dominant light alloying elements are still actively debated, largely due to experimental difficulties in precisely measuring the properties of Fe-rich alloys and liquids under core conditions and our lack of understanding of Earth accretion and core formation history.

Recent advances in high-pressure and synchrotron techniques have permitted both static and dynamic pressure experiments on crystalline iron alloys under P-T conditions found at Earth's center. Numerous static and dynamic studies have reported high-pressure density and sound velocity of solid-iron-based, light-element-containing

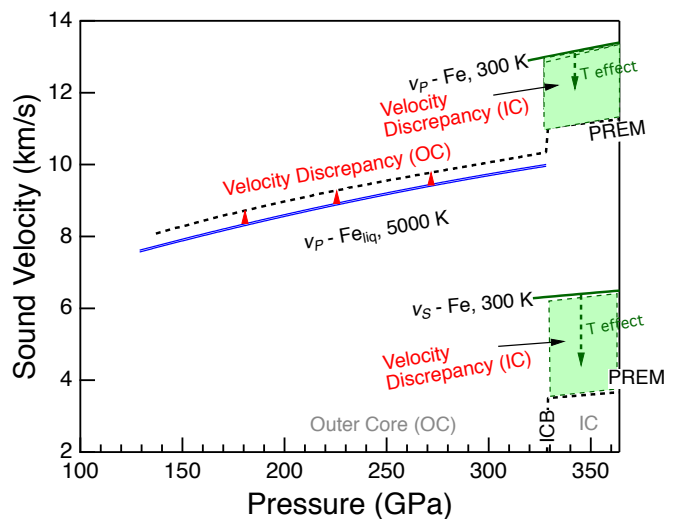
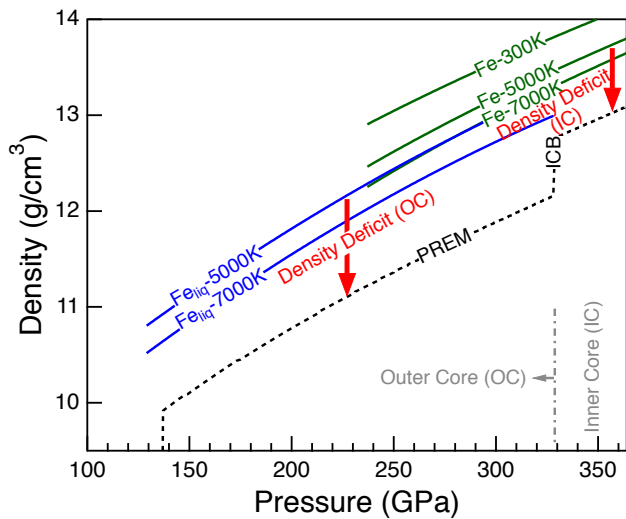


FIGURE 18. Comparison of density and sound velocity of solid and liquid Fe with PREM values. Figure courtesy of B. Chen (University of Hawaii)

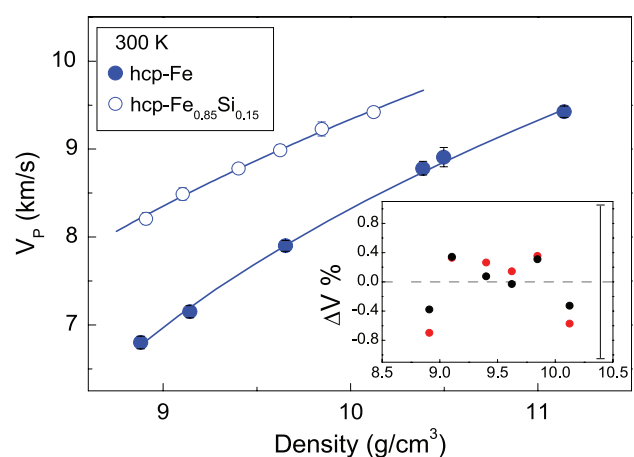
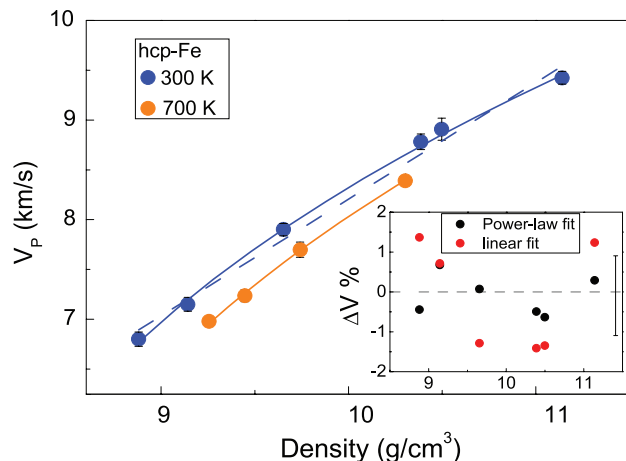


FIGURE 19. Effect of pressure and temperature on iron and iron-silicon. The nonlinear behavior is a test of the extent of validity of Birch's law. From Mao et al. (2012)

alloys and liquids as candidate components for the solid IC and liquid OC, respectively. High P-T laboratory investigations of the elastic and viscoelastic properties of candidate iron-light-element alloys and liquids serve as fundamental input to constrain the identity and abundance of light elements.

The studies of iron have been extended to Fe-Si and Fe-C, Fe-Ni alloys using synchrotron techniques such as momentum-resolved inelastic X-ray scattering. Compressional sound velocity phonons are measured directly from powder samples at pressures exceeding one megabar and temperature up to 1000 K, using external heating. Despite reduced signal intensity, the validity of Birch's law (a linear relationship of the compressional velocity of a suite of rocks and minerals with density) can be tested under extreme pressures and temperatures.

The richness of the vibrational properties that are revealed through nuclear resonant inelastic X-ray scattering (NRIXS) experiments can be fully exploited to derive quantities such as the thermal expansion coefficient, vibrational entropy, shear and compressional sound velocity, and iron isotope fractionation. Accessing this information at extreme pressures and temperatures exceeding 2 Mbar and 3000 K on a routine basis has the potential to provide further constraints on terrestrial cores. Current achievements include development of a new method of determining melting (Figure 20) with reduced uncertainty of ± 100 K and measurement of the thermal expansion coefficient and Grüneisen parameter at pressures up to 1.7 Mbar.

Compared with experimental data on the physical properties of crystalline iron alloys, there is a remarkable lack of data on the elastic and viscoelastic properties of iron-rich liquids due to experimental challenges. Liquid properties are usually investigated at pressures under 10 GPa, far below expected OC conditions, and only cover less than

one-tenth of pressures found at the top of the OC. This lack of data on iron-rich liquids and great challenges facing experimental investigation under relevant conditions at Earth's core are expected to continue into the foreseeable future. The most promising approach to establishing a systematic data set on density, sound velocity, viscosity, and structure of iron-rich liquids in previously unexplored regions of pressure, temperature, and composition space involves robust lower-pressure experiments combined with exploratory advanced experiments supported by computational simulations up to core conditions. The systematic high-accuracy, low-pressure data will be used to benchmark and validate the reliability of the theoretical predictions, and high pressure-temperature calculations will be used to estimate and predict the liquid properties under core conditions where experiments are extremely difficult and data are sparse. Such methodology significantly reduces errors introduced in long extrapolations. The liquid properties determined from both experiments and computations will allow stringent tests of various composition models for the outer core.

The core density deficit, the difference between the inferred density of pure iron at core conditions and the seismically determined density of the outer core, is an important factor limiting concentration of allowable light elements such as C, S, and Si. It is likely that these elements, when mixed with Fe, or Fe-Ni alloys, comprise the geochemical model of the inner core. The current debate about the extent of core density deficit is tied to our limited knowledge of the (1) melting point of iron and its alloys at those pressures, (2) thermal expansion coefficient, (3) thermal pressure, (4) sound velocities of candidate alloys (Figure 21), and (5) effect of temperature on the electronic contribution to vibrational entropy, among others. A combination of two separate inelastic X-ray scattering (IXS)

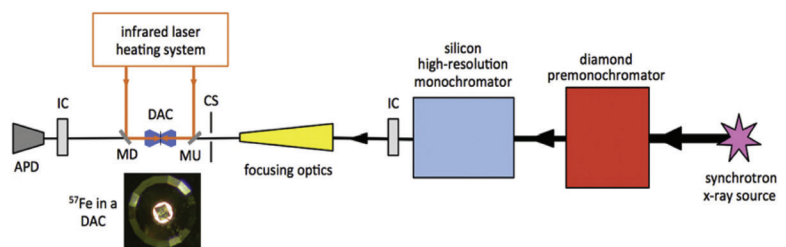
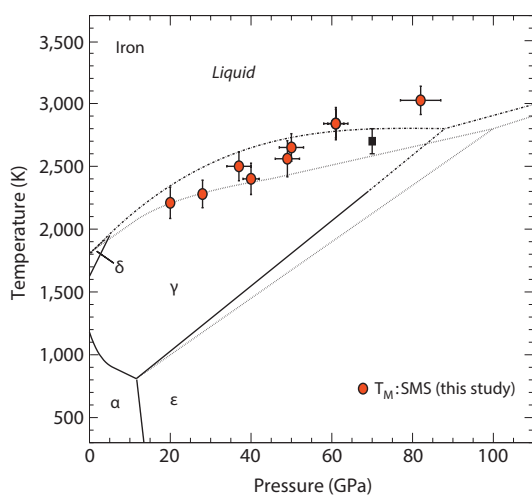


FIGURE 20. (left) Melting of iron at high pressures using synchrotron Mössbauer spectroscopy and (top) the associated setup for melting experiments at sector 3-ID-B of the Advanced Photon Source. The 14.4 keV X-rays are monochromatized to a bandwidth of 1 meV using a high-resolution silicon monochromator. The sample is in a water-cooled diamond anvil cell (DAC). An infrared laser fast temperature readout spectrometer and associated optics are located above the sample area. Delayed photons are collected by an avalanche photodiode detector (APD). Figures from Jackson et al. (2013), reproduced with publisher's permission

techniques (HERIX and NRIXS) addresses these questions, and it is likely that it will do so with more rigor in the future. Measurements of Debye, compressional, and shear sound velocities; thermal expansion coefficient as determined by slope of vibrational entropy (via phonon density of states) with volume; and melting point using synchrotron Mössbauer spectroscopy (SMS) through accurate determination of recoil-free fraction all contribute toward solving the core density deficit problem.

Iron Isotope Fractionation

Did core formation fractionate isotopic ratios, in particular, those of Si and/or Fe? Terrestrial basalts have non-chondritic Fe isotopic compositions, and Si isotopes have a BSE value that is non-chondritic, which could reflect partitioning of these elements into the core. It has long been thought that pressure was not a variable that could alter isotopic ratios, and that isotopic fractionations would be

negligible at high temperature. However, recent work at both high pressure and temperature has proven both of these statements to be wrong. To understand the extents to which Si and Fe are fractionated isotopically between metal and silicate, the isotopic ratios in each phase must be measured with reasonable accuracy. At high pressure, this is difficult as there is not enough material to measure, and proving isotopic equilibrium is challenging. However, recently, NRIXS has made this measurement feasible by either determining the force constant or using kinetic energy derived from measured phonon density of states. The isotopic ratios are directly comparable to the measured force constants so that phases can now be probed for their isotopic ratios at high pressure. Furthermore, the issues surrounding the accuracy of such measurements have recently been addressed, paving the way for more systematic studies under high pressure and temperature conditions in the near future.

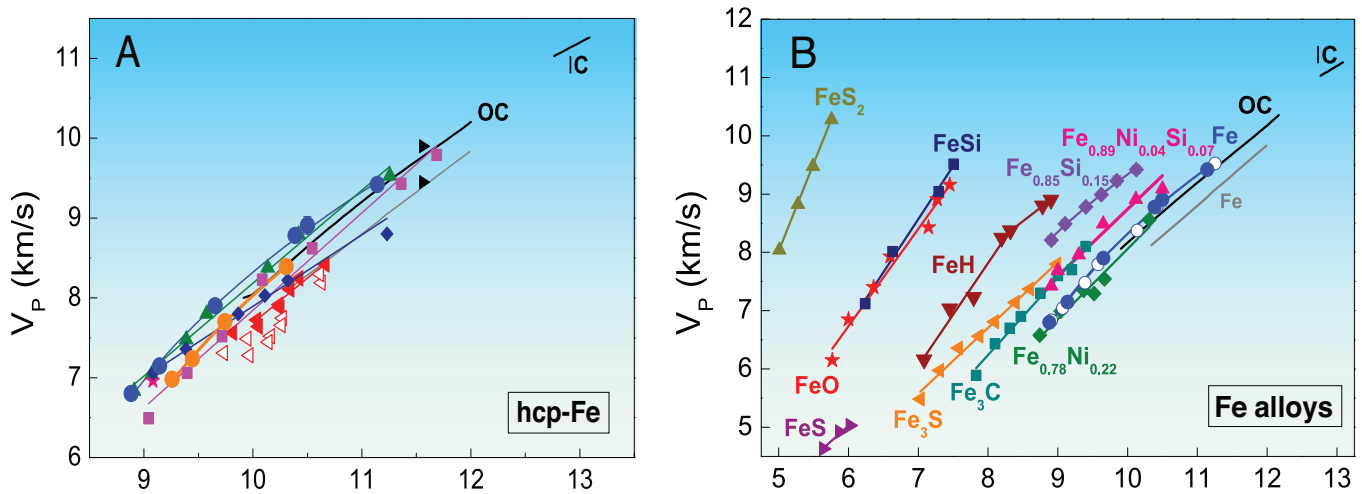


FIGURE 21. Compressional sound velocity of (A) iron and (B) various iron alloys in the pressure range of Earth's core. From Mao et al. (2012)

5. Experimental Technology and Infrastructure

Many significant innovations in mineral physics experimental techniques are enabled by the ability to produce starting samples, process quench products, or modify the pressure-generating device with the use of advanced fabrication techniques and instrumentation. The samples are in most cases extremely small, often much smaller than the thickness of a human hair. Many experiments that are capable of retrieving valuable information about sample properties rely on knowledge and control of sample geometry and surroundings on a micron, or even submicron, scale. Major advances in this area have been made in the last decade. In the multi-anvil press, standardized cell assemblies have been designed and made available through COMPRES, allowing a wide range of new laboratories to quickly come up to speed with their in-house multi-anvil infrastructure. Thermal gradients have been reduced through modeling and experimentation, and cells with large sample volumes have been developed for sample synthesis. In the diamond anvil cell, various innovations in double-sided laser heating with shaped laser beams and pulse control have improved the stability and uniformity of temperature, allowed pressure and sample diffraction to be measured more reliably at the hotspot, and enabled access to much higher temperature regimes than previously possible. The quality of high-pressure, room-temperature equation of state measurements has vastly improved with the development of the GSECARS/COMPRES gas-loading system. The routine loading of soft noble gases such as helium and neon, has reduced the degree of nonhydrostaticity, leading to more accurate and precise measurements of bulk moduli for mantle and core materials.

5.1. HEATING TECHNIQUES

In general, there are two main methods for generating high temperatures in the DAC at high pressures: laser heating and electrical resistive heating. Laser heating typically uses infrared lasers and directs the laser down the compression direction of the DAC. Laser heating is effective at generating temperatures up to 6000 K, but suffers from axial and radial temperature gradients. Advances, such as double-sided heating and beam-shaping optics producing flat-topped beam profiles, have led to great improvements in reducing

temperature gradients in the DAC, however, even currently achievable gradients are still quite substantial. Furthermore, fine temperature control is difficult to achieve with laser heating, and reliable measurements of temperatures below ~1100 K are challenging. Electrical resistive heating has the advantages of thermal stability and uniform temperature within the sample chamber. Previously, this technique was limited to temperatures below 1100 K, however, recent advances using graphite foil resistance heaters have pushed the achievable temperature range to nearly 2000 K. The main drawbacks to this technique are the tedious nature of building the foil heater assembly and inconsistent heater performance (i.e., power-temperature relationship) due to the fact that each heater is made individually. Computer numerical control (CNC) machining has been used successfully to fabricate ring-shaped graphite heaters that exhibit a high degree of consistency in heater performance. Simplification and standardization of graphite resistance heating parts, similar to what has been done for multi-anvil cell assemblies, will allow broader use of this technique in the mineral physics community. These advances have the potential to open doors for robust and reproducible resistive heating studies in temperature regimes that used to be accessible only through laser heating, improve our ability to accurately measure P-V-T equations of state, and allow high P-T deformation experiments to be conducted using radial diffraction in the diamond anvil cell. Coupling high-temperature graphite resistance heating with microfabrication techniques to create diffusion couples will potentially allow measurement of diffusion coefficients through the entire pressure range of Earth (Figure 22).

Fabrication of controlled-geometry samples for laser-heated diamond anvil cell experiments using nanofabrication techniques and facilities, though already noticeably successful, is still in its infancy, with room to grow and advance (Figure 23). Using a combination of deposition, photolithography, etching, and sample recovery, “double hot-plate” samples of metals and oxides have recently been fabricated for equation of state studies. These techniques, in conjunction with chemical-vapor deposition (CVD) diamond growth, can also allow for creation of “designer” diamond anvils with the capability of measuring magnetic and electrical transport properties at

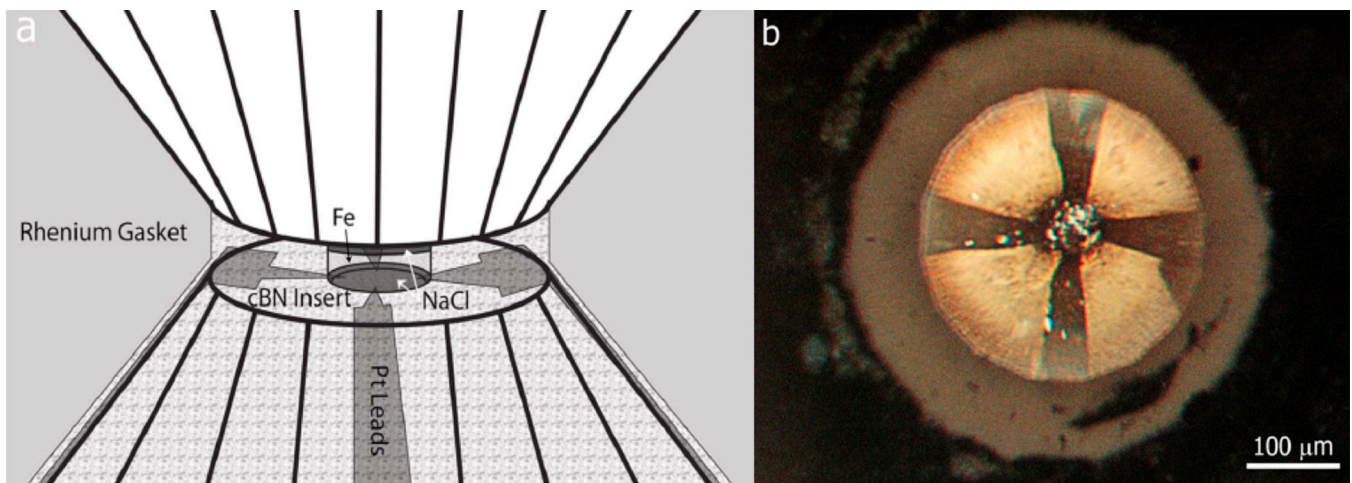
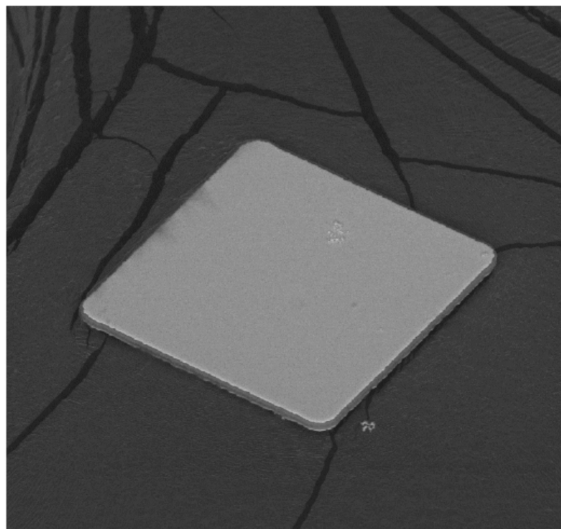


FIGURE 22. Schematic (left) and photograph (right) of a designer anvil with deposited platinum electrodes. From Seagle et al. (2013), reproduced with publisher's permission



| | | | | | |
|----------|---------|--------|------|------|--------|
| HV | WD | HFW | det | spot | 40 μm |
| 15.00 kV | 18.1 mm | 124 μm | BSED | 4.0 | SEMCAL |

FIGURE 23. Ni/SiO₂/Ni double hot-plate sample for use in a laser-heated diamond anvil cell. The Ni layers are 200 nm thick and the SiO₂ layer is 1 μm thick. This is one of ~10,000 identical samples that were fabricated using sputtering, photolithography, and etching. Figure courtesy of J. Pigott (The Ohio State University)

core pressures. When combined with laser and FIB milling, samples with more complex, Earth-like compositions can be created. Deposition and photolithography can also be used to deposit thermocouples for both diamond anvil cell and multi-anvil cell experiments. FIB technology coupled with nanofabrication capabilities will play a pivotal role in making near-term scientific advances such as quantifying the thermal conductivity of iron and iron alloys at core conditions. Additionally, easier access to a FIB and electron microscopy centers will permit detailed studies of the partitioning of elements between lower mantle phases, silicates, and iron, and liquid and solid iron.

5.2. MICROFABRICATION

Increased collaboration between the mineral physics and materials science communities has led to the incorporation of FIB technology into high-pressure geoscience research. FIB technology provides very unique advantages in the quest to address key questions in deep Earth research. The spatial resolution and milling capabilities are especially suited to the dimensions of samples that are encountered in DAC experiments. FIB samples can be used in complementary analytical techniques, such as transmission electron microscopy, energy dispersive spectroscopy, and X-ray fluorescence, for studies of element partitioning and diffusion.

In addition to the suite of possible analyses that can be performed on slices made with a FIB, procedures have been developed for fabrication of samples specifically tuned to high-pressure experiments. Trenches have been milled to contain metal samples, and single crystals can be cut, polished, and oriented for Brillouin spectroscopy. The use of a FIB in sample preparation opens doors for fabrication of natural and synthetic single crystals with a wide range of compositions. Furthermore, manufacturing of tailored bicrystals for the study of interfaces and grain boundaries should be possible. Thus far, the mineral physics community has broadly relied upon access to facilities that house FIBs, often in materials science departments. A FIB devoted to high-pressure research and widely available to the COMPRES community will lead to the scientific and technical advances needed to move the field forward in the next decade. The community would greatly benefit from easy access to a user-based FIB with a dedicated technician located at or near a synchrotron beamline for post-experimental analysis and pre-experiment fabrication.

5.3. LARGE-VOLUME PRESS TECHNIQUES

For a number of years there has been a well-recognized need and desire for an openly accessible multi-anvil press that would provide large-volume synthesis of materials and samples at very high tonnages. A press with large tooling for large anvils that allows concomitant increases in the size of pressure media, furnaces, and samples would open new possibilities for the US high-pressure community. Synthesis of large samples of well-characterized high-pressure phases for distribution throughout the community would become possible and would permit direct interlaboratory comparison of results, improve the reliability of the results, and open new research opportunities for laboratories that have been sample-limited. Another application would be creating large nano-polycrystalline diamonds for use as larger and tougher anvils for diamond anvil cells. This type of novel anvil has been used with amazing success in Japan and Europe to extend the pressure range accessible to both diamond anvils as well as large-volume press experiments. A third example application is growing large single crystals of high-pressure phases, which makes an array of new property measurements possible, such as single-crystal neutron diffraction, ultrasonic sound velocities, and direction-dependent rheological properties.

The extension of in situ multi-anvil techniques to higher pressures, up to 60 GPa or even up to a megabar (100 GPa), is a longstanding goal in the United States that is now attainable with a concerted community effort. The use of a six-axis press, with the force on each axis independently controllable and with a set of eight sintered diamond anvils inside, provides the uniform force environment that is necessary to achieve these pressures. The pressures are so high that many phenomena will not be quenchable, thus this press would be best utilized at a beamline. This approach would make the study of Earth materials under extreme pressures and highly stable and uniform temperatures possible. Also, the device would form a better bridge between the diamond anvil cell and multi-anvil cell methods, enabling better data consistency verification and improving the overall accuracy of pressure and temperature measurements as applied to Earth. Extending the pressure range of multi-anvil cell experiments together with improvements in laser and resistance heating for diamond anvil cell experiments can lead to a full, accurate description of the thermal equations of state of lower mantle and core phases. This is essential for accurate compositional, elastic, and rheological models of Earth's interior. Additionally, the accessibility of a high-tonnage press for sample synthesis can expand the compositional

space of samples, allowing, for example, for thermal equation of state measurements as a function of Fe and Al content for bridgmanite, ferropericlase, and calcium-silicate perovskite. Constraining the modal percent of each phase is important for quantifying the amount of heat-producing elements in the lower mantle.

The availability of well-characterized starting materials is critical to the experimental attainment of Earth mantle assemblages. Mineral physics laboratories are limited to obtaining samples from existing chemical companies (which do not cater specifically to the research community) or to synthesizing their own more complex samples, which can differ markedly from samples of other laboratories. The mineral physics community should think very carefully about the possibility of creating a centralized sample synthesis facility to address sample availability issues. Silicate and oxide samples produced by gel synthesis and oxide mixing techniques, with controlled oxygen fugacity furnaces and glassmaking facilities (high-temperature splat-quench and levitation techniques), would greatly benefit the community. Ideally, this facility would also contain instruments (i.e., sputter tool, contact aligner, plasma etcher) needed to generate nanofabricated metal and oxide samples. A facility dedicated to mineral physics synthesis could be contained at a single site or consist of a coordinated network of facilities hosted at multiple institutions. The production of community-wide samples could result in reproducible data and promote "round-robin" projects where multiple laboratories or beamlines work on samples from a common source (the olivine elasticity round-robin being a notable recent example).

5.4. NEUTRON DIFFRACTION

Another area of mineral physics research that has advanced significantly in the last few years is neutron diffraction. Neutrons have unique capabilities compared to synchrotron X-rays when applied to in situ, high-pressure experiments. For example, neutrons allow probing of magnetic structures, discrimination between isotopes, and investigation of the structure of light elements such as hydrogen. One major reason that neutron diffraction is not more widely adopted by the mineral physics community is the low attenuation of neutrons, which necessitates relatively large sample volumes. Recently, a large-volume diamond anvil cell was constructed that allows measurements of the compression behavior of D₂O ice to pressures above 90 GPa. These types of large-volume diamond anvil cells require large anvils. Natural diamond is prohibitively expensive, however, large synthetic diamonds grown by CVD can be economically feasible. Production of large

CVD diamonds would allow for neutron diffraction at high pressures, facilitating studies of light elements at high pressure and temperature.

5.5. DYNAMIC COMPRESSION

Impact phenomena and shock processes are of major importance in geophysics and planetary science. Studies of equations of state, phase transformations, melting, strength, and other phenomena at high dynamic pressure have long played an important role in understanding the composition and physical state of the interior of Earth and other planets. Dynamic compression studies also uniquely provide the capability to study impact and cratering processes that are so important in planetary formation and evolution. Laboratory shock experiments have traditionally been carried out by high-velocity plate impact using powder or light gas guns. More recently, new techniques for the generation of shock waves using lasers or pulsed power systems have been developed. Taken together, these methods are now capable of producing loading durations ranging from nanoseconds (lasers) to microseconds (guns).

Dynamic compression techniques can often achieve substantially higher pressures than static techniques, but shock waves are inevitably associated with entropy production and consequent heating. Ramp compression is a new technique that results in lower temperatures and allows higher states of compression to be achieved under dynamic loading. Both shock and ramp loading involve many orders of magnitude higher strain rates than static compression.

In recent years, new experimental facilities and techniques in dynamic high-pressure science have emerged (e.g., **Figure 24**). They have enabled experiments to be conducted at extreme pressures corresponding to those of the deep interiors of giant planets, and conditions of large-scale planetary impacts to be reproduced. New synchrotron and free electron laser facilities are providing access to high brightness X-ray sources, which enable novel in situ probing of the complex structural and rheological response of geological and planetary materials. Key characteristics of existing and developing facilities in the United States are provided below.

The Omega laser at the University of Rochester and the National Ignition Facility at Lawrence Livermore National



FIGURE 24. Experimental sample chamber at the Matter in Extreme Conditions beamline of the Linear Coherent Light Source. From https://portal.slac.stanford.edu/sites/lcls_public/Instruments/mec/Pages/default.aspx

Laboratory are able to deliver kilojoules to megajoules of laser energy onto millimeter-sized targets for up to ~10 nanosecond durations. At Omega, the typical pressures investigated by shock or ramp loading techniques range from 100–1000 GPa, and samples can be probed with in situ, time-resolved X-ray diffraction. Recent advances emerging from this facility include the first experimental determination of the rock salt-to-cesium chloride phase transition in magnesium oxide under shock and ramp loading. The National Ignition Facility has the potential to reach multiterapascal pressures in geological materials, as recently demonstrated by a ramp compression study of diamond to 5 TPa, a pressure corresponding to that inside Jupiter’s core.

The Z machine at Sandia National Laboratory is a pulsed power system capable of producing shaped current pulses and induced magnetic fields that can be used to generate pressures above 600 GPa or to accelerate flyer plates to tens of kilometers per second. The loading time scale for Z experiments is up to hundreds of nanoseconds. Recently, Z has been used to study impact vaporization of iron up to ~500 GPa, which has applications to understanding the response of planetary cores to high-velocity impacts at the late stages of planetary accretion.

The Linear Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center is a hard X-ray free electron laser (FEL) that provides unprecedented X-ray brightness. The LCLS can deliver monochromatic photons tunable up to 11 keV with ~100 femtosecond pulses producing 10^{12} – 10^{13} photons per pulse. At the Materials in Extreme

Conditions (MEC) beamline, samples may be dynamically compressed using pulses from a Nd-YAG laser system focused to a diameter of ~200–400 micrometers (Figure 24). The facility enables the study of dynamics of phase transitions and other phenomena in geological materials from ~10 GPa up to multimegabar pressures.

The Dynamic Compression Sector (DCS) is a new user facility dedicated to dynamic compression of condensed matter at the Advanced Photon Source, Argonne National Laboratory (Figure 25). The facility enables time-dependent changes under dynamic compression to be studied at peak stresses from ~5 GPa to over 200 GPa and at time durations ranging from tens of nanoseconds to microseconds. The focus is on time-resolved, in situ X-ray diffraction and imaging measurements. Loading platforms at the DCS will include both conventional guns (powder and light gas) as well as a high-powered laser. The coupling of dynamic compression with high-brightness, high-energy, tunable X-rays at a premier synchrotron facility will provide important new capabilities for carrying out crystallographic measurements under in situ conditions and for directly imaging ongoing deformation processes in real time. The integration of synchrotron and free electron laser X-ray sources with dynamic loading platforms provides novel capabilities to record a sequence of diffraction patterns or spatially resolved images during dynamic events. This is a major advance over existing dynamic techniques that are limited to indirect observations of surface wave profiles or samples recovered after release from high pressure.

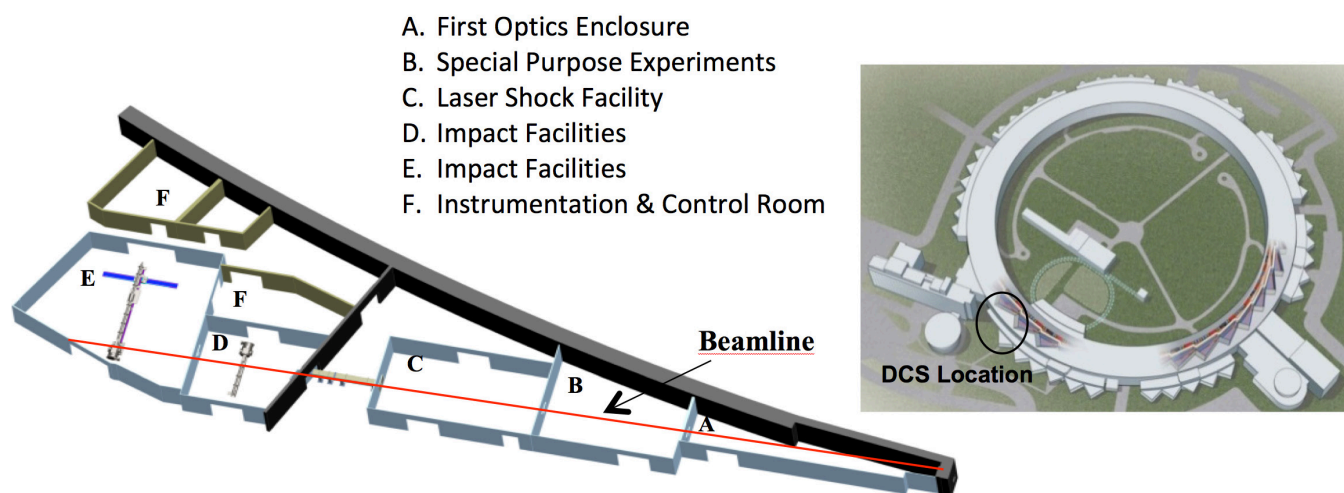


FIGURE 25. Overview of the Dynamic Compression Sector of the Advanced Photon Source. *Figure courtesy of DCS*

5.6. COUPLING HIGH-PRESSURE CELLS WITH ENERGETIC ION BEAMS

Relativistic heavy ion beams provide a unique means of accessing physical regimes far from thermodynamic equilibrium. Heavy ions deposit substantial quantities of kinetic energy (up to several GeV) into nanometer-sized volumes of a material within an exceedingly short interaction time (sub-femtosecond), which results in extremely high energy densities (up to tens of eV/atom). These ion-matter interactions can result in novel kinetic pathways through equilibrium and non-equilibrium states that trigger complex structural modifications within highly localized damage zones. In a recently developed approach, this highly ionizing radiation was combined with pressure by irradiating pressurized samples in a DAC with relativistic projectiles produced by one of the world's largest ion accelerators. The use of such high ion beam energies is essential because ions are first required to traverse a millimeter-thick diamond anvil (of a DAC) before reaching the pressurized

sample. Over the past decade, experimental protocols of this type have been continuously developed to routinely expose samples to static pressures up to 1 Mbar, and ion fluences up to 1×10^{13} ions/cm². High temperatures of up to 500°C have also been incorporated into these experiments through the use of resistive heating (**Figure 26**).

The coupling of extreme energy deposition from swift heavy ions with high pressure and temperature leads to exciting applications at the interfaces of materials research, nuclear science, and geoscience. This experimental approach can be used to study the behavior of materials under extreme conditions, form and stabilize novel phases, manipulate the physical and chemical properties of solids at the nanoscale, and investigate the effects of radioactive decay events on compressed and heated minerals from Earth's interior (e.g., nanoscale simulations of fission-track formation under crustal conditions and phase transitions of radiation-damaged minerals resulting from meteorite impact).

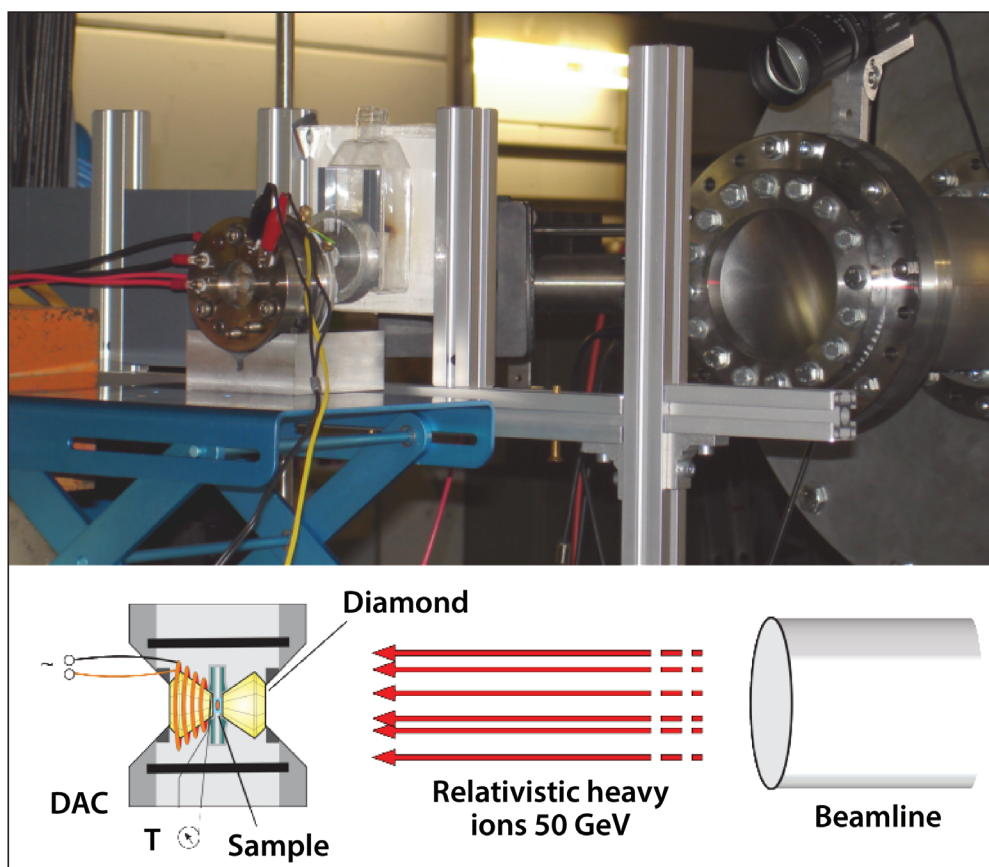


FIGURE 26. Photo (top) and schematic (bottom) of the experimental setup for exposing pressurized heated samples in a DAC to a beam of relativistic ions. Typical ion projectiles are ²³⁸U, ²⁰⁷Pb, and ¹⁹⁷Au with kinetic energies of about 50 GeV. For the irradiation, the DAC is placed in air, 45 cm behind the beamline window. *Figure courtesy of M. Lang (University of Tennessee, Knoxville)*

6. Cyberinfrastructure and Information Sharing

One of main factors that has shaped how scientific investigations are conducted today compared to a decade ago is the ease of access and exchange of data, information, and resources enabled by cyberinfrastructure and the Internet. Researchers in the mineral physics community rely on, and take advantage of, these resources in almost every single step of their work. Mineral physicists need to grapple with three issues related to cyberinfrastructure.

Key questions include:

- How can we most efficiently retrieve information and interpret experimental data?
- How do we bridge the gap between experiments and computer simulations?
- How do we share data within and outside the mineral physics community?

6.1. SOFTWARE FOR AUTOMATED DATA ANALYSIS

Synchrotron radiation user facilities are critical resources that enable state-of-the-art research and training in mineralogy, mineral physics, and environmental science. Access to these facilities is very competitive (scientific merit-based peer review process), and time allocated for experiments is always very constrained. Most beamlines at the synchrotron facilities are oversubscribed with experiment proposals at 200–300% with respect to available beam time. Investments in cyberinfrastructure that increase the ease, efficiency, and reliability of the experiments will maximize the benefit of the beam time to the scientific community, may decrease the amount of time necessary to conduct the projects, and enable future experiments that are impossible today.

The most popular and fundamental type of experiments conducted at synchrotrons is X-ray diffraction, which produces detailed information about crystal structure, symmetry, chemical bonding, and density of minerals and other crystalline solids. Modern synchrotron-based diffraction experiments are typically conducted using area detectors, where the data are recorded in the form of digital diffraction images. Data analysis software that enables efficient and reliable processing of these digital images is a critical component, allowing retrieval of mineralogical information

from experiments. Most non-diffraction experiments such as inelastic X-ray scattering have an even more dire need for development of reliable, automated, and easy-to-use data analysis software, because they are more specialized and have a smaller community of potential code developers.

Ongoing upgrades and construction of state-of-the-art large-scale user facilities in conjunction with the rapid development of new experimental capabilities have led to unprecedented accumulation of data during experiments. Over the past decade, the collected data per experimental run increased from a few hundred megabytes per day to as much as several terabytes. We can now measure phenomena at temporal and environmental conditions that have previously been unreachable. However, the lack of tools to inspect and evaluate the collected data at close to real time imposes severe limitations on the planning of measurement strategies. The growth in the amount of data and the increasing data rates pose a significant challenge for analysis, but also open unique opportunities to the scientific community. There is a well-defined and strongly pronounced need for collaborative development of well-documented reusable open source software libraries for automated data analysis. Community organizations such as COMPRES provide a perfect framework for coordinating such efforts and assuring their sustainability.

The increasing amount of published data in our field opens new opportunities for data mining, rediscovery (re-analysis of legacy data with new software tools and algorithms), and statistics-based research if the data and metadata are shared in a consistent manner. One of the most successful examples of the impact of mined data and data sharing in the mineral physics community is the development of effective ionic radii by Shannon and Prewitt (1969). The article has been cited over 6800 times and standardized the evaluation of changes in crystal structures.

6.2. FIRST PRINCIPLES COMPUTATIONS

First principles quantum theories facilitate all of the mineral physics research discussed above. Recent computational innovations include capabilities to model electronic, liquid, and thermoelastic properties of mantle minerals,

and the development of algorithms that can identify new polymorphs. These calculations fill critical gaps in our systematic mineral physics knowledge database and provide means to develop a more complete understanding of atomic-scale processes that control high-pressure structural, electronic, and thermodynamic phenomena. Indeed, these results often inspire experimentalists to go in new directions and look for experimental verifications of daring theoretical predictions. Examples include determination of the post-perovskite structure, prediction of a larger-than-expected thermal conductivity of liquid iron, prediction of spin transitions in iron-bearing mantle minerals, description of defect structures and storage capacity of volatiles in mantle minerals (**Figure 27**), extension of melting temperatures beyond experimental reach, and description of the structural evolution of melts with pressure and temperature in an early magma ocean.

To broaden the scope of first principles calculations to facilitate new discoveries requires increasing access to these tools to a larger community of mineral physicists and increasing the computational capacity of the community to address larger and more complex systems. Increased access can be facilitated by improving the knowledge base of our graduate students and postdocs through workshops and short-term visits, and by improving the usability of these codes for those without a strong background in computational details and the approximations involved in the quantum mechanical calculations.

Larger calculations, calculations with a large number of configurations, and calculations that include dynamic processes such as deformation, diffusion, melting, and liquid

properties require as much as a processor-year of supercomputer time. Increased computational resources, including dedicated supercomputer time for mineral physics research, will expand the reach of computationally based discoveries.

Although software for performing first principles calculation is widely accessible, researchers without strong backgrounds in quantum mechanics and computational experience find it challenging to use these tools. Efforts such as the Virtual Laboratory for Earth and Planetary Materials (VLab) are being pursued to bridge this gap, make computational tools more accessible to experimenters, and leverage the aggregated computational power of grid systems to solve intrinsically high-throughput problems that had been practically intractable in materials computations for Earth and planetary sciences applications. For example, VLab provides an easily accessible and user-friendly Internet launch pad for these complex distributed calculations (**Figure 28**). The development of workflows for high-throughput calculations and their deployment in the Internet transmuted VLab into a science gateway and opens great opportunities for seamlessly merging these computational capabilities into the future comprehensive mineral physics database.

6.3. DATA SHARING

Understanding Earth's inner workings (e.g., volcanism, plate tectonics, magnetism, volatile cycles) as well as surface mineralogy requires reliable petrologic models of the interior. Such models are derived from the information about bulk chemistry of the planet, high-pressure and

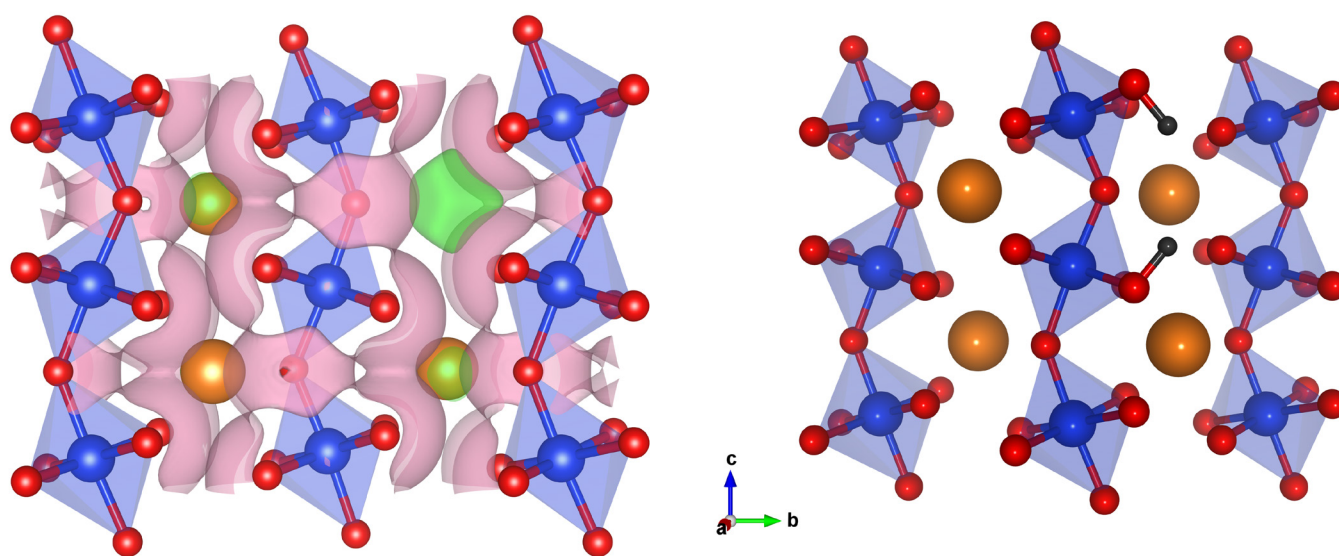


FIGURE 27. Predicted stable hydrogen defect structure of hydrous post-perovskite (hy-ppv) at 120 GPa. (left) View of electron isosurfaces of ppv with Mg-vacancy looking down the a-axis. Pink and green isosurfaces contour regions of high and low density, respectively. (right) Predicted hydrogen defect in ppv. Atom positions are shown as oxygen (red), silicon (blue), magnesium (orange), and hydrogen (black). *Figure courtesy of J. Townsend (Northwestern University)*

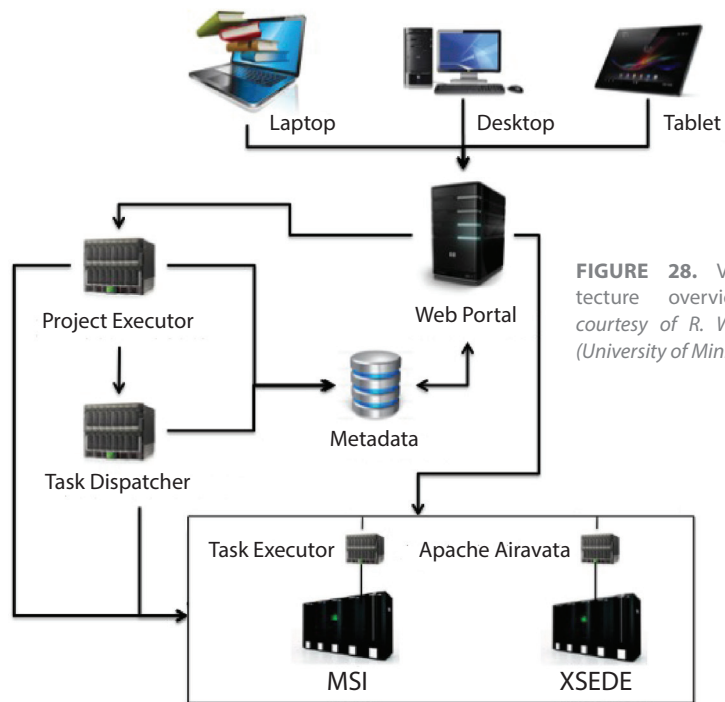


FIGURE 28. VLab architecture overview. *Figure courtesy of R. Wentzcovitch (University of Minnesota)*

high-temperature phase equilibria, and thermodynamic properties of the relevant mineral phases and solid solutions, constrained by geophysical observations. There already exists a range of excellent free academic software tools (e.g., *Perple_X*, *MELTS*) that permit researchers to carry out thermodynamic phase equilibria calculations and produce petrologic/mineralogic models that predict the dominant rock types as a function of depth and also provide information about acoustic wave velocity profiles that can be correlated with seismic observations. This software relies on the availability of comprehensive databases of thermochemical and elastic properties of relevant mineral phases. Such databases currently exist only as static compilations, are limited by the particular consistency criteria that their authors emphasized (e.g., thermodynamic constants that were chosen to best reproduce acoustic velocities for each mineral may not equally well reproduce phase equilibria), and do not offer proper ways of estimating the uncertainties of geophysical models.

There is an urgent need for an easily accessible, reliable, and critically evaluated online database of thermodynamic data that would be available to the mineral physics community, but more importantly, to other Earth science communities that are the major data consumers. Such a database would need to allow easy incorporation of new results coming out of mineral physics labs worldwide, and would define information and quality standards necessary to evaluate internal consistency as well as maintain interfaces with other knowledge databases (e.g., the petrology/geochemistry database *Library of Experimental Phase Relations* and the *American Mineralogist*

Crystal Structure Database).

In the last two decades there has been very rapid and dramatic development in experimental methodology. In addition, mineral physics experimental papers that report numerical data often have taken very different approaches, for example, in the variety of pressure and temperature reference scales used. These aspects make it very difficult for researchers from outside the field to understand and properly assess and use these data. A very important task related to creating a mineral physics database is to properly include this type of metadata, as well as assess and indicate the uncertainties and sources of errors that are not explicitly explained in the papers. To make such database truly comprehensive is a very large task that needs to be thoroughly planned and discussed by a panel of experts. It will require interfacing and close collaboration with community organizations and facilities such as *COMPRES*, *GSECARS*, and *HPCAT*. Efforts in this direction are currently under way, using testbed infrastructure, hosted by *IEDA*, an established and multidisciplinary data center facility. To be effective and widely used, the database will need to be easily and conveniently accessible online and include appropriate search and manipulation tools. A framework like *IEDA* can provide access to these features and include support of cyberinfrastructure experts to define and create new services. Within this endeavor, it will be critical to initiate outreach efforts to increase community involvement and build a consensus about data standards, formats, and critical database services/mechanisms, and prepare a case for a more comprehensive focused database development effort after completion of the current project.

7. Conclusions

The 2014 planning workshop and this report convey a picture of a very progressive and dynamic field that continues to benefit from significant technological innovations and breakthroughs, driving the science in new exciting directions. Mineral physics is intimately connected to, and relevant for, mainstream geophysics, petrology, and geochemistry, and has great potential for producing new materials that may satisfy some of most important technological needs of our society.

We are fortunate to have organizational framework at our disposal that enables strategic planning and investments in a widely shared and unique infrastructure. The majority of the new directions and opportunities identified in this report are worthwhile investments with a low-risk/high-reward ratio, but they require some capital equipment and a long-term commitment to focused development and stewardship. Well-established and tested resource management mechanisms provided by our community organizations assure that selection of investment priorities for the next decade will be conducted carefully and with the best interest of the whole scientific community at heart.

Investing in mineral physics is like opening a door to a new dimension of the universe. Explicit rewards are hard to predict, but the long-term benefit of gaining knowledge about how exactly nature harnesses extremes of pressure and temperature and how this information can help our society is potentially immense.

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Acronyms

| | |
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| APS..... | Advanced Photon Source |
| BSE | Bulk silicate Earth |
| COMPRES | Consortium for Materials Properties Research in Earth Sciences |
| CMB | Core-mantle boundary |
| CVD | Chemical-vapor deposition |
| DAC..... | Diamond anvil cell |
| DCS | Dynamic Compression Sector |
| ERDA | Elastic Recoil Detection Analysis |
| EoS | Equations of state |
| FIB | Focused ion beam |
| FTIR | Fourier transform infrared |
| GSECARS..... | GeoSoilEnviro Center for Advanced Radiation Sources |
| HERIX | High-resolution inelastic X-ray scattering instrument |
| HPCAT..... | High Pressure Collaborative Access Team |
| IEDA..... | Interdisciplinary Earth Data Alliance |
| IXS | Inelastic X-ray scattering |
| IC..... | Inner core |
| LCLS | Linear Coherent Light Source |
| LLSVP | Large low shear velocity province) |
| LPO | Lattice-preferred orientation |
| NDC | Nanodiamond composites |
| Nd-YAG | Neodymium-doped yttrium aluminum garnet |
| NRIXS | Nuclear resonant inelastic X-ray scattering |
| NSLS | National Synchrotron Light Source |
| OC | Outer core |
| ppv..... | Post-perovskite phase |
| PREM | Preliminary Reference Earth Model |
| PX ² | Partnership for eXtreme Xtallography |
| RDA..... | Rotational Drickamer apparatus |
| SIMS..... | Secondary ion mass spectrometry |
| SMS | Synchrotron Mössbauer spectroscopy |
| TZ | Transition zone |
| ULVZ..... | Ultra-low velocity zone |
| VLab..... | Virtual Laboratory for Earth and Planetary Materials |
| V_p | Compressional wave velocity |
| V_s | Shear wave velocity |

