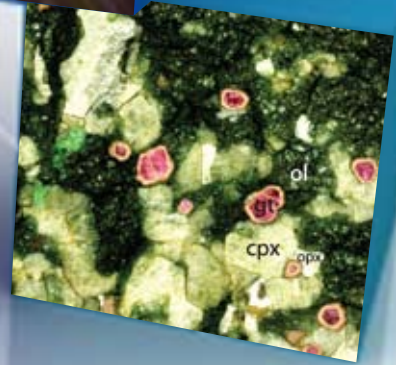
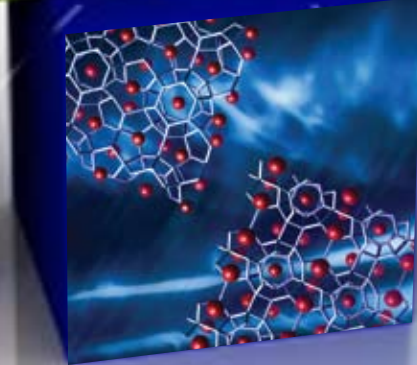
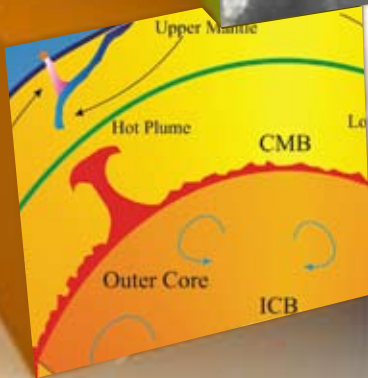
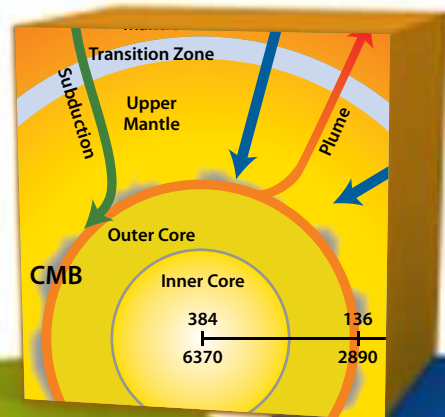


# Understanding the Building Blocks of the Planet

THE MATERIALS SCIENCE OF EARTH PROCESSES



Long-Range Planning for High-Pressure Geosciences Workshop

March 2-4, 2009, Tempe, Arizona



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This report is drawn from the many presentations and discussions at the Long-Range Planning for High-Pressure Geosciences (LRPHPG) Workshop held in Tempe, Arizona, on March 2–4, 2009. The workshop was attended by 87 members of the mineral physics and geophysics research communities from 39 institutions. Initial drafts of this report were openly available and the high-pressure geosciences community commented on them.

The participant list for the LRPHPG Workshop can be found at: [http://www.compres.us/index.php?option=com\\_content&task=view&id=97&Itemid=123](http://www.compres.us/index.php?option=com_content&task=view&id=97&Itemid=123)

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# Executive Summary

The field of high-pressure geosciences is dedicated to increasing our knowledge of the materials that make up the overwhelming majority of planet Earth—those that reside below the surface and are compressed by the overlying burden. It is from the interior that the planet's atmosphere and hydrosphere were originally degassed, and melting processes at depth created (and continue to create) our ocean basins and continents. Thus, the starting points for Earth's habitable environment—its atmosphere, its surface—originate from our planet's voluminous interior. The deep interior produces the forces that generate virtually all non-weather-related natural hazards: earthquakes, volcanic eruptions, and tsunamis. Its impact on the surface is, perhaps, best illustrated by the annihilation ~251 million years ago of ~90% of Earth's life due to the environmental consequences of a massive volcanic eruption whose outpourings covered a sizable fraction of Asia. In short, the planet's interior has been an integral and controlling influence on Earth's evolution—and its effects are dictated by the physical and chemical properties of the materials of the interior, which are the domain of the high-pressure geosciences.

The challenges associated with simulating Earth's interior through both experiment and theory are formidable. Probing and synthesizing materials at the conditions of the interior, which are critical for understanding the properties of materials at depth, require extraordinarily high pressures and temperatures. Correspondingly, state-of-the-art approaches are necessary to theoretically calculate material properties under these conditions. The high-pressure geosciences community has spearheaded the development of new techniques to probe materials at high pressures (and has seen its techniques adopted by a broad range of other scientific disciplines), deployed emergent technologies, including those developed

at national facilities, and conveyed this high-level expertise to new generations of students. From making better and larger diamonds to understanding the physical properties of hydrocarbon clathrates (which may make up the largest natural gas reservoirs of the planet), the high-pressure geosciences community has also played a key role in developing and understanding materials of direct societal importance—and particularly those materials that have required high pressures to manufacture.

A 2009 workshop on frontiers in high-pressure geosciences, funded by the National Science Foundation (NSF), considered promising research directions in this field over the next decade. This two-day workshop featured nine plenary talks and breakout discussion sessions on four themes:

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

Workshop participants reviewed the impact the field of high-pressure geosciences has had on other subdisciplines of the earth sciences, including seismology, geodynamics, and petrology. They also discussed the future of high-pressure geosciences: what are the next major breakthroughs of our community, and what infrastructure will be necessary to achieve them? This COMPRES workshop was the second one focusing on long-range plan for high-pressure earth sciences. The first, "A Vision for High-Pressure Earth and Planetary Sciences Research: The Planets from Surface to Center," was held on March 22–23, 2003 in Miami, Florida, and led to the 2004

Report on “Current and Future Research Directions in High-Pressure Mineral Physics ” (often called the Bass Report).

This report describes what the high-pressure geosciences community does, the broad rationales for the science done by the field, the technical developments that the discipline has made, and where the future directions of the field likely lie. Predicting the future is difficult for this vibrant and fast-moving field: the last decade has seen new and unexpected discoveries that have changed the views of the deep reaches of our planet, including the recognition of novel electronic and structural properties of Earth materials at the extreme conditions of the interior. With new and improved techniques and infrastructure, the community is poised over the next decade to continue to produce dramatic new discoveries and truly engender a profound understanding of the deep Earth’s critical role in producing our habitable planet.



# Chapter 1 | Introduction

When viewed from the perspective of Earth's interior, our planet is overlain by a vanishingly thin atmosphere, and covered by an ocean that is tiny relative to the massive rocky interior. Indeed, the habitable zone of the planet occupies only the thinnest of veneers at the surface of our planet—and, like all veneers, its existence and viability depend directly on what lies beneath. The discipline of *high-pressure geosciences* is concerned with the properties of the part of our planet that lies beneath the surface, of which almost none is accessible to direct sampling via drilling (which is able to scratch only the uppermost ~0.2% of the planet), and which is compressed to extraordinary pressures by the burden of many kilometers of overlying rocks. Why are geoscientists concerned with this vast yet inaccessible region? It is the deep materials of the planet that drive the flows that produce plate tectonics. Our ocean and atmosphere originated from degassing of the deep planet and they continue to be cycled through the interior, and the core-generated magnetic field protects our surface from energetic particle bombardment. In short, the habitable environment of Earth's surface is a direct consequence of phenomena directly associated with Earth's deep interior—indeed, it is not an exaggeration to say that our hydrosphere, and hence our biosphere, exists by permission of the planet's interior.

Beyond the importance of the interior to the evolution of the surface environment, the extreme pressure and temperature conditions within the planet give rise to a suite of phenomena that impact the dynamics and structure of the planet that can *only* be understood through high-pressure experiments and theory. Materials transform to far denser structures under the pressures and temperatures of the interior, including producing economically important compounds like diamond. The solid interior is able to flow, generating plate tectonics, our continents, and the topography of

the planet. Volcanism originating from deep within Earth is responsible for giant eruptions in Earth's history, including the massive volcanic outpourings in Siberia 251 million years ago that killed 95% of the planet's life and fundamentally changed the nature of the planet's biota. And, our deep interior likely contains far more water, carbon, and certainly sulfur than exists at Earth's surface. The exchange between the surface and interior reservoirs of volatile components fundamentally impacts our climate over short (as was seen late last century by the eruption of Mt. Pinatubo and the associated decline in planetary average temperature of about 1°C) and long time scales (as illustrated by our planet's likely fluctuations from largely iced over to temperate ~750 million years ago), and moderates the volume of our ocean.

Thus, the vast bulk of our planet has a profound effect on our surface environment. It is the principal goal of the high-pressure geosciences community to probe the properties and processes deep within our planet. The knowledge that is garnered from such studies of the interior has applicability across not only the geosciences, but also through much of the physical sciences. These impacts extend to the neighboring earth science disciplines of seismology, geodynamics, geomagnetism, and geochemistry, and also more broadly to materials science, condensed matter physics, and solid-state chemistry. For example, geoscientists are now able, using constraints on sound speeds in Earth materials, to interpret the images of wavespeed variations in Earth's interior generated by seismologists; the knowledge of how solid rock flows at extreme conditions is crucial for the geodynamic understanding of how our silicate mantle convects; and comprehensive studies of iron and its alloys at high pressures have illuminated the major driving forces for the magnetic-field-producing geodynamo of Earth's core. In short, the entire discipline of high-

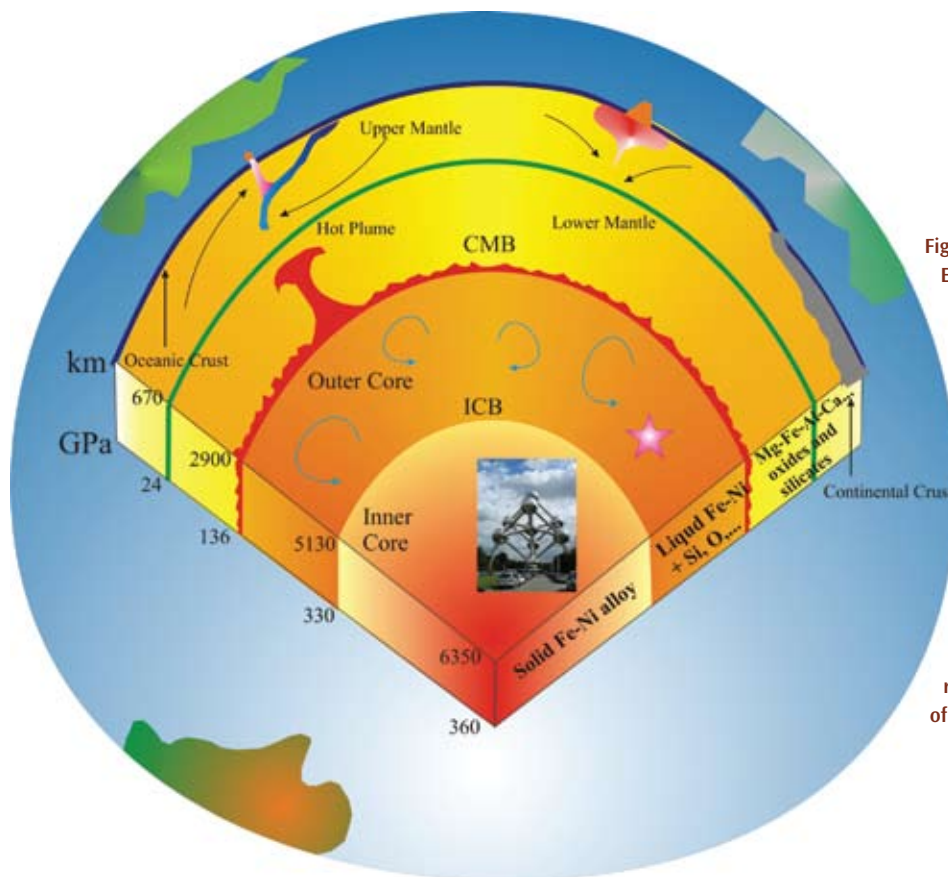


Figure 1.1. Schematic cross section of Earth's interior, illustrating compositions, depth ranges, and pressures of different layers. Dynamic features are also illustrated, including subducting ancient ocean floor (in blue), and upwelling plumes (in red). Inset illustrates the crystal structure of the phase of iron likely to be present in the inner core. Relevant temperatures at different depths are near 2000 K at the 670-km depth seismic discontinuity, 4000 K at the planet's core-mantle boundary (CMB), and roughly 6000 K at the center. Courtesy of J.F. Lin, University of Texas at Austin.

pressure geosciences is motivated by an overarching goal of understanding the ongoing physical and chemical evolution of our planet. Notably, the effects of the high-pressure geosciences community are not isolated within disciplines of the earth and planetary sciences. Many of the tools developed in the high-pressure geosciences to examine materials at extreme pressures have been adopted in wholesale fashion across the scientific community as *the* techniques for probing matter and synthesizing new materials at extreme conditions. Hence, the high-pressure geosciences community already exemplifies one of the primary recommendations of the 2009 NSF-GEO Vision Report: to “Reach out in bold new directions, engaging and incorporating other disciplines.”

Why have the experimental and theoretical techniques of the high-pressure geosciences community proven so valuable? Simply put, their measurements and calculations are extremely challenging, and high-pressure geoscientists have pushed the frontiers of technique development for synthesis

and characterization of materials at extreme conditions. The vast bulk of the planet is at enormously high pressures, and the goals of the community have been to not only create apparatuses that simulate the conditions of having tens, hundreds, and thousands of kilometers of rock piled on our samples as overburden (generally at extremely high temperatures), but also make meaningful measurements on samples under these conditions. Because pressure is force per unit area, pressures can be maximized by making samples small—in the high-pressure community, millimeter-sized samples are considered “large-volume”—and inferring the properties of a complex aggregate of materials (sometimes called rocks) at the multiple-micron scale under extreme conditions requires intense and often highly focused probes. Facilities at the Department of Energy's national laboratories have enabled microsamples to be examined with light ranging from x-rays to the far-infrared, as well as intense streams of neutrons. Alternatively, high-velocity bullets can be shot at

larger samples and the properties of the shock-compressed target measured very, very quickly, before the sample catastrophically decompresses. Here, the challenges are primarily related to the microsecond or less—and sometimes substantially less—time scales of the experiment. Finally, theoretical treatments of Earth materials require calculations on systems that are both chemically and structurally complex, and which often possess different structures that lie close in energy to one another. Hence, rigorous, accurate, and often very-large-scale theoretical calculations are required for the systems of interest in the high-pressure geosciences.

The high-pressure geosciences community has deployed its techniques to generate a broad suite of new and unanticipated results over the last decade that have both illuminated the processes and properties of materials that occur within the planet's interior, and provided insights into the

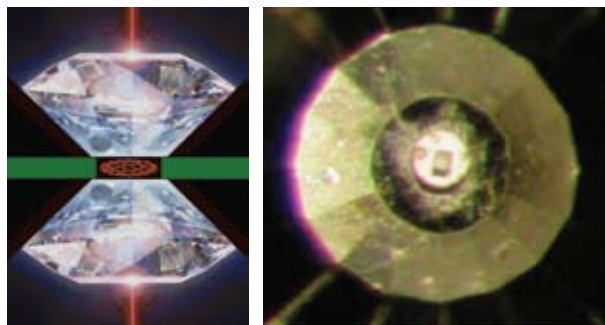


Figure 1.2 (left) Schematic of a diamond anvil cell. Two gem-quality diamonds are truncated at their tips, and compressed together at a metal gasket that contains a sample. The red vertical line illustrates that the sample can be optically accessed by visible light, or probed by lasers. Vertical scale of the picture is approximately 8 mm. This type of apparatus is capable of generating pressures that span most of the depth of the planet. Image courtesy of Hawaii Institute of Geophysics. (right) View along the axis of force through the diamonds of a sample (small blocks within the sample chamber, which is illuminated by transmitted light, filled with a transparent pressure medium, and surrounded by a metal gasket). Dimensions of the sample chamber are  $\sim 0.1$  mm. Image courtesy of J. Jackson, Caltech.

complex interactions between our surface environment and the deep planet. The community's recent achievements include:

- Discovered fundamental pressure-induced changes in the electronic properties of iron, one of our planet's most abundant elements; at extreme conditions, its electronic configuration shifts from high spin to low spin. This shift results in paradigm-changing effects on the density, seismic velocity, and viscosity of the materials in Earth's deep mantle.
- Constrained water and carbon sequestration deep within the planet, with relevance to the genesis of our planet's ocean, atmosphere, and climate.
- Identified a transition to a previously undiscovered "post-perovskite" phase at the deepest depths of our silicate mantle—a phase whose presence likely modulates the heat flow out of Earth's core and, hence, controls the energy that produces Earth's magnetic field.

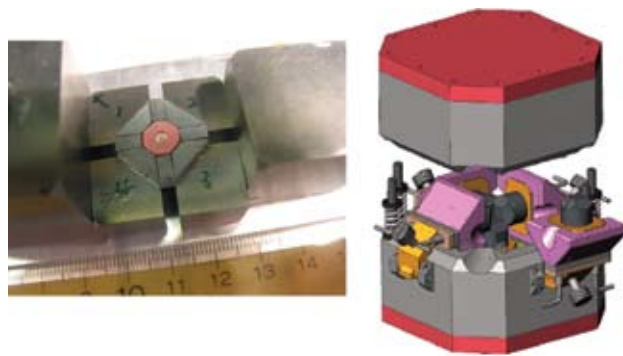


Figure 1.3. (left) Large-volume press assembly. The sample is contained within a furnace assembly at the center of the numbered tungsten carbide cubes; the diamond-shaped region is gasketing. A second set of cubes is oriented on top of the assembly prior to compression, and the resultant cubic apparatus is then hydraulically compressed. Dimensions across the edge of the blocks are  $\sim 3.5$  cm. Prior to compression, a second set of blocks is placed on top of the assembly. Such assemblies can routinely access conditions that correspond to  $\sim 700$ -km depth in the planet. One of the challenges for our community is to substantially extend the routine pressure range of this apparatus. Photo courtesy of Mineral Physics Institute, Stony Brook University. (right) Schematic of a recently designed large-volume press assembly (called D-DIA-30), designed particularly for deformation experiments at high pressures. The cubic assembly is inserted into the central portion of the apparatus, and controlled differential strains on the sample can be generated through independent motion of the hydraulic rams. Vertical dimension of the apparatus is approximately 1 m. Image courtesy of Y. Wang, University of Chicago.

- Determined the viscosity of solid rocks in situ at high pressures and temperatures, providing fundamental experimental constraints on the vigor of mantle convection and, hence, on plate tectonics itself.
- Established the chemical systematics necessary to recognize rocks from the deepest depths ever observed, followed rapidly by the discovery of such rocks.

One of the primary focuses of the high-pressure geosciences community lies in understanding the complex structures of Earth and planetary materials that occur at both moderate and extreme conditions. Such materials often have technologic uses or are valuable analogues for technologic materials and, therefore, the high-pressure geosciences community maintains a significant materials-oriented component. Recent economically relevant achievements include:

- Probed the properties of clathrates and hydrogen-rich materials. The former is likely one of the primary reservoirs of subsurface natural gas, and the latter have major implications for energy storage.
- Synthesized large diamonds at low pressure using chemical vapor deposition (CVD) technology. This accomplishment builds on the long-standing impact of our discipline on the synthesis of ultra-hard materials, which has had a profound effect on the industrial abrasives industry, and is the result of the need for large, pure, low-cost diamonds for high-pressure experiments. It will have applications for coatings, electronic devices, and many other industrial applications.
- Examined the capability of novel oxide structures as media for the long-term confinement of nuclear waste. The recognition that some minerals can effectively retain radionuclides for long periods is venerable, but characterizing the roles of chemistry, pressure, temperature, and radiation damage on the inertness of possible confining materials has allowed the tuning of material properties to maximize their retention ability.

These discoveries, which are both interdisciplinary in their impact and which hinged on experimental and theoretical innovations, are illustrative of a range of future goals of the high-pressure geosciences community. Specifically, generating our science increasingly requires improved collaboration, synergies, organization, and access to community facilities. Our discipline has produced highly successful enterprises designed to facilitate cutting-edge experimental science for individual investigators at national particle accelerator facilities. These groups include the NSF-funded CONsortium for Materials Properties Research in the Earth Sciences (COMPRES) and, at the Advanced Photon Source APS), portions of the GeoSoilEnviro Consortium for Advanced Radiation Sources (GSECARS), the High-Pressure Collaborative Access Team (HPCAT), and the High-Pressure Synergetic Center (HPSynC). To successfully sustain our community into the future, we anticipate that ensuring general access to state-of-the-art computational facilities will be a priority, as will exploring new models for ensuring successful utilization and access



Figure 1.4. (left) Piston-cylinder-type apparatus. The height is about 1.5 m and the sample, which is typically a few millimeters on a side, is contained within the central gold-colored column. These apparatuses have typical pressure limits that correspond to 100-km depth in the planet, and have been extensively used to constrain magma chemistries and fluid-rock interactions in the uppermost region of the planet. Image courtesy of Rockland Research. (right) A shock wave gun. The gun's length is ~15 m. In effect, this piece of equipment is a cannon that fires a gas-driven projectile into a sample, and the sample is intensively monitored while it is compressed to high pressures during the shock event. Pressures that span Earth's entirety can be accessed by shock-wave techniques. Photo courtesy of S. Stewart, Harvard University.

to national facilities and experimental, computational, and analytic infrastructure that are necessary but beyond the scope (and desirability) of a single principal investigator to maintain.

Our collective focus on the behavior of materials that make up Earth and other planets leads to an intrinsic interdisciplinarity and broadly interactive character of our field within the earth sciences. For example, seismology, with its focus on faulting and wave speeds, depends upon our studies of the mechanics of failure and the elastic properties of materials; geodynamics hinges on our characterizations of the viscous flow of materials; geomagnetism depends on our determinations of the electromagnetic properties of materials; petrology relies on characterizations of mineral/melt equilibria; planetary science incorporates the equations of state and behavior under shock-loading that we determine in modeling the interiors and impact-history of planets; and, ultimately, the planet's climate is controlled by the exhalations from its interior that, modulated by the surface environment, have generated our atmosphere.

Although we could view our discipline as central to each of these areas of inquiry, a more accurate portrayal is that we provide *an overarching framework* for how the planet's materials behave, a framework that supports all of our adjoining disciplines within the earth sciences.

In this report, we describe both our recent achievements and the areas that we see as ripe for our community to make the next generation of advancements in our understanding of the interior—the very guts—of Planet Earth. The degree of difficulty associated with probing Earth materials at pressures corresponding to those generated by tens, hundreds, or thousands of kilometers of piled rock, and particularly at simultaneous temperatures of thousands of degrees Kelvin, is extraordinary. Over the last several decades, our community has marshaled a combination of forces, from our innovative and continuously developing high-pressure and high-temperature experimental technologies, to state-of-the-art theoretical approaches, to the formidable strength of national particle accelerator facilities, to accomplish our goals

of improving understanding of our planet. Although we have made enormous progress, many of the discoveries produced new questions that we could not have anticipated a decade ago, and many pivotal issues remain unsolved or controversial. Our view is that with an integrated approach coupled with technical advances, we can see our way toward truly enhancing our understanding of the deep Earth, and ensuring that we fundamentally understand our piece of the complex interrelationships that govern the evolution of our planet's habitable environment.

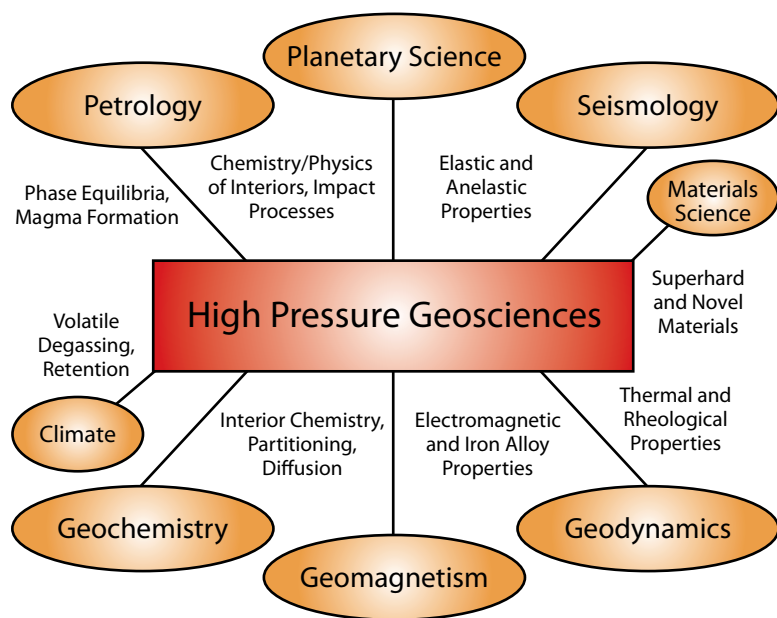


Figure 1.5. Schematic of linkages between high-pressure geosciences and neighboring disciplines. For each discipline, the data/results of primary interest and overlap from high-pressure geosciences are labeled. After Liebermann (2005). Original design by A. Lattimore, Stony Brook University, redrawn by J. Adams, Geo Prose.

# Chapter 2 | Earth's Habitable Surface: A Consequence of the Planet's Interior

The ocean basins and continents, overlain by the ocean and atmosphere, are fundamental characteristics of Earth's surface—they are features that set Earth apart from the other terrestrial planets. Indeed, each of these features is crucial to the habitability of the planet's surface, and the deep Earth has controlled their genesis. In the case of the ocean basins, their depths are a result of the greater density of the oceanic crust relative to continental crust. The oceanic basaltic crustal layer is produced through upwelling and melting of dense mantle beneath mid-ocean ridges. Correspondingly, the lower-density continental crust is predominantly generated by entrainment of water-rich rocks of the ocean floor to depth through subduction, followed by the release of water, and comparatively low-temperature generation of silica- and water-rich melt above the subducted slab. It is this type of water-assisted melting that not only

generates continental crust, but also the explosive volcanism of the Ring of Fire surrounding the Pacific. Above the crust are the ocean and atmosphere—crucial to our planet's habitability, with their existence likely being a direct consequence of degassing of volatile materials from Earth's interior. Volcanic degassing, which is well known to impact the sulfur content of the atmosphere on monthly and annual time scales, has been a primary contributor to our ocean and atmosphere. Hence, the linked processes of silicate melting, volcanism, and volatile degassing have played a principal role in producing the habitable environment of Earth's surface.

The continent-ocean basin dichotomy of Earth's surface hinges on both the melting processes that occur at depth within the planet, and the ability of Earth's interior to retain—and, under some circumstances, release—water. Indeed, despite our planet's

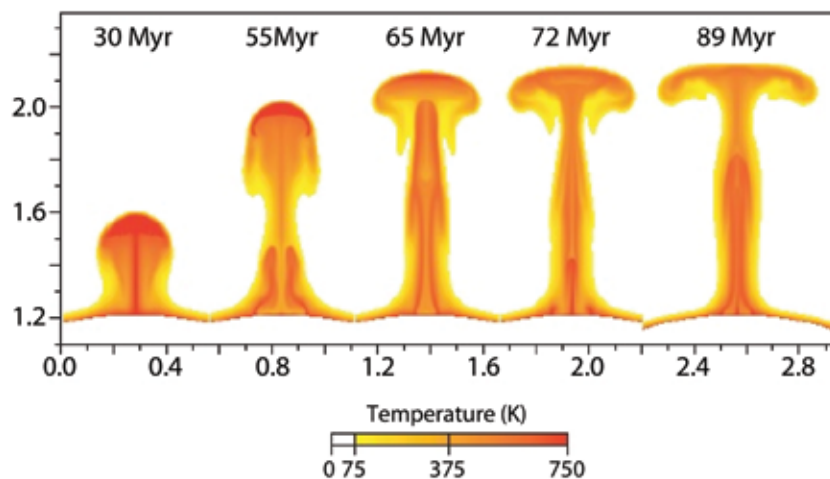


Figure 2.1. Fluid dynamic model of the thermal signature of a mantle upwelling from the core-mantle boundary, which could be connected to flood basalt generation. The colors represent temperatures above those of the surrounding mantle. Here, the spatial dimensions are expressed as multiples of 2885 km, the thickness of the mantle. The production of a flood basalt would occur as the rising plume head approaches Earth's surface (at 2.2 on the vertical axis). From a high-pressure geosciences perspective, the key issues are the quantity and nature of the melt generated at different depths at suites of different temperatures within thermal upwellings. Reprinted by permission from Macmillan Publishers Ltd: *Nature*, Lin and van Keken (2005), copyright 2005.

average land-surface elevation of over 2 km below sea level, there is an abundant portion of the planet that sits above the waterline. Thus, the principal topographic features of our planet—our high-standing, exposed continents—are generated by deep melting of the planet. The effects of melting on the surface environment are not solely confined to the generation of continents and ocean basins. Dramatic volcanic events that involve immense outpourings of magma from Earth’s mantle have occurred sporadically in Earth history; perhaps the best-known of these “flood basalts” are the Siberian Traps. This set of eruptions ~251 million years ago released ~4 million cubic kilometers of basaltic magma onto the planet’s surface, a volume more than sufficient to cover the combined areas of Alaska, Texas, and California with lava to depths of more than a kilometer. The effects of such a massive eruption on the surface environment are still poorly understood, but a clear indication of its impact is derived from the synchronous extinction of 95% of marine species and 70% of all terrestrial vertebrate species. The mechanism for the extinctions likely resides in the voluminous amount of gases—principally sulfur- and carbon-bearing—that would have accompanied such an eruption. Beyond atmospheric climatic changes, a large influx of such gases to the atmosphere would have also probably acidified the near-surface ocean. The Siberian Traps, which came as close as any known event in Earth history to destroying life on the planet, may appropriately be viewed as *Death from the Deep Earth*—and understanding of the physical and chemical processes that give rise to deeply derived magmatism is thus of major interest. Indeed, melting is the primary means not only by which the planet’s crust formed, but also by which the planet segregated into different compositional layers. Hence, understanding the process and effects of melting at depth within the planet is one of the key goals and major recurrent themes of the high-pressure geosciences community.

With respect to the ocean and atmosphere, both water and carbon dioxide share a common trait: each can be stably bound into rocks and thus transported



Figure 2.2. Flood basalt exposure at the Snake River Canyon, WA, showing sequential lava flows emplaced over about 1 km of vertical relief. This set of basaltic flows are part of the Columbia River Basalts, which are widely thought to have been produced by the same mantle upwelling that currently produces the subterranean heat in the Yellowstone region. Photo courtesy of V. Camp, San Diego State University.

into, or retained within, the planet. In the case of water, a broad suite of hydrated phases, from low-pressure clays and layered structures such as talc and micas, to more exotic hydrated phases stable only at high pressures, and even water stably dissolved into the structure of normally water-free phases, each can provide stable, solid hosts for water over a range of pressure and temperature conditions. The recognition that amounts of water equivalent to that of the ocean or more could be sequestered in nominally water-free minerals within Earth’s deep interior represents an unexpected discovery of the high-pressure community.

The amount of atmospheric carbon dioxide represents the main difference between the atmospheres of Mars, Earth, and Venus. Venus has an atmosphere that is ~96% carbon dioxide and a suffocating atmospheric pressure of about 93 atmospheres, while Mars has about the same percentage of atmospheric carbon dioxide, but a pressure of only ~0.007 atmospheres. For comparison, Earth has an atmospheric partial pressure of carbon dioxide of about 0.0004 atmospheres. The contrasts between the terrestrial planets indicate that they have markedly different degrees to which carbon dioxide is retained within, and cycled

into, each planet's interior. These differences among planetary carbon cycles exercise a fundamental control on the atmosphere, climate, and habitability of each of the terrestrial planets, and probing the portions of the carbon cycle that reside within the solid portion of the planets represents a primary goal of the high-pressure geosciences community.

In contrast to the many possible forms in which water can be stored at depth, carbon dioxide may be sequestered at depth within the planet primarily as CO<sub>3</sub>-bearing carbonates—in essence, the equivalent of deep-Earth limestones. The ambiguity that emerges with carbon storage at depth involves the degree of oxidation of the planet's interior. The existence of diamonds and (possibly) abiogenic methane within Earth's mantle each show that the degree of oxidation of the mantle fundamentally influences how carbon is stored deep within the planet. The usual viewpoint is that zones that have been affected by subduction (and hence that have indirectly interacted with the surface) are likely more oxidized, while regions that retain a chemical signature of core formation are more reduced. Hence, the oxidation state of a parcel of material in Earth's mantle likely reflects the processes and chemical interactions to which it has been exposed—and producing means for determining the oxidation state at depth could provide a valuable forensic tool to illuminate the chemical history of our planet's interior. Indeed, the oxidation state of different mantle regions likely controls the genesis of perhaps our planet's most aesthetic major economic mineral—diamond.

The precise amounts of water that are retained at depth is uncertain but, as long as the effects of water on mineral properties are well characterized, they can be inferred for different regions based on observations of seismic wave velocities or electrical conductivity at depth. Indications are that at least the equivalent of an ocean of water is likely sequestered at depth within the planet, and perhaps substantially more. Because the ocean accounts for only ~0.025% of Earth's mass, even a relatively small amount of water retention at depth within solid crystalline

phases can yield a reservoir that dwarfs our near-surface hydrosphere. The net observation here is that the deep Earth's likely storage capacity for water is large relative to the size of the ocean.

Deriving constraints on how water can be stored within Earth's mantle, through both theory and crystallographic and spectroscopic experiments on materials synthesized in wet environments at the conditions of Earth's interior, has been an area of major advances for the high-pressure geosciences community over the last decade. The key unknown parameters have been the amounts of water delivered to the surface (through volcanism) relative to rewatering of the interior (through subduction of water-rich materials) throughout Earth history. The balance between these two fluxes exercises a fundamental control on the volume of water at the surface, and determination of their relative rates is crucial for understanding the geologic history of water at the planet's surface. Hence, our community is producing data that address one of the most long-standing questions of not simply science, but also humanity: why do we have an ocean?

As with water, the amount of carbon present at depth is difficult to determine, but is certainly far greater than the modest amount present within our atmosphere. The carbon dioxide reservoir of the near surface is dominantly sequestered in carbonate rocks—rocks that have taken up the slowly released, over geologic time, voluminous amount of volcanic carbon dioxide degassing from the planet's interior. The interest in this slow bleed of carbon dioxide from the interior is not casual: it is the steady accumulation of deep-Earth-generated carbon dioxide within the atmosphere ~750 million years ago that pushed Earth out of the so-called “snowball Earth” climate that appears to have produced global glaciations, including sea ice at equatorial latitudes. Hence, the deep Earth carbon reservoir has been responsible for keeping our planet from remaining an iced-over planet with life confined to small and peculiar niches. The Cambrian evolutionary explosion of multicellular organisms 540 million years ago was likely made possible by the equable climate produced by steady



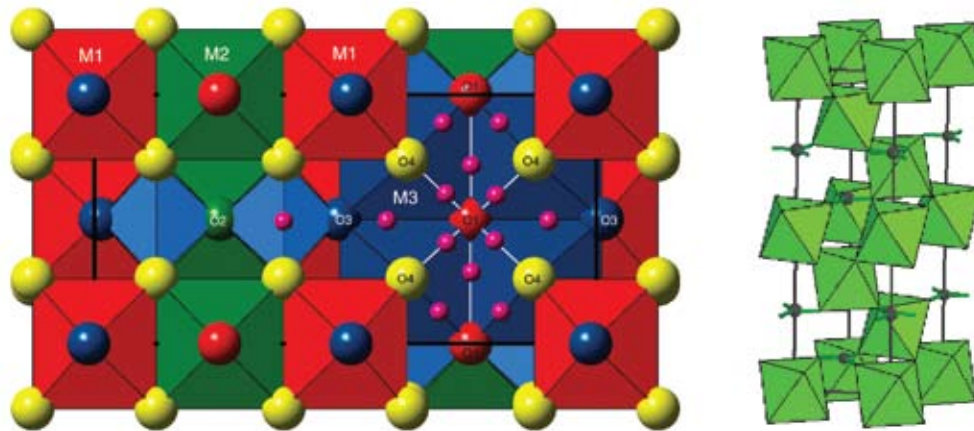


Figure 2.3. Crystal structures of the two crystalline phases that are likely to be the largest hosts of water and carbon dioxide in planet Earth. (left) Crystal structure of hydrous-(Mg,Fe)<sub>2</sub>SiO<sub>4</sub>-wadsleyite, which is the dominant phase within Earth's mantle between 400- and 520-km depth. Large balls represent different oxygen sites, and red and green octahedra are typically occupied by magnesium or iron cations, while blue tetrahedra contain silicon. Pink balls show the possible sites for hydrogen substitution in this phase. This phase was predicted to be a major water carrier on theoretical grounds two decades ago, with the prediction subsequently being verified by experiment; an intense amount of effort continues to be dedicated to probing the properties of this material. (right) Crystal structure of MgCO<sub>3</sub>-magnesite. The grey balls indicate carbon, and the octahedra represent magnesium ions that are octahedrally coordinated by oxygen. This phase is, with diamond (which is present under non-oxidizing conditions), the probable host for carbon from shallow depths to near 2000-km depth within Earth's mantle. Recent work indicates that near this depth, magnesite transforms to a denser phase that contains carbon with four neighboring oxygens; the significance of this transformation for the planet's carbon budget is a topic of active inquiry. Images courtesy of J. Smyth, University of Colorado.

greenhouse degassing. Among the most critical roles played by the surface environment (when it is not iced over) has been the sequestration of degassed carbon dioxide from the interior, and the conversion of a small portion to atmospheric oxygen (and complementary organic carbon). In this sense, there is a direct feed-through of deep Earth carbon into the planet's biosphere and, after decay, eventually back into the rock record.

The effects of the planet's interior on life, and surface habitability, are clear. Yet, the issue of to what depth life can exist within Earth's interior is an area of active inquiry. Life has long been known to persist to the pressures present in the deepest ocean: at the base of the Marianas Trench, pressures exceed 0.1 GPa (1 kbar), but life appears to thrive at these depths. The question that we pose is how deeply might life extend to substantially greater pressures within the solid Earth in places such as between grains, or in

fractures. The techniques developed by the high-pressure geosciences community—which include optical access to high-pressure cells and spectroscopic techniques that can detect metabolic products—have proved particularly valuable in this quest for the deepest possible organism. Although life clearly cannot exist at the temperatures and pressures present in the vast majority of the planet, there are indications that some single-celled organisms can survive and even conduct metabolic processes at pressures corresponding to depths of ~30 km. The ability of life to persist—and perhaps thrive—at moderately high pressures also has implications for the possibility that life could exist in protected locations in other parts of the solar system. Possible locales include the water layer that lies beneath the ice of the Jovian moon Europa, or within deep aquifers on Mars. The study of life under such extreme conditions hence incorporates not only geobiology, but also planetary science.

The high-pressure geosciences community has been critically concerned with how carbon (in its many possible chemical forms) is retained and processed within the deep Earth. Among the primary results is that, under oxidizing conditions, carbon can be retained in carbonate phases throughout the depth range of Earth's mantle, while more reducing conditions result in diamonds. The widespread appreciation that deep carbon represents a major (and, by mass, the dominant) player in our planet's carbon cycles represents one of the true achievements of our field. But, the chemistry and phase equilibria of carbon at depth are complex, and we have not yet approached a full understanding of this critical carbon reservoir.

## Key Questions

- How has Earth's interior controlled the surface budget of carbon and water through the planet's history?
- Are there hidden reservoirs of hydrogen and carbon at depth?
- What is the oxidation state of Earth's interior?
- What are the properties of the molecular fluids  $\text{CO}_2$ ,  $\text{H}_2\text{O}$ , and  $\text{CH}_4$  at high pressures and temperatures?
- What are the melting relations and phase equilibria of hydrated and carbonated materials at all mantle conditions?
- How does carbon behave over a wide range of deep Earth conditions, including as a function of pressure, temperature, and oxidation?
- To what depths within the planet can single-celled life persist, and to what conditions can it thrive?

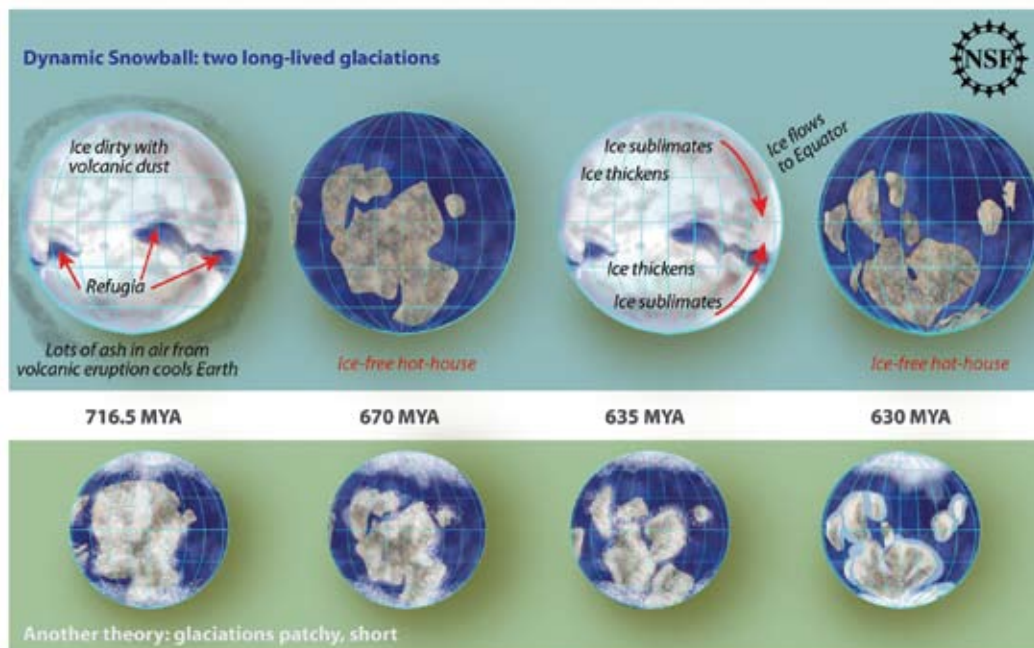


Figure 2.4. Two possible scenarios for how equatorial glaciation of a snowball Earth might have occurred between 716.5 and 620 million years ago. In the top scenario, glaciers encompass both the polar oceans and most of the supercontinent Rodinia twice in this era, with hotter (and mostly ice-free) periods following the glacial periods. In the lower scenario, ice coverage is confined to the equatorial continent and the polar ocean regions during the coldest periods. In these scenarios, ash- and sulfur-emissions from volcanic events generate catastrophic climatic cooling, while long-term accumulation of carbon dioxide from volcanic degassing ultimately produces sufficient greenhouse warming to defrost the planet. Credit: Zira Deretsky, National Science Foundation.

# Chapter 3 | The Magnetic Field, Earth's Core, and the Deep Mantle

## The Magnetic Field and the Habitability of Earth's Surface

Earth's magnetic field is often thought of simply as a navigational tool, producing reliable compass directions at the planet's surface. However, the effects of the presence of a magnetic field on biologic systems are profound. The energetic cosmic ray flux at Earth's surface is dramatically reduced by having a field—and Earth's is the strongest among the terrestrial planets. This reduction in energetic particle flux decreases the mutation rate from charged particles that are deflected by the planet's dipolar magnetic field. Thus, the magnetic field contributes significantly to the habitability of the planet's surface, and has for at least the last 3.5 billion years. From a technologic perspective, the magnetic field provides protection from what can be an electromagnetically harsh solar environment. Frequently, the effects of solar flares disrupt the Canadian and Scandinavian electrical distribution systems—a direct consequence of the orientation of field lines near Earth's poles. But, such disruptions are minor compared to more extreme solar events. For example, the largest coronal mass ejection on record, the 1859 Carrington event, was sufficiently severe that it generated auroras at the equator and induced fires in telegraph offices. The magnetic field acts as a protector against both major and minor solar events, with their prospectively profound effects on our electrical infrastructure. Indeed, the magnetic field's effect on extraterrestrial energetic particles can be viewed as similar to that of the ozone layer's role in screening damaging ultraviolet radiation.

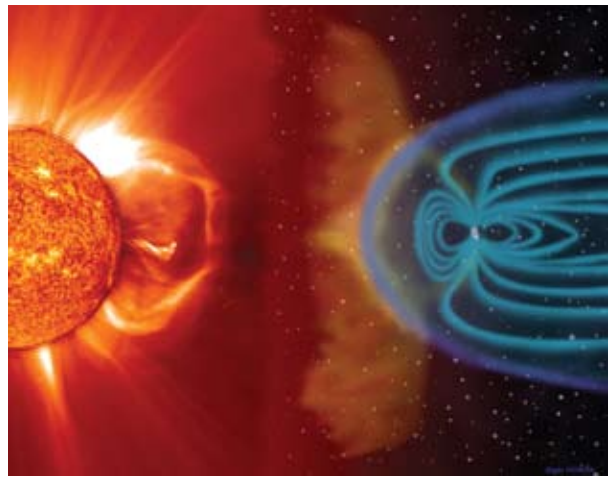


Figure 3.1. Composite illustration of the interaction of a solar coronal mass ejection with Earth's magnetic field. The interactions of such ejections with Earth's field depend on their polarity relative to that of Earth's, and on past deflection of the field by previous energetic events. Distances are not to scale. Courtesy of S. Hill, NASA.

It has long been appreciated that the magnetic field is generated by fluid motion within Earth's electrically conductive, iron-rich liquid outer core (conventional solid-state ferromagnets are annihilated at the high temperatures of the core). Although the dipolar character of the field is clearly produced by the effects of rotation on the fluid core, rotation alone is insufficient to drive a long-term magnetic field. Improving our insights into the composition and dynamics of Earth's core, and hence the energetics and drivers of Earth's geodynamo—which includes how our magnetic field is produced—is among the primary goals of high-pressure geosciences.

## Iron Alloys—The Phase Relations of Earth’s Innermost Interior: Constraints on Temperature, Composition, and Phase

The properties of Earth’s core materials are pivotal in understanding the magnetic field generation process. Seismologic observations yield a strong starting point for inferences about the state of material within the planet’s core. The recognition of the core as being composed of a central solid inner core and liquid outer core provides a compelling case that liquid-solid phase equilibria are critical for the core’s evolution. Moreover, the combination of high-pressure measurements of elastic properties and densities, the velocities of seismic waves and densities in the core, and the cosmochemical abundance of elements leads to the robust conclusion that the core is an iron-nickel alloy. Yet, it is an impure alloy, with about 10 wt% of a lighter alloying component in the outer core and roughly 5 wt% of a lighter material in the solid inner core. The precise identity of these lighter alloying components has been a major

unsolved question in geophysics, as well as one of the primary sources of uncertainty in our knowledge of the bulk composition of our planet. The most likely major components of the light-alloying component are sulfur, oxygen, silicon, carbon, and hydrogen, with minor roles likely being played by elements such as phosphorus and nitrogen. Moreover, if elements with long-lived radioactive isotopes (potassium is the most common suggestion) are present in even minor abundance in the core, then the magnetic dynamo could be partially driven by radioactive heating. Our knowledge of the elastic and chemical properties of alloys of each of these elements with iron has mushroomed over the last decade, but these properties are often characterized at pressures and/or temperatures that fall substantially short of those present within the core. Indeed, measurements of properties at the extraordinary pressures and temperatures of Earth’s core remain among the scarcest and most challenging experiments and calculations in the earth sciences.

Even knowledge of the temperature of Earth’s core remains uncertain. Although the top of Earth’s core is generally thought to be around 4500 K with the central temperature of the planet near 6000 K, these values hinge on both the identity of the lighter alloying component(s) and the melting relations of this composition at Earth’s core conditions, and might differ by ~1000 K from these estimates, generating a large uncertainty in our knowledge of the overall heat budget of our planet. In concept, the interface between the solid inner core and liquid outer core should represent a fixed point in pressure and temperature space—but the location of that fixed point depends on the composition of the coexisting liquid outer and solid inner core, and hence the compositional uncertainty associated with the core maps directly into a range of possible temperatures for this solid-liquid interface. Thus, our constraints on the thermal state of this region of the

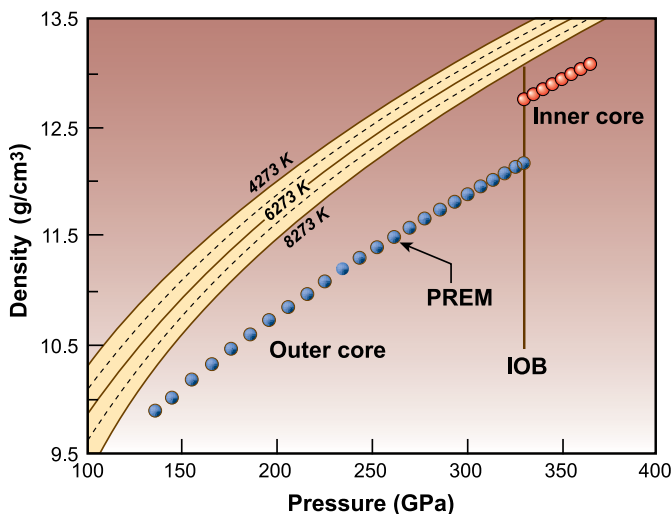


Figure 3.2. Illustration of the requirement for a lighter alloying component within both the outer and inner core. Brown lines represent the estimated density of hexagonally close-packed iron at different temperatures, and the blue and red dots show the seismically derived (Preliminary Reference Earth Model, or PREM) constraints on density within the inner and outer cores. IOB denotes inner core-outer core boundary. From: Figure 2 in Fiquet et al. (2008); reproduced with permission from the Mineralogical Society of America.

planet depend directly on theoretically and experimentally determining what phases are present in the suite of elastic-property-permitted possible core compositions.

With the limited data available on the core of the planet, each empirical observation becomes of unusual value in determining the properties of this most remote region of the planet. Recently, the inner core has been observed to be both laterally heterogeneous and seismically anisotropic. The observation of anisotropy within the inner core—faster wave velocities along polar paths relative to equatorial paths—provides a strong indication that oriented crystallites, or inclusions, are present within the inner core. The most parsimonious interpretation for the presence of this anisotropy is that the solid inner core flows (as does most of the solid silicate mantle), and the crystals within the inner core become oriented within this flow field. The phase of iron that is generally inferred to be present within the inner core has hexagonal

symmetry, and hexagonal crystals are prone to such preferred orientation. Yet, the seismic anisotropy also has an apparent variation in magnitude between hemispheres within the inner core, and may be absent in the very center of the planet. The physical origin of such a pattern is controlled by how much the velocities of iron at inner core conditions vary depending upon crystal orientation. In short, do these anisotropies imply large differences in orientation, or fairly modest degrees of crystal orientation? Thus, what these preferred orientations imply for the dynamics of the inner core hinge on the material properties of iron at core conditions. It is one of the aspirations of the field of high-pressure geosciences to experimentally and theoretically constrain the material properties of iron at the simultaneous high pressure and temperature properties of Earth's inner core.

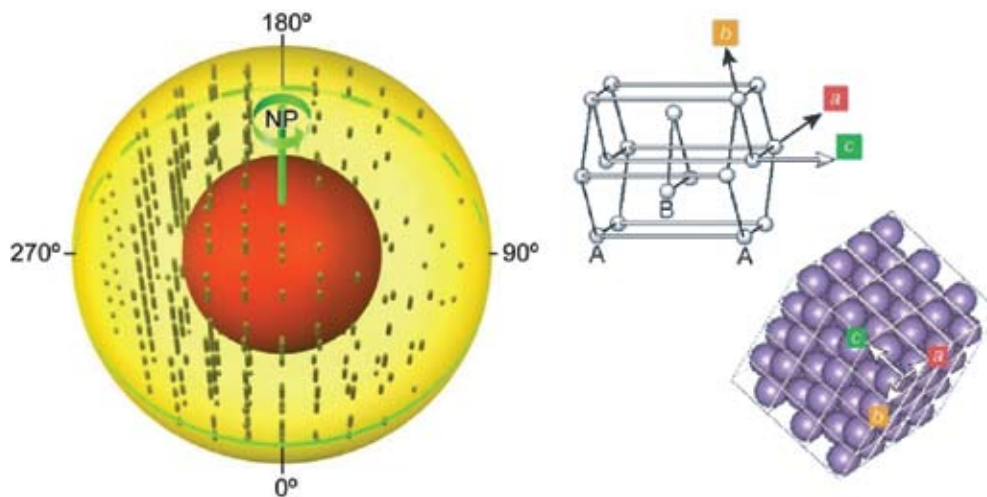


Figure 3.3. (left) Image of the inner core, with length of markers representing how much faster seismic waves travel along the axis of the marker relative to the average for that depth within the inner core. The red innermost core at the center has no detectable anisotropy. Courtesy of X. Song, University of Illinois at Urbana-Champaign. (right) Crystal structure of hexagonal close-packed iron, which is widely viewed as the dominant phase within the inner core. Theoretical calculations indicate that seismic waves would travel faster in the a-b plane relative to along the c-axis in this material; high-pressure experiments on analogues and on iron at lower pressures confirm this general trend, and generate a natural explanation for the anisotropy in terms of a heterogeneously textured inner core. Yet, the origin for why the texturing would be heterogeneous remains elusive. Reprinted by permission from Macmillan Publishers Ltd: *Nature*, Jephcoat and Refson (2001), copyright 2001.

## Transport Properties of Iron Alloys: Implications for the Sustainability and Energetics of the Geodynamo

The power requirement to produce our planetary-scale magnetic field is about 1 Terawatt (or about a factor of ten less than that of all power used by humans on Earth). This figure is a lower bound, as the efficiency of the generation process is ill constrained. The energy required to run the geodynamo has several likely sources: (1) outer core fluid flow driven by cooling from the mantle above; (2) presuming that the solid inner core is growing with time, release of latent heat of fusion at the inner core-outer core boundary; (3) exclusion of a light alloying component during solidification of the iron-enriched inner core, and buoyant rise of the light material; and (4) heat generated by any radioactive elements dissolved within the core (with  $^{40}\text{K}$  being the most commonly suggested candidate).

The first of these sources, heat flow out of the top of the core, is largely controlled by the thermal conductivity of the core and mantle—in essence, the rate at which heat can be delivered into the overlying

mantle from the core. Not only does this core-derived heat help drive the geodynamo, but it also plays a key role in driving mantle convection (and hence plate tectonics), through heating the convecting mantle from below. Moreover, the magnitude of iron's thermal conductivity controls the sustainability of Earth's magnetic field given that fluid flow is required to generate the geodynamo. Thermal conductivity, while a conceptually simple parameter, is difficult to measure at extreme conditions. One of the goals of the high-pressure community over the next decade is to improve our ability to both measure and theoretically calculate this parameter at deep-Earth-relevant conditions.

Two of the other possible energy sources for the geodynamo, latent heat release and buoyant rise of crystallization-excluded lighter-alloying enriched material, each depend on the growth of the solid inner core with time. Seismologic studies have demonstrated that the material of the inner core is textured, and may be zonally heterogeneous. How such structures might arise hinges both on the physical and chemical processes occurring during core crystallization, and on any convective stirring that occurs in the solid inner core. The former processes depend entirely on the phase equilibria of the core alloy (which in turn is dictated by its composition), and on the nucleation and growth of iron crystallites at the ultra-high pressure and temperature conditions of Earth's inner core. In comparison, inner core convection is controlled by the competing transport properties of viscosity and thermal conductivity of solid iron alloys at core conditions.

Thus, we see that the thermal conductivity of core materials—how efficiently these iron-rich materials conduct heat—is crucial for constraining a range of broad-reaching problems, including Earth's heat flow budget, the convective vigor in the outer and inner cores, and the timing of the formation of the inner core. Measurements of thermal conductivity at extreme conditions are very challenging. Although a few measurements have been conducted using the coupling of light with thermal waves within the

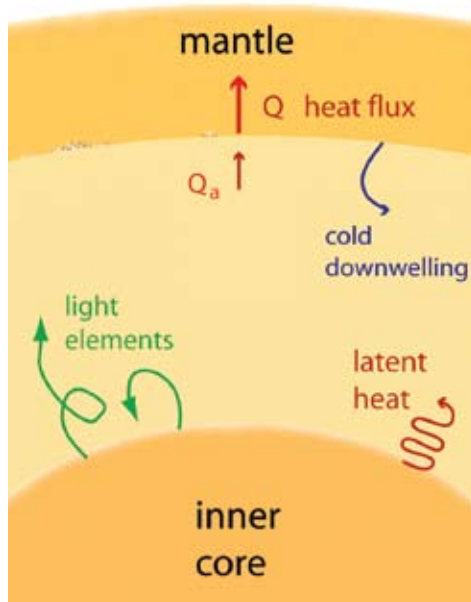


Figure 3.4. Illustration of the thermal and chemical buoyancy effects on core convection. Courtesy of B. Buffett, University of California at Berkeley.

sample (such as impulsive stimulated scattering), a range of other time-resolved measurements, including time-domain thermoreflectance and femtosecond broadband optical spectroscopy, will likely be increasingly deployed over the next several years. The stakes in accurately constraining thermal conductivity are high. From the perspective of the history of Earth's magnetic field, the key question that will be determined by accurate thermal conductivity measurements is: how long has Earth had a solid inner core? Because the inner core plays a key role in determining the convective style of the core and in generating the driving forces of the geodynamo, its growth history is critical for understanding how our magnetic field has evolved through time. Our present uncertainty of a factor of two or three in the thermal conductivity at core conditions (which, in light of the extreme conditions and difficulty of the measurement, is an excellent achievement) causes fundamental differences in our models of the evolution and timing of inner core formation, with estimates varying between ages of ~1.5 billion years to ~4 billion years for the onset of inner core crystallization.

The possible presence of radioactive elements (especially potassium-40, but less plausibly uranium and/or thorium) within the core, whose decay would generate heat that would contribute to the geodynamo, also lies in the firmly testable domain. Both experiments and theory have provided some tantalizing hints that, in marked contrast to their lower-pressure behavior, radioactive elements may dissolve in iron alloys at high pressures. If this is the case, then the fundamental process of radioactive decay of long-lived radionuclides may play a key role in producing Earth's magnetic field. The presence (or absence) of radioactive elements within the core may ultimately be observationally determined through a fortuitous synergy between the fields of astrophysics and geophysics. Radioactive decays produce neutrinos, thus, neutrino detectors, which are usually deployed within mines near Earth's surface, should be able to resolve whether there is a significant source of geoneutrinos—and hence radioactive elements—within Earth's deepest interior.

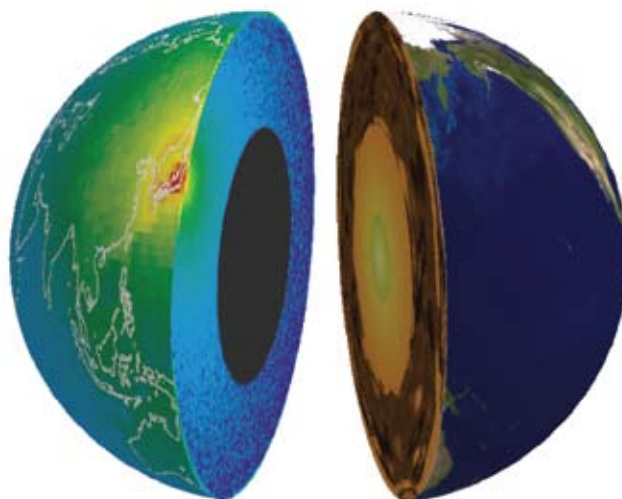


Figure 3.5. (left) Sources for geoneutrinos at the Kamland neutrino detector in Kamioka, Japan (redder colors indicate that higher fluxes of neutrinos are detected from these regions), juxtaposed with an image of seismically generated deep Earth structure (right). Reprinted by permission from Macmillan Publishers Ltd: *Nature*, Araki et al. (2005), copyright 2005.

The need for more information on the properties of iron alloys at core conditions—their phase equilibria, their melting (and crystallization) behavior, their solid and liquid viscosities, and their thermal and electrical conductivities—is thus driven by a desire to understand the chemical and physical properties of Earth's core, and hence the planet's geodynamo. Significant new constraints on core alloys have emerged over the last decade, but the underpinning questions require suites of experiments and complex calculations at the conditions of Earth's deepest interior—and these are among the most challenging of enterprises.

It is not solely with an eye to constraining the genesis of Earth's magnetic field that the physical and chemical properties of the outer core are of interest. The chemistry of the core likely reflects the manner in which the earliest Earth accreted from smaller bodies. The key questions here include: (1) how much did Earth's core material react with the silicate portion of the planet? and (2) what fraction of the bodies that accreted to form the bulk of Earth were themselves differentiated into core and mantle? In this sense,

the composition of Earth's core may provide one of the few records of the long-ago objects that merged together to form our current planet.

The reaction of iron-rich material with the silicate mantle would cause water within the silicates to react with iron, forming rust at low pressure, and iron oxide and iron hydride at higher pressures. Each of these processes would lead to water loss from the silicate Earth-ocean-atmosphere-climate system, either through hydrogen release and escape from the atmosphere, or through sequestration of hydrogen within Earth's core. Hence, the process of core formation controlled the water budget that the earliest Earth retained, and thus the reservoir of water available for formation of the planet's ocean.

### The Deepest Mantle: The Container of Earth's Core

The composition of Earth's core may also evolve through time by interactions with the mantle. In effect, the mantle acts as a ceramic thermos around the core—but the degree to which the ceramic interacts with the molten iron of the core is unclear. Certainly, the lowermost ~300 km of the mantle is among its most structurally complex regions, and hence, mirrors the complexity of the uppermost few hundred kilometers (which are affected both by plate tectonics and the deep roots of continents). Because of its distinctive and complex character, this zone is distinguished from the overlying mantle, and is referred to as the D'' (D double-prime) layer. The features that are likely present in the lowermost mantle include a new high-pressure silicate phase known as post-perovskite—a phase that only becomes stable within the deepest lowermost mantle, and whose existence may explain a long-enigmatic discontinuity in seismic wave velocities a few hundred kilometers above the core-mantle boundary. Additionally, the crystal structure of this phase could explain the robust anisotropy of seismic wave propagation (in which waves propagating with different orientations travel with different velocities) observed within D''.

Although we've come a long way in our understanding of the deep mantle, major issues remain. The current estimates of the dependence of the pressure/depth of the phase transition on temperature indicate that in hot regions, this transition may not occur, and lower-density perovskite could be juxtaposed with cooler post-perovskite. Such a scenario explains the regionally variable character of the seismic discontinuity that has been associated with the post-perovskite transition; but it also poses a suite of dynamical issues. In particular, the role that hot regions containing the less-dense perovskite phase play in driving mantle upwellings is a topic of intense scrutiny. Moreover, the temperature at the top of the outer core could be sufficiently high that a lens of perovskite may exist directly above the core, underlying the denser post-perovskite phase. The dynamic implications of such an inverted-density scenario are also complex, and their exploration will require a cross-disciplinary effort that incorporates improved constraints on the conditions under which this transition might occur within the planet.

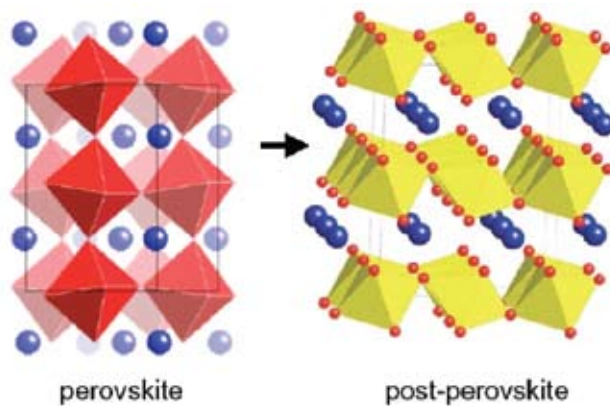


Figure 3.6. Crystal structures of the  $(\text{Mg,Fe})\text{SiO}_3$ -perovskite and post-perovskite phases. The blue atoms are silicon, while the red and yellow polyhedra are the oxygen neighbors of the magnesium ions, and the red atoms in post-perovskite are oxygens. Within post-perovskite, seismic waves propagate more rapidly along the directions defined by the layers of yellow polyhedra, and more slowly perpendicular to these layers. Reprinted by permission from Macmillan Publishers Ltd: *Nature*, Duffy (2008), copyright 2008.



The discovery of this new phase ranks as one of the major advances in the high-pressure geosciences over the last decade. Its discovery has galvanized interest across the fields of geodynamics, seismology, and the high-pressure geosciences community. The synergies that have arisen between these fields in conjunction with the possible presence of the post-perovskite

phase of  $(\text{Mg,Fe})(\text{Si,Al})\text{O}_3$  has provided constraints on the possible heat flow out of the core (and thus the driving force for the geodynamo), as well as producing new paradigms for how mantle plumes—the isolated upwellings that give rise to non-tectonic volcanic features such as the Hawaiian Islands—might form in the lowermost mantle.

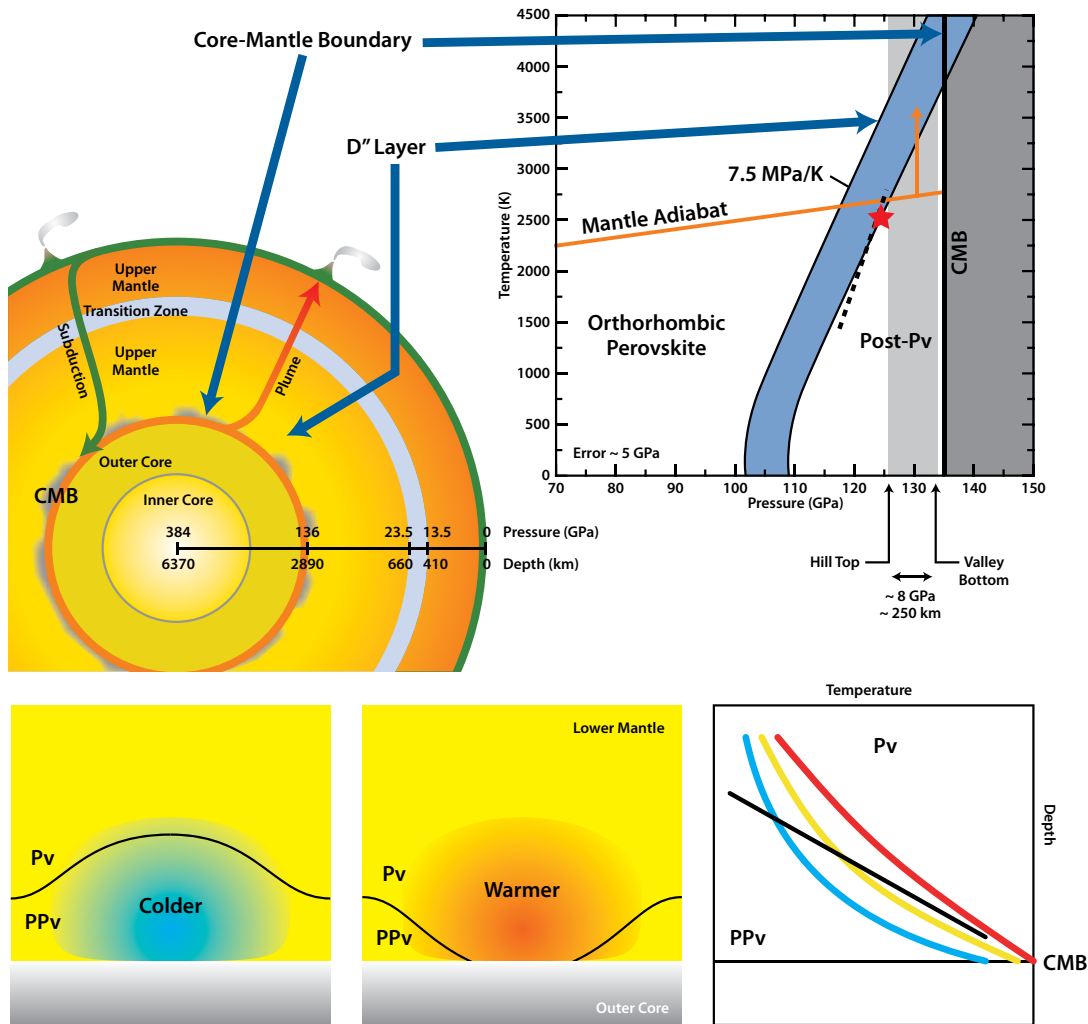


Figure 3.7. Diagrams of the possible effects of variable temperature on the occurrence of the post-perovskite phase transition. (top) Theoretical phase boundary between perovskite and post-perovskite, compared to the temperature distribution in normal, convecting mantle (mantle adiabat). The thermal boundary layer near the core-mantle boundary can produce hot, downward deflections of this boundary, while colder regions will be associated with an upwarped boundary (right and center panels of lower figures). In the right panel of the lower figure, the red, gold and blue lines represent a hot, normal and cold temperature distribution in the deep mantle, and the black line represents the pressure-temperature slope of the perovskite to post-perovskite transition. Note that because the top of the outer core is nearly isothermal, the possibility exists that a thin layer of perovskite is present over the entire surface of the core-mantle boundary. Top figure from: Lay et al. (2005). Bottom panels from: Figure 5a in Shim (2008).

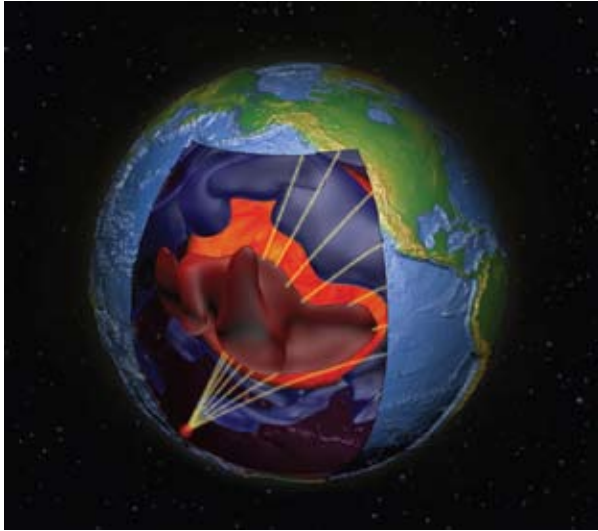


Figure 3.8. Contoured image of seismic velocity anomalies in the lowermost mantle; the red region is the large, low-shear velocity province (LLSVP) below the Central Pacific, and the blue regions are seismically fast zones that may be associated with ancient subduction of oceanic crust. The core is shown as the orange underlying ball. The yellow lines represent paths traveled by earthquake waves from a near-surface source (red dot) that interrogate the LLSVP. Courtesy of E. Garnero, Arizona State University.

However, the post-perovskite phase, and its likely seismic signature, is far from the only anomalous features near the base of the mantle. For example, two large, low-shear velocity provinces (LLSVPs) lie in almost antipodal positions beneath Africa and the Southwest Pacific. These features, which extend ~1000 km above the core-mantle boundary are zones characterized by seismic shear wave velocities that are a few percent lower than the surrounding “normal” mantle. Their compressional velocities are slightly depressed as well, but are far short of their shear velocity anomaly. The current understanding of the change of seismic velocities with temperature implies that, if we attribute the shear wave velocity depression of these features simply to them being hotter than their surroundings, then their temperature would be elevated by order 1000 K. Not only would such a dramatic temperature anomaly be expected to have a larger signature within the compressional wave velocity of these features, but if LLSVPs were purely thermal features, they would be expected to dominate

mantle convective flow, producing massive upwellings and perhaps associated volcanism. Rather, it seems that these features—each roughly the size of the largest asteroid, Ceres—differ in composition from their surrounding material. Indeed, current indications are that they may be slightly denser than their surroundings. This difference in composition is consistent with the seismic observation that the sides of these features, where they can be interrogated, appear to be fairly sharp, a probable signature of a chemical, rather than solely thermal, difference. But, we do not yet understand either the chemistry of these features, or how they might have arisen—and these are major challenges for our community to constrain. Are they primordial, dating from Earth’s earliest formation, or have they been generated over time by a yet-unrecognized deep Earth process? And, however they were generated, what does their presence imply for our canonical view of mantle convection?

Not all velocity changes near the core-mantle boundary span such large regions. Ultra-low velocity zones (ULVZs) are found in the lowermost 10–25 km of the mantle—these regions involve decreases in seismic velocity of 10–30%. Such strongly depressed velocities are found essentially nowhere else in Earth’s mantle (indeed, they are comparable to the difference in velocity between Earth’s highly silicic, buoyant crust and its underlying mantle), and our community has aggressively launched efforts to explain ULVZs. Two primary options exist: these zones could be areas of partial melting of the mantle, or they could be areas where the iron content is dramatically increased above that of normal mantle. In the former case, these regions would represent the largest silicate magma chambers on the planet, existing directly above the core, and characterized by melts that, unlike near-surface magmas, are so dense that they sink rather than rise. In the case of iron enrichment, ULVZs would be features that are transitional in composition between the core and mantle. It has long been appreciated that chemical reactions occur between silicates and molten iron, but the length scale over which these reactions operate is uncertain, and hinges on the diffusion

rates at this hot, ceramic-molten metal interface. Our community is addressing these challenges through a tandem approach using both high-level theory and state-of-the-art high-pressure experiments. The goal is to determine both the behavior of iron within silicates at extreme conditions and the properties of silicate liquids at ultra-high pressure conditions.

### Key Questions

- What are the light-alloying components of Earth's core?
- What is the temperature of Earth's core?
- What are the transport properties (particularly thermal conductivity and viscosity) of iron alloys at core conditions, and hence what is the likely age and growth rate of the inner core?
- What are the magnitudes of different heat sources within Earth's core, including its radioactive element content?

- How do variations in chemistry and temperature affect the depth (or pressure), thickness, and amplitude of the post-perovskite transition in the lowermost mantle?
- What are the temperatures and chemistries of the two large, low-shear velocity provinces in the deep mantle?
- With respect to ultra-low velocity zones, what are the properties of silicate melts at core-mantle boundary conditions, and how, and at what level, can the core enrich the mantle in iron at Earth's core-mantle boundary?

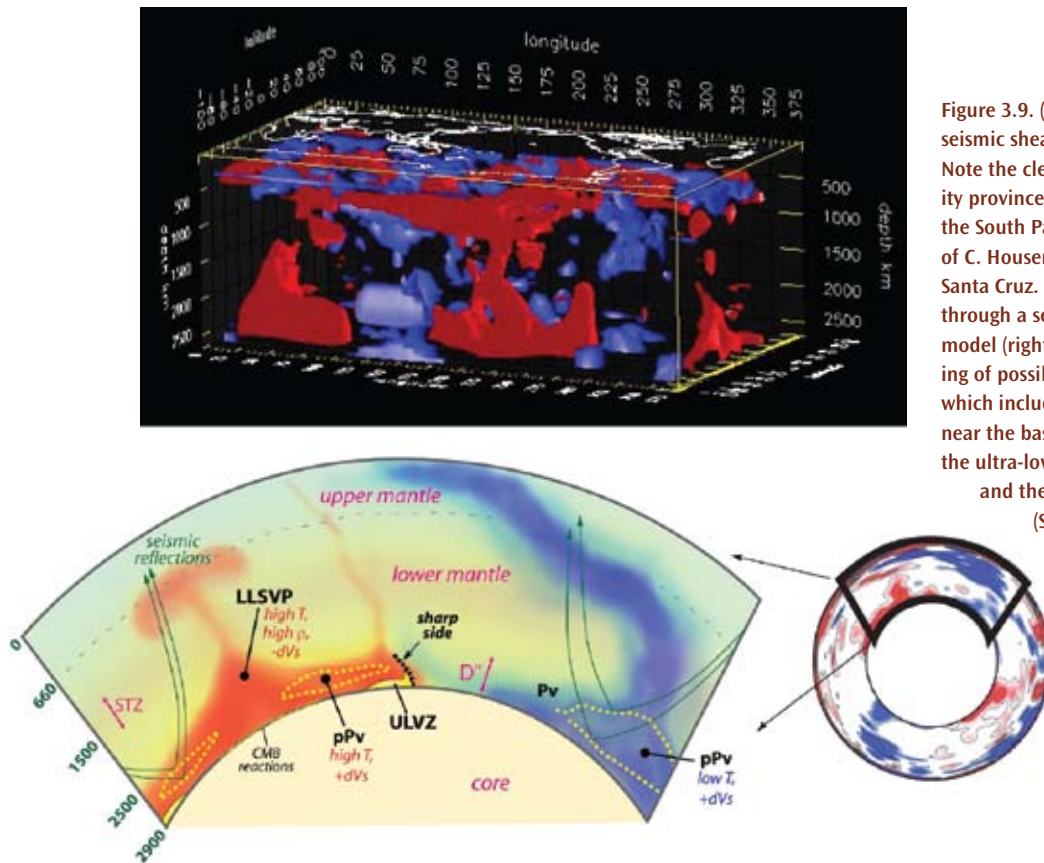


Figure 3.9. (top) Contoured global seismic shear velocity anomalies. Note the clear large, low-shear velocity province (LLVSP) features beneath the South Pacific and Africa. Courtesy of C. Houser, University of California, Santa Cruz. (bottom) Cross section through a seismic tomographic model (right) and interpretive drawing of possible features present, which include LLSVPs, post-perovskite near the base of the mantle (pPv), the ultra-low velocity zone (ULVZ), and the spin-transition zone (STZ). From: Figure 1 in Garnero and McNamara (2008). Reprinted with permission from AAAS.

# Chapter 4 | The Third Dimension of Plate Tectonics

Development of the plate tectonic paradigm is surely the prime achievement of the geosciences in the 20<sup>th</sup> century. It provides a comprehensive understanding of how the surface of our planet evolves, and explains processes ranging from the driving force of seismic failure, to mountain building, to most volcanism. The surficial lateral motion of plates is well understood from a wide range of geodetic and geologic measurements. What remains an enigma, however, is the third dimension of plate tectonics. This third dimension includes the ultimate fate of subducting slabs, features that exert a downward pull that translates to lateral forces, and their interaction with Earth's internal system. By the same token, the manner in which upwellings—mid-ocean ridges and non-tectonic volcanism—are sourced from great depths lies also at the cutting edge of our understanding of the deep planet. Moreover, how the planet progressed from having an early, likely largely molten uppermost few hundred kilometers (or more) of the mantle 4.5 billion years ago to its current, generally well-characterized near-surface system in which plates overlie a mostly solid (but actively convecting) mantle remains fraught with uncertainties. Hence, deriving constraints on how the interaction between the deep Earth and the plate tectonic system has evolved throughout Earth history represents one of the high-pressure geoscience community's principal challenges.

In tandem with seismic probes of the planet's interior, geochemical examination of rocks generated at and extracted from depth, and geodynamic simulations, the tasks for the field of high-pressure geosciences involve constraining the composition, minerals, viscosity, density, and temperature at

depth, which in turn map into the buoyancy forces that drive upwellings and downwellings within the planet. Ultimately, the most basic reason that cold slabs sink and hot materials rise involves the thermal expansion of Earth materials—their decrease in density with increased temperature. The rate at which they move is, in turn, also controlled by the viscosity of the material through which the upwellings and downwellings migrate. But, temperature is not the only property that produces positive and negative buoyancy. Compositional shifts, such as iron enrichment or depletion, and changes in phase (which are often correlated with composition) can also control whether material is buoyant. A classic example of such effects involves the mineral garnet. At pressures corresponding to depths of ~50 km, this mineral becomes abundant within subducted oceanic crust, at which point this formerly buoyant crustal material becomes denser than its surrounding mantle—an effect produced by the abundance of aluminum within basaltic oceanic crust.

## Thermoelasticity and Seismic Mapping of the Planet

The primary evidence that can be brought to bear to understand the nature of the mantle convection, which ultimately drive plate tectonics, involves variations in seismic wave velocities, and discontinuities in seismic wave velocities within Earth's interior. Such seismic data on Earth's interior usually include the velocity of both compressional and shear waves (so-called “body waves,” as opposed to surface waves, which primarily sample the uppermost few hundred kilometers of the planet). Compressional waves

have particle motions in the same direction as wave propagation (akin to sound waves), while shear waves have particle motions perpendicular to the direction of propagation.

One of the major challenges for high-pressure geosciences involves determining the dependence of seismic wave velocity on pressure, temperature, composition, frequency, and even crystal orientation of the materials of Earth's interior. Seismic waves typically have frequencies of about 1 Hertz and wavelengths on the order of kilometers, far in excess of the dimensions of high-pressure samples. Hence, experiments that directly constrain wave velocities are conducted using either ultrasonic sound waves (often in the megahertz range), or laser light (Brillouin spectroscopy, usually in the gigahertz range). But, velocities also depend on the elastic properties of Earth materials—how materials respond to compression or shearing while held at high pressures. So, measurements of density as a function of pressure and/or temperature (under static, or zero frequency conditions) can yield elastic moduli that can be compared with either seismic measurements or the results of high-frequency experiments. Thus, such experiments can be used to validate that high-frequency results can be extrapolated to seismic frequencies.

In instances where there is a frequency dependence of velocity (i.e., dispersion), or where attenuation of waves can be measured, then these

provide prima facie evidence that anelastic behavior is occurring within the material—that is, a portion of the energy of the waves is being absorbed as they travel through the material. Such anelasticity can be constrained in the seismic frequency band from the attenuation of seismic waves, and strong attenuation provides an indication that grain size or partial melt effects are present within the mantle. Evaluating the relative magnitude of these different effects requires a sequence of challenging measurements, often in a range that approaches the low frequency of seismic waves. While progress has been made in this area,

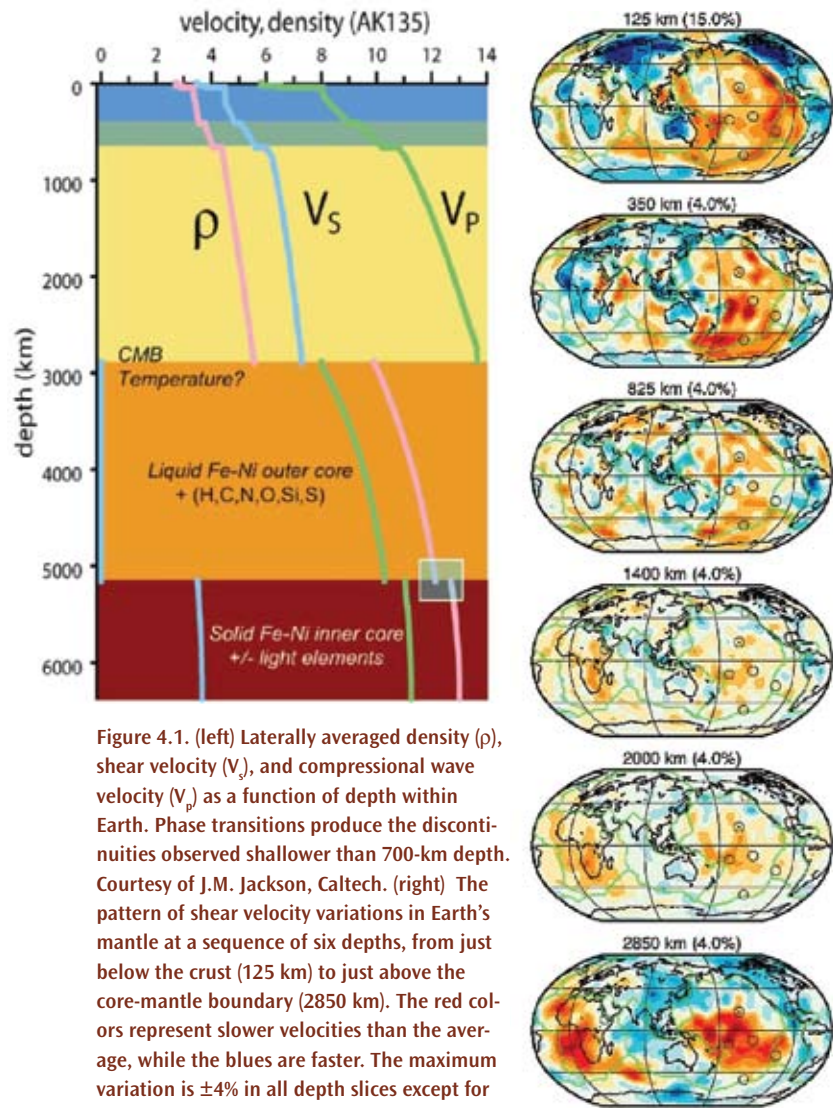


Figure 4.1. (left) Laterally averaged density ( $\rho$ ), shear velocity ( $V_s$ ), and compressional wave velocity ( $V_p$ ) as a function of depth within Earth. Phase transitions produce the discontinuities observed shallower than 700-km depth. Courtesy of J.M. Jackson, Caltech. (right) The pattern of shear velocity variations in Earth's mantle at a sequence of six depths, from just below the crust (125 km) to just above the core-mantle boundary (2850 km). The red colors represent slower velocities than the average, while the blues are faster. The maximum variation is  $\pm 4\%$  in all depth slices except for the shallowest depth, where the variations are  $\pm 15\%$ . From: Ritsema et al. (2004).

the ability to fully interpret seismic maps of mantle attenuation remains incomplete, and a primary future goal is to better constrain anelastic effects within Earth's mantle.

Within the elastic regime, the challenges are to map out the relative variations of compressional and shear wave velocity so that, for example, regions in the planet of higher temperature (and hence lowered wave velocities) can be distinguished from zones with enriched iron contents (which would also be characterized by lower wave velocities, but often have different ratios of shear to compressional wave velocity depression). Obviously, tradeoffs exist with respect to enrichments in other elements as well (e.g., water content), and distinguishing different compositional signatures from one another and from the characteristics of thermal anomalies represents a primary challenge. In this sense, the overall field of *thermoelasticity* provides the basis for determining what the complex variations in seismic velocities in the deep Earth mean, and how they map into variations in temperature or chemistry at depth. This effectively provides the means by which the characteristics of rocks—what types of rocks they might be and how hot they are—can be determined remotely through a combination of seismic observations and high-pressure measurements and calculations. It is this ability to meaningfully probe and interpret results from regions of the planet that we can never view or sample that has enabled high-pressure geoscientists to geologically map the third dimension of plate tectonics, resolving the motion of solids at depth that drives our plate tectonic system, and compositional variations that have a complex interplay with the fluid dynamics of the deep Earth system. The capability to describe the forces that drive mantle convection allows the time dependence of mantle flow to be addressed, and hence permit constraints on the likely history (or fourth dimension) of plate tectonics on Earth. Indeed, the results that we derive, which can constrain both the chemical and thermal buoyancy (whether positive or negative) of regions of the deep Earth, ultimately feed directly back into our

understanding of the history and dynamics of Earth's interior—the dynamics that, from beneath, continue to drive our plate tectonic engine.

## The Transition Zone and Mantle Phase Transitions

Earth's mantle is divided into two main parts: the upper mantle, extending down to ~400-km depth, and the lower mantle, which begins near 700-km depth. The transition zone lies between these two depths. The samples that we have from these regions decrease progressively in abundance with depth. From the upper mantle, we have abundant samples that were entrained in volcanic upwellings, while from the massive lower mantle, there might exist a few isolated samples of a few tens of microns in dimensions embedded within diamonds. From the transition zone, occasional rock fragments have made their way to Earth's surface. Within the transition zone, the common minerals of the upper mantle—olivine (also known as the gemstone peridot) and pyroxenes—convert to a suite of spinel- and garnet-related as well as more complex crystal structures (dubbed ringwoodite, majorite, and wadsleyite, respectively) before ultimately converting to silicate perovskites and a simple magnesium-iron oxide at the top of the lower mantle. The pressures at which these transitions initiate, and the width of the pressure interval required for them to proceed to completion, depend on both temperature and, to a lesser extent, composition. Therefore, seismic characterizations of the depth and sharpness of these discontinuities can, when coupled with accurate laboratory measurements of these transitions, provide a particularly accurate gauge of the temperature and composition through this critical region of the planet. It is in the transition zone region that downwelling slabs can be markedly deflected, with some even becoming nearly horizontal, and where their seismic signature appears to dramatically broaden—a likely indicator of increased viscosity at depth.

The underpinning causes of deep earthquakes, those that occur between ~350- and 684-km depth (the depth of the deepest earthquake ever recorded), may well be connected to the phase transitions that occur within the transition zone. These events are always associated with ancient subducted material. However, they occur at depths below which the normal brittle fracture that generates near-surface seismic events is likely completely suppressed by pressure. Therefore, mechanisms different from standard low-pressure faulting are likely required to explain why these deep events occur. The idea that these events are associated with how phase transitions proceed within subducted slabs (with the transitions likely impeded by the low temperatures present in these environments) has provided a possible suite of solutions to this long-standing dilemma (faulting within metastable material that is converting to its high-pressure/temperature phases). Hence, exploration of the linkages between phase transitions and seismic failure is motivated by the importance of understanding the deeper portion of the planet's seismicity.

Although the general nature of the transitions that give rise to the seismic discontinuities within the transition zone are known, their precise temperature and composition dependences remain areas of extraordinarily active inquiry. Future progress on this topic awaits refinement of pressure scales for materials used as pressure/temperature standards in many experiments (which include MgO, gold, and NaCl). Indeed, as our understanding of the transition zone has become more nuanced, complexities that we could not have envisioned a decade ago have shifted our interpretations of the behavior of different regions of the transition zone—for example, water and partial melting may each play a major role in the depths at which these transitions occur in different regions. And, tantalizing hints have emerged that phase transitions in the low-temperature cores of subduction zones may be dramatically deflected, with major potential implications for the buoyancy forces associated with subduction and hence the driving force of plate tectonics itself. The diversity of structural richness that we are beginning to recognize in

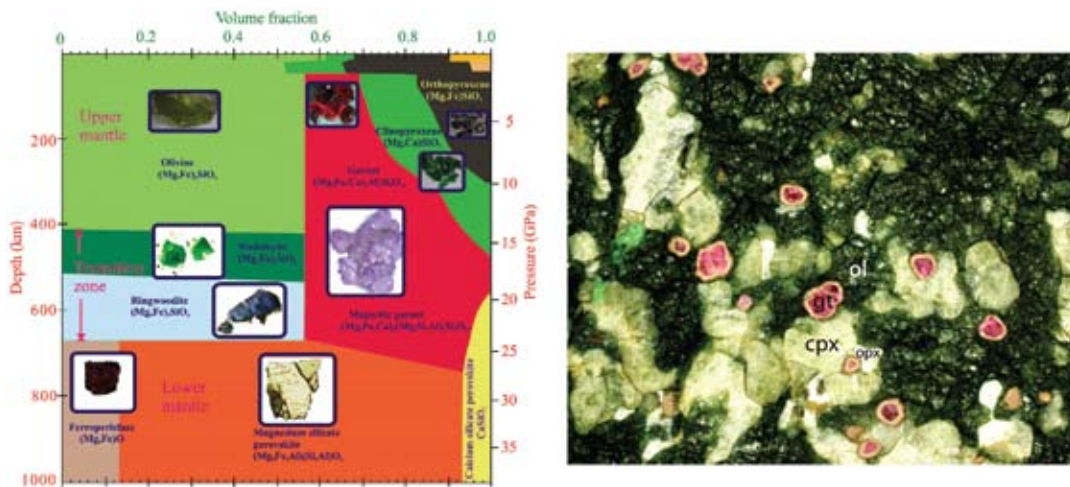


Figure 4.2. (left) Phase assemblages within peridotite, the widely inferred composition of Earth's upper mantle, illustrating the phases present at depth within the planet. The work conducted by the high-pressure geosciences community in constraining this phase diagram over this pressure range at variable temperatures has been extensive; work at higher pressure/deeper conditions is far sparser, due to the experimental difficulties in conducting such work. From: Figure 1 in Frost (2008); reproduced with permission from the Mineralogical Society of America. (right) Cross section through a peridotitic rock that was entrained to the surface in a volcanic upwelling, with olivine (ol), garnet (gt), clinopyroxene (cpx), and orthopyroxene (opx) labeled. Courtesy of H.W. Green, University of California, Riverside.

this region of the planet furnishes another example of the crucial synergies that have arisen between improved seismic characterization and an enhanced understanding of the properties of Earth materials at extreme conditions.

## Deeper Transitions?

In addition to the transition to the post-perovskite phase that occurs near the core-mantle boundary, the iron contained within silicate minerals has been discovered to undergo a transition that involves the pressure-induced pairing of iron's *d*-electrons at depths

in the mid-lower mantle: the high-spin to low-spin transition. Although there were long-standing suspicions that such transitions might occur in Earth's mantle, proof of their existence was achieved only in the last few years. These discoveries were enabled by state-of-the-art x-ray sources and spectroscopic experiments at national facilities (such as those in the DOE national laboratories in the United States, as well as in Japan and Europe), coupled with high-level first principles theoretical investigations. In tandem with the discovery of the changes in spin state, a new generation of experiments on the magnetic properties of minerals at extreme conditions was initiated involving synchrotron-based measurements of the Mossbauer effect, in which light is absorbed or emitted at the energies of transitions in the nuclei of atoms. These energies are dependent

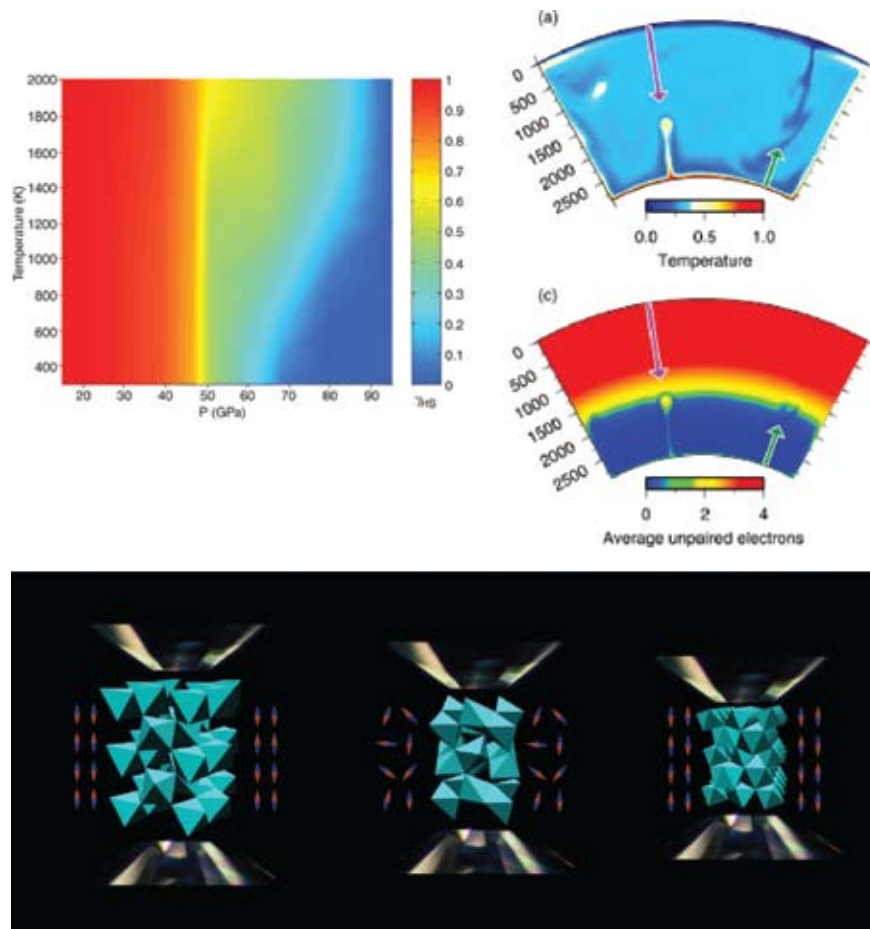


Figure 4.3. (Top left) Experimental constraints on the gradual change in iron spin state in (Mg,Fe)O. Red represents electronic configurations in which iron is in a high-spin state (scale is in terms of fraction of iron that is in a high-spin state), blue represents an electron-paired, or low-spin state of iron, and intermediate colors represent intermediate spin states. The occurrence of spin transitions over an approximately 40 GPa pressure range, or 1000-km depth range, is unique among major transitions in mantle minerals, and was entirely unexpected. From: Figure 3 in Lin et al. (2007); reproduced with permission from AAAS. (Top right) Possible geodynamic implications of gradual spin transitions. Here, the rising of a hot upwelling (indicated by the purple arrow) is enhanced by the spin transition, as hot material accesses the low-density, high-spin structure at higher pressures; correspondingly, a cold downwelling's vertical velocity is also enhanced (green arrow). From: Bower et al. (2009). (Bottom) Artist's interpretation of deep-mantle mineral magnetism. Two opposing diamond anvils symbolize increasing pressure under which the magnetism in  $\text{Fe}_2\text{O}_3$  first disappears but then surprisingly reappears at very high pressure. The occurrence of such complex magnetic phase transitions is expected to profoundly affect our understanding of planetary magnetic records. Courtesy of S.-H. Shim (after Shim et al., 2009).



on the magnetic and structural environment around the atom. These atomic nucleus-oriented experiments have produced some highly unexpected and conceptually challenging results. As with many discoveries, the recognition of these spin transitions generated a broad suite of previously unanticipated questions, including: (1) should these transitions exhibit a seismic signature (and, if so, what might it be)? (2) what are the effects of these transitions on mantle heat transport? and (3) how does the temperature dependence of these transitions affect the vigor of thermal upwellings and downwellings? These questions represent extremely active areas of inquiry, and this discovery has driven a high level of interdisciplinary attention and collaborations between high-pressure geosciences and the seismology and geodynamics communities. The discovery of these new states of iron illustrate the type of new insights that the community has garnered, and believes it can continue to garner, from new technologies as they come on line.

Although the high-pressure geosciences community has achieved a general understanding of mantle mineralogy, our certainty about the chemistries and complete mineral assemblages present within different mantle rocks decreases as one goes deeper into Earth's mantle—and this uncertainty impacts our understanding of geochemical processes likely to occur at depth within the planet. Hence, a principal goal of our community is to understand how different elements partition between minerals (and coexisting melts) within the deep mantle, and to determine the stability range and chemistry of important minor phases. As simple examples, potassium-carrying minerals appear to be present in small abundance in a range of mantle rocks at depth. Yet, even with their small abundances, such minerals are major players in determining the likely concentrations of radioactive, heat-generating elements present within the silicate mantle. However, the composition, chemistries, and stability range of such minerals are not well constrained.

Correspondingly, the presence of water-bearing minerals (with water either dissolved as a defect within nominally dry minerals, or water actually bound as a fundamental part of a mineral's crystal structure) is a well-documented possibility within Earth's upper mantle. The effects of such water on the seismic velocity of water-bearing assemblages and on the chemistry of melts produced at upper mantle depths remain areas of active inquiry. Moreover, the role of water, and the ability to retain water, within the deeper mantle remain obscure. A major goal of our community is to conduct accurate chemical, phase, and elasticity characterizations on mantle assemblages across the entire range of mantle pressures, temperatures, and possible chemistries—in essence, we wish to understand the nature and properties of the rocks that make up the bulk of our planet.

### **Thermal and Electrical Conductivity of Mantle Minerals: How Does the Mantle Homogenize and Transport Heat and Electrons?**

The ability of Earth materials to transport heat and electrical charge influences phenomena as disparate and key as the cooling rate of the planet and the ability of the magnetic field to be transmitted through Earth's ceramic mantle. Indeed, the mobility of electrical charge and the ability of heat to be transported are material parameters that influence in a fundamental way our understanding of Earth's inner workings.

Thermal conductivity governs how heat is transported from Earth's core, into the mantle, and subsequently out of the mantle into the crust and to the surface. Electrical conductivity, which governs how electrical charge is carried through Earth materials, is very sensitive to temperature, composition, and the presence of highly conducting fluids or minor phases. Knowledge of these properties under the extreme conditions of Earth's interior from core to crust is crucial for unraveling key questions concerning the planet's origin, evolution, composition, volatile budget, and the genesis and nature of plate tectonics.

Zones with highly elevated electrical conductivity occur in the crust related to magmatic/volcanic structures, and in parts of the mantle that may contain volatiles or hydrous partial melts. At deeper depths, structures at the core-mantle boundary, such as ultra-low velocity zones that exist in patches at the core mantle boundary, may also be highly electrically conducting and may affect Earth's magnetic field. The overarching question that emerges from such heterogeneities is: what is Earth's electrical conductivity—from core to crust, and how is it affected by changes in temperature, iron content, volatile content, partial melt, and/or fluids?

Electrical conductivity at depth can be determined by methods that include magnetotellurics, geomagnetic depth sounding, and satellite magnetic measurements. In the future, long-term satellite measurements may be able to provide a full global three-dimensional conductivity structure of Earth. Interpreting these results properly depends on accurate determination of electrical conductivity values of candidate Earth materials under extreme conditions and also upon having models of defect and ionic concentration and mobility to extend the results to unmeasured conditions and compositions. This combination of measurements and observations may be able to answer the issue of the water (hydrogen) content of Earth's interior—a topic that is crucial for our understanding of water cycling between the surface and interior, and the evolution of Earth's hydrosphere. The presence of small amounts of water in a mineral's structure can cause a great increase in its electrical conductivity. Furthermore, a reasonably precise mantle electrical conductivity model is necessary to fully interpret magnetic field observations and to properly infer conditions in the core—conductivity within the mantle acts as a partial screen for Earth's magnetic

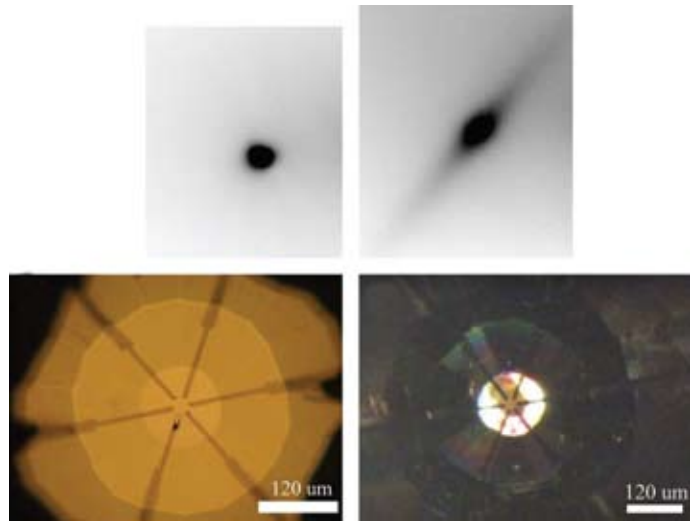


Figure 4.4. (top) An example of one means of measuring thermal conductivity. A reverse-color image of a laser-heated spot on two different orientations of graphite; in the image on the right, the beam is impinging on a high thermal conductivity crystallographic direction in graphite, and heat is being transported away from the circular laser spot. From: Figure 6a in Kavner and Nugent (2008). (bottom, left) Vapor-deposited electrical leads on a diamond anvil for electrical conductivity measurements. Here, with the exception of small tabs within the sample, the leads have been coated with a layer of vapor-deposited diamond. (bottom, right) A sample of (Mg,Fe)O in transmitted light at high pressures with its electrical conductivity being measured by a multiprobe technique. From: Figure 1 in Lin et al. (2007).

field, and reconstructing the nature of the screen can allow accurate reconstructions of the field at the top of the outer core.

Thermal conductivities of mantle materials are crucial for determining how heat is transferred between zones that do not exchange heat via fluid motion (through convective transport). Hence, the thicknesses of boundary layers—like those between the core and mantle, between cold subducted slabs and surrounding mantle, and between the convecting mantle and the surface—hinge on the thermal conductivity of mantle materials. Transport of heat can occur via different mechanisms, including through interatomic vibrations in crystals (lattice conductivity) and through radiative conductivity—heat transport via light. Naturally, the latter mechanism depends on the transparency of minerals at high pressures and temperatures—and the optical properties of

the complex crystals of Earth's mantle. Experiments to constrain both lattice and radiative thermal conductivities at the conditions of Earth's interior are at the cutting edge of current techniques—and our community has only begun to systematically characterize the dependence of this vital transport property on parameters that include pressure, temperature, chemistry and grain size. The goals here are to achieve an understanding of how heat leaves the core and enters the mantle, the temperature and conditions of the core-mantle boundary region, and how rapidly subducted slabs/cold convective downwellings thermally equilibrate with the surrounding mantle. The anticipated outcomes are to establish the boundary conditions on mantle convection, and hence provide constraints on how plate tectonics itself operates.

### **Chemical Diffusivity and Viscosity: How Does the Mantle Mix and Flow?**

The properties of chemical diffusion and viscosity (rheology) each control mantle mixing at different length scales. Over time, chemical diffusion can cause rocks to locally reach equilibrium with each other over scales of millimeters to many meters, effectively blending and homogenizing materials with different compositions, provenances, and histories. Viscosity, on the other hand, exercises a fundamental control on the vigor and length scale of convective motion within the solid mantle, and therefore dictates how material is mixed into Earth's mantle at length scales greater than meters. Although mantle viscosity is known to be roughly  $10^{20}$  times that of water from a wide suite of observations, including ongoing vertical rebound of northern Canada and Fennoscandia from glacial loading and modeling of Earth's gravity field and plate rates, its dependence on depth is not well constrained in the deep planet. Moreover, possible lateral variations in viscosity are important for understanding how the deep mantle flows (or, in solid state parlance, how it creeps). For example, in the upper mantle, the viscosity structure of the oceanic

mantle likely plays a principal role in determining that mid-ocean ridge volcanism is narrowly confined to the ridge crest.

With respect to diffusion, experimental measurements of atomic diffusion rates in minerals have only recently become possible at pressures extending deeper than the top of the lower mantle. There are now experimental data on transition zone minerals (wadsleyite, ringwoodite) and lower mantle minerals ( $\text{MgSiO}_3$  perovskite,  $(\text{Mg,Fe})\text{O}$ -ferropericlase) at pressures up to 35 GPa (corresponding to a depth of  $\sim 1000$  km), including diffusion of Si and O, which probably are the rate-limiting ions in the high-temperature creep deformation responsible for mantle flow. These advances have been enabled by the development of large-volume pressure cells with uniform temperature and low shear stress (but high pressure) over a large volume ( $\sim 1 \text{ mm}^3$ ), and by the development of isotopic and chemical probes with high spatial resolution, such as secondary ion mass spectrometry (SIMS and nano-SIMS), Rutherford Back-Scattering (RBS) techniques, and analytical transmission electron microscopy (ATEM). The high-pressure geosciences community is at an unusual time of convergence between excellent (and recently developed) nanoscale materials characterization techniques and an unprecedented sophistication of high-pressure experimental design.

Complementary computational studies of diffusion in minerals have also made significant advances. Classical molecular dynamics studies can now be conducted on systems containing a billion atoms for times up to a nanosecond—although this seems brief, it is orders of magnitude longer than characteristic molecular vibrational time scales, and hence is viewed as essentially accessing steady-state behavior. Such simulations open the possibility of simulating actual diffusive hopping of atoms in minerals, rare events that require a large number of atoms and long simulation times to acquire the statistics necessary to calculate diffusion coefficients. First-principles simulations are now capable of accurately determining the energy required for an atom to hop to an adjacent vacant site

and the energy of vacancy formation, from which the diffusion coefficients can be calculated. In MgO, for example, there is excellent agreement between first-principles simulations and experiments on the absolute diffusion rates and the pressure and temperature dependence of cation and anion diffusion.

With respect to viscosity, measurements of the flow of materials at controlled high pressures and temperatures, and at a known differential stress or strain, have long been viewed as among the most challenging of experiments at extreme conditions. Yet, new technical developments have significantly extended the range over which flow properties can be determined; many of these advances have profited from funding of Grand Challenge grants from the NSF Division of Earth Sciences. The development of large-volume presses designed to measure deformation and apparatuses that rotationally shear a sample while it is held at high pressures enable measurements of deformation and fabric development with a well-controlled strain rate, temperature, and chemical environment at pressures extending into the mantle transition zone (up to 17 GPa, corresponding to a depth of ~500 km, with prospects of measurements to 25 GPa, or 750-km depth). Development of higher-pressure diamond anvil cell techniques coupled with radial x-ray diffraction measurements, which effectively measure the response to shear stress within high-pressure samples, provide information on material strength and slip mechanisms under very high pressures, but to date largely provide information at low temperatures and relatively high stresses. Similar to diffusion measurements, tandem advances in analytic methods and in high-pressure techniques are enabling experimentalists to push the frontiers of viscosity measurements at extreme conditions. The prospect exists, in the foreseeable future, for constraining the viscosity of Earth materials throughout the conditions of Earth's mantle.

## Properties of Planetary Fluids— Magmas and Metasomatism

The most popularly recognized manifestation of Earth's deep heat is volcanoes. Less-widely appreciated is that magmas also provide the medium through which Earth has differentiated to its current layered structure of crust, mantle, and core, and that magmas are ultimately the origin of the geochemical differences between subducted slabs and their surrounding mantle. For example, the continental crust on which the human race resides is produced through subduction-generated entrainment of hydrous minerals to depth followed by their decomposition and release of water under the high temperatures of Earth's interior. This ascent of water from the slab into the overlying mantle and water-induced melting is an expression of the importance of not only magmas, but fluid in the deep Earth. Moreover, magmas represent perhaps the most prevalent samples of the planet's interior. Determining what types of magmas, and their chemical characteristics, are generated from different source rocks at different pressure and temperature conditions yields fundamental insights into not only how and where magmas are generated, but also the nature of the rocks themselves at depth. From a surface-oriented perspective, magmatism and metasomatism (the process of alteration of rocks in Earth's interior by fluids) are critical parts of the cycling of both carbon dioxide and water between the interior and the surface (and vice versa). The physical and chemical properties of magmas and fluids are hence of major interest not only as the principal mechanism of Earth differentiation, but also as a key part of how (and whether) volatiles are retained or released from the interior.

From the point of view of Earth's history and evolution, magmas were almost certainly more prevalent in the past than in the present. This conclusion is a simple consequence of Earth's net cooling (largely through plate tectonic processes) through time. The current paradigm of lunar formation through collision of an approximately Mars-sized object with Earth ~4.5 billion years ago essentially dictates that a large

portion of the early Earth was melted, and that the properties of melts at high pressure controlled Earth's earliest evolution. A planet with much of its uppermost few hundred kilometers (at a minimum) melted poses unusual challenges in modeling the crystallization history and dynamics of a magma ocean. Our terrestrial magma ocean certainly played a fundamental role in setting the stage for subsequent Earth evolution, including the initiation of plate tectonics. In contrast, an early magma ocean also occurred on our moon, and no plate tectonics resulted on this smaller body. Although provocative experimental and theoretical results have been generated, the constraints on the properties of an almost entirely molten planet—which includes the chemistry and density of the first solids to crystallize from a melt, and the thermodynamic, transport, and textural properties of a largely melted system—remain in their infancy.

An overarching goal for the field of high-pressure geosciences is to develop a precise understanding of the melting relations (as well as both major and minor element chemistry of melts) of the likely range of mantle assemblages throughout the depth range of Earth's mantle, and from wholly molten systems to the partial melting of materials that predominate today. However, simply constraining the compositions of melts that are generated is only a part of the problem (albeit a large one). For example, the density of magmas control whether they ascend or descend within Earth, and a broad suite of evidence has been gathered that indicates that silicate melts at a range of depths within the planet may sink—and hence never be observed at Earth's surface. Such sinking melts may well give rise to regional (and gigantic in comparison to the scales of crustal magma chambers) zones of partial melt both above the 400-km seismic discontinuity, where olivine transforms to the complexly structured wadsleyite phase, and within the ultra-low velocity zone that lies above parts of Earth's core-mantle boundary. Moreover, both the melts' viscosity and surface tension control how, and in what manner they are able to ascend—whether these melts will predominantly travel along grain boundaries,

wetting the surrounding rock as they travel, or whether they ascend through channels or via bulk ascent of a magmatic blob (or diapir). The viscosity of high-pressure melts is also critical in determining the rates of flow, and hence the speed of cooling, of a magma ocean early in Earth's history. Therefore, as with their corresponding solids, the thermoelasticity of melts (particularly their density, thermal expansion, and compressibility) and their viscous behavior are of key importance for our understanding of the evolution of our planet.

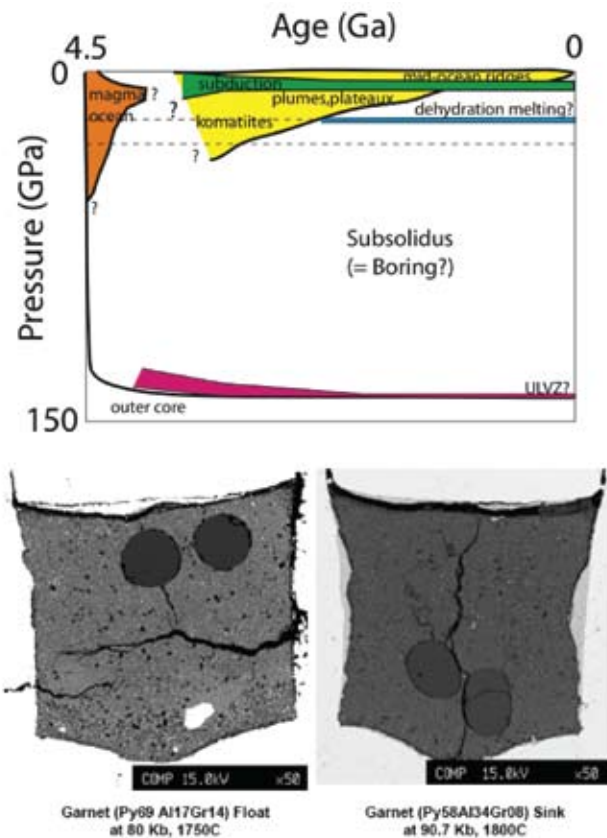


Figure 4.5. (top) Evolution of melt distribution and types of melting as a function of depth through Earth's history. Dotted lines denote the pressures of the 400- and 670-km discontinuities. Courtesy of P. Asimow, Caltech. (bottom) The float-sink method for determining the density of melts, and whether they are positively or negatively buoyant. Here, at modestly different pressure conditions corresponding to ~240- and 270-km depth in Earth, respectively, garnet spheres float (left) or sink (right) within a basaltic melt. The density of the melt is bracketed, and the melt on the left is more dense than this particular garnet chemistry. Courtesy of C. Agee, University of New Mexico.

The role of water-rich fluids is similarly of primary importance. Aqueous fluids represent a major means of element transport within both Earth's crust and within the region of the mantle that overlies subducting slabs—and underlies Earth's subduction-induced volcanic Ring of Fire. Indeed, water is known to greatly lower the melting temperatures of Earth materials, and both the properties and behavior of aqueous fluids, and their precise relationship with the genesis of silicate melts, is not only of interest to the high-pressure geosciences community, but also of major societal interest. Such water-facilitated volcanism is the root cause of almost all life-threatening volcanism on the planet. The underpinning geochemical influences and signatures of the flux of water within both magmas and rocks are fundamental to our understanding of the process of metasomatism and, while significant progress has been made in these areas, the pressure and temperature ranges over which detailed information is available on the interactions of aqueous fluids with rocks remain relatively modest. Novel and unexpected new insights have been garnered from modest extensions in the pressure range of experiments on aqueous solutions. For example, at deep crustal conditions, aqueous fluids and silicate melts form a smooth, entirely miscible continuum of chemistries with one another. The precise manner in which water interacts with rocks within Earth's interior represents a deeper extension of the well-known field of crustal hydrology, with relevance for the cycling of water and the transport of elements within Earth's interior.

### **Linkages Between the Deep Earth and the Lithosphere: Deeply Derived Magmas, Heat Sources, and Metamorphism**

The deep Earth and the lithosphere (crust plus upper mantle) cannot be viewed in isolation from one another. In addition to the generation of both continental and oceanic crust from materials at depth, and the subduction of the lithospheric tectonic plate back into the planet's depths, a range of other means

of exchanging mass and heat between the interior and the near-surface layers have been identified. In fact, both rocks and magmas can move between the deep interior and surface (and vice versa) in ways that are still being probed and discovered. These processes include the genesis of peculiar carbon-rich magmas, as well as high-temperature magmas that were primarily generated early in Earth's history, and massive flood basalt eruptions that almost certainly emerge from considerable depth in the mantle. From the perspective of the interchange of rocks, the recently recognized ability of nominally buoyant continental crustal rocks to be dragged to depths of several hundred kilometers and returned to the surface containing mineralized signatures of their journey to depth represents one of the most provocative and challenging-to-explain recent discoveries in the geosciences.

Among magmas erupted at Earth's surface, only a small number originate at depths greater than a couple of hundred kilometers. These magmas function as carriers of our deepest rock samples. Such magmas include kimberlites—the dominant diamond-bearing ore deposit of the planet. Kimberlites are narrow, pipe-like, CO<sub>2</sub>-driven eruptions that, through the refrigerating decompression of gas on ascent from depth, erupt at temperatures cold enough that diamonds (whose stable phase at ambient pressures is graphite) are metastably retained. From ballistic analyses, their eruption velocity is estimated to be of order of hundreds of kilometers per hour—a rate commensurate with a gas-driven eruption. Other carbon-rich magmas that emerge from depth and have considerable economic interest include carbonatites—very-low-viscosity carbon-rich melts that provide the major economic reservoirs of strategic elements such as niobium. These carbon-rich melts are thought to be the first melts derived from slightly carbonated mantle material. The low viscosity of these melts allows them to percolate rapidly upward along grain-to-grain contacts within the mantle, geochemically interacting with the column of mantle material that they traverse. The manner in which kimberlitic and carbonatitic magmas are produced

is intimately tied to the processing of carbon within the planet and the genesis of diamond and other ore deposits, and are topics of both long-term and ongoing active inquiry. The ability to produce accurate constraints on how carbonate-rich melts are formed and how they move within Earth's deep interior will be markedly improved by recently developed micro-analytic capabilities that the high-pressure geosciences community aspires to make broadly accessible over the next decade.

The record of magmas erupted at Earth's surface provides us with an opportunity to sample the entire range of magma types and eruptions through time. Indeed, there is ample evidence that magmas in the past differ from those erupted today. Before 2.2 billion years ago, lavas called komatiites were far more

common in the geologic record. These magmas are far higher in their MgO content relative to today's basalts and can loosely be viewed as a composition intermediate between the basalt that makes up today's ocean basins and that of the underlying mantle. The mechanism initially proposed for generating such magmas involved higher temperatures within the ancient Earth—perhaps 200–400 K hotter than today. Recently, however, it has been appreciated that the same effect could be generated by such magmas being substantially wetter than most of today's usual basalts. The key issue that arises here is: how have Earth's volcanic effluxions changed through time, and what do these changes tell us about the planet's evolution? An enhanced understanding of how the mantle melts under a broad suite of deep Earth conditions

would lead to a marked improvement in our ability to interpret our ancient rock record in the context of our planet's evolution.

The most massive eruptions of the last 300 million years of Earth's history are flood basalts, which are huge eruptions, spanning as much as  $4 \times 10^6$  km<sup>3</sup> in the case of the Siberian Traps—an event whose eruption was synchronous with the Permian-Triassic mass extinction of 251 million years ago. Within the United States, the last such eruption produced the Columbia River Flood Basalts, initiated about 17 million years ago. Although their volume is over an

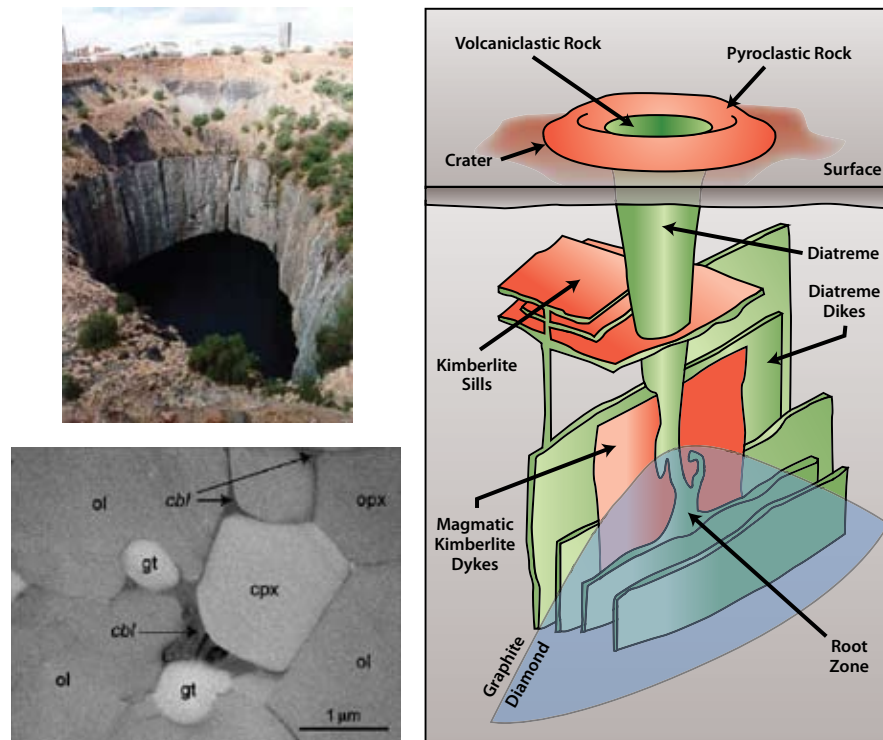


Figure 4.6. (top left) The Kimberley Big Hole #1, which at surface depths is a mined-out kimberlite pipe. The structure in background is the 15-story DeBeers diamond sorting building. Courtesy of M. Billen, University of California, Davis. (bottom left) An experiment determining the composition and location of carbonate-rich melts in a mantle assemblage at high pressures. Gt indicates garnet, ol is olivine, cpx is clinopyroxene, opx is orthopyroxene, and cbl is the carbonatite liquid. Courtesy of R. Dasgupta, Rice University. (Right) Schematic of the inferred deep structure of kimberlite pipes, extending from the diamond stability field near 150-km depth to the surface. Redrawn from: <http://www.ags.gov.ab.ca/minerals/diamonds/diamonds.html>.

order of magnitude less than the Siberian Traps, they still cover a large portion of the states of Washington and Oregon to depths of hundreds of meters.

Approximately 18 such flood basalt occurrences are recorded in the geologic record. The volume of even the smallest of flood basalts indicates that extensive melting of a large portion of Earth's upper mantle took place under a fairly confined geographical area. Hence, a large heat source at depth is likely also required to generate these features—and the origin of this heat has been argued by some to lie very deep in Earth's mantle, and perhaps even at its interface with the core. Regardless of its precise origin, the means by which such massive volcanic events are generated is clearly tied to how Earth's mantle melts. Thus, a comprehensive database on both the melting of mantle materials at high pressures and temperatures, and the physical and textural properties of melt/rock aggregates at extreme conditions, would lead to great advances in understanding the production of such enormous (and, for the biosphere, massively destructive) volcanic events.

Although buoyant magmas are well known to ascend from depth, it came as a surprise when buoyant continental rocks found in a few locations (the Himalayas, Alps, and Norway) were recognized as having clearly descended to depths of several hundred kilometers, probably by being entrained in a descending flow (and then subsequently exhumed). Evidence for this descent includes both the presence of high-pressure phases (including, in some instances, microdiamonds) that can only exist at depths of 150 km or more, as well as the compositions of coexisting mineral phases that can only occur at deep depths. These environments, subjected to ultra-high-pressure metamorphism, provide an unusual tectonic conundrum—what sorts of environments are required to push (or pull) a block of buoyant material down to deep depths, and then allow it to return to the surface? And, what constraints do these observations place on rheological and other transport properties of the crust and mantle? Related issues also arise that bear fundamentally on the processing

of continental crust, such as: how much continental material is pulled down into Earth's mantle and does not return to Earth's surface, being ultimately remixed back into the mantle? The recycling of oceanic crust through subduction has long been appreciated, but the idea that a mechanism may exist for potentially entraining coherent blocks of continental crust back into the mantle produces a new paradigm for potential two-way flow (genesis from the mantle, and perhaps occasional return) between the geochemical reservoirs of continental crust and the deep mantle.

### Key Questions

- What do variations in seismic wave velocities imply for the composition and temperature field at all depths through the mantle, and hence for the overall pattern of mantle convection?
- What are the melting and phase relations of mantle materials from the near surface to the core-mantle boundary, and what are the chemistries and physical properties of melts generated at different depths within the planet's interior?
- What does the history of magmatism on Earth reveal about the changing state of Earth's interior?
- How does the electronic state of iron change in different minerals at high pressures—and what is the effect of such changes on the physical properties of materials at depth within the planet?
- What are the magnitudes and causes of anelastic effects (i.e., attenuation and dispersion) on seismic wave velocities within Earth?
- How are thermal and electrical conductivities altered by pressure, temperature, and composition within the planet?
- Given constraints on temperature and composition, what is the three-dimensional distribution of viscosity within Earth's mantle?
- How do aqueous and carbon-rich fluids behave at depth, and how do fluids and rocks interact, particularly in subduction-related environments?
- How is buoyant continental material entrained to deep depths and returned to the surface?



# Chapter 5 | Other Planets, Other Interiors

The other planets of our solar system, their moons, and the burgeoning and surprising number of recently discovered extra-solar planets present remarkable opportunities for examining what processes and events govern planetary evolution. Studies of other planetary bodies yield insight into how our planet was generated—the sole known habitable planet, with stable liquid water at the surface, an equable temperature and, of course, life. Each object in the solar system has arrived at its present state due to a complex interplay between size, composition, its particular evolutionary and accretionary history, and their distance from the sun. Indeed, the planets of our solar system span from gas giants, Jupiter and Saturn, with possible rocky/iron cores of many Earth masses overlain by a liquid mix dominated by hydrogen, helium, carbon, nitrogen and oxygen, to almost water-free objects like Io and Mercury, to “minor” planets such as Ceres and Pluto, which are probably ice and rock-dominated. The larger terrestrial planets (Venus, Earth, Mars, as well as the Moon) have most frequently been the focus of the high-pressure geosciences community, because the lessons learned from experiments on Earth materials can most readily be applied to these bodies. Yet, the field of high-pressure geosciences is well suited to address the complementary effects of planetary size (and thus interior pressure) and composition, and hence to draw key inferences on planetary evolution.

## Terrestrial Planets and Large Moons

Our other terrestrial planets (defined as those planets that are, like Earth, primarily composed of rock and iron), Mercury, Venus, and Mars, each have some degree of commonality with Earth, but also some truly remarkable differences. For example, Mercury is the only other terrestrial planet with an actively generated magnetic field. Its overall density implies that it is far more enriched in iron (or, alternatively, depleted in silicates) relative to any of the other terrestrial planets. In effect, it is a core with an approximately 400–800-km thick silicate veneer (in contrast to Earth’s ~2900-km thick mantle). As an example of the insights that are brought to bear, the high-pressure geosciences community constrained the melting behavior of iron alloys and produced an unusual and provocative picture of the coupling of the core’s thermal evolution with the forces that could drive the fluid flow that generates the Mercurian magnetic dynamo. In effect, solidifying iron within Mercury’s core could descend, or “snow” through the liquid of its core. With respect to the silicate fraction of Mercury, questions arise that are, as with Earth, anchored in the melting behavior of silicates within planets. Is its surface enriched in silica, as are continents on Earth or the white highlands of the Moon, or is it formed from basalt, as is Earth’s ocean floor and the darker portions of the Moon?

A notable synergy exists between new missions, such as the recent Messenger probe, and research on the material properties of planetary interiors. As observations improve, the level at which detailed questions can be posed that require answers from the high-pressure geosciences community is enhanced. Indeed, one of the primary challenges in the era

following Messenger's first Mercury fly-by is to interpret the widespread evidence for highly explosive, volatile-rich volcanism observed at the surface of what has been widely inferred to be a dry and nearly geologically inactive planet.

Venus, in contrast to Earth and Mercury, does not have a magnetic field, and essentially all of its near-surface CO<sub>2</sub> appears to be present in its atmosphere. The ~90 bars of CO<sub>2</sub> in the Venusian atmosphere provide a principal comparison with our own atmosphere, which presently has an atmospheric partial pressure of CO<sub>2</sub> of about 0.0004 bars (or, ~0.0003 bars, prior to the injection of anthropogenic CO<sub>2</sub> into the atmosphere). On Venus, the feedback loop between high (~700 K, or ~800°F) surface temperatures and high CO<sub>2</sub> content of the atmosphere has produced a materials-driven environmental catastrophe for the closest proxy to Earth in the solar system. In short, the decarbonation temperature of carbonates, for which the high-pressure geosciences community has documented the pressure dependence, is exceeded in Venus' near-surface environment. Hence, there are no limestones (the dominant carbon dioxide-bearing rock type near Earth's surface) in the

Venusian crust, only degassed CO<sub>2</sub> in its atmosphere. Moreover, Venus appears to have almost entirely volcanically resurfaced itself ~600 million years ago. The straightforward inference here is that volcanism of the type that produced the Siberian Traps and perhaps the Permo-Triassic boundary's enormous extinctions on Earth occurred, but on a far larger scale (and has perhaps occurred several times) on Venus. Again, voluminous melting of this type involves pervasive and relatively deep mantle melting. Understanding the chemistry and physical properties of melting of Earth and planetary materials at depth is hence of key importance in controlling the evolution of Venus.

The water and carbon reservoirs of Mars remain enigmatic. The degree and manner in which these elements are stored at even shallow depths is unclear. Yet, the compositional constraints on Mars' interior are more robust than those of either Venus or Mercury, as a number of meteorites (meteorite classes known as shergottites, nakhlites, and chassignites) were blasted off of Mars by large impact events and ultimately landed on Earth. Hence, Mars is the only other planet from which we clearly have samples of its volcanic rocks. The net results from these

samples appear to be that the mantle of Mars is more oxidized than that of Earth, and also has a higher iron content. As with Venus, deeply derived thermal events are likely critical in driving Martian volcanism. The largest volcanic edifice in the solar system, Olympus Mons, a volcano three times higher and far more massive than Earth's Mt. Everest or Mauna Loa, is a dominant topographic feature on the red planet. And, there is evidence that Mars once had a magnetic field, but it shut

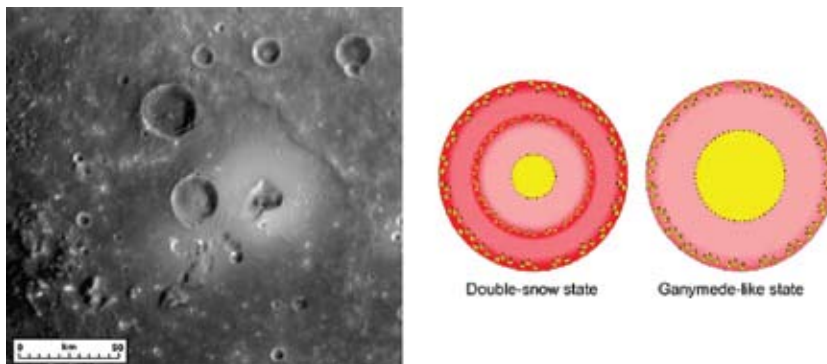
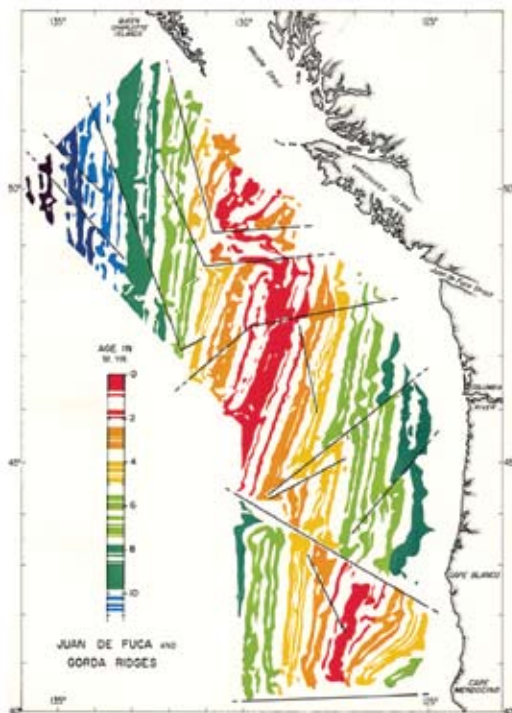
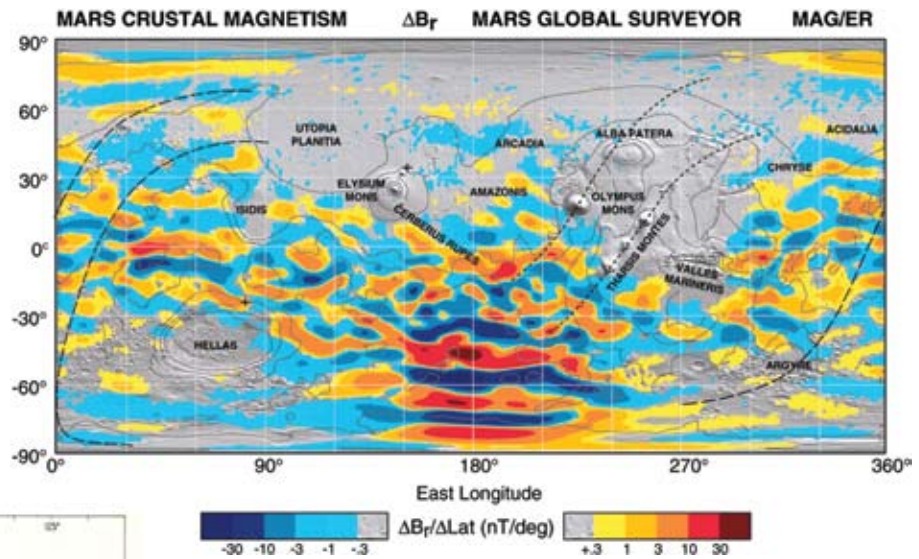


Figure 5.1. (left) Image of a possible explosive eruption on Mercury, as taken by the Messenger probe; the noncircular indentations are attributed to volcanic vents, while the circular features are due to meteoritic impacts. Image from NASA ([http://science.nasa.gov/media/medialibrary/2008/07/03/03jul\\_mercuryupdate\\_resources/kidney.jpg](http://science.nasa.gov/media/medialibrary/2008/07/03/03jul_mercuryupdate_resources/kidney.jpg)). (right) Possible physical behavior of the cores of Mercury, Mars (the double-snow state), and Ganymede. Yellow represents crystallized iron that, due to pressure-induced shifts in the melting relations of the iron-sulfur system, could crystallize at different depths. Shades of red indicate sulfur content. Deeper reds imply greater sulfur content, and hence lower density. From: Figure 3 in Chen et al. (2008).

Figure 5.2. (right) Martian magnetic lineations, possibly produced by a reversing field coupled with ancient formation of new crust via spreading. Red zones are positive polarity and blue zones are negative polarity. Newer crust in the northern hemisphere shows no signs of such lineations. From: Figure 1 in Connerney et al. (2005). (below) Terrestrial magnetic lineations off the Pacific Northwest, where colored regions are zones of normal polarity (after Vine, 1966).



by high-pressure mineral transformations near the Martian core-mantle boundary. The latter possibility, changes in the crystallization behavior of the core, can be understood from experiments on the melting behavior of iron alloys at high pressures. From such constraints, the possibility that the core of Mars might contain solidifying zones within its liquid layer has been proposed.

The key commonalities in our approach as high-pressure geoscientists to our neighboring terrestrial planets are that, first, we aspire to understand how carbon and water are processed, and possibly cycled, between their interiors and near-surface reservoirs. Second, we wish to better constrain the melting processes that have occurred on the other planets. The bulk compositions of Mercury and Mars differ from that of Earth, so their magmas are/were generated from interiors whose compositional flavor differs from that of the terrestrial samples we typically examine. Third, we wish to understand the origin or lack of magnetic field on these different planets. They all have iron-rich cores, and the underpinning thermal and chemical effects that can either produce or squelch planetary magnetism are areas that the high-pressure geosciences community is uniquely suited to address.

off long ago. The reasons for its demise are unclear, but undoubtedly stem from changes in the pattern of convective flow within the Martian core (which studies of tidal deformations show continues to contain liquid). Such changes in fluid flow could have been induced by shifts in heat flow at the Martian core-mantle boundary or changes in the crystallization pattern of the Martian core. The former is likely associated with large volcanic upwellings of the type the high-pressure geosciences community strives to understand—and that may be influenced

## Solar System Satellites and Minor Planets

The satellites and minor planets of the solar system provide a variety of unusual and unique challenges and opportunities. Our own Moon, likely generated by the splash from a Mars-sized impact on the proto-Earth, is a unique example—a body with an immensely hot origin whose subsequent evolution (including its depletion in water and carbon) is entirely a history of magmas and impacts, which are both high-pressure phenomena. The Jovian moon Io, whose ongoing volcanism is driven by Jupiter-induced tidal heating of its interior, is the source of the most sulfur-rich magmatism in the solar system—and the manner in which tidal thermal pumping of Io’s interior has produced eruptions of such peculiar chemistry is a topic of active study. Correspondingly, the large icy satellites, which include Saturn’s Titan and Jupiter’s Ganymede, Callisto, and Europa, have water/ice fractions varying from a few percent in the case of Europa to about 40% in the case of Ganymede. Each of these objects poses notable opportunities for the high-pressure geosciences community: both Titan

and Ganymede are larger than Mercury (although less massive), and they have more water than any of the terrestrial planets. Indeed, the pressure at the base of the ~1000-km-thick ice layer on Ganymede is over 10 times that of the deepest spots within Earth’s ocean. The properties of saline and ammonia-bearing fluids under high-pressure conditions likely have implications for possible deep-water layers beneath the ice of these moons. Moreover, Ganymede has a strong internally generated magnetic field, and hence a molten iron-rich core. Ganymede’s interior thus remains quite hot, providing a possible source of heat that could produce melting deep within its ice layer.

Beyond the large moons, even the minor planets—Ceres, Sedna, Eris, Quaoar, and Pluto (and Pluto’s possible doppelganger, Neptune’s moon Triton), spherical bodies with radii between ~450 and 1500 km—show evidence for geologic processes in their near-surface environment, with water-bearing minerals having been detected at Ceres’ surface, and major dark and light regions being present on Pluto’s surface. In these instances, low-temperature and modest pressure (maximum of thousands of bars) processes are likely to be prevalent. Yet, the ingredients (ammonia- and probably methane-rich) and temperature range (cryogenic at modest pressures) differ markedly from those usually examined for terrestrial applications. Hence, these bodies offer differing ice chemistries and total ice/rock ratios than occur on Earth. Understanding the properties of relevant compositions under pressure can lead to important clues about how such bodies may resurface themselves, how “cryovolcanism”—volcanism dominated by icy components—might occur in such bodies, and whether the crucial ingredient of life—liquid water (albeit perhaps extremely impure brines)—might exist at some depths on such bodies.

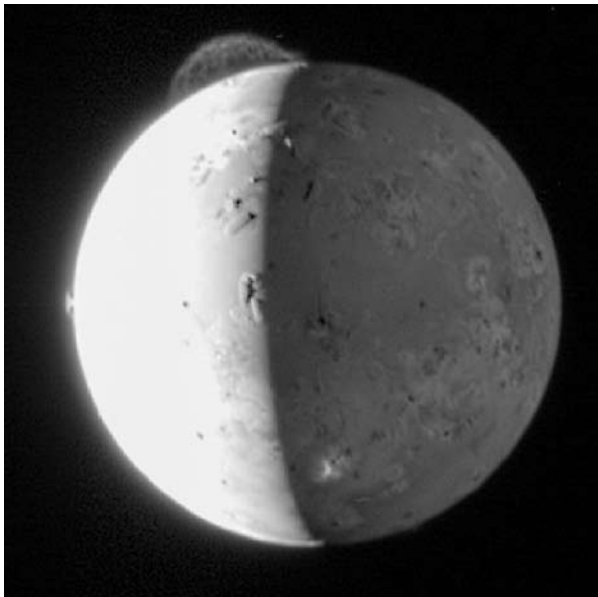


Figure 5.3. An eruption plume rising ~330 km above the surface of Io from the Tvashtar volcanic feature on March 1, 2007, observed by the New Horizons flyby of Jupiter. Photo from NASA ([http://www.nasa.gov/mission\\_pages/newhorizons/news/jupiter\\_images.html](http://www.nasa.gov/mission_pages/newhorizons/news/jupiter_images.html)).

## Large Planets: H-rich Systems at Ultra-Extreme Conditions

The largest planets of the solar system, Jupiter, Saturn, Uranus, and Neptune, access almost stellar ranges of pressure and temperature. Indeed, the conditions in the interiors of the largest of these bodies likely access the boundary between “normal” matter and plasma—a partially ionized fluid. The pressure at the center of Jupiter (~4000 GPa) is over 10 times that at the center of Earth, and the temperature is roughly three times as high (15000–20000 K). Even the smallest of these bodies, Uranus, has a central pressure of 800 GPa and a temperature near 8000 K. Therefore, the experimental challenges presented by such bodies are formidable. Nevertheless, because hydrogen is the dominant element within both Jupiter and Saturn (and abundant within Uranus and Neptune as well), the goal of understanding the high-pressure and high-temperature behavior of these planets coincides well with one of the long-standing goals of the high-pressure physics community: documenting the conditions under which the simplest atom, hydrogen, undergoes a transition to a metallic state. For Jupiter and Saturn, this transition is of key importance: the powerful magnetic fields of these planets are likely generated within a convecting metallic hydrogen-rich fluid, rather than the iron-rich fluids that generate the magnetic fields of Mercury and Earth. For comparison, the magnetic fields of Uranus and Neptune likely arise from fluid flow within a high-temperature, electrically conducting “ice” layer composed primarily of a mixture of fluid water, ammonia, and methane.

Beyond the metallization of hydrogen, major issues remain almost unprobed due to the extreme conditions within these planets. These issues include: the nature of rocky cores under these conditions; the

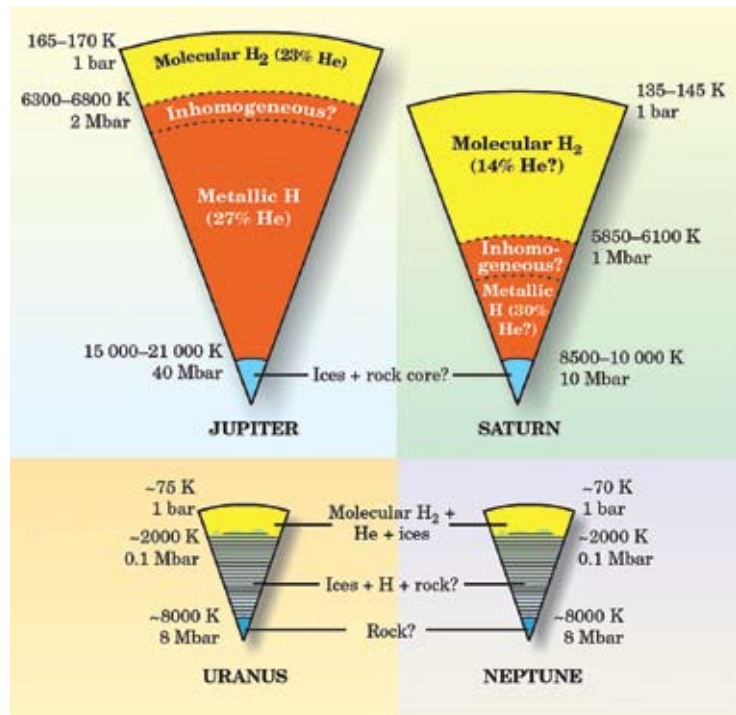


Figure 5.4. Inferred internal structures of the giant planets of our solar system. The existence of rocky cores within each of these bodies is inferred, and the depth of the transition to metallic hydrogen remains uncertain. Reprinted with permission from Figure 4 in T. Guillot (2004), copyright 2004, American Institute of Physics.

interaction between hydrogen and the second most abundant element, helium, within Jupiter and Saturn; how complex mixtures of ammonia, methane, and water such as are present within Uranus and Neptune behave at extraordinarily high pressure and temperature conditions; and how rocky material might be eroded or dissolve within an overlying, hydrogen-rich fluid layer. Indeed, a major internal energy source within these bodies may be progressive unmixing of denser helium from lighter hydrogen as these planets cool. Moreover, at the center of these bodies may lurk rocky/iron-rich cores with masses an order of magnitude greater than that of Earth. Whether such material reacts with and can become suspended within the H-He rich interior is enigmatic. There is sufficient uncertainty within the dependence of volume (or density) on pressure and temperature of these planets’ constituents at the extreme conditions of their interior that it is difficult to resolve whether or not a

large internal core is even required. The issues raised by these giant planets are fundamental to determining the nature of most of the planetary mass within our solar system. Improving our understanding of the state of the interiors of these bodies will require a synergistic effort between dynamic (shock-driven) and static experiments coupled with state-of-the-art theory.

### Exoplanets: New Frontiers of Size, Thermal Regime, and Composition

The eight planets of our solar system represent a profoundly limited sample of the 381 planets known as of mid 2009. Of course, 373 of these planets orbit around other stars, and this selection is observationally biased toward those that are close to their host star and/or that are relatively massive. This bias is simply a result of their means of detection: whether from the Doppler shift generated by the gravitationally induced motion of their host star, from light decreases during transits across their host star, or from gravitational microlensing, big and close-in planetary bodies are more likely to be detected. So, bodies the size of Jupiter (or larger) in orbit closer

than the Earth-Sun distance to their host star are now common objects among the known planets. Although we have observational constraints on the composition and internal structure of the eight planets of our solar system, the constraints on exoplanets are far sparser. Mass and distance from their host star are usually known, as is the eccentricity of their orbit. For about 70 objects, there are also constraints on their radius, and hence the mean density of the planet can be established.

Even with limited data, these new worlds already pose new planetary regimes that could not have been envisioned a decade ago. For example, large objects with rapid and highly eccentric orbits, and thus likely extreme tidal heating, have been commonly observed—the so-called “hot Jupiters” among planets. There is even the plausible suggestion that some of these planets may have emerged in stellar systems with markedly different elemental concentrations than are present in our own. For example, in lieu of the domination by oxygen-bearing minerals in our near-to-the-sun terrestrial planets, carbon/carbide-dominated phases might dominate within planets in other systems. In short, observational constraints of

these planets are rapidly improving (with, for example, the first images of an exosolar planet having recently been obtained). Future enhancements in satellite-based detection of exoplanets from missions such as the recently launched Kepler spacecraft will provide far more data on which to test predictions of characteristics such as mass-radii relations for exoplanets with markedly varying starting compositions. Hence, our ability to interpret the nature, and perhaps even the likely formation history, of the panoply of planets in our galaxy will hinge on an already-emergent interplay between the high-pressure geosciences field and astronomy/astrophysics. The key ingredient here will be our ability to produce, through both experimental and

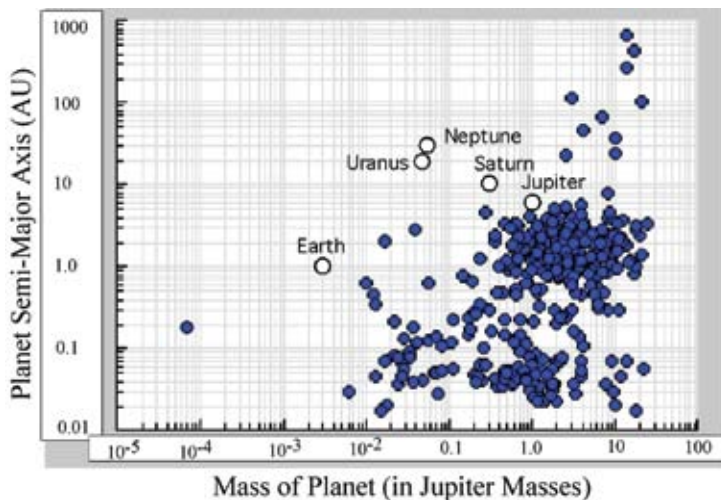


Figure 5.5. Relation between the masses of exoplanets and their distance from their host star. Blue circles represent the 373 exoplanets characterized to date. A subset of planets within our solar system are also shown for reference. Data are from the continuously updated Encyclopedia of Exoplanets at <http://www.exoplanet.eu>.

theoretical approaches, a broad suite of compositional and thermal properties for possible exosolar planets that can be used to characterize, distinguish, and constrain the rapidly growing numbers of these bodies.

## Key Questions

- How are water and carbon dioxide sequestered within the terrestrial planets?
- How do the differing compositions of the silicate mantles of other planets influence melting and crustal generation of these bodies?
- What are the interplays between the phase relations of iron and its alloys and the generation or lack of magnetic fields on different planetary bodies?
- What are the interactions between rocky and icy layers within satellites? Under what chemical and thermal conditions are deep-water-rich fluids (“oceans”) likely to be generated, and how is cryovolcanism generated?
- What are the properties of the complex mixture of materials present within the giant planets of the solar system? How is the metallization of H-rich fluids and high conductivity of water/ammonia/methane-rich fluids affected by different compositions and conditions? What is the solubility of helium in hydrogen at extreme pressures and temperatures, and at what conditions do silicates become entirely soluble in iron?
- What are the effects of novel chemistries and extreme temperatures and pressures, such as may be present in some exoplanets, on planetary structure and density? From a structural perspective, how variable is the compendium of exoplanets?

# Chapter 6 | The Invisible Frontier: Creating the Conditions of Earth and Planetary Interiors

At the crux of high-pressure geosciences is the ability to both generate and simulate the high pressures associated with the interiors of Earth and other planets—and often to generate these high pressures while heating samples to temperatures of thousands of degrees. The task here is conceptually simple, but operationally difficult: to simulate the compression produced by the equivalent of loading a material with anywhere from kilometers to thousands of kilometers of rock, while simultaneously cooking the material at ultra-high temperatures. To achieve these extraordinary conditions, high-pressure geoscientists have pioneered a wide-range of experimental technologies and computational approaches oriented toward addressing our fundamental queries: What resides within planets, and how does their interiors govern the evolution of their surfaces?

The process of achieving extraordinary pressure and temperature conditions is, of course, iterative and continuously evolving: new technologies, materials, or designs are often brought to bear. Moreover, accessing these extreme pressures, and often temperatures, is only half the task. The other half is to usefully interrogate geomaterials either after they are quenched from high pressure and temperature conditions or, more directly but significantly more difficult, while they are actually held in situ at enormous pressure and temperature. Our community has continuously introduced new probes and refined older ones, including spectroscopy, calorimetry, elemental analysis, and measurements of electrical and thermal conductivity and deformation, as well as state-of-the-art diffraction and scattering techniques, to address

the broad suite of chemical, elastic, and dynamic issues associated with planetary interiors. These new developments regularly translate from high-pressure geosciences to high-pressure materials science and solid-state physics and chemistry.

In tandem with our experimental and analytic developments, we have applied and developed rigorous theoretical techniques to computationally characterize how Earth materials behave under extreme conditions. But, our analytical work hinges on our ability to generate extraordinary pressures and temperatures. Experimental comparisons are critical for assessing the robustness of theoretical approaches. Loosely, the high-pressure geosciences community has used three separate approaches to simulate the conditions of planetary interiors: (1) “static” experiments, in which a compressed sample is held at high pressures for periods of time; (2) “dynamic,” or shock-loading experiments, in which a sample is essentially hit by a high-velocity bullet or explosion-induced shock waves, and interrogated while the sample is compressed (and its temperature is increased) by the shock wave over time scales that range from nanoseconds to, in a few instances, as long as a millisecond; and (3) theoretical approaches, which computationally simulate the effects of pressure and temperature on materials, often using quantum mechanical methods of simulating bonding interactions in materials under extreme conditions.



## Static High-Pressure Techniques

The desire to generate progressively higher pressures has been a long-standing aspiration of physical scientists—and geoscientists have long recognized the importance of high-pressure experiments in addressing the nature of, and processes present within, Earth's interior. Yet, the generation of high-pressures is inordinately challenging. Indeed, even in the nineteenth century, Michael Faraday and others, through studies of heated liquids in enclosed volumes, fully appreciated the difficulties and hazards of generating high pressures in a macroscopic volume. Because pressure is force per unit area and the strength of any material prior to deforming or breaking is finite, there has been a progressive and natural trend toward miniaturization of static high-pressure experiments to minimize the force necessary to achieve a given pressure. But, as the pressure of Earth's interior varies over 6.4 orders of magnitude, different high-pressure apparatuses are particularly suited to different problems. Where comparatively modest pressures (a few thousands of bars, or fractions of a GPa) are required, hydrothermal bombs—steel chambers that might be characterized as ultra-heavy-duty pressure cookers—are commonly used. At somewhat higher-pressure conditions (up to  $\sim 5$  GPa, corresponding to depths of 150 km in Earth), steel and tungsten carbide piston-cylinder devices have been used. Both hydrothermal bombs and piston-cylinders have been, and continue to be, extensively used in quench studies (and, indeed, much of our knowledge of the development of rocks in Earth's crust and shallow upper mantle is generated by piston-cylinder work). Such apparatuses remain the workhorses for detailed geochemical and petrologic

studies of relevance to the crust and shallow upper mantle. Yet, they share the common problem that the samples are surrounded by large and thick pieces of sealed metal. Therefore, in situ interrogation of samples while they are held at high temperatures and pressures is difficult.

Two families of apparatus have dramatically extended both the pressure range of static experiments and have allowed samples to be probed while held at simultaneous pressures and temperatures: the multi-anvil press and the diamond-anvil cell. The multi-anvil (or “large-volume”) press relies on simultaneous hydraulic compression of a cubic or tetrahedral assembly composed of tungsten carbide or sintered diamond composite blocks with truncated corners. In cubic cells, the sample sits within a tube (often surrounded by a cylindrical furnace) at the center of an octahedron compressed by the ram-driven blocks. The advantages of this technique include: (1) a fairly uniform high pressure and temperature environment; (2) high-intensity x-ray beams can be directed between the blocks (if separated by low absorbance material), and the sample can be x-rayed for either imaging or diffraction/spectroscopy during a high-pressure and high-temperature experiment; (3) small (of order a cubic



Figure 6.1. (left) View from above, with top anvil assembly removed, of a multi-anvil press. The sample assembly is sitting in the square region between the four visible hydraulically driven anvils (a fifth provides the base of the central square). Scale across the picture is approximately 0.7 m. Photo courtesy of Y. Wang, Advanced Photon Source. (right) Representative hydraulic press in which multi-anvil assemblies are compressed. The bottom anvil assembly (steel-colored object on left) has been slid out of the press. This is a 2000-ton Sumitomo Industries Press currently installed at Stony Brook University. Photo courtesy of R. Liebermann, Stony Brook University.

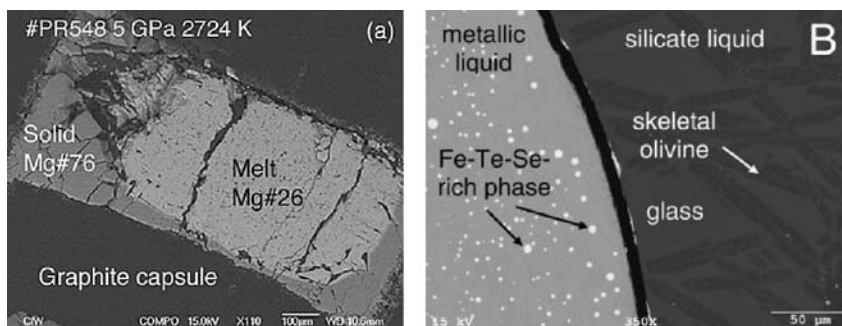
millimeter) but macroscopic high-pressure samples can be quenched from high pressures and high temperatures and characterized at ambient conditions, allowing determinations of phase assemblages and chemical transport properties; (4) by applying differential stress to the sample, deformation experiments designed to probe the viscous flow of Earth's interior (and hence the driving mechanisms of plate tectonics) are conducted; (5) by introducing transducers in to the sample assembly, ultrasonic sound wave velocities can be measured; (6) electrical conductivity can be characterized by introducing leads into the samples; and (7) liquid density and viscosity are constrained by imaging falling (or rising) spheres.

With these capabilities, the multi-anvil press has produced much of the insight into the phase transitions and melting processes undergone by Earth material down to ~700-km depth (or ~25 GPa). The “routine” pressure range for this apparatus has typically topped out at these pressures, but there are significant possibilities that this range could be extended possibly by using sintered diamond anvils. One of the major technical goals of our community is to construct a multi-anvil press that can regularly access pressures corresponding to most of the depth range of Earth's mantle (1500–1800-km depth, or ~50–60 GPa). Promising indications that such a

pressure range is feasible have emerged from our Japanese colleagues, but significant technical challenges remain to produce an instrument that can routinely generate such extreme conditions. The production of higher pressures in multi-anvil apparatuses may ultimately involve a considerable bridging and cross-fertilization between the technology of the diamond anvil cell and that of the large-volume press. Active areas of inquiry include how to minimize anvil deformation at extreme conditions, and the usage of multiple stages of anvils to generate very high pressures. The anticipated scientific benefits of such an instrument include rigorously quantifying melting relations of Earth materials at significantly greater pressures than have been conducted to date, and refining our knowledge of the different phases present at great depths within Earth's mantle.

Far more extreme conditions of pressure and temperature can be achieved using the opposed anvil configuration of the diamond anvil cell. Although there are many different designs of this apparatus, they all share the common feature of two gem-quality diamonds (typically a few millimeters in size and a fraction of a carat in weight) with their points lopped off, and the two small surfaces aligned parallel with one another. The diamond anvil cell takes advantage of extremely small areas (typical lateral dimensions

of samples vary between 10 and 500 microns, and thicknesses between 5 and 50 microns) and the extreme hardness of diamond to generate extremely high pressures. Samples are mounted between the anvils and are usually contained within a metal gasket. Force is applied mechanically at the back faces of the diamonds and, because of the small dimensions, only fairly modest forces are required.



**Figure 6.2.** (left) Cross section of a quenched multi-anvil press charge with coexisting solid  $(\text{Mg}_{0.76}\text{Fe}_{0.24})\text{O}$  and liquid  $(\text{Mg}_{0.26}\text{Fe}_{0.74})\text{O}$  equilibrated at 5 GPa and 2724 K. 100-micron scale bar is shown at the bottom. From: Figure 1a in Zhang and Fei (2008). (right) Fine-scale structure of coexisting quenched iron-rich liquid and quenched silicate melt from a charge run at 1.9 GPa and 2233 K, illustrating that fine-scale chemical variation can be ubiquitous in high-pressure charges. Scale bar of 50 microns is at the bottom. Reprinted from Figure 3b in Rose-Weston et al. (2009), copyright 2009, with permission from Elsevier.

With this apparatus, pressures in excess of those within Earth have been generated, albeit not routinely; however, pressures in excess of 1 million bars (100 GPa), corresponding to depths of roughly 3000 km in Earth, are achieved fairly routinely.

The diamond cell truly provides a window on the materials of Earth's interior. Because of diamond's transparency, one can optically view the sample while it is held at high pressures. And, this transparency enables probing of the sample using any type of electromagnetic radiation that can penetrate through a few millimeters of diamond—which is much of the electromagnetic spectrum. Indeed, spectroscopic probes that use light, ranging from x-rays and gamma-rays, to visible light, to the infrared, can each be deployed. Only portions of the ultraviolet and a few limited regions in the infrared are entirely inaccessible. The high-pressure geosciences community has pioneered the application of x-ray diffraction and scattering techniques, as well as Mossbauer, infrared, Raman, and Brillouin spectroscopies on samples held at extreme conditions. Subsequently, these methods have been used extensively in materials chemistry and solid-state physics. Using such techniques, the structure, wave velocities, and thermodynamic behavior of materials throughout the pressure range of much of the planet's interior can be constrained. Perhaps most importantly, diamond's transparency allows high-intensity lasers to be focused into the sample, producing local heating to temperatures of many thousands of degrees, truly simulating the pressure and temperature regime of much of Earth's interior. The laser-heated diamond cell has allowed our community to interrogate materials at conditions down to our planet's core, and hence has produced an unprecedented level of insight into the physical and chemical properties of the deepest reaches of our planet.

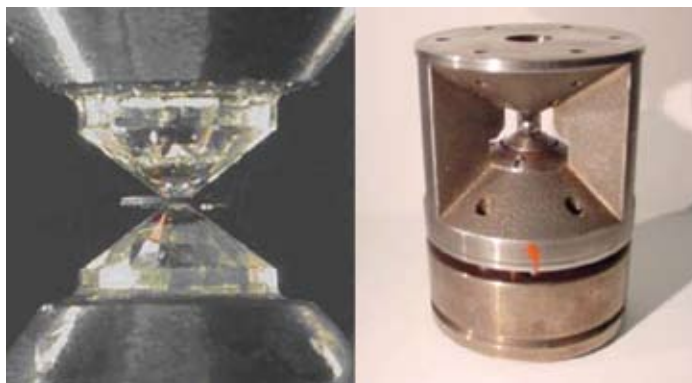


Figure 6.3. (left) Close-up view of the diamonds and metal gasket (center) within a diamond anvil cell. Vertical dimension of picture is  $\sim 1$  cm; total flat portion of the anvil tips is  $\sim 500$  microns. Photo courtesy of H.-R. Wenk, University of California, Berkeley. (right) Diamond anvil cell; diamonds sit at the apex of the two cones. This particular cell allows both parallel and perpendicular (through the gasket) access to the sample relative to the vertical axis of force. Photo courtesy of J. Jackson, Caltech.

Yet, challenges associated with the diamond cell remain: improvements in our ability to characterize pressure and temperature at extreme conditions are ongoing, with an ultimate aspiration to routinely generate conditions that are as accurately constrained as those produced in larger pressure-generating apparatuses. Furthermore, efforts are underway to optimize our capabilities to maintain and characterize single-crystal samples (which often shatter under differential stress) under extreme conditions, but this work presents a few difficult-to-surmount technical challenges. And, given the strong interest in simulating the interiors of giant planets (exo- or otherwise), there is the long-term goal of enhancing the pressure and temperature ranges that can be routinely accessed using the diamond anvil cell—an area in which the U.S. high-pressure geosciences community has led the world.

The ability to accurately probe both the structure and chemistry of samples at the microscopic scale, and reproducibly construct tiny and complex cell assemblies, is vital for our science. However, pressure apparatuses are, by their nature, limited in the size sample that they can generate. The community has deployed electron microscopic techniques, micro-focus spectroscopies, and fine-scale high-intensity

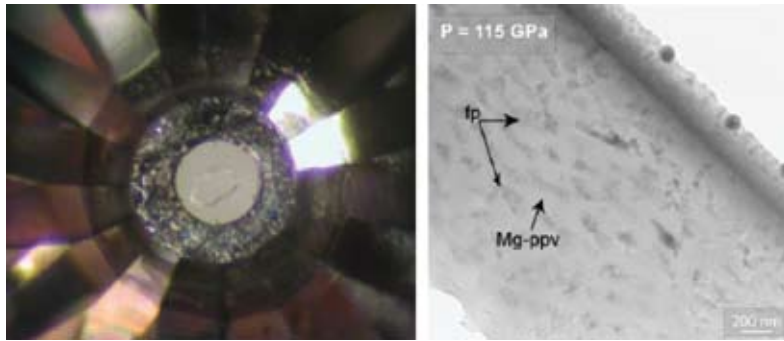


Figure 6.4. (left) View through the diamond anvil into a pressurized sample. The grey-speckled annulus is the metal gasket, and the mineral sample (center oblong feature) is held within a liquid pressure medium. Sample diameter is ~200 microns. Photo courtesy of T. Duffy, Princeton University. (right) Electron microscope image of a quenched, laser-heated diamond cell charge synthesized at 115 GPa and 2200 K; light regions are (Mg,Fe)SiO<sub>3</sub>-postperovskite (Mg-ppv: likely the dominant mineral at Earth's core-mantle boundary) and dark regions are (Mg,Fe)O-ferropericlasite (fp). The contrast is produced primarily by the different iron contents of the two phases, and the scale bar of 200 nm is in the lower right. Reprinted from Figure 2b in Auzende et al. (2008), copyright 2008, with permission from Elsevier.

x-ray probes, but future development hinges on making better measurements at smaller scales. Improving our ability to characterize and interrogate our samples at the nanoscale is one of the community's highest priorities. Many in situ probes require the use of complex cell assemblies, such as microcircuitry deposited on the diamond tip (so-called "designer anvils") or embedded in multi-anvil assemblies. Improvements in fabrication techniques, such as the ability to grow diamonds at very low pressures using chemical vapor deposition, have allowed such cell assemblies to become increasingly useful. These chemical vapor deposition techniques have been optimized by members of the high-pressure geosciences community. The prospects for creating cell assemblies incorporating microelectronic probes is becoming well within reach, and the high-pressure geosciences community fully expects a greatly enhanced need for nanofabrication in the future. Therefore, the development of the infrastructure to achieve reasonably routine access to such capabilities is a major area of emphasis.

## Shock-Loading Techniques

The intense work on static high-pressure experiments notwithstanding, the conditions in deep planetary interiors and those created during bolide impacts exceed those achievable in static experiments. Higher-pressure conditions can be achieved through mirroring the natural impact process by firing high-velocity projectiles at samples, by detonating explosives near materials, or by hitting them with a high-intensity laser beam. One of the challenges in such experiments lies in probing the

samples during the brief time over which they are dynamically compressed. Such dynamic pressure loading (shock waves) can provide critical observations in regimes extending from Earth's deep interior to the conditions within Jupiter and extra-solar planets. Shock waves have the advantage of simultaneously generating deep planetary ranges of temperature and pressure—the impact of the projectile not only pressurizes the sample, but also produces heating. Such experiments can also explore material properties in the high-strain-rate regime of planet-forming collisions and during the shock metamorphism of meteorites, thereby constraining the conditions of the early solar system.

Born during the Manhattan Project, conventional shock-wave research on geologic materials has primarily used "explosive" or "two-stage light-gas gun" techniques. Indeed, extensive data sets on how minerals and rocks responded to shock compression have been produced over the last five decades. The data sets have yielded extensive insight into the elastic and thermodynamic properties of these materials under extreme pressure and temperature conditions. In particular, shock-wave measurements have produced primary constraints on what mixes of iron and

light elements match the density of the outer core, and on the density and thermodynamics of silicate melts in the deep mantle. Much of the information about the properties, density gradient, and thermodynamics of a possible early magma ocean on Earth have been derived from shock experiments. Shock-loading experiments on silicate melts and liquefied gases (such as deuterium and hydrogen) have been an area of major recent focus for shock-wave experimentalists—these ongoing experiments are extremely challenging, but are motivated by their uniqueness and value for understanding planetary interiors *and* fundamental physics.

Moreover, shock-generated high-pressure minerals are found in meteorites. In many instances, the only natural occurrences of high-pressure phases that we know to be present in Earth's interior are within meteorites. Meteorites carry perhaps the most robust record of the early stages of planet-forming processes. The pressure, temperature, and impact duration (related to size and velocity of the pre-collision planetismals) experienced by these samples of the earliest solar system can be inferred by comparisons with

laboratory-created shocked samples. A systematic approach combining shock-recovery studies, examination of naturally shocked meteorites, and physics-based modeling of pressure, temperature, duration, and retrograde transformation will provide requisite constraints for understanding the early solar system.

Over just the last several years, these “conventional” shock-wave techniques have been complemented by laser-driven shock-wave experiments. In such experiments, an extraordinarily high-intensity laser pulse is typically fired at a coating on a sample, which explosively vaporizes and sends a shock wave into the sample. This revolution in technology is poised to significantly expand the opportunities available to our community, particularly as such experiments can be conducted on pre-compressed samples held within a diamond cell. Laser-driven shock-wave experiments are rapidly extending the regimes of pressures and temperatures that can be accessed. “Pulse shaping” of the shock front and manipulation of the initial conditions through precompression of the sample allow access to a broader range of thermodynamic states, many of which are currently inaccessible to static experiments.

Additionally, laser-driven shock experiments could potentially reduce both the considerable cost per data point relative to conventional shock-wave experiments, and enhance the rate at which shock experiments can be conducted. Equation-of-state measurements, sound-velocity measurements, temperature measurements, and sample recovery have all been demonstrated using such laser-driven techniques, and future expansion of the types of measurements that can be conducted is anticipated.



Figure 6.5. (left) Cross section of a simulation of an impact of a Mars-sized object with the proto-Earth during planetary accretion. Such an impact is widely thought to be responsible for the formation of the Moon through jetting off of debris from Earth and the impactor. Figure courtesy of J. Melosh, Purdue University. (right) Space Shuttle view of the Manicouagan impact structure in Canada. Diameter is ~100 km. This feature was generated by an impact 214 million years ago. Such impacts can induce major shifts in both the climate and biosphere, and one aim of dynamic compression experiments (coupled with fluid dynamic modeling of large impacts) is to constrain the likely effects of such large impacts. Photo courtesy of J. Spray, University of New Brunswick.

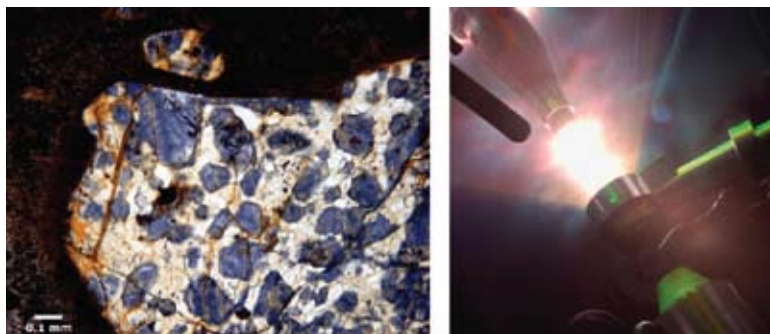


Figure 6.6. (left) The high-pressure phase of  $(\text{Mg,Fe})_2\text{SiO}_4$ -olivine (popularly called peridot) within the Taiban meteorite; the presence of the blue ringwoodite, a material stable only at depths greater than 520 km in Earth, demonstrates that the rock was shocked to extremely high pressures. Such shocked meteorites provide not only the sole natural occurrences of many high-pressure phases, but also provide a record of processes in the early Solar System prior to planet formation. Courtesy of E.R.D. Scott, University of Cambridge. (right) Time-integrated picture of a laser-driven shock experiment. Here, a diamond cell (center, at end of light beam) holds a pre-compressed sample of He, and a high-intensity laser is fired at the back surface. Analytic equipment is at the lower right. The experiment was conducted at the Omega Laser Facility at the University of Rochester. From: Figure 1 (right) in Jeanloz et al. (2007).

A number of scientific problems are well suited to laser-driven shock studies. These problems include constraining the physical properties of the interiors of giant Jupiter-class planets, which consist principally of hot and highly compressed H and He at conditions well above those accessible through static experiments. In particular, under what conditions do these elements become metallic? Under what conditions do metallic H and He form a solution in the interior, under what conditions might they unmix, and how do these affect the planet's thermal state? Laser-driven shock techniques may render the conditions in the interior of these planets experimentally accessible and thus answer such fundamental questions.

The discovery of large, possibly rocky super planets in other solar systems has produced an additional set of questions that can be addressed only through shock compression. For example, do rock-forming minerals from Earth's interior dominate the deeper parts of superearths or are they replaced by entirely different phases with different physical properties? The answers to such a question could be generated by synergistic technologic developments. For example, the prospect exists that future fourth-generation

synchrotron x-ray light sources (sources more intense than the current second- and third-generation sources present at Argonne, Lawrence Berkeley, and Brookhaven National Labs), in combination with shock facilities, could permit the structural examination of matter shock compressed to conditions present in the interiors of giant rocky and gas planets. Such in situ, x-ray-under-shock experiments have been conducted on a few isolated occasions. Rendering such marriages of demanding high-pressure experiments and advanced analytic techniques both more routine and widely

available represents a primary goal for the high-pressure geosciences community.

### Theoretical Approaches to High-Pressure Geosciences

The accurate numerical simulation of complex materials under extreme conditions is among the most notable challenges of condensed-matter physics. Such simulations are crucial for the high-pressure geosciences, because computations can provide predictions of unforeseen behavior, illuminate the underpinning physical origin of observed phenomena, and access conditions that are either difficult or impossible to access experimentally. The pace of developments in the high-pressure geosciences has accelerated with the establishment and expansion of theoretical groups throughout the world. The contributions made by first-principles computations have not only complemented experiments, but have forged ahead in the domain of terapascal (TPa) pressures (thousands of GPa) and temperatures of  $10^{5-6}$  K. These extreme conditions have, in turn, provided motivation and targets for new national experimental facilities such as the

National Ignition Facility (expected to be operational in 2010), as well as for nascent techniques like laser-driven shock studies.

The theoretical challenges associated with geomaterials include: large and complex unit cells containing many different atoms, large numbers of possible different phases that materials could adopt that lie close in energy to one another, amorphous (liquid) materials that require large (and long) simulations to achieve equilibrium, correlated solids such as iron-bearing minerals, and the quantum behavior of hydrogen in hydrous and nominally anhydrous phases. Hence, chemically and structurally complex geologic materials provide unusual computational challenges for theoretical approaches that are most commonly tested and deployed in binary or ternary systems. Yet, even in systems containing only one component, the effects of pressure have often produced unexpected results, from Wigner and Huntington's 1935 quantum-theory-based prediction that hydrogen might become a monatomic metal under compression, to the recent discovery that alkali metals become transparent insulators at high pressures.

Theoretical approaches used in the high-pressure geosciences to date span a broad range and have evolved over the last several decades from an initial widespread use of empirical potentials, to the now far-more-frequent approaches that are rooted in first-principles quantum mechanics and molecular dynamics. Our community has used techniques such as density functional theory, linear-response-based techniques, quantum Monte Carlo approaches, linear scaling algorithms coupled with *ab initio* methods, and molecular and lattice dynamics incorporating first-principles-derived potentials to explore the properties of geomaterials. Moreover, the high-pressure geosciences have evolved a highly complementary relationship between theoretical and experimental work, with

theory providing new insights that drive experimental work, and vice versa. Over the last several years, examples of this interplay include: (1) theoretical characterization of the structure of the key post-perovskite phase of  $\text{MgSiO}_3$  that likely dominates Earth's deepest mantle; (2) quasi-harmonic computations of free energies, enabling calculations of phase boundaries and thermodynamic properties; (3) calculations of the properties of melts at high compression, which have provided insights into both prior shock experiments and the likely thermal state of a possible magma ocean on Earth; and (3) achieving the ability to find the minimum energy structure of complex geomaterials at extreme conditions through variable cell shape molecular dynamics and evolutionary algorithms, which have provided constraints on the structure of experimentally observed phases.

One of the main challenges of condensed matter physics that currently occupies a major role in high-pressure geosciences is the theoretical treatment of strongly correlated systems, such as iron-bearing minerals. Strongly correlated systems are

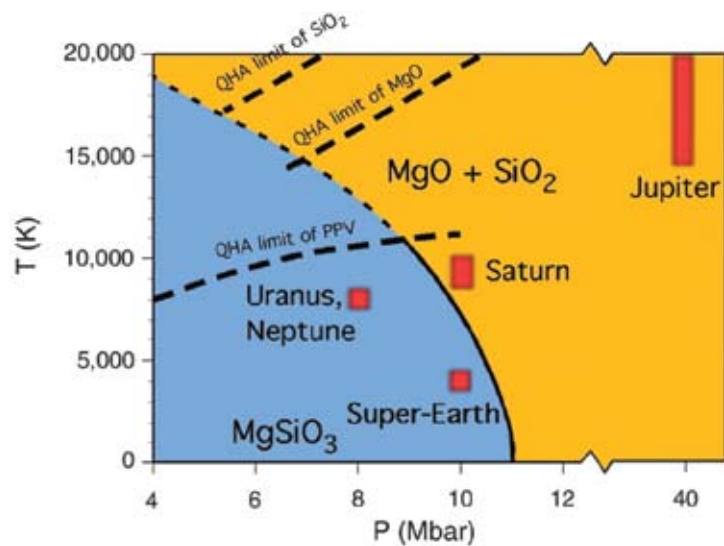


Figure 6.7. Theoretical calculation of the pressure and temperature range in which the  $\text{MgSiO}_3$ -post perovskite phase breaks down, at ultra-high pressures and temperatures, to its constituent oxides. Such a break down is likely to occur within the giant planets of our solar system. Dotted lines denote the upper limit of applicability of the quasi-harmonic approximation (QHA) used in the calculation. From: Figure 3 (left) in Umemoto et al. (2006), reprinted with permission from AAAS.

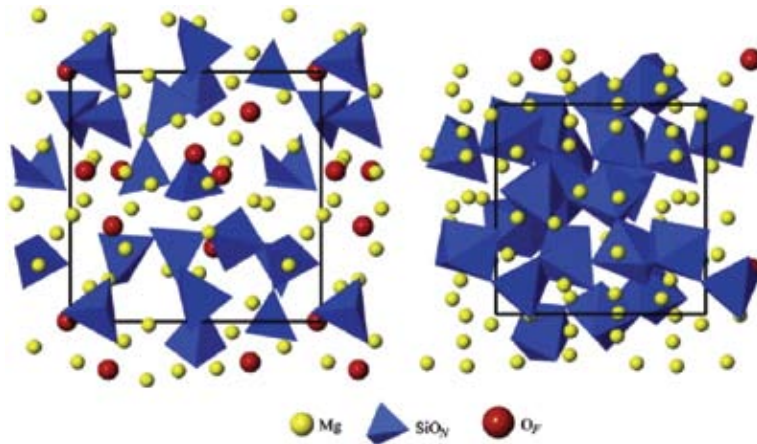


Figure 6.8. Results of a molecular dynamics calculation on the effect of compression on  $\text{Mg}_2\text{SiO}_4$  liquid at 3000 K. The left panel shows results of a simulation at the liquid's ambient-pressure volume, while the right shows the structure under a volume compression of 50% (corresponding to a pressure of  $\sim 160$  GPa). The bonding environment of the silicon atoms is markedly changed, from being tetrahedrally coordinated with respect to oxygen to being predominantly octahedrally coordinated at high compressions. Red circles are oxygen ions that are not bonded to a silicon. Reprinted from Figure 1 in DeKoker et al. (2008), copyright 2008, with permission from Elsevier.

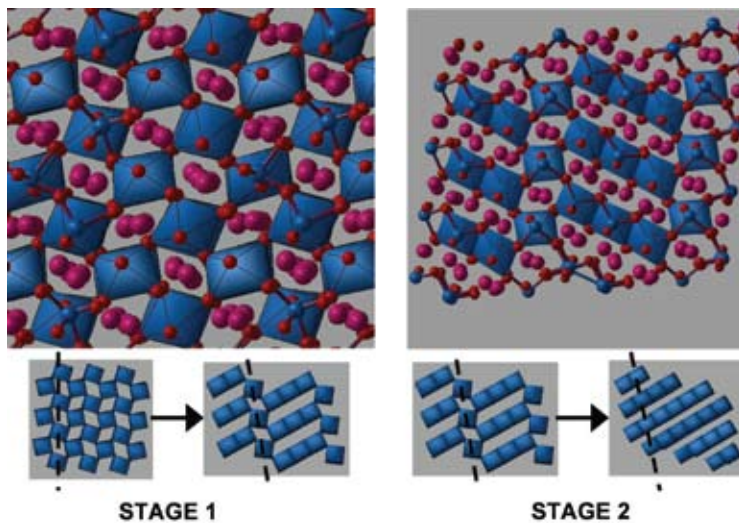


Figure 6.9. Illustration of possible transformation (and potential deformational) mechanism from  $\text{MgSiO}_3$ -perovskite (large upper left panel, with blue polyhedra being silica octahedra and purple spheres being magnesium atoms) to post-perovskite, as calculated using a metadynamic technique. Small panels show octahedral configurations during the transformation. Upper right panel shows an intermediate structure between perovskite and post-perovskite, with transitional zones being associated with stacking faults. The small panel on the far right shows the final octahedral configuration of the post-perovskite phase. Dotted lines in the small panels show preferred slip planes. Modified from: Oganov et al. (2005).

those in which the electrons cannot be treated in isolation, or as subject to a mean field induced by their surroundings. As such, these systems present particular theoretical challenges, and lie at the frontier of current developments in condensed-matter theory. Because of the abundance of iron in the minerals of Earth's mantle, description of the physical properties of the mantle depend on an accurate treatment of this problem. Crossovers in spin state have been observed in lower mantle phases and their consequences for mantle properties are being explored. Quantum Monte Carlo techniques and dynamic mean field theory are also expected to contribute significantly to these problems, and an active dialog between experiments and theory is currently taking place.

Advances in the theoretical domain of high-pressure geosciences have often proceeded via tandem improvements in both software and hardware. Obviously, continued development of high-pressure geosciences theory hinges on both improvements in, and availability of, continuously evolving hardware and software. The challenges for the community include ensuring that investigators can access both state-of-the-art techniques and computational infrastructure. Over the next decade, there are a number of areas where dramatic advances in theoretical approaches are anticipated. For example, even with high-powered supercomputing, the size and time scale of theoretical simulations remain limited. The ability to



conduct longer-time-scale simulations of materials (which are currently limited to  $\sim 10^{-9}$ – $10^{-12}$  seconds) will likely be achieved as computational power increases. Longer-length-scale simulations that can incorporate crystal defects critical for viscous flow, such as dislocations, will likely become progressively more feasible. And, simulations of amorphous materials, like silicate melts, will similarly benefit from such larger scales. Such larger-scale calculations hold the prospect for moving theoretical predictions more fully from the structural and the thermodynamic domain toward accurate simulations of transport properties, including solid and liquid rheology. Such expanded calculations will also improve the ability to theoretically treat highly multicomponent systems, and prospectively enable the mechanisms and kinetics of phase transitions and reactions to be accurately characterized. In short, advances in approaches and infrastructure have begun to move high-pressure geosciences theory into entirely new domains—and this richness of new achievements is fully anticipated to continue.

- Deploy laser-shock studies more broadly within the high-pressure geosciences.
- Improve and extend theory, hardware, and computational approaches to model the structures and properties of geomaterials, including enabling dynamic, kinetic, and mechanistic studies, and improving treatments of both strongly correlated and weakly bonded systems.

### Key Technique-Oriented Goals

- Markedly expand the pressure range over which our community is able to conduct large-volume ( $\sim$ cubic millimeter) high-pressure experiments.
- Improve the characterization of pressure and temperature conditions within diamond anvil cells, and increase their routine pressure and temperature limits.
- Enhance our ability to create and utilize nano-scale chemical and structural probes of high-pressure samples.
- Access and routinely utilize nanofabrication techniques to construct high-pressure sample assemblies.
- Expand and improve conventional shock wave techniques in the study of geomaterials, including taking advantage of synchrotron-based characterizations of shock-loaded materials.

# Chapter 7 | Broader Impacts: New and Complex Materials at High Pressures

The field of high-pressure geosciences is naturally concerned with Earth materials—and a key goal of our discipline is to explore the societal, technological, and industrial utility of these or related materials. The application of pressure often results in materials adopting new crystal structures, or allows compounds to form that cannot be produced at low-pressure conditions. Thus, high pressures have been used to generate materials that are extremely hard or have novel electronic or chemical properties. In many instances, such new materials can be quenched to ambient pressures, and hence any novel or unusual physical properties may prospectively be used. Examples of the types of materials for which high pressures have found considerable applications include not only ultra-hard materials, but also materials used for radioactive waste disposal and possible hydrogen storage materials. In fact, one of the primary and until recently largely unrecognized fossil fuel reservoirs of the planet, natural gas clathrates, require moderate pressure to access their stability range.

## Ultra-Hard Materials

The classic example of the societal utility of high-pressure geosciences is, of course, the well-known high-pressure mineral diamond. First synthesized in the early to mid 1950s, the manufacture of artificial diamond represents one of the early achievements of modern high-pressure experimental techniques—techniques unambiguously applied to simulate the conditions under which diamond formed within Earth's interior. Continuing this long-standing and

industrially important area of research, the investigation and discovery of “super-hard” materials has been one of the major endeavors of not only high-pressure geoscientists, but high-pressure materials scientists and solid-state physicists in general. The underlying concept here is simple: materials with compact, three-dimensional networks of strong bonds tend to be hard, and the effects of high pressures are often to generate such bonding environments.

The diamond-manufacturing industry today produces well over 100,000 kilograms per year of diamond, which substantially exceeds the amount of diamonds that are mined. Such diamonds are routinely used not only for the construction and drilling industries through diamond-bearing saws and drill bits, but, because of the high thermal conductivity of diamond, are used within the semiconductor industry as well.

In the domain of super-hard materials beyond diamond, the focus of the high-pressure geosciences community has been, for the most part, two-fold: first, discovering new, very hard materials that might either be more easily synthesized, or perhaps even be harder or tougher than diamond; and second, improving the means by which diamond itself might be manufactured. In the first case, workers in our discipline have discovered and/or characterized a wide array of nitrides, carbides, borides, and oxides that approach diamond in their resistance to compression and potentially in hardness as well. In many of these cases, high pressures are necessary to synthesize the phases that are potentially of use as super-hard materials.

High-pressure researchers have also engaged in searching for new types of super-hard materials that might have highly desirable material properties, preferable to those of diamond. For example, although extraordinarily hard, single-crystal diamond also fractures readily; such fracture is a common type of failure for high-pressure anvil experiments. Recently, it has been recognized that diamond- and silicon carbide-containing nanocomposites may have unusually high fracture strength while retaining much of the hardness of diamond. This discovery illustrates the value of our community's ongoing search for hard materials with highly desirable physical properties.

In terms of improvements in diamond manufacturing, our community has also spearheaded efforts to improve chemical vapor-deposition techniques for metastable diamond growth at low pressures. This work has been pursued at least partly with the goal of producing larger single-crystal diamond anvils to accommodate larger samples for ultra-high-pressure experimentation. As the cost of high-quality diamonds (such as are required for anvils) increases exponentially with size, the size of high-pressure anvils has been limited by simple economics. Synthesis of larger diamonds obviously has applications that extend well beyond anvils for high-pressure devices, including high-speed electronics that require rapid temperature dissipation, and extending to diverse purposes such as producing high-strength and high-transparency windows for spacecrafts and deep-sea submersibles.

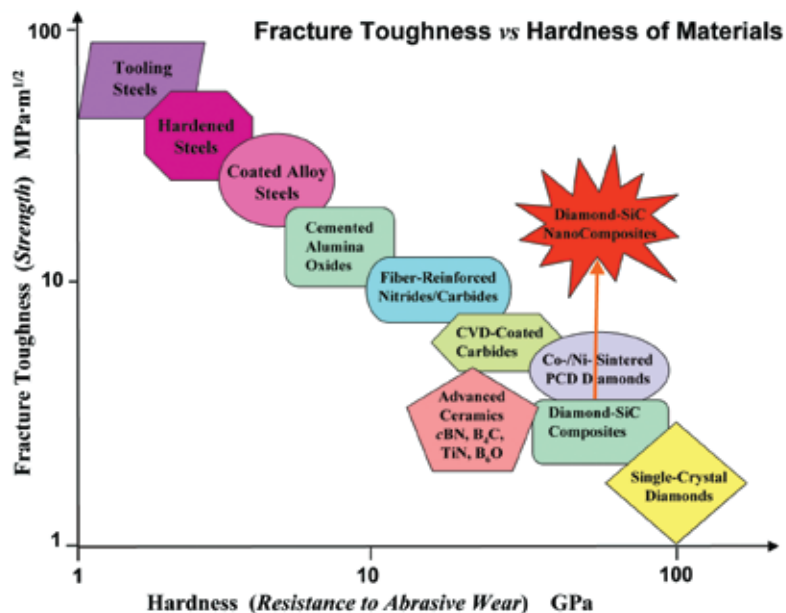


Figure 7.1. Trend in hardness of differing materials relative to their resistance to fracture. In general, fracture toughness decreases with hardness for many materials. However, nanocomposites can differ substantially from this trend, and hence may have both industrial uses as well as applications within high-pressure devices. Image courtesy of Y. Zhao, Los Alamos National Laboratory.

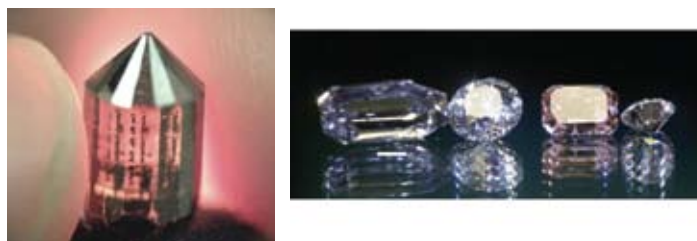


Figure 7.2. (left) Five-carat synthetic diamond produced by chemical vapor deposition at pressures below 1 bar. The diamond was cut from a larger, 10-carat stone. (right) Sequence of synthetic, gem-quality diamonds, with the second and fourth from the right being cut as anvils. Photos courtesy of Carnegie Institution of Washington.

## Radioactive Waste Immobilization

The geosciences community has long recognized that some minerals are highly effective at retaining actinides and other radioactive elements. The importance of this property is straightforward: if medium- or high-level radioactive waste can be sequestered within mineral/rock matrices at geologic time scales, then the considerable health hazard of radioactive pollutant mobility within the environment can be

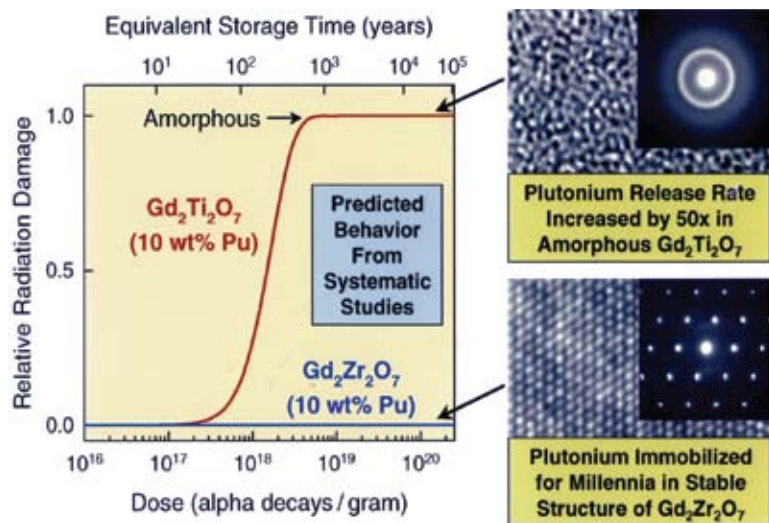


Figure 7.3. (left) The radiation damage undergone by two pyrochlore-structured phases containing 10 wt% plutonium, illustrating the marked difference in radiation damage in the two phases as a function of radiation dosage and the corresponding storage time over which such dosages would be accumulated. (right panels) Transmission electron microscopy of the radiation amorphized material (top) and crystalline material (bottom). Insets are diffraction rings from the amorphized materials and spots from the crystalline lattice. Reprinted with permission from Ewing et al. (2004), copyright 2004, American Institute of Physics.

averted. In effect, isolating radioactive materials within synthetic rocks, minerals, or ceramics is akin to simply inverting the usual extraction processes of elements, through creating high-grade, water- and radiation-resistant ores of these elements. The advantages of such storage are multifold: radioactive materials are immobilized, can be prospectively recoverable from their storage media, and are localized within secure “hard-rock” storage facilities.

Yet, the retention of radioactive materials is not simple. Energetic radioactive decay of elements produces radiation damage within host minerals, generally as a zone within the crystal that has had its crystalline order disrupted, or amorphized, by accumulated decay events. The amorphization of materials through radiation damage has significant similarities to pressure-induced amorphization, and our community has expended considerable effort to design and optimize the performance of waste isolation materials. The conceptual issues posed by such materials represent classic problems in crystal chemistry: what

structural sites are most suited to retain different radioactive elements, and what crystal structures are most resistant to damage? The societal issues addressed by these lines of research are long standing, and are incredibly important from an environmental perspective: how long and how safely can we store different forms of radioactive waste?

## Energy Storage and Climatic Issues

The development of improved means to effectively store hydrogen at relatively high densities is critical for the economic viability of hydrogen storage and delivery. One of the principal limitations of hydrogen as a fuel, and in turn for

the prospects of a “hydrogen economy,” involves the expense and inefficiency of hydrogen storage. Simply put, liquid hydrogen is both relatively low density (70 g/liter) and cold (20 K)—and liquefaction, boil off, and transport each limit the viability of hydrogen as a primary fuel. Pressure provides a natural means for achieving high densities, and hence our community has probed new methods by which hydrogen can be retained in abundance within crystalline phases at modest pressures. These potential storage means have included new types of clathrates—a broad designation for materials whose lattice is composed of one type of molecule, but in which other molecules or atoms can be trapped within holes in the structure. Among hydrogen-bearing clathrates, some phases are, at low temperatures, recoverable to ambient pressure. The prospect of such approaches to hydrogen storage may lead to their widespread utility.

The interest of the high-pressure geoscience community in clathrates is not, however, solely generated by hydrogen storage. The largest untapped natural

gas reservoirs of the planet are methane clathrates formed at the water-loaded high pressures of the continental shelves. The size of the submarine methane clathrate reservoir is not well characterized, but estimates are often of the order of trillions of tons, a remarkable amount that dwarfs by a factor of 10 or more the sizes of the well-known continental natural gas fields. Within these deposits, the characteristic chemistry of the methane clathrates is  $\sim 8\text{CH}_4 \cdot 46\text{H}_2\text{O}$ ; structurally, they bear many similarities to ice itself. Although clathrates have long been known, their extraordinary abundance in the shallow marine continental shelf environment (and their prospective economic importance) has reinvigorated studies of these complex molecular crystals. Notably, because of the abundance of hydrogen within these structures, state-of-the-art neutron diffraction methods, pioneered by high-pressure geomaterials scientists have been, in addition to a suite of spectroscopic techniques, among the primary probes of these materials.

While they may prove to be an important energy source in the future, the detailed stabilities of clathrates are also of critical environmental importance. If methane, one of the most effective greenhouse gases, is released in abundance from marine clathrates destabilized by warming ocean water, its atmospheric concentration could dramatically increase. Tantalizing hints exist that such destabilization, and short-term marked increases in the temperature of the planet, could have occurred  $\sim 55$  million years ago in conjunction with a long-term warming process. The Paleocene-Eocene Thermal Maximum appears to have produced a global temperature increase of  $\sim 6^\circ\text{C}$  that lasted for  $\sim 20,000$  years, with the initial time scale for clathrate destabilization and methane release being perhaps as short as 1000 years. Such a large temperature change dramatically affected the planet's biota. Evidence of previous environmental catastrophes may be retained in clathrate deposits beneath the ocean floor. Hence, there are both robust environmental and economic rationales for probing how

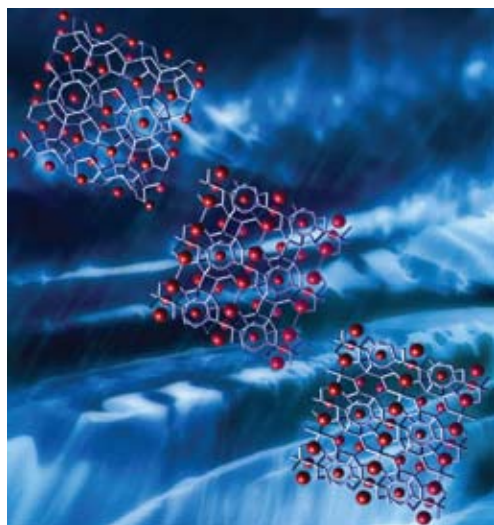


Figure 7.4. Images of different, closely related clathrate phases. The matrix is formed from water molecules. The red spheres are sites in which guest atoms or molecules (in this instance noble gases) can reside. In this image, the precise structure of these different polymorphs was resolved using neutron diffraction under pressure. Image courtesy of C. Tulk, Oak Ridge National Laboratory.



Figure 7.5. (left) Combustion of methane-ice clathrates. Photo courtesy of the Naval Research Laboratory. (right) Release of methane bubbles from the Hakon Mosby mud volcano at 1250-m depth in the Barents Sea. At this location, methane clathrates have been found to exist within 2 m of the seafloor. Reprinted from Figure 2a in Sauter et al. (2006), copyright 2006, with permission from Elsevier.

clathrates respond to changes in pressure, temperature, and composition. The high-pressure geosciences community continues to aggressively pursue studies of these novel and societally important materials.

Finally, the monotonic increase in atmospheric CO<sub>2</sub> concentration since the start of the industrial era has motivated widespread discussion of mechanisms for large-scale carbon sequestration. Because of the volumes of CO<sub>2</sub> involved, and the simple observation that Earth—through both organically and inorganically generated carbonates—already sequesters approximately the equivalent of 90 bars of CO<sub>2</sub> within its crust (for reference, our current atmospheric partial pressure of CO<sub>2</sub> is ~0.0004 bars), virtually all nonbiologic means of sequestration involve geologic settings. Many of the proposed techniques for carbon sequestration incorporate burial of carbon contained within solid-state materials, generation of carbonates from reaction of rock with injected CO<sub>2</sub>, or high-pressure CO<sub>2</sub>-water interactions. For example, the Norwegian North Sea Sleipner CO<sub>2</sub>-injection project involves inserting supercritical liquid carbon dioxide at a pressure near 100 bars at the rate of about 1 million tons per year into an underground saline aquifer ~1000 m beneath the ocean surface. In many pressurized environments, juxtaposed CO<sub>2</sub> and water react to form solid clathrates. Clearly, the experimental and theoretical simulation of what happens chemically to sequestered CO<sub>2</sub> (and at what rate) lies in the domain of the high-pressure geosciences. Hence, improvements in the ability to conduct larger-volume high-pressure experiments, with in situ characterization of reactions and their products, will facilitate the assessment and evaluation of proposed geologic means of carbon sequestration.

## Key Prospects

- Synthesize a greater variety of super-hard materials at high pressures, including those with novel electronic or thermal properties.
- Use high pressures as a guide for improving available means of nuclear waste sequestration.
- Use high-pressure experiments and theory to improve possible avenues of efficient hydrogen storage.
- Achieve better constraints on clathrate properties, and on the kinetics and thermodynamics of clathrate formation and breakdown

# Chapter 8 | Future of the Field: Building our Community

Three aspects of the high-pressure geosciences community have enabled us to achieve its past successes: personnel, infrastructure, and imagination. To achieve the community's goals as it moves forward, we need not only to ensure that the facilities and shared resources used continue to be both state of the art and readily accessible, but also that the curricular contributions and educational outreach of the community advance as new knowledge is gained. The infrastructure-oriented aspects of the community include (1) maintaining, upgrading, and replacing national x-ray and neutron facilities; and (2) ensuring appropriate support and access for high-pressure experimental needs at these facilities. Moreover, some community requirements are most readily achieved via centralized facilities or infrastructure. These needs might include larger presses, nanofabrication/analysis facilities, and, for theoretical calculations, centralized software and/or hardware repositories. All of the achievements with respect to scientific infrastructure rely, however, on a talented and creative user base.

Our community fully embraces the fact that the future of high-pressure geosciences lies in the hands of our present and future students. Maintaining a robust student population trained in high-pressure techniques is critical for our future scientific progress. Our recent success at moving students into the professoriate has been excellent: the high-pressure geosciences has placed over 30 of our Ph.D. students into new faculty positions at research universities in the last decade. Yet, sustaining our successes in developing human infrastructure will involve overcoming a variety of challenges, including those posed by shifting demographics and cultural attitudes. The high-pressure geosciences community takes these

challenges seriously, and has a longstanding track record of reaching out to students through education and outreach efforts, and collaborating with existing curricular initiatives in the earth sciences (e.g., the “Teach Mineral Physics Across the Curriculum” project described below). Going forward, the goal is to continue and expand these efforts while updating techniques and strategies to reflect our increasingly “online” and virtually connected culture.

## Recommendations for New Community Experimental and Computational Infrastructure

The high-pressure geosciences community has long embraced the recommendation of the 2009 NSF-GEO Vision report that geoscientists should “invest wisely in and responsibly manage the next generation of tools, technologies, and techniques, including advanced computation to enable cutting-edge research.” This dictum has been key to the past success of the community, and will certainly remain vital for the future. The new science that the community aspires to conduct involves a range of next-generation capabilities and technologies and hence requires that a range of technical challenges be surmounted. These new directions include: (1) reaching higher pressure and temperature conditions, and achieving high pressures and temperatures within larger sample volumes; (2) improving the ability to probe samples, both in situ at high pressures and temperatures, and quenched from these conditions, at the nanoscale; (3) making the transition from “point” measurements on high pressure and temperature samples to full-scale imaging of the spatial variations in sample properties;

(4) augmenting the ability to address issues of extrapolating among different time scales (e.g., from the experimental, in the femto- to megasecond range to those of planetary processes in the 0.01 to 100 petasecond range); (5) enhancing capabilities to probe the properties of heterogeneous phases and complex assemblages (and particularly interfaces and grain boundaries); and (6) achieving the precisions, accuracies, and resolutions in high pressure and temperature work that are enjoyed at ambient conditions. While these represent an ambitious set of goals, considerable progress has been made on each of these challenges over the last decade—and it is a robust expectation that the community’s rate of progress will be enhanced in the coming years.

Future progress in these areas hinges, as it has in the past, on access to state-of-the-art particle accelerators, which have dramatically decreased the spatial scale at which we are able to probe samples, enhanced the rate at which we are able to probe/image samples, and permitted better (and faster) time-resolved

measurements. In short, access to improved probes—whether involving x-rays, neutrons, or infrared radiation—has markedly improved our capabilities, and new generations of particle accelerators are, as is described below, critical parts of the high-pressure geosciences’ vision for the future. However, these more energetic and better-resolved probes represent only a portion of what is needed to produce advances in the high-pressure geosciences. There are several critical areas in which the high-pressure community needs to make major scientific advances.

### Larger-Volume, Higher-Pressure Experiments

From the experimental side, achieving larger volumes at high pressures and temperatures is a primary goal. Such larger volumes are expected to allow better controls on the chemical environment, more uniform conditions of pressure and temperature, more readily interrogated samples and, for deformational experiments, more accurately controlled stresses and strain rates. The production of a larger-volume,

higher-pressure facility for the community thus holds the prospect of a quantum leap in the caliber of data collected at extreme conditions. Moreover, such developments will extend large-volume experiments into pressure ranges that correspond to depth extents of the planet previously inaccessible by such experiments. There are indications that the time is ripe for rapid developments in this arena. Improvements in sintered diamond technology have produced stronger and larger anvils than previously available, and the understanding of how to more efficiently generate pressures in large-

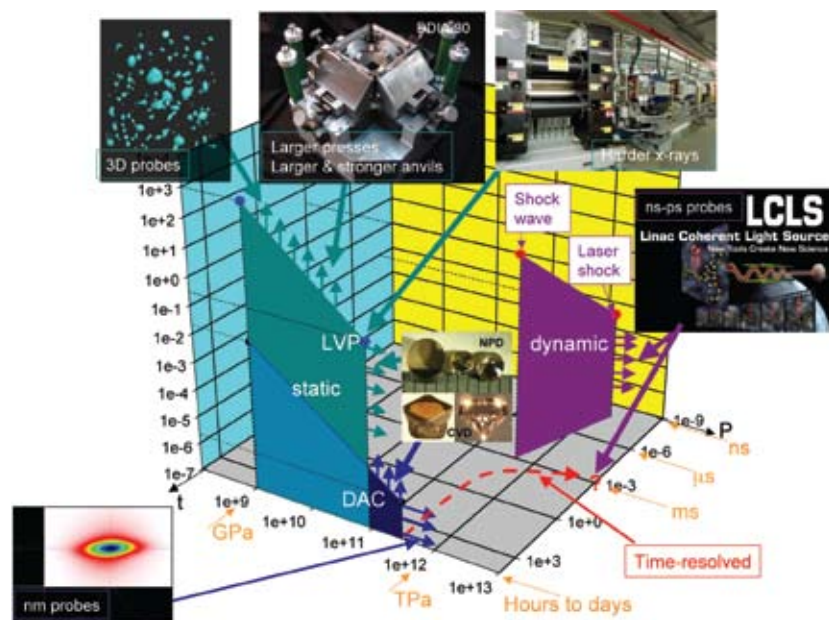


Figure 8.1. Pressure, temperature, and volume (in  $\text{mm}^3$ ) range of different high-pressure techniques, including the large-volume press (LVP), diamond anvil cell (DAC), and shock techniques. Possible means through which different ranges of pressure, volume, and time could be accessed are labeled by the insets. Courtesy of Y. Wang, University of Chicago.



volume apparatuses has progressively grown. Even with these developments, the likely effort associated with constructing such an apparatus transcends that which could be expected in any individual laboratory, and hence producing such a larger volume press will require a community-based effort.

### *Access to Nanocharacterization and Nanofabrication Facilities*

In addition, improving access to, and availability of, nanocharacterization and nanofabrication equipment for the high-pressure geosciences community is another key goal. The controlling factor here is that large sample volumes at extreme conditions are difficult to achieve. Hence, microanalysis can lead to not only constraints on material behavior in the tiny samples that are necessitated by ultra-high pressure and temperature conditions, but also to richer and more nuanced information being produced from larger, lower-pressure samples. Indeed, the ability to analyze materials at the nanoscale provides a key bridge to resolving the effects of the markedly different time scales between experiments and planetary behavior, as phenomena happening at the nanoscale on the experimental time scale may occur at the macroscale in the geologic time frame. Similarly, the ability to construct custom-designed micro-experimental charges offers the prospect of conducting complex, targeted experiments on electronic, magnetic, or transport properties at extreme conditions.

### *Creating Infrastructure for Theoretical Work*

For theoretical tools, a principal component of future progress involves access to, and development of, state-of-the-art computational codes. While development of new theoretical approaches will obviously continue, the high-pressure geosciences community is generally well poised to spearhead or take advantage of breakthroughs in theoretical techniques. Hence, a major goal is to ensure that a reliable, accessible, and user-friendly computational infrastructure for high-pressure geosciences exists that will strengthen the work of investigators not connected to a major

computational facility. Such a facility will also make it easier for new investigators to become established. This infrastructure might take the form of a virtual organization providing transparent access to computational resources, software, post-processing tools for analysis and visualization of results, collaborative capabilities, and, most importantly, training and support. A wide suite of governmental agencies continues to significantly invest in computational hardware that is made available to users, and therefore hardware infrastructure in and of itself does not currently represent a limiting issue for the high-pressure geosciences community. The materials simulation community has initiated such virtual organizations, and high-pressure geosciences goals include, where appropriate, effectively using such efforts, making them user-friendly for the geosciences community, and, where necessary, developing similar virtual efforts. For example, the theoretical community has devoted considerable effort to ensuring widespread availability of codes for the simulation of materials. Some of packages are free, while others are commercially available. User plus developer communities for some code packages number in the hundreds of researchers in academia and industry, and are at the cutting edge of developments in the field of materials simulations. In some instances, experienced development teams are available to deliver tutorials on computational methods of importance to the high-pressure geosciences. The availability of technically adept staff (akin to a theoretical version of beamline scientists) to support the use of powerful and popular software would likely enhance its use by the high-pressure geosciences community. The key aspect here is to enable all potential investigators, irrespective of their experience level, to use state-of-the-art theoretical techniques to address high-pressure problems.

### *Thermodynamics, Elasticity, and Transport Properties Databases*

There is also a broad-based need in the high-pressure geosciences to construct reliable, readily accessible state-of-the-art databases on the properties of

mineral, melt, and fluid assemblages at the extreme conditions of Earth's interior. One of the values of such an infrastructure is that it would supply our neighboring disciplines—geodynamics, which relies on thermal buoyancy forces, petrology with its dependence on rock chemistries, seismology, which hinges on the elastic properties of minerals, geomagnetism, which depends on core properties and the conductivity properties of the planet—with ready access to information that the high-pressure geosciences can provide. The challenge of constructing such a database (or databases) lies in the intrinsic chemical complexity and extreme thermodynamic conditions of the planet's interior. The most viable means of constructing such a database involves combining the best information from both the experimental and theoretical domains to construct a consistent and comprehensive database for use by the entire geophysics community. The ambition is to create a web-based and interactive database that would also fulfill a pedagogical function in offering hands-on experience in thermodynamics or elasticity of minerals to both beginners in the high-pressure geosciences community, and users in other disciplines.

### **Maintaining and Enhancing Access to State-of-the-Art Beamlines**

The net goals of both experimental and theoretical high-pressure geoscientists are to better understand the petrology, deformational behavior, elastic properties, and chemical behavior of plausible Earth materials over the depth and pressure range of both our own and other planets, and to be able to simulate the interactions and structure of fluids and melt-fluid aggregates at pressures ranging from those of the crust to the core. The high-pressure geosciences has both helped develop and taken advantage of new and in some instances previously unanticipated techniques to pursue novel approaches to problems. In the last few years, these techniques have ranged from nanoscale tomography, to laser-driven shocks, to nuclear resonance x-ray spectroscopies. Such creative

and serendipitous developments will, of course, continue. Ensuring that the infrastructure and human capital exist to fully take advantage of such developments is a clear priority for the community.

In the context of infrastructure, the ability to probe samples in situ under high pressure and temperature has been a crucial development in advancing the field of mineral physics. Large accelerator-based facilities produce infrared, x-ray, and neutron beams with sufficient intensity to allow rapid, spatially resolved measurements of samples held at high pressures. The tremendous advances in such sources over the last three decades has enabled fundamentally new types of measurements, resulting in major advances in our understanding of the properties of materials at extreme conditions. X-ray diffraction and spectroscopy experiments can now be performed at the pressure and temperature conditions of the core-mantle boundary. There remain, however, significant limitations on pressure, temperature, sample size, and probe intensity that restrict what can be done. New light sources coming online and others in the planning stages will enable dramatic improvements in the spatial and temporal resolution of experiments conducted by our community. Here, we give general overviews of the new and soon-to-be-built sources to which the high-pressure geosciences community has, or aspires to have, significant access.

#### ***Spallation Neutron Source***

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory has the most intense neutron beam among research facilities worldwide, and our community has ensured that a beamline at this source was dedicated to high-pressure research (Spallation Neutrons at Pressure, or SNAP). The dedicated SNAP beamline for high-pressure research was developed by a team of geoscientists and commissioned in early 2008. Neutrons are ideal for studies of materials containing hydrogen (or deuterium), such as water in deep Earth minerals, or new materials for hydrogen storage. This is a simple consequence of the neutron scattering cross section of hydrogen and deuterium

(which, for comparison, have small x-ray scattering cross sections). Neutrons are also the preferred probe for studying electron spins, and we will now be able to probe the magnetic properties of materials at conditions of the deep Earth. Neutrons are also highly useful for examining the texture, or anisotropy, of samples, and the structure of amorphous materials. The primary dilemma with neutrons in high-pressure research is that they require a fairly large sample size (on the order of  $1 \text{ mm}^3$ ) to generate useful diffraction data. Therefore, improvements in generating higher pressures within larger-volume samples are expected to immediately enhance the capabilities of conducting neutron scattering under extreme conditions.

### Advanced Photon Source

The Advanced Photon Source (APS) at Argonne National Laboratory is the nation's brightest source of hard x-rays (that is, high energies above about 25 kiloelectron volts). It has a number of specialized facilities for high-pressure research, including those at GSECARS, HPCAT, and the nuclear inelastic x-ray scattering beamline 31D. Using these beamlines, researchers can conduct not only x-ray diffraction experiments at high pressures and temperatures, but can also make a broad suite of other measurements. These measurements include x-ray emission spectroscopy (for iron spin-state studies), x-ray Raman scattering (for low-Z electronic structure), nuclear resonance scattering (for iron electronic structure and phonon densities of states), and ultrasonic measurements (for sound speed determinations under

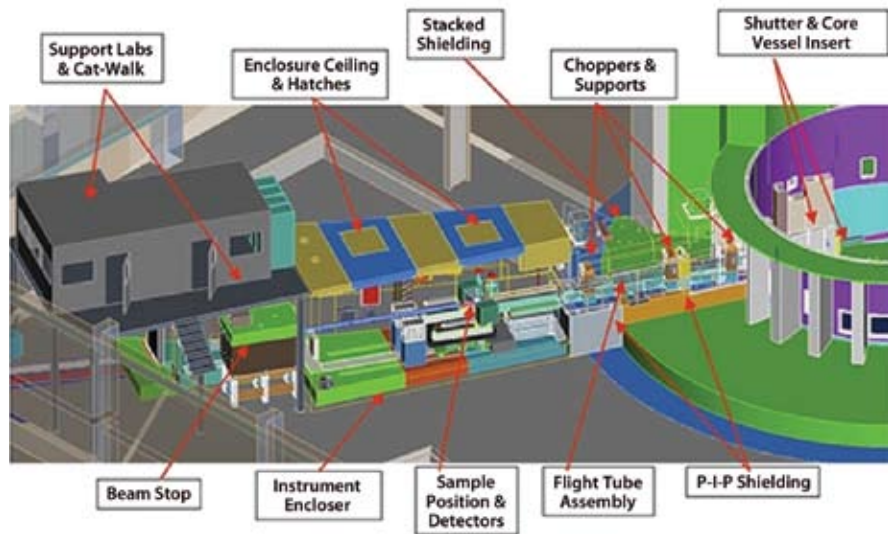


Figure 8.2. Schematic of the now-complete high-pressure beamline at the Spallation Neutron Source. Horizontal dimension is approximately 30 m, and the high-pressure device is mounted at the location labeled “sample position.” Courtesy of C. Tulk, Oak Ridge National Laboratory.

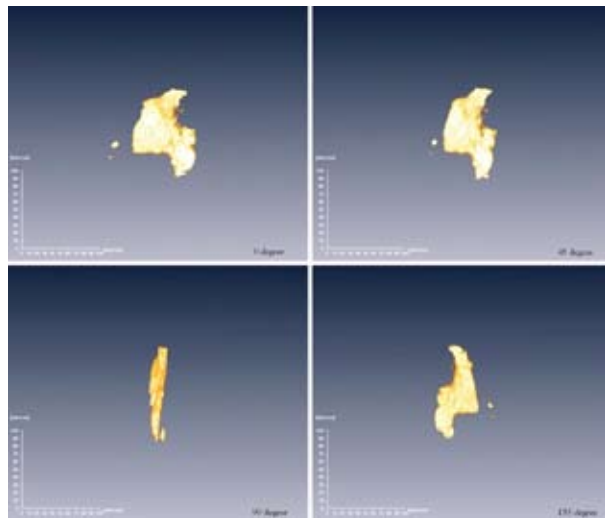


Figure 8.3. Tomographic images of a sample of amorphous Se held at a pressure of 10.7 GPa within the diamond anvil cell, and measured at the HPCAT facility of the Advanced Photon Source at Argonne National Laboratory. Because of the accuracy with which the three-dimensional image of the sample can be reconstructed, the volume of the sample can be determined as a function of pressure from the 3-D imaging alone. From: Figure 4 in Liu et al. (2008).

deep-Earth conditions). The APS beamlines are being upgraded over the next several years to use new optimized undulator sources and improved optics, which

will greatly increase the x-ray beam quality available for high-pressure research. In short, the prospects for improved spectral and spatial resolution are excellent.

### National Synchrotron Light Source

The National Synchrotron Light Source (NSLS) is the home of the first U.S. dedicated high-pressure diamond cell line in 1990, the first multi-anvil beamline in 1992, and the first infrared beamline in 1999. These beamlines, operated by COMPRES, continue both to foster creative science and spawn new techniques. X-ray diffraction and imaging capabilities enable a wide range of experimental studies at NSLS. A new synchrotron, NSLS II, is currently under construction and is anticipated to replace NSLS-I in 2015. This facility will increase the beam brightness by nearly five orders of magnitude compared to the existing high-pressure beamlines at NSLS-I. It will be the premier source in the country for performing experiments below x-ray energies of 25 keV and above 50 keV, depending on the insertion device. Improved

capabilities will result for diffraction, imaging, x-ray Raman scattering, x-ray emission spectroscopy, and nuclear resonant scattering.

### Advanced Light Source

The Advanced Light Source (ALS) at Lawrence Berkeley Laboratory is a third-generation synchrotron facility with a major commitment to high-pressure research. In particular, facilities are available for high-pressure/high-temperature x-ray diffraction studies in diamond anvil cells on the dedicated beamline 12.2.2, with both conventional (along the axis of force of the diamonds) x-ray diffraction and radial (perpendicular to the axis of force) diffraction capabilities. Both laser-heated and resistively heated cells are used; multiple temperature measurement systems have been deployed (conventional and four color) for characterizing both the temperature and its distribution within laser-heated samples. High-pressure experiments are conducted on a beamline that uses a superbend source, with energies in the 6–40 keV range.

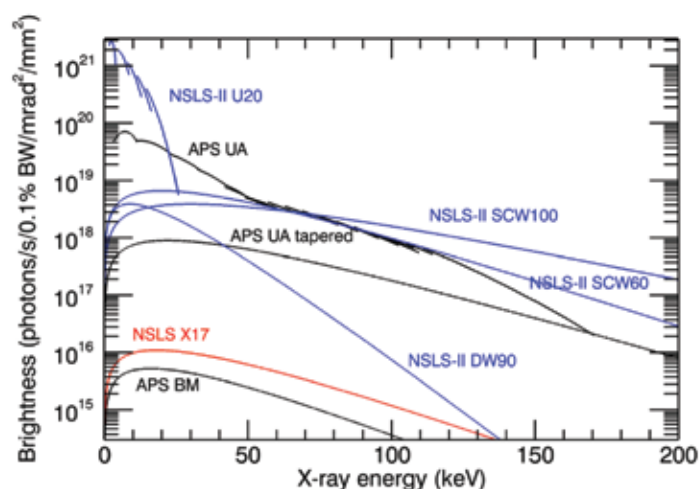


Figure 8.4. (left) Brightness of synchrotron x-ray sources at the National Synchrotron Light Source (NSLS) and the Advanced Photon Source (APS). Sources include the NSLS-II 20-mm period undulator tuning curve; NSLS-II superconducting wiggler 100-mm period, 6T field; NSLS-II superconducting wiggler 60-mm period, 4T field; NSLS-II damping wiggler, 90-mm period; NSLS X17 superconducting wiggler; APS 33-mm period undulator tuning curve; same APS undulator with gap tapered from 10.5–12.5 mm, modeled as a wiggler source; and APS bending magnet. Courtesy of M. Rivers, Advanced Photon Source. (right) Artist's conception of the NSLS-II ring storage building that is currently under construction. Circumference of ring is 792 m. Courtesy of Brookhaven National Laboratory.

### Energy Recovery Linac

The brightness of storage ring sources is ultimately limited by the equilibrium horizontal beam size that results from the competition between energy loss and focusing as the electron beam orbits for many revolutions. Linear accelerators, on the other hand, can produce beams whose sizes are limited only by the brightness of the electron gun. Producing a high-intensity x-ray beam from a linear accelerator (linac) is prohibitively expensive in energy consumption unless the beam energy can be recovered within the linac itself.

Such an energy recovery linac (ERL) has been proposed by a group from Cornell University. This proposed source would have a much smaller electron beam size, and a two-to-three order of magnitude increase in brightness compared to storage ring sources. It would also have much shorter pulse lengths, permitting fast, time-resolved experiments that can use repetitive pump-probe methods. Such a source would be ideal for 20 keV high-pressure experiments, permitting a further order-of-magnitude decrease in beam size or a factor of 100-fold increase in intensity at the same size, even compared to NSLS-II. Such a source would truly represent the next generation in beamline technology beyond the upcoming set of new synchrotrons. A conceptual design for this instrument is likely to be submitted in 2010 and, if approved, construction would probably take about five years. Hence, the possible ERL construction lies well within the planning horizon of the high-pressure geosciences community.

### Linac Coherent Light Source

The Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator is the nation's first hard x-ray free-electron laser (FEL). It is a fundamentally new type of x-ray source with a peak brightness that

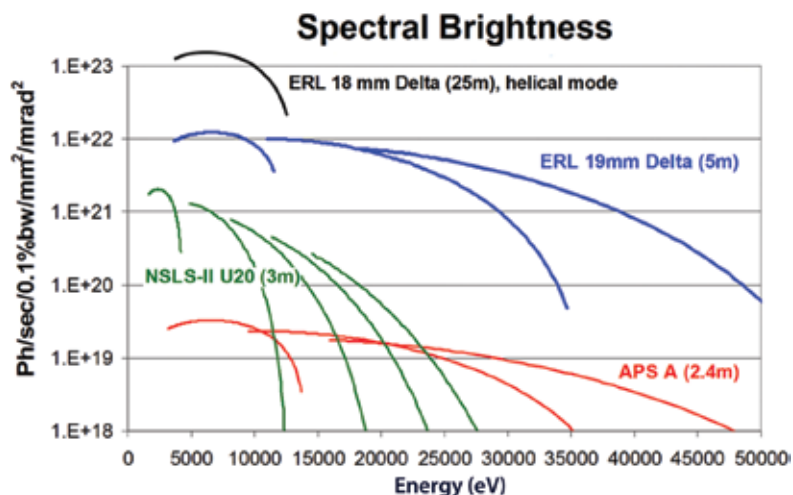


Figure 8.5. Prospective brightness of an energy recovery linear accelerator (ERL) relative to that accessed currently by the Advanced Photon Source (APS), and by the National Synchrotron Light Source-II (NSLS-II) after its completion. Courtesy of M. Rivers, University of Chicago.

is nearly eight orders of magnitude greater than storage ring sources such as APS or NSLS-II. It delivers a tremendous number of coherent photons ( $10^{12}$ ) in a single extremely short pulse (40 fs) with a low pulse repetition rate (<100 Hz). It will permit entirely new classes of experiments, such as prospectively capturing a complete diffraction pattern during a laser-driven shock wave, or allowing studies of highly excited states and nonlinear phenomena. Indeed, each x-ray pulse from LCLS has sufficient intensity to produce an x-ray pattern from a shocked material that is comparable to those generated statically within the laser-heated diamond anvil cell at third-generation synchrotron sources. The LCLS source is completely coherent in the spatial domain, which means that the source is diffraction-limited in its size and angle. First light for this facility was achieved in September 2009, and one of the beamlines is designated as a Matter at Extreme Conditions beamline.

### Facilities Overview

Over the last several decades, the high-pressure geosciences community has leveraged access to superlative national facilities to generate a broad suite of novel discoveries and new insights into Earth's

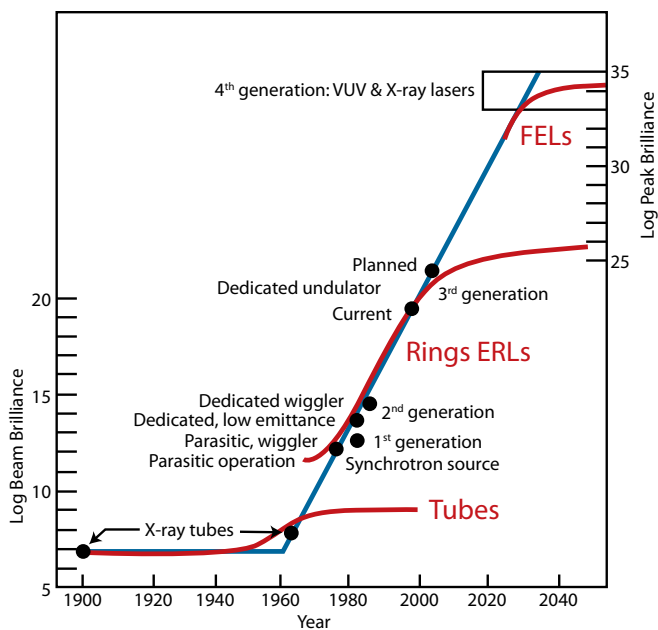


Figure 8.6. Increase in brilliance of x-ray sources with time, with orders of magnitude jumps in intensity being associated with shifts in x-ray generation technology. Courtesy of M. Rivers, University of Chicago.

internal structure using innovative experimental techniques. As new facilities are constructed and older facilities upgraded, it is a critical community-wide goal to maintain and enhance access to this improving set of high-intensity beam sources. Moreover, assuring that adequate technical and infrastructure support is available so that the community can make optimal use of these national assets represents a vital and complementary priority. Such support is currently made available to the community through consortia and collaborative research teams such as COMPRES, GSECARS, and HPCAT. The combination of access to, and support at, state-of-the-art facilities, coupled with the high-pressure geosciences' long-standing pattern of creativity and scientific innovation, has provided a highly successful recipe for international scientific leadership in the high-pressure geosciences. And, it is a recipe that is anticipated to remain successful well into the future.

## Improving Educational Materials and Community Outreach/Recruitment

The field of high-pressure geosciences is intrinsically interdisciplinary. Within the earth sciences, high-pressure practitioners span the subdisciplines of mineral physics/mineralogy, geochemistry, and petrology. Beyond the earth sciences, the expertise of high-pressure geoscientists has considerable overlap with condensed-matter physics, solid-state chemistry, and materials science. Such interdisciplinarity has both advantages and disadvantages. Although there is no formal course or curriculum that a typical undergraduate would encounter that deals primarily with the high-pressure geosciences, recruits to the field may emerge from many different scientific disciplines. Hence, the outreach and educational focuses of the community have been on working toward injecting high-pressure geosciences into the K–16 curriculum wherever possible, and pursuing student recruitment from a range of different backgrounds and disciplines.

Accomplishments in education and outreach include both organized efforts (e.g., through COMPRES) and the distributed efforts of community members working at their home institutions. The Consortium has worked with other earth science organizations to promote inquiry-based education and outreach by participating in nationwide collaborations between scientists, educators, materials developers, government agencies, and other stakeholders. These efforts include collaborations with the seismologically oriented EarthScope, the Digital Library for Earth Systems Education (DLESE) projects, and the Science Education Resource Center (SERC) at Carleton College. In the last case, taking advantage of interactions with pedagogically oriented faculty at Montana State, community members have contributed a sequence of ready-to-lecture modules for “Teaching Mineral Physics Across the Curriculum” at the undergraduate level.

The high-pressure geosciences community has also aggressively promoted opportunities for high school students and undergraduates to become involved in high-pressure research. Members of the high-

pressure earth sciences community have sponsored a variety of Research Experiences for Undergraduate Programs under the aegis of NSF, and COMPRES has supported internships for undergraduates working at high-pressure-oriented beamlines. In addition, a large fraction of high-pressure researchers actively engage undergraduates in their research by supporting them with their regular research grants. Many of these students present papers at American Geophysical Union meetings, appear as coauthors on publications, and some go on to research careers in science. Through these efforts, the community has exposed large numbers of undergraduates and in some cases high school students to high-pressure geoscience.

As with the other physical sciences, the representation of minorities and women in the high-pressure geoscience community is currently inadequate. The community has actively sought to recruit minority members for years and is continuing to work aggressively in this area. New efforts in minority recruitment include participation by NSLS in the Historically Black Colleges and Universities (HBCU) Interdisciplinary Consortium for Research and Education Access in Science and Engineering (INCREASE). The goal of the INCREASE program



Figure 8.7. Undergraduates working under the aegis of NSF's Research Experience for Undergraduates Program at the control center of the multi-anvil cell beamline at the National Synchrotron Light Source. Interlocked door to the x-ray hutch is present in the background. Photo courtesy of G. Gwanmesia, Delaware State University.

is to engage faculty from HBCUs in research using synchrotron facilities and to train students from these institutions in synchrotron research. By working with student-faculty research teams, the program aspires to create continuity between the student's research experience and the rest of their educational experience. The program will also develop curriculum for a two-course sequence in basic synchrotron science to be taught at HBCUs. Members of the high-pressure geosciences community have been actively seeking funding for such initiatives from programs in the NSF Directorate of Geosciences such as "Opportunities for Enhancing Diversity in Geosciences."

The inherently interdisciplinary nature of high-pressure experimental geoscience poses particular challenges for traditional higher-education structures, which typically discourage training in interdisciplinary fields by focusing program evaluation criteria on metrics tied to departments and through competition for resources among departments. Graduate students training to work in experimental high-pressure geoscience typically require significant course work that is not offered within geoscience programs. In this way, the discipline is constantly pushing the leading edge of U.S. universities' efforts to move toward interdisciplinarity. Members of our community are currently working on an effort to define a community-wide set of learning goals for graduate students to assist faculty in planning their students' training. The combination of skills needed for high-pressure geoscience research serves as a strong foundation for professionals in a wide suite of industries, including those related to petroleum and high-technology materials. Indeed, significant numbers of our graduates enter these fields.

### Future Educational Directions

Going forward, we envision a three-pronged approach to building a diverse mineral physics work force. Our primary educational focus is in higher education. The current trend is toward diversifying undergraduate geoscience education to include

courses in climate and environmental science. This expansion of scope of traditional geoscience majors dictates integrating high-pressure geoscience topics into existing courses for geoscience majors, rather than introducing them in new courses. Information about high-pressure geosciences is far more likely to be included in the curricula of existing courses if non-high-pressure-oriented faculty have easy access to interesting, well-formatted materials that tie directly into their existing courses. Therefore, one strategy instituted by our community involves developing such modular curricular materials. For example, materials discussing high temperature and pressure rock deformation fit naturally into structural geology courses, and materials discussing the deep carbon and nitrogen cycles can readily be included in courses covering Earth history and environmental science. Naturally, there are ample opportunities to incorporate materials into introductory mineralogy and igneous and metamorphic petrology courses. An additional area with considerable potential is modular materials for introductory classes. These modules can describe the relevance of high-pressure experimental work to topical questions, such as the origin of plate tectonics, volcanism, the origin of Earth's ocean, or the connection between processes of core formation and the amount of carbon and hydrogen available to the biosphere.

Faculty members who are high-pressure geoscientists frequently integrate discussions of their research into their teaching. Yet, few students actually have the opportunity to engage in research at major facilities. Accordingly, expanding virtual access to synchrotron facilities could facilitate introducing a far broader suite of students to cutting-edge science, and is likely to be particularly effective with the current generation of socially networked, Internet-oriented students. Indeed, some instructor/researchers have begun using Skype, video cams, and other existing technology to connect to their classes while on the beam line—in essence, producing “virtual access” to laboratory experiments and facilities.

The community must also continue to vigorously pursue efforts to increase the numbers of minorities and women within its ranks. This task will require continued engagement in enterprises such as the INCREASE program recently initiated at NSLS, as well as improving our community's interfacing with organizations such as the Society for Advancement of Chicanos and Native Americans in Science (SACNAS). In short, the recruitment of minority and women graduate students is a long-standing challenge in the physical sciences. Among the most empirically successful recruitment interactions are those that involve well-established “pipelines” between particular undergraduate institutions and individual research groups or departments. A challenge for our community is to establish pipelines that extend throughout our discipline, through interactions with institutions that incorporate substantial diversity in their student body.

### Future Community-Building Goals

- Maintain and ensure access and technical support for the high-pressure geosciences community at existing and future national experimental facilities.
- Improve and increase our educational outreach to the K–16 community through curricular contributions, organized programs, and individual efforts.
- Develop a larger volume, higher-pressure community facility.
- Ensure community access to nanocharacterization and nanofabrication facilities.
- Construct an easily accessible, web-based database of thermodynamic, elastic, and transport properties of mineral, melts, and fluids.
- Develop infrastructure for easy access to, and technical support for, community members to use state-of-the-art theoretical codes.



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# Acronyms

ALS.....	Advanced Light Source (Lawrence Berkeley National Laboratory)
APS .....	Advanced Photon Source (Argonne National Laboratory)
ATEM .....	Analytical transmission electron microscopy
COMPRES.....	Consortium for Materials Properties Research in the Earth Sciences
CVD .....	Chemical vapor deposition
DLESE .....	Digital Library for Earth Systems Education
DOE .....	US Department of Energy
ERL.....	Energy recovery linac
FEL .....	Free-electron laser
GSECARS .....	GeoSoilEnviro Consortium for Advanced Radiation Sources
HBCU .....	Historically Black Colleges and Universities
HPCAT.....	High-Pressure Collaborative Access Team
HPSynC.....	High-Pressure Synergetic Center
INCREASE .....	Interdisciplinary Consortium for Research and Education Access in Science and Engineering
LCLS .....	Linac Coherent Light Source (Stanford University)
LLSVSP .....	Low-shear velocity province
NSF.....	National Science Foundation
NSLs.....	National Synchrotron Light Source (Brookhaven National Laboratory)
PREM.....	Preliminary Reference Earth Model
RBS.....	Rutherford Back-Scattering
SACNAS .....	Society for Advancement of Chicanos and Native Americans in Science
SERC .....	Science Education Resource Center at Carleton College
SIMS .....	Secondary ion mass spectrometry
SNAP .....	Spallation Neutrons at Pressure
SNS.....	Spallation Neutron Source (Oak Ridge National Laboratory)
ULVZ .....	Ultra-low velocity zone



COMPRES | the Consortium for Materials Properties Research in Earth Sciences

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