Current and Future Research Directions in High-Pressure Mineral Physics
High-Pressure Mineral Physics

The field of high-pressure mineral physics is highly interdisciplinary, encompassing the full range of chemical, physical, and biological processes that take place at high pressures beneath the surfaces of planets. These processes influence magnetism in Earth’s core at over 1.3 million atmospheres of pressure, and methane production by microbes at high pressure in ocean sediments. In the broadest sense, the goals of mineral physics studies are to understand how planetary systems operate, from the center to the surface, and to understand the processes involved in planetary evolution. This is done by examining the properties of minerals under extreme high pressure and temperature conditions, by performing computer simulations to understand the behavior of planetary materials at the most fundamental atomistic level, and by studying the interactions among the components of the entire Earth system—be they chemical reactions among minerals or biologically mediated interactions.

This field has witnessed numerous discoveries and breakthroughs during the past decade. Along with breakthroughs come not only the ability to understand more-complex phenomena, but also the ability to confront exciting challenges. In light of these recent achievements, the challenges for the future, and, consequently, the immense prospects for discovery in the field of mineral physics, it seems timely to describe them in a single document. This report is organized to take the reader on a journey from Earth’s center to its surface, and then beyond to the other planets and moons in our solar system, all from the perspective of high-pressure mineral physics.

Finally, no description of high-pressure mineral physics would be complete without mentioning the role that technology plays in our research. This is a field that has distinguished itself through technological innovation and invention. In trying to understand the interiors of planetary bodies, Earth and planetary scientists have been the leaders in pushing forward the boundaries of extreme conditions that can be attained in the laboratory. They have been central players in the use of synchrotron radiation and neutron scattering for understanding the states of matter at high pressures and temperatures. High-pressure mineral physics is an area that by its very nature thrives on inventing new tools to understand Earth, and to see deeper and deeper into the interiors of planetary bodies.

Earth cover figure courtesy of Edward Garnero, Arizona State University.
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Diamond Anvils, Multi-Anvil Apparatus, and Growing Big Diamonds: Tools of High-Pressure Science

Diamond is the hardest and toughest substance known to man. As such, it is the material of choice to use as a pressure-generating “anvil” in high-pressure devices. Diamonds have been used as anvils to attain the highest pressures ever achieved in the laboratory. However, the rarity of large natural diamonds and their great expense has limited such ultra-high-pressure experimentation to extremely small samples. Obtaining larger diamond anvils is the key to performing a range of experiments that require larger samples, such as neutron scattering experiments. Recent breakthroughs in the growth of synthetic diamonds in the laboratory indicate that a new generation of high-pressure equipment using large diamond-anvils may soon become a reality.

A research team at the Carnegie Institution of Washington and the Los Alamos National Laboratory has reported a major breakthrough in growing diamonds from chemical vapor deposition. They found that these high-pressure-temperature annealed crystals are the hardest diamonds ever tested. See Yan, C-s., H-k. Mao, W. Li, J. Qian, Y. Zhao, and R. J. Hemley, 2004, Phys. Stat. Solidi, (a) 201, R25.

The natural diamond anvils in these different styles of high-pressure cells are approximately 1/4 carat in weight. Scaled-up devices would be used with the large synthetic diamonds of over 1 carat in weight to do a new generation of high-pressure experiments using larger samples. Photo courtesy of Dmitry Lakshtanov, Stanislav Sinogeikin, and Jay Bass, University of Illinois, Urbana-Champaign.

T-25 multi-anvil, high-pressure module installed in a 1000-ton press on GSECARS beamline at the Advanced Photon Source of the Argonne National Laboratory. Using this apparatus, pressures in excess of 25 GPa and temperatures over 2000 K can be obtained in samples of 1 cubic millimeter volume. Photo courtesy of Yanbin Wang, University of Chicago.
The interiors of Earth and other planets cannot be directly observed. No borehole has ever pierced Earth’s thin crust due to the high temperatures and pressures existing at depth. Yet we know a great deal about Earth’s interior, and what we have learned over the last 10 years in particular has been astonishing. The simple layered models depicted in textbook diagrams (e.g., Figure 1A) are being replaced with more sophisticated models that show the complexity and dynamics of Earth’s interior (e.g., Figure 1B). The features of this internal system give us clues as to how the interior works—for example how material moves, how heat is transported, and what it is made of—and how Earth evolved to this state.

Earth’s interior continues to affect society in very direct and profound ways. Earthquakes and volcanic eruptions result from chemical reactions and motions in Earth’s mantle, the stony region from a few tens of kilometers depth beneath the continents to almost 3000 km in depth. Buried at shallow levels beneath the ocean floor and preserved by high pressures in the sediments are the greatest known deposits of hydrocarbon energy resources—clathrates. Clathrates are also a potential major contributor to global warming and underwater landslides that can generate tsunamis. At much greater depth, motions in Earth’s metallic core are responsible for the magnetic field at the surface, which is the basis for navigation. Computer simulations of liquid metal flow in the outer core that can generate a magnetic field like Earth’s have just been achieved in recent years. We now know that Earth’s mantle likely contains far more water and carbon dioxide than is present in all the world’s oceans and atmosphere combined. Direct evidence of carbon reservoirs in the mantle can be seen in diamonds. This most valuable of gemstones originates hundreds of kilometers beneath the surface. Thus, mantle processes have probably had a strong influence on the quantity of carbon dioxide—a major greenhouse gas—present in the atmosphere. The common thread that unifies these diverse phenomena is that they involve processes in materials at extremely high pressure and temperature conditions.

Figure 1. A. Simplified depiction of Earth’s layers. B. Modern view of the mantle. Seismically fast regions are shown in blue, slow regions are red. Red regions are likely hotter and more buoyant than average mantle, while blue regions are likely cold and dense. Figures courtesy of Edward Garnero, Arizona State University. B also from Grand, S.P., 2002, Mantle shear-wave tomography and the fate of subducted slabs, Phil. Trans. R. Soc. Lond. A, 360, 2475-2491.
Only a few isolated pieces of deep-Earth rock have ever been found. These are relatively small pieces of the mantle brought to the surface over a billion years ago during the most violent volcanic eruptions in Earth history. These are the same rare rocks (kimberlites) in which diamond deposits are found. As valuable as these clues are, they tell us only about a relatively shallow part of Earth’s interior.

Nevertheless, the last decade has brought unprecedented advances in understanding Earth’s interior and other planetary bodies in our solar system. These advances have come through the development of instruments that simulate the incredibly high pressures and temperatures existing in planetary interiors (see box opposite page 1). This growth in the high-pressure field has in turn been largely stimulated by the availability of U.S. national research facilities, in particular high-energy radiation sources (e.g., synchrotron x-rays, infra-red radiation, neutrons) that allow us to probe the properties of matter at extreme pressures and temperatures. These sophisticated facilities have presented extraordinary opportunities for understanding Earth and other planets. The technology for performing an entirely new generation of experiments is now within our reach. We will be able to “see” the complex interiors of planets with a clarity that could not be imagined only a decade ago.

This report is an outgrowth of the discussions and results of a workshop on A Vision for High Pressure Earth and Planetary Sciences Research: The Planets From Surface to Center held on March 22-23, 2003 in Miami, Florida. The National Science Foundation’s (NSF) Division of Earth Sciences commissioned and supported this workshop, and the NSF-funded Consortium for Materials Properties Research in Earth Sciences (COMPRES) organized it. Fifty-six scientists attended the workshop (Appendix 1), convened by Jay Bass and Donald Wiedner.

The stimulus for the workshop was the rapid growth of the field of high-pressure mineral physics, the numerous scientific discoveries made in recent years, and the enormous prospects for future scientific breakthroughs. In addition, it was recognized that there is a rapidly increasing demand on centralized national facilities for experimentation and computation in high-pressure mineral physics. COMPRES was formed in part as a response to these developments, with the mission of identifying promising research opportunities, promoting the development of new technology, providing coordinated oversight of certain centralized facilities, and providing education and outreach for the high-pressure Earth and planetary sciences community. The Miami workshop was held to identify the most promising areas for future scientific discovery, and areas that are ripe for future technological breakthroughs. This document is intended to be a statement by the high-pressure Earth science community on the status of our field and some of its most exciting and challenging directions for the near future.
The Core and Core-Mantle Boundary

One of the greatest achievements of high-pressure science has been the ability to reach pressures and temperatures of Earth’s core in the laboratory (Figure 3). This pressure regime is from 1.3 million atmospheres (1.3 Mbar) at the boundary between the mantle and core, to 3.3 Mbar at Earth’s center. The magnitude of such pressures far exceed anything known through human experience.

Although Earth’s core is not directly accessible to us, a detailed and fascinating picture of this region has been revealed during the last decade. Seismological studies have shown that the solid inner core at Earth’s center is anisotropic, with faster seismic velocities in N-S directions than along equatorial paths. Earth’s inner core may also be “super-rotating,” with a speed that is faster than the surrounding mantle and crust. If so, this superrotation may be key to understanding how magnetic forces couple with the iron-rich core and how the geomagnetic field is generated.

At the upper boundary between the rocky mantle and the liquid outer core (the core-mantle boundary or CMB), scientists have detected a far more complicated structure than previously thought. This CMB structure is, in fact, suggestive of large-scale chemical reactions and the presence of iron-rich silicate liquids where the core and mantle are in contact. Alternatively, the properties of the CMB may also reflect a phase transition, or new atomic structures for phases with different properties than those of the overlying mantle. The CMB region may be as complicated as the interface between the solid Earth and the atmosphere. Understanding the cause of the CMB structure appears to be crucial for understanding the dynamics and evolution of our planet. Due to possible chemical and physical interaction between the mantle and core, and/or

Figure 3. Summary of the pressures and temperatures that can be attained by “static” experimental techniques, compared with the expected pressures and temperatures in Earth (the geotherm). With static techniques, samples are compressed by two or more anvils, as in the Large Volume Press (LVP, six anvils), or the Diamond Anvil Cell (DAC, two diamond anvils). A goal for the next decade is to simultaneously attain the pressures and temperatures at Earth’s center and at the deeper portions of the giant planets. Figure courtesy of Guoyin Shen, University of Chicago.
Simulating Core Pressures and Temperatures with the Laser-Heated Diamond Cell

Advanced technologies of high-pressure experimentation have made it possible to simulate material properties and reactions under extreme conditions equivalent to those in Earth's core. Rapid progress in computational mineral physics has also contributed to a better understanding of materials properties under these conditions. The laser-heated diamond anvil cell is one of the main experimental tools for reaching the pressures and temperatures conditions in Earth's core for long time periods, allowing a variety of measurements to be made. High-powered lasers produce the greatest temperatures under static, high-pressure conditions.

Major questions about the core that are being pursued with the diamond anvil cell and theoretical calculations include:

**Heating Up The Core.** One of the first quantum mechanical calculations on mineral properties conducted ~30 years ago suggested a significant solubility of potassium in iron under core conditions. Recent experimental studies under high pressure support this notion. These results suggest that substantial heating in Earth's core is possible, which affects the history of Earth's magnetic field.

**Core Anisotropy.** Both theoretical and experimental studies have been performed on the elastic anisotropy of solid iron under Earth's inner core conditions. Results indicate substantial elastic anisotropy, but the nature of elastic anisotropy appears to be sensitive to temperature.

**Core-Mantle Boundary.** The properties of silicate minerals such as perovskite at core-mantle boundary layer conditions have been investigated both experimentally and theoretically. Both results show that a phase transformation in this mineral to a highly anisotropic structure provides a possible explanation of the properties of the core-mantle boundary.
To simulate conditions in Earth’s core, the sophisticated laser-heating system at the Advanced Photon Source, Argonne National Laboratory, heats to high temperatures (up to thousands of degrees Celsius) samples that are compressed to high pressure in diamond anvil cells (left). This particular system is used for Nuclear Inelastic X-ray Scattering (NRIXS) experiments to measure the physical properties of deep-Earth materials containing iron atoms. It is being used extensively to study the properties of possible core materials.

In this Nuclear Inelastic X-ray Scattering (NRIXS) experiment with laser heating, x-rays come from the right and hit the sample at high pressure and temperature (left). The sample is buried within the copper cooling block near the center of the photo. From this experiment, which is only possible with the most modern synchrotron facilities, seismic velocities on core materials can be measured. This new type of experiment is being carried out at the Advanced Photon Source. (Photos courtesy of Wolfgang Sturhahn, Argonne National Laboratory)
high pressures and temperatures. For example, to understand the cause of seismic anisotropy of the inner core and how core material deforms in response to various forces, we need to know the elastic constants of iron under inner core conditions. These have been measured and calculated for the first time only within the last few years. Theoretical studies on the energy budget of the core-mantle system suggest that a large amount of heat is expected to be generated in the core. Indeed, it is this heat that drives fluid motion in the outer core and generates Earth’s magnetic field. Both theoretical and experimental studies now suggest that the quantity of radioactive elements that can be dissolved in iron may be very different at deep-Earth conditions. A better understanding of this problem is critical for understanding the generation of the geomagnetic field as well as the history of this planet as a whole.

**Core Energetics**

Heat from the core drives the geodynamo, generates the magnetic field, and is largely responsible for much of the tectonic activity and movement of continents on the surface. The ultimate source of all this heat is not completely understood, but much of it comes from radioactive decay. At the same time, we suspect that the core is cooling, and that as a result the inner core has crystallized and is growing larger with time. In many cases this view of core evolution is based on enormous extrapolations of data obtained at much lower pressures than are found in the core, and in other cases our views are shaped by plausibility arguments. We are now in a position to directly obtain a new generation of physical property and geochemical measurements on core materials under actual core pressures and temperatures.

**Key Questions**

1. How much potassium and other radioactive elements can be present in the core, and where does all the heat emanating from the core come from?
2. How old is the inner core and how quickly is it growing?
3. What is the energy source that drives the geomagnetic dynamo?
4. Did the core segregate from the mantle early in Earth history or did it evolve separately? What effect did this possible core segregation have on the chemical evolution of the mantle?
5. Did the cores of other planetary bodies such as Mars and Venus evolve in a different way, due to differences in core compositions and melting points?
6. How does the melting temperature, $T_m$, vary with composition, and how did differences in core melting temperatures affect the evolution of other planets, such as Mars and Venus?

**Structure and Dynamics of the CMB**

The core undoubtedly has some interaction with the overlying mantle at the CMB. Yet it is not known whether the strange seismic properties of isolated patches in the bottom 200 km of the mantle and the CMB (known as the D" region) are due to reaction of mantle material with the core below, the sinking of dense materials through the mantle to pile up at the CMB, or phase transformations in silicate minerals under the pressures and temperatures of the CMB. Depending on the melting point of iron alloys and the concentration of radioactive elements in the core, there may be a huge change in temperature at the CMB, which stimulates convective upwellings and hotspot plumes like Hawaii.

**Key Questions**

1. Is D" a graveyard of cold, dense material that was once at the surface and then was subducted back into the mantle, sinking to the CMB? Or is D" a region of the mantle that has reacted chemically with core materials? What phase transformations in mantle minerals occur at CMB conditions, and what are the seismic properties of these phases?
2. How hot is the molten outer core, and how big is the temperature jump at the CMB? The answer to these questions will tell us the heat flux out of the core.
3. How big is the lateral variation in heat flux from the core, and how does it affect the dynamo action (geomagnetic reversals)?

4. Is the mantle partially molten at the CMB?
   • What are the melting temperatures of lower mantle rocks?
   • What would be the effects of temperature and compositional variations be on lateral heterogeneity in seismic wave velocities and density? That is, how does seismic structure depend on chemical composition and temperature at CMB conditions?
   • What is the thermal conductivity of the mantle, and how much is the flow of heat out of the core impeded at the D’ layer?

Composition and Structure of the Outer Core

It is well known from shock wave and diamond anvil experiments that the core is not dense enough to be made of pure iron. Some unknown light elements must be alloyed with iron, and these will likely have a strong effect on the melting point of the core. Even the solid inner core seems to have some lighter material dissolved in it.

Key Questions
1. What light elements are present in the outer core, and how are they distributed? Is there any variation in the concentration of the light elements between the bottom and top of the outer core?
2. How do light elements affect the physical and chemical properties of the outer core, in particular the melting point, density, elasticity, seismic velocities, and electrical conductivity?

Inner Core Structure

The inner core has crystallized out of a cooling molten iron alloy, and is growing with time. This growth has likely affected the properties of the magnetic field over Earth history. In fact, magnetic forces may actually speed up the rotation of the inner core with respect to the rest of Earth.

Key Questions
1. How does the inner core affect the geodynamo? It appears that the core and Earth’s magnetic field are strongly linked through the observation of inner core superrotation. Little is known beyond that, although this interaction certainly has an effect on the magnetic field through time. Electrical conductivity and viscosity (strength) measurements on iron will be important in this regard.
2. Is there any significant heat flux from the inner core?
3. Is there partial melting (a mushy zone) in the inner core? We do not know if the inner core is completely solid or whether it includes some molten material between grains. Matching seismic velocities and seismic constraints on attenuation is very important.
4. What is the crystal structure of the solid inner core phase? We have learned much about the properties and crystal structures of iron at core conditions, but we are just starting to appreciate how small amounts of impurities mixed with iron can change both its properties and structure. It has long been presumed that a simple hexagonal form of iron (hexagonal closest-packed iron) is its stable structure in the inner core. However, other structures are possible (such as the body-centered cubic, or BCC structure that is stable under normal conditions), especially for the actual alloy of the inner core. The most pressing questions to be answered next are:
   • Is a BCC body-centered phase of iron alloy stable in the inner core?
   • What effect will the crystal structure have on observable properties of the core, like the elastic anisotropy of iron under inner core conditions?
5. How large are the grains of inner core material? This will be important for understanding seismic attenuation and flow within the inner core.
6. How great is the inner core’s viscosity and how strongly coupled are the inner core and the mantle (can one rotate with respect to the other)?
7. Is the inner core convecting or flowing?
Subduction and Mantle Processes

Subduction is the process by which cold slabs of brittle oceanic lithosphere plunge down into Earth’s interior. These subducting slabs consist of old basaltic oceanic crust that has been altered and hydrated, with cold and chemically depleted mantle underlying the crust, and a thin veneer of sediments. Subduction is the mechanism by which crustal and upper mantle material is recycled back into the mantle, and this process expresses itself in ways that greatly impact life on the surface. Most earthquakes and subaerial volcanoes occur at convergent plate margins where subduction is active. While plate tectonics provides a general framework for understanding how subduction relates to volcanoes and earthquakes, the mechanisms by which they are generated at subduction zones are just beginning to emerge.

Studies of subduction processes and the mantle into which subducted material is delivered will continue to be a focus of high-pressure studies over the next decade. Trying to understand the origin of intermediate- (70-300 km depth) and deep-focus (300-700 km depth) earthquakes, and developing models of subduction-related volcanism, will be primary goals. Some of the key related issues to be addressed include: the efficiency of recycling volatiles like water and carbon dioxide into the mantle; identifying mineral reservoirs for volatiles in the deep mantle; magma generation and migration; the ultimate fate of subducted slabs; the composition and structure of the mantle; convective flow of material in the mantle; and core-mantle boundary interactions.

Deep Earthquakes

To generate earthquakes, large differential stresses must be exerted on brittle, cold material. For these reasons, most earthquakes occur at relatively shallow levels. As lithosphere is subducted to greater depths and is heated by the surrounding mantle, its strength decreases as it warms, becoming softer and ductile. Seismicity should cease when slabs are hot enough to flow like heated plastic instead of rupturing in a brittle fashion. Yet earthquake activity persists to depths of about 700 km in the mantle, much deeper than calculations and laboratory experiments would predict. The problem of why intermediate and deep-focus earthquakes occur is one of the great unsolved problems in geophysics today (Figure 4).

A number of hypotheses have been proposed for the origin of deep earthquakes. The interiors of slabs may remain cold enough that the mineral olivine persists metastably to depths below 400 km. The atoms in this metastable olivine may suddenly rearrange to form the stable β (beta) and γ (gamma) high-pressure minerals (called wadsleyite and ringwoodite, respectively), thereby generating an earthquake in the process. Alternate hypotheses include shear instabilities in stable materials at high pressure, runaway heating from a central nucleation site of failure, or the sudden dehydration of hydrous (water-bearing) minerals, such as serpentine, under high-pressure conditions. None of these mechanisms satisfactorily explains all of the observational information on deep-focus earthquakes; however, the technology needed to generate differential stresses and deform rocks under pressures and temperatures for intermediate-focus earthquakes has just recently been developed. A great deal of additional laboratory study on the deformation and failure of rocks is required before deep-Earth seismicity can be fully understood. Developing such instrumentation is a first-order priority for the high-pressure community.

Volcanism and Melts

Aside from presenting a serious natural hazard, volcanism is the mechanism by which new crust is formed, and it has been perhaps the most important process involved with formation of the atmospheres and oceans. It has also likely exerted a significant influence on climate change through time by delivering greenhouse gases to the atmosphere. Most volcanism occurs at mid-ocean ridges on the seafloor far beneath the ocean surface, and this is the mechanism by which new oceanic crust is created. On the surface of the continents, most present-day volcanism
is related to subduction, occurring along continental margins near subduction zones and on numerous island arcs such as Japan.

Ocean water alters the basalt of the upper crust, forming hydrated minerals such as serpentine, which contain abundant water. Along with entrained sediments, these wet subducting materials are the first to melt as they are warmed by the surrounding mantle. The water and carbon dioxide in volcanic gases clearly show that they result from the formation of wet subduction-zone magmas. Exactly how these melts make their way to the surface, how quickly they travel, and how their chemistry is altered along the way are poorly constrained. Yet all of these things affect the properties of the magmas we ultimately see on the surface, the eruptive styles of volcanoes, and the hazards they pose to society. The atomic structures of silicate melts are key to understanding their behavior, physical properties, their volatile content, and the migration of melts from their point of origin at high pressure to the surface.

High-pressure experiments and computer simulations to determine the properties of silicate melts will be an active area of investigation in the future. Neutron scattering is a particularly effective experimental tool for investigating melt structures and properties. As more intense neutron sources such as the SNS (Spallation Neutron Source) come on line in the next few years, the development of new generations of large-volume diamond anvil cells and multi-anvil high-pressure devices for neutron-scattering experiments could lead to important breakthroughs in research on magmas.

Interestingly, not all magmas may rise to the surface. This counterintuitive situation results from the fact that melts are very compressible and their density increases more rapidly with pressure than for most crystalline solids. Thus, below a critical depth, silicate magmas may actually sink rather than float to the surface. This curious concept could have profound consequences for the evolution of the early Earth, its possible chemical stratification, and for the sequestering of elements and volatile compounds at depth. There are at present very few experimental studies of the properties of silicate melts at high pressures—especially their density and elastic properties. However, the development of new tools for conducting such studies promises to be an area of emphasis in the coming decade.

Figure 4. Generalized view of a lithospheric slab subducting through the upper mantle, into the lower mantle. The distribution of earthquakes in the subduction zone and slab are shown by red and black filled circles. Figure modified from Green, H., 1994, Solving the paradox of deep earthquakes, Sci. Amer., September 1994, p. 65. Original figure © Roberto Osti Illustrations.
Volatiles at Depth

Water has a great effect on mineral properties, such as seismic velocities, anisotropy, strength, and viscosity, to name a few. As a potentially vast source of water and CO₂, volatiles in Earth’s mantle may have had a huge impact on climate change throughout geologic time. Therefore the presence or absence of water and carbon in Earth’s deep interior has become a central issue in high-pressure research, and will be an area of intense investigation for the foreseeable future.

In its earliest history, 4.5 billion years ago, Earth was hotter than at present. As a result, convection of mantle rocks was extremely rapid and it is likely that a large portion of the initial volatile inventory of the deep Earth was lost early on through volcanism. The impact of a planet-sized body with Earth in a moon-forming event would have produced additional heat and loss of volatiles from the interior. Yet we know that volatile elements such as hydrogen and carbon still reside at depth. Rocks from the interior such as kimberlites contain diamonds (made entirely of carbon), as well as hydrous phases. There is also abundant water and carbon dioxide in volcanic gasses. These volatiles may be residual from Earth’s early accretion, or they may have been recycled into the mantle through subduction. We do not know what fraction of the subducted volatile inventory quickly returns to the surface at volcanoes, but current estimates indicate that it is low, about 15 percent. The remainder may be redeposited in the mantle at great depth. Thus, the mantle may well be Earth’s largest reservoir of water and carbon.

Where would this water reside? We now know that minerals we normally think of as “dry,” so-called nominally anhydrous minerals, can in fact accommodate significant quantities of hydrogen (water) locked up in their crystal structures. The uppermost mantle minerals, garnet and pyroxene, could accommodate multiple oceans of water in their structures. Even more water could be present in the transition zone between 410 and 660 km depth. A major recent discovery is that the primary minerals in this depth range, the high-pressure forms of olivine named wadsleyite and ringwoodite, can accommodate up to three weight percent of structurally bound water. Even the small amounts of water in the densest phases of the lower mantle (perovskites and magnesiowustite) could amount to several oceans worth of H₂O.

Key Questions

A number of intriguing questions are raised if the mantle is a reservoir for potentially vast quantities of volatiles.

1. What are all the possible phases in which water could be retained at depth?
2. If there is water in the mantle, is it from subduction recycling, or is it primordial?
3. What subduction-zone minerals can retain water and carbon until they are in the transition zone where they can be readily absorbed by minerals there?
4. When mantle rocks rise above 410 km depth, do saturated minerals dehydrate, thus releasing dense aqueous melts that are recycled to depth at mantle downwellings? That is, is the 410 km seismic discontinuity a dehydration boundary or “water filter”?
5. Can we identify volatiles in the mantle using seismic prospecting techniques? Answering this question will require knowledge of the elastic properties of hydrous phases, especially at high pressures and temperatures.
6. Do volatiles affect the properties of seismic discontinuities, such as their widths, depths, and the velocity jumps across them?
7. What are the densities and elastic properties (including seismic properties) of aqueous silicate melts or solutions at high pressures?
8. How do small amounts of water affect the rheologic properties of high-pressure minerals and the patterns of convection in the deep Earth?

The Mantle

Earth’s mantle, a nearly 3000-km-thick shell of stony material between the crust and the metallic core, accounts for approximately seven-eighths of Earth’s volume. Knowledge of the composition and mineralogy of the mantle is therefore essential for understanding Earth’s total inventory of elements, and the evolution of Earth through time.
It is now well established that with increasing pressure, upper mantle minerals such as (Mg,Fe)$_2$SiO$_4$ olivine, garnet, and pyroxene transform to denser mineral phases. These transformations are associated with major jumps in seismic velocity, called discontinuities, at depths of 410 and 660 km. Additional subtle discontinuities with smaller velocity jumps may occur at other depths as well. Transformations to a perovskite-structured phase with the formula (Mg,Fe)SiO$_3$ is generally associated with the major seismic discontinuity at 660 km depth. This phase, along with (Mg,Fe)O and perovskite-structured CaSiO$_3$, are thought to account for the bulk of the lower mantle deeper than 660 km. This basic sequence of phase transformations is now well established and provides a basis for understanding the prominent seismic structures of the mantle. The 410 and 660 km discontinuities are often taken as the boundaries of the “transition zone” in the mantle. These discontinuities are the most prominent seismic features between the shallow crust-mantle boundary (Moho) and the core-mantle boundary at about 3000 km depth. They provide major clues as to the chemical, thermal, and dynamic state of the mantle.

What is more difficult to ascertain is the degree to which the mantle might be chemically heterogeneous, with an onion-like structure of chemically distinct layers. Yet the extent and nature of chemical heterogeneity in the mantle is crucial for understanding the patterns of convection that drive plate tectonics, Earth’s internal thermal structure, and the planet’s evolution through time. Seismic studies of the upper mantle reveal a highly heterogeneous region in terms of temperature and composition (Figure 1B). Continents appear to have massive roots of cold, chemically distinct material that extends perhaps hundreds of kilometers beneath the surface. Some subducting slabs appear to be trapped and floating on the 660 km discontinuity, whereas others seem to penetrate directly into the lower mantle. Thus, the patterns of flow, recycling, and mixing in the mantle seem to be uneven and complex (Figure 5). Whether such complexity extends to yet greater depths is highly uncertain. We do not at present know whether seismic velocity discontinuities involve changes in chemical composition as well as changes of phase, or whether the mantle is roughly homogeneous on a gross scale. Even more difficult to discern are lateral variations in composition and temperature. Seismic studies have indicated the presence of large superplume structures extending upwards over a thousand kilometers or more from the core-mantle boundary. Whether these structures result from temperature or a chemically distinct diapir is as yet unknown. A new generation of velocity measurements on lower mantle phases at the extreme high pressure-temperature conditions of the lower mantle will be necessary to answer these questions (see box on p. 12-13).

Figure 5. A conceptual view of a stratified Earth’s mantle. Two cold blue slabs penetrate the 660 km discontinuity (dashed line), and sink through the lower mantle. They deform a dense layer in the lowermost mantle without penetrating through it. Other subducting slabs, such as that beneath the back arc on the right, do not penetrate into the lower mantle and float on top of the 670 km discontinuity. See Kellogg, L.H., B.H. Hager, R.D. van de Hilst, 1999, Compositional stratification in the deep mantle, Science, 283(5409), 1881-1884. Figure from http://www-geology.ucdavis.edu/%7Ekellogg/mantle.jpegs courtesy of Louise Kellogg.
The Mantle Transition Zone and Deep Earth Chemistry

Perhaps the most prominent features within the mantle are rapid jumps in seismic velocities—or discontinuities—at 410 and 660 km depth. These discontinuities mark the upper and lower boundaries of the “transition zone,” a region in which seismic velocity and density increase very rapidly with depth. Various features of the transition-zone discontinuities, such as their size, sharpness, and variation in depth around the globe, are among the most important clues available on the chemistry of the deep mantle. Mineral physicists are obtaining the type of information that is needed to interpret the seismic structure of the transition zone. Indeed, the use of high-pressure laboratory data to analyze seismic features is one of our most powerful tools for understanding the current state and evolution of the deep Earth.

Laboratory experiments have established that transition-zone discontinuities are associated with phase transitions in the major minerals of the upper mantle: olivine, pyroxene, and garnet. When the crystal structure of a mineral changes due to high-pressure phase transitions, the characteristic seismic wave speeds of the minerals change as well. What we do not know is whether transition-zone discontinuities are associated with changes in chemical composition, or just changes in crystal structures to high-pressure forms.

Key to understanding the seismic structure of the transition zone and, indeed, the entire mantle, is measuring seismic wave speeds of minerals at high pressures and temperatures. Today, measurements of wave speeds (or elastic properties) are done using a variety of sophisticated techniques, for example: (1) Brillouin laser light scattering from atomic vibrations (figures right-hand page), (2) generating ultrasonic waves in crystals (figures below), and (3) by synchrotron x-ray techniques (figures below and on p. 5). Extending these techniques and others to higher temperature and pressure conditions is a primary goal for the future.

Techniques for Studying the Mantle

Synchrotron x-ray experiments with a multi-anvil high-pressure press like the T-25 shown at right. Eight cubic anvils compress the a sample at their center (shown in red). X-rays are used to monitor the sample size and for x-ray diffraction, while a transducer transmits sound waves into the sample for measuring their speed. Figure courtesy of Baosheng Li, Stony Brook University.
Laser light going into a diamond anvil cell to measure velocities by Brillouin scattering. Photo courtesy of Jennifer Jackson and Jay Bass, University of Illinois, Urbana-Champaign.

Schematic diagram of a Brillouin spectrometer used to measure sound velocities $V_p$ and $V_s$ in the laboratory using laser light scattering. Figure courtesy of Stanislav Sinogeikin, University of Illinois, Urbana-Champaign.

Laser heating in the diamond cell while measuring seismic velocities using Brillouin scattering. Figure courtesy of Stanislav Sinogeikin and Jay Bass, University of Illinois, Urbana-Champaign.
Recent seismic studies have shown that the lowermost 200 km of the mantle, the so-called D” region, is among the most heterogeneous regions of the planet. This thin layer above the core-mantle boundary (CMB) displays a high degree of lateral variability in its velocity structure. Isolated patches of lens-shaped low-velocity material seem to float on top of the core-mantle boundary. It seems possible that chemical reactions are taking place in D” between the silicate mantle and the iron-rich metallic core. This may be a region where slabs ultimately descend and are reassimilated into the mantle, making the CMB a “slab graveyard” (Figure 7). Alternatively, core-mantle interactions may lead to pockets of iron-rich silicate melts that are too dense to rise very far upwards. High-pressure studies of the stable phases that may exist in D” and the chemical reactions between silicates and metals are in their infancy, but will do much to shed light on the possible reasons for the existence of D”. For example, researchers in Japan have recently discovered a post-perovskite phase that exists under D” conditions (Figure 6). Measurements of the elastic properties, densities, attenuation, and viscosity of both crystalline phases and melts appropriate to the D” region are of the utmost importance.
Near-Surface Processes

The near-surface environment—primarily the atmosphere, hydrosphere, biosphere, and deeper levels that directly interact with them—is affected to a surprising degree by deep-Earth and high-pressure processes. In a practical sense, we might define the relevant environments as those that we experience on the surface or that can be directly sampled, for example, by drilling. Over the past several years there has been increasing awareness of the continuous interaction between Earth’s deep interior and its oceans and atmospheres. The deep Earth is indeed the source of the planet’s oceans and primordial atmosphere, and continues to affect climate on many time scales. Understanding the precise nature of these interactions and the rates at which they occur will be an area of intense activity within the high-pressure community for the foreseeable future.

Closer to the surface, modest pressures stabilize what is likely the planet’s largest hydrocarbon reservoir, and one which has not yet been exploited.

Earth’s oceans, while appearing vast at the surface, only represent a small feature on the skin of the planet: in total, the oceans amount to less than 1/1000th of Earth’s mass. How did the planet’s oceans arise? It is likely that much of Earth’s earliest atmosphere and water was lost about 4.5 billion years ago when the impact of a Mars-sized body upon Earth formed the Moon, melting and vaporizing a large portion of the planet. Yet 3.7 billion-year-old rocks show clear signs that liquid water was present at Earth’s surface. Current theories for how our planet generated an ocean involves degassing of water from Earth’s interior. Indeed, it appears likely that the amount of water/hydrogen bound into Earth’s interior is at least equivalent to, and may dwarf, that within the planet’s oceans. How that water (or hydrogen) is retained in the interior, and how abundant it is, are issues that can only be resolved through work on materials at high pressures.

At plate margins, water is reintroduced into the planet by subducting water-containing minerals formed in the oceanic crust and overlying wet sediments. Water vapor is degassed from the interior in explosive volcanic events at these plate margins (e.g., Mount St. Helens, Figure 8) and at hot springs and fumaroles associated with volcanic activity. Taken together, degassing and subduction form a large-scale hydrologic cycle that has been pumping water and gases onto the surface and then recycling them. The underlying question that emerges from studying these processes is whether Earth’s oceans are decreasing or increasing in volume with time. Such changes in ocean water volume are anticipated to take place over long time scales (tens to hundreds of millions of years), but are fundamental for interpreting the sedimentary geologic record.

Carbon Dioxide

Like the oceans, Earth’s initial atmosphere was degassed from the interior, probably very early in Earth history. The composition, and even the pressure, of this earliest atmosphere are poorly constrained. The best guesses are that the Hadean atmosphere was dominated by CO₂, perhaps even more than one atmosphere of this well-known greenhouse gas. For comparison, today’s atmosphere has an abundance of CO₂ of only about 0.0003 atmospheres. Part of this early CO₂ atmosphere was fixed into rocky form through either weathering or biologic processes, while another portion was converted (through photosynthesis) into the present-day oxygen within our atmosphere. As with water and the genesis of Earth’s oceans, one of the basic scientific challenges for high-pressure Earth sciences is to determine the recycling and sequestration processes of carbon within the deep Earth.

The importance of carbon dioxide degassing from Earth’s interior extends well beyond the fundamentally important problem of the genesis of Earth’s atmosphere. Even the small (and growing) amount of carbon dioxide in the present-day atmosphere has a profound effect on Earth’s climate due to the efficiency of CO₂ as a greenhouse gas. It has been estimated that over most of the previous 600 million years, the CO₂ content of the atmosphere has been 4-15 times the present value.
The most prominent mechanisms for release of this CO₂ involve the deep Earth: either enhanced volcanic degassing and/or greater subduction of carbonate-rich sediments into the deep Earth. Subduction puts carbonate sediments in proximity to hot mantle material where decarbonation reactions release CO₂. This general conceptual framework immediately raises a number of critical issues for understanding interactions between the deep Earth and the atmosphere.

**Key Questions**

1. What is the efficiency of CO₂ degassing from different types of subducted materials?
2. To what degree do different types of major volcanic events carry carbon from Earth’s deep interior and inject it into the atmosphere?
3. What is the distribution, manner of sequestration, and average content of carbon at depth? What minerals hold carbon in the deep Earth and where?

High-pressure studies will provide insight into long-term planetary climatic changes through studies of the behavior of greenhouse gasses such as CO₂ within Earth’s deep interior.

**Magmas: Tapping Deep Reservoirs of Water and Carbon**

Our oceans and atmospheres, and indeed the carbon present in life itself, is ultimately derived from Earth’s interior—delivered by magma to the surface. While there are strong indications that magmas dramatically change their structure, density, and chemical properties at high pressures, our knowledge of the interplays between the microscopic structure of magmas and the solubility of gasses at depth is in its infancy. How microstructural changes depend on the temperature, pressure, and chemical composition of the magma (including the presence of carbon and water) remains ill-defined. Understanding these relationships is important for understanding how water and CO₂ are delivered to the surface, the rate at which this delivery occurs, and whether it is likely to increase or decrease in the future.

It has long been assumed that the magmas we see at Earth’s surface reflect the composition of Earth’s outermost skin. In some cases this is clearly not true. For example, diamonds (composed entirely of carbon) were formed deep within Earth’s mantle and carried rapidly to the surface in rare, unusually violent eruptions. Under some conditions, nearly pure carbonate magmas, called carbonatites, may erupt. Carbonatites resemble molten washing.
soda more than molten rock. These magmas are of considerable geologic interest because they may be revealing vast reservoirs of volatile material at depth, and because they provide most of the planet’s economic deposits of several technologically important elements such as tantalum and niobium.

The conventional wisdom is that most magmas originate in Earth’s uppermost mantle and lower crust. Whether the more common (and less violent) magmas erupting at the surface today have some link with the deepest parts of the mantle is, however, not known. Experiments at high pressure may well show that magmas (and thus, new crustal material) can, in fact, be derived from throughout Earth’s silicate mantle, dramatically altering our ideas about Earth’s average composition and deep-seated heterogeneity.

Kimberlites deserve additional comment as an extreme example of how rocks from Earth’s interior can be emplaced at the surface. In the case of these diamond-rich deposits, they are driven upward by CO₂ at velocities of perhaps hundreds of kilometers per hour, cooling as they rise and expand. Through this process, diamond is preserved instead of reverting to graphite as it normally would at magmatic temperatures. Kimberlites are of interest not only because they are the primary source of diamonds (they are in fact named after the Kimberley diamond mines in South Africa), but because they represent the deepest magmatic materials known. However, their chemical composition is very different from common notions of what the mantle is made of. As such, they will continue to be a subject of future study by the high-pressure community.

**Key Questions**

1. What circumstances lead to the eruption of kimberlites?
2. Do kimberlites represent a large region of the mantle with kimberlite composition, or are they isolated anomalies? The answer to this question will have far-reaching implications for understanding mantle composition and the possibility of chemical stratification within the mantle.
3. From what depths did kimberlites originate, and have they resided over a range of depths before rising explosively to the surface?
4. At what rates have kimberlites risen? Has their speed of ascent changed with depth, or are they restricted to only the upper couple of hundreds of kilometers as often thought?

Answers to these questions will tell us much about the composition of the interior, and in particular the size of the mantle reservoir of CO₂ and water.

**Clathrates**

Degassing of CO₂ from Earth’s interior may have played a significant role in warming Earth’s climate, but it is not the only greenhouse gas that can be retained in geologic materials. There has recently been a growing interest in clathrates, or solid gas hydrates. Clathrates can be thought of as a combination of a gas and normal water ice that forms a single solid substance at low temperatures and high pressures. The water molecules in clathrate hydrate form an ice-like structure that traps small molecules (guests) such as methane in nearly spherical cavities. The interest in clathrates is motivated by an increasing recognition of its abundance in Earth’s subsurface and on icy bodies of the solar system, its possible economic importance as a source of fuel, and its potential role in both climate change and natural hazards. Large volumes of methane are sequestered by this solid along deep continental margins and below regions of permafrost (Figure 9).

Global estimates of the methane in clathrates indicate that it may be the largest sources of hydrocarbon on Earth. The release of methane from this clathrate reservoir has been suggested as a source of variation in atmospheric methane during glacial/interglacial cycles in the recent past. These suggestions have fueled speculation about future releases of methane in response to global warming.

**Key Questions**

Among the critical questions about clathrates to be addressed in the coming years are:

1. What are the stability fields of clathrates, especially methane and CO₂ clathrates? The answer to this question will help predict how much of a change in sea level (and hence a drop in pressure at the ocean bottom) or change in ocean temperature would lead to a release of greenhouse gases into the
1. Burning methane clathrate, perhaps the most abundant energy source in the world. Figure from http://www.gashydrate.de/.

atmosphere. It would also help to predict where underwater avalanches in the ocean floor might occur.

2. What are the kinetics of clathrate formation and decomposition, and under what conditions would methane be released into the atmosphere? This affects calculations of global warming and the rates at which atmospheric gasses can make their way back into ocean sediments.

3. What are the physical properties of clathrates, in particular their elastic properties? This information will determine the speed of seismic waves in clathrates, which are needed to interpret geophysical surveys for regional inventories of clathrate or to model the response of the clathrate reservoir to changing environmental conditions. Knowledge of the elastic properties is essential in prospecting for clathrates using seismic techniques, just as the petroleum industry prospects for oil and gas.

4. Are there further high-pressure phase transitions in clathrates? Phase transitions would change all of the physical and chemical properties of clathrates, affecting calculations of their abundance, stability, and release into the environment.

Experimental studies using neutron sources, such as the Spallation Neutron Source now under construction at Oak Ridge National Laboratory (Figure 10), will be invaluable for determining the properties of clathrates. This is because these water-based compounds are made of light elements, in particular hydrogen, making them extremely difficult to study using x-rays. Neutrons are far more sensitive to the hydrogen atoms in a material and interact strongly with them. Until now, the use of neutron scattering under high-pressure conditions has been quite limited. The mineral physics community is already developing new types of diamond-anvil and multi-anvil high-pressure devices that will be suitable for use with neutron scattering.

**High-Pressure Geobiology**

The origin of the methane within clathrates is likely biologic. Yet, until the recognition of these deposits over the last ~15 years, mankind was unaware of this large reservoir of organic carbon. Indeed, the distribution of organics and biota within Earth’s subsurface is critical to understanding global carbon cycling. Although the extent of near-surface carbon cycling has been extensively studied, the deep subsurface contributions to the hydrocarbon content of the planet remain unconstrained.

The existence of a deep biosphere has been hypothesized since very early times, but only since the 1950s, with the isolation of deep-sea microbes specially adapted for growth at high pressures, were the first direct clues to the existence of deep life recognized. The physical limits (pressure and temperature) on the existence of a biosphere remain open questions, as these hold important clues to the extent of carbon reservoirs within Earth’s subsurface, as well as clues to the viability of life in planets and planetary bodies. There is now a growing awareness that life can exist under extreme high-pressure conditions that were previously thought to be unimaginable, extending the depth range of what we think of as the biosphere.

Recent field studies have pointed towards the presence of a significant diversity and mass of biology in the deep subsurface. However, most interpretations on the extent of biologic interactions with geologic systems are at best guesses. To get a clearer picture of the extent of geobiological interaction as well as better constrain the kinetics and viability of these biological processes, a focus towards laboratory-based, high-pressure geobiology studies is essential. With the expertise available to study materials and their properties at extreme pressures, the high-
pressure community is well poised to not only open new frontiers in high-pressure geobiology, but also take a lead in the further development of this aspect of high-pressure science.

**Goals of the High-Pressure Community Relevant to Near Surface Processes**

- Constrain the rates at which water and carbon are cycled into, and out of, the Earth.
- Determine how the mantle releases carbon to the atmosphere/hydrosphere, and what climatic effects it might have.
- Determine the effect of pressure on life, mechanisms of life’s survival at high pressure, and the metabolic processes of life at high pressure.
- Determine the non-biologic origins of organic material.
- Determine the ways in which diamonds grow within Earth.
- Determine the properties of natural fluids at high pressures.
- Simulate in the laboratory the fluids that are characteristic of the subduction process, and compare them with exhumed natural samples.
- Improve constraints on the genesis of carbon-rich magmas.
- Determine how the structural properties of melts control their properties at high pressures.
- Determine the properties of the clathrate hydrocarbon reservoir.
- Determine the interrelationship between the deep biosphere and the clathrate reservoir.

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*Figure 10. Spallation Neutron Source (SNS). Photo courtesy of Oak Ridge National Laboratory.*
The overarching intellectual issue and challenge for planetary scientists is to understand how planetary bodies form and evolve, and to determine their current structures and dynamics. Specific questions and many of the experimental challenges differ from those posed for Earth studies because the range of compositions and thermodynamic conditions in the solar system is much greater than for Earth. The data returned from spacecraft, and the ongoing explosion of new information about extrasolar planets, enable us to address fundamental questions, but only if we can improve our understanding of material properties and processes at relevant temperatures and pressures.

The universe consists mostly of hydrogen and helium, with minor amounts of heavier elements created through nucleosynthesis in massive stars. However, the most abundant elements also tend to be the most volatile, and the weak gravitational fields of smaller bodies (such as Earth) make it difficult to retain these light elements. It is convenient to divide the elements into three groups:

- Gases are those that do not condense (i.e., do not form solids or liquids) under conditions plausibly reached when planets formed;
- Ices are those that form volatile compounds and condense, but only at low temperatures (beyond the asteroid belt);
- Rocks are those that condense at high temperatures and provide the building blocks for the terrestrial planets.

From this “elemental” grouping we can identify four kinds of bodies in the solar system: The gas giants with their strong gravitational fields (Jupiter and Saturn), the ice giants (Uranus and Neptune), the solid ice/rock bodies (Europa, Ganymede, Callisto, Titan, Triton, Pluto, and many smaller bodies), and the terrestrial bodies (Mercury, Venus Earth, Moon, Mars, and Io). Below we discuss the intellectual challenges in understanding each of these classes of bodies.

**Gas Giants**

The gas giants (Jupiter and Saturn) are fluid, predominantly hydrogen planets. All of the recently discovered extrasolar planets are comparable in mass to Jupiter and are, accordingly, almost certainly of similar composition to Jupiter, since no material other than hydrogen is of sufficient abundance. At the outset, we pose central questions for these bodies.

**Key Questions**

1. How do gas giants form? Do they have rock/ice cores and if so, how large are their cores?
2. What is their radial structure? Are there first-order phase transitions (e.g., metallization of hydrogen or a plasma phase transition)?
3. What are the dynamics of these planets (heat flow, magnetic field, convective state)?

The first question is perhaps most central because we believe that the presence of a core is related to the process whereby planets form. This leads immediately to the problem of how to detect a core from our remote vantage point. Observations by spacecraft missions and telescopes give us information on atmospheres and the near surface environment, while celestial mechanics tell us their total mass, average densities, and the distribution of mass inside a planet. If we know how the density of surficial material increases with pressure and temperature inside the planet (that is, if we know the pressure ($P$) – volume ($V$) – temperature ($T$) equation of state), then we can tell how much core material would be needed to obtain the right planetary mass and density. Therefore, detection of a core requires knowledge of the behavior of the overlying hydrogen. We believe that the mass of the Jovian core is only ~ 3 percent or less of Jupiter’s mass, but this estimate is sensitive to the equation of state of hydrogen. Consequently, how well the internal structure of the gas giants is understood relies primarily on a better understanding of hydrogen and hydrogen-helium mixtures. The thermodynamic conditions of greatest interest for these planets are probably $P \sim 0.3$ to 10 megabars and temperatures of a few thousand Kelvin. Much of this regime is colder than the conditions probed by conventional shock-wave experiments, but hotter than that achieved in static experiments thus far. Nearly isentropic (at
constant entropy) compression experiments using shock reverberation techniques, or magnetic compression techniques, show much promise for determining material properties under the relevant P-T conditions.

Key Experiments

1. Improve determination of P-V-T equations of state for hydrogen. Phase transitions can cause a sudden increase in density, so they are important to identify, as well as the mixing properties with other cosmically abundant materials, especially helium and water.

2. Determine derivatives of the equation of state. Of particular importance is the Gruneisen parameter, which determines how temperature increases with pressure (or depth). These properties are essential for determining the thermal structure of the interior and its convective state.

3. Determine transport properties, especially electrical conductivity, for a broad range of pressure, temperature, and compositions.

Key experimental approaches:

1. Extend diamond anvil cell techniques to higher temperatures and pressures, which is especially difficult for hydrogen.

2. Further use and develop shock-wave techniques, which can produce isentropic or nearly isentropic compression.

Ice Giants

The ice giants (Uranus and Neptune) are less well understood than Jupiter and Saturn and are also probably more complicated because all the cosmically abundant classes of materials are significantly represented. The greatest need is a better understanding of water and its mixing properties with other materials (hydrogen, other ices, especially methane, and rock).

The conditions of interest are slightly lower pressure (0.1 to several megabars) but at temperatures of several thousand K (well into the fluid regime, even if water forms a high-melting-point ionic solid). The conditions of interest are slightly lower pressure (0.1 to several megabars) but at temperatures of several thousand K (well into the fluid regime, even if water forms a high-melting-point ionic solid).

Water Ices

Most of the moons of the outer planets, Jupiter, Saturn, Uranus, and Neptune, lack a rocky crust but are surfaced by hard, rigid ices of various kinds that behave like rocks. These planet-sized ice/rock satellites are the most water-rich solid bodies in the solar system. For example, Jupiter’s moon, Ganymede, is larger than Mercury and the pressure at the base of its uppermost ~1000 km-thick ice layer is ~15 times the pressure in the deepest parts of Earth’s oceans. Therefore, the high-pressure properties of water, ices, and their interactions with rocky material are of critical importance to the chemical evolution of ice-dominated bodies in outer solar system. Models of the present structure of these bodies are uncertain. For some, whether they are differentiated bodies or not depends on whether radiogenic and accretional heat were sufficient to allow differentiation into a rocky core and an icy mantle. The depth and thickness of their internal layers depend on these thermodynamic phase boundaries among various forms of H$_2$O-ice (e.g., I, II, VI, VIII), which are unknown in most cases. Therefore, a starting point for understanding the inner structure of icy satellites like Titan is a full understanding of the phase diagram of H$_2$O-ice.

Key Questions

1. What are the phase boundaries between the low-temperature (i.e., ~70 K at 0 GPa, ~300 K at 10 GPa), high-pressure
phases, including hydrogen-disordered phases. These boundaries are still unknown.

2. What are the energy barriers and transition rates for structural transitions? Because metastability is the norm in H₂O-ice, rather than the exception, transition rates are important for determining the lifetime of metastable phases that might be abundant in these objects.

3. What are the properties of aqueous fluids at pressures of 1-2 GPa and temperatures of hundreds of degrees Celsius, and what chemical reactions occur between these fluids and rocks of meteoritic chemistry? These are each critical areas of experimentation for understanding the internal evolution of some of the most novel bodies in our solar system.

**Clathrate Studies**

Clathrates on solid ice/rock bodies are the same type of clathrates that exist in Earth’s ocean sediments. They consist of modified water-ice structures in which there are available sites for other molecules. However, on the ice/rock bodies the most interesting possible molecules are hydrogen, carbon monoxide, carbon dioxide, and nitrogen, in addition to methane as on Earth. Noble gases are also of interest (though not highly abundant) because they may be detected in atmospheres and thereby provide diagnostics of formation and evolution involving clathrate decomposition and outgassing. Because clathrate stability fields are typically bounded above by temperatures that are comparable to or not much larger than the melting point of water ice, it is unlikely that they are present in gas giants or ice giants, but they could be important for the large icy moons. Perhaps of greatest interest is the “high” pressure (pressures of a few GPa or less) stability of various clathrate phases involving methane and other gases. These may be relevant to understanding the origin of methane on Titan. The rheology of clathrates is also of interest because they will affect convective flow and heat transport (they appear to be significantly stiffer than water ice).

**Terrestrial Bodies**

As with ice/rock bodies, the evolution of the terrestrial planets depends on knowing the phase diagrams (e.g., stability fields of different phases, melting curves) and the rheologic or flow behavior of relevant materials. The needed phase diagrams that remain to be worked out experimentally must cover a much wider range of compositions than those for Earth (e.g., including relatively sulfur-rich mixtures). Perhaps the biggest gap in knowledge concerns the rheology of relevant materials and mixtures of phases as in the case of the ice bodies; this gap is likely to be filled in the near future by experiments using new high-pressure deformation apparatus such as the D-DIA (Figure 11).

**Rheology**

One of the central issues for all planetary bodies is the rheologic properties of the materials within their interiors. Models of the dynamics and evolution of planetary interiors have now reached a stage where one can incorporate some aspects of realistic rheologic laws as constrained by laboratory experiments and theoretical mineral physics. These models show that mantle dynamics and the evolution of Earth and other terrestrial planets depend critically on such laws. Realistic models thus need accurate rheologic properties that take into account, for example, mineralogy, water content, and grain size. Thus far, experimental studies of the rheology of mantle materials have been focused mainly on olivine at low pressure. Although olivine may indeed be the major phase in Earth’s upper mantle, the mineralogy of other planets might be dominated by other minerals (e.g., pyroxenes), which could have very different rheologic behavior. Moreover, virtually no quantitative data are available for the rheologic properties of deep mantle minerals, except for some very recent pioneering efforts. The rheologic properties of more than 90 percent of Earth’s mantle are unconstrained by laboratory studies. Techniques are now being developed for quantitative rheologic experiments under pressures and temperatures equivalent to the mantle transition zone and deeper. These techniques will enable us to explore the rheologic properties of the entire mantle, providing insight into the dynamics of the whole Earth. Phases likely to exist at great depth, such as perovskites and magnesio-wustite, urgently need to be investigated. The rheology of materials relevant to other planetary bodies is similarly crucial yet poorly constrained.
**Ices**

The rheology of water ice and related ices remains imperfectly understood yet of great importance for understanding convection and tidal dissipation in these solid ice/rock bodies. In particular, the competition and balance between grain-size-sensitive (GSS) and dislocation creep in ice needs more consideration. Grain growth is promoted in GSS creep and grain-size reduction is promoted in dislocation creep. Therefore, for materials where both mechanisms produce measurable strain, it is entirely possible that steady-state deformation in some portions of the ice/rock bodies (e.g., the ductile layer of the Europan ice shell) there will be significant contributions (>10 percent) to the strain rate from both mechanisms. H₂O exists in a number of distinct ice phases, depending on pressure and temperature, and GSS creep in many of these water ice phases also needs to be measured in the lab. An analogy may exist between ice I and olivine, where very important viscosity differences exist between GSS and dislocation creep. Measuring GSS creep at more extreme conditions is a monumental task technically, but it is a long-range vision for high-pressure planetary sciences.

**Two-Phase Systems**

Subduction of oceanic lithosphere is difficult to initiate on Earth, and subduction is even more difficult to initiate on planets that do not have plate tectonics. Laboratory experiments on dry rocks predict a lithospheric strength that is too high to allow subduction. Small stresses on the San Andreas Fault and small stress drops during earthquakes are also difficult to reconcile with these experiments. Water or melt are factors that are believed to be responsible for the reduction in rock strength. The rheology of two-phase systems (rock-water, rock-melt) and associated processes such as dehydration embrittlement and shear localization are critical for understanding subduction. The rheology of two-phase systems is also important for understanding core formation and extraction of magma onto planetary surfaces. We need to continue studying the rheology and dynamics of two-phase systems both experimentally and theoretically.

**Microstructures**

Increasing attention is being given to rock microstructures because they affect rheology and also because deformation modifies them. Particularly important are grain size and the preferred orientation of crystallographic axes (lattice-preferred orientation). Grain size strongly influences rock viscosity whereas lattice-preferred...
orientation controls the nature of seismic anisotropy from which the geometry of flow can be inferred. The importance of grain-size evolution on convection patterns has been studied through numerical modeling. We now have evidence of seismic anisotropy from the crust to the inner core, but its geodynamic significance can only be understood when the factors controlling anisotropic structure formation are known. Recent laboratory studies have shown that microstructure development is highly sensitive to stress state and chemical conditions (e.g., water content). Currently available data on microstructural evolution are limited to low-pressure conditions and most data are for single-phase materials.

Grain growth is now recognized as an important process in mantles of terrestrial planets. Grain growth affects planetary evolution through the feedback among grain size, viscosity, and mantle convection, and can also control the existence or absence of convection in planetary interiors. Although grain growth in one-phase systems has been studied to a limited extent, grain growth in multi-phase systems has not been well understood either for low- or high-pressure phases. Some aspects of microstructural evolution such as grain-growth kinetics are totally different between single-phase and multi-phase materials. Further progress on these issues is needed to improve understanding of terrestrial planet dynamics. Both experimental and theoretical studies of coarsening in realistic mineral assemblages is needed.

**Impacts in the Solar System**

Impacts and collisions are major processes in the formation and evolution of planetary bodies. Collisions have generated a wide range of pressures and temperatures throughout the solar system’s history, from early accretionary encounters to present-day events, resulting in catastrophic disruption. Recently, craters have been used as a powerful probe of material properties. The morphology of impact structures reflects properties beneath planetary surfaces, providing precious information about internal composition and structure, such as the depth to the subsurface ocean on the Jovian moon, Europa (Figure 12).

Current investigations focus on the cumulative chemical and physical alteration of planetary bodies as a result of billions of years of collisional evolution. Recent studies have shown how energy deposited from impact events on Mars and Titan has melted ground ice and possibly formed transient habitats containing liquid water.

Advances in understanding all planetary bodies are constrained by the limited measurements of the phase diagrams and thermodynamic properties of the large range of chemical compositions found in the solar system. Critical aspects of fundamental processes remain poorly understood, including the kinetics of shock-induced melting and solid-solid phase transformations.

To understand the evolution of the solar system and to utilize craters as a remote-sensing tool, planetary scientists rely upon dynamic, high-pressure experiments that measure the high-pressure and high-temperature material properties of rocks and minerals. Increasingly, data obtained from both shock and static compression experiments are combined to formulate the necessary equations of state and dynamic rheology (strength) models. Further developments of in situ measurements of shock processes are required, such as x-ray and neutron diffraction and Raman spectroscopy, which are under active development using static techniques. Invention of new experimental techniques that enable widespread use of isentropic or arbitrary compression paths will bridge the fields of shock and static compression, providing access to phase spaces previously unattainable, such as the second critical point of water.
Progress in high-pressure Earth and planetary sciences is closely tied to technological innovation and infrastructure development. Researchers are continually pushing forward the limits of pressures and temperatures that can be achieved in the laboratory, adapting new types of experimental probes for high-pressure experiments. Examples of the latter are the recent developments of using inelastic x-ray scattering techniques to determine the electronic structures and sound velocities of core and mantle materials at high pressures. Inventing technology to perform new types of experiments in higher pressure-temperature regimes is the lifeblood of our science. Listed below are some technologies and experimental capabilities that are critical to develop in the coming decade, along with some experiments that need to be performed to advance understanding of planetary interiors.

**Needed Technology Development**

- Experimental equipment and techniques for measuring the crystal structures and seismic properties (or equivalently, elastic properties) of deep-Earth crystalline phases and melts under pressure and temperature conditions spanning the mantle and core.
- Development of large-volume devices for determining phase equilibria at pressures to 60 GPa. This would expand the current capabilities by approximately a factor of two.
- Apparatus to perform high-pressure rheology experiments to 30 GPa and beyond.
- High-pressure devices for synthesizing large quantities of samples at >30 GPa. This will involve the development of new anvils for multi-anvil presses with superhard materials.
- Computer simulations of the properties of deep Earth crystalline phases and melts.
- High-pressure devices for synthesizing large quantities of samples at >30 GPa. This will involve the development of new anvils for multi-anvil presses with superhard materials.
- Improved x-ray tomography equipment for use with high-pressure samples.

**Properties of Core Materials – The Ultimate in Extreme Earthly Conditions:**

The development of experimental facilities for measuring the physical and chemical properties of Earth materials under core conditions (P>135 GPa, T>3000 K) are among the most difficult technical challenges in our community because the pressures involved are so high. Properties that are key include the densities, equations of state, thermal conductivity, kinetics of chemical reactions, and plastic flow. Relatively large sample volumes will be needed to characterize many of these properties. New techniques for measuring these properties will need to be developed, including the measurement of rheologic and elastic properties under these extreme conditions.

**New X-Ray Probes:**

High priority areas are the development of inelastic x-ray scattering to measure sound velocities at ultra-high pressures, free-electron laser x-rays under shock conditions, and the development of optics for inelastic x-ray scattering with multi-anvil apparatus. Dedicated beam-lines to perform state-of-the-art inelastic x-ray scattering experiments are necessary at national facilities.

**Neutrons:**

Neutrons are the best way to probe the structures of hydrous phases, and to determine the structural properties of silicate melts and aqueous solutions. New high-pressure equipment must be developed to utilize the next generation of neutron scattering facilities, such as the SNS. Ultra-high-pressure experimentation at SNS will involve scaling up the types of equipment used for x-ray experiments, including techniques for growing large diamonds. High-priority objectives include:

- Large-volume diamond-anvil cells for determining the structures of minerals by neutron scattering to 100 GPa.
- Paris-Edinburgh class high-pressure cells for pressures to 20 GPa and high temperatures of 2500° C for x-ray and neutron beam-lines.
- Focused ion beam instruments for preparing precision electron microscopy samples and nano-machining.

**Computational Mineral Physics:**

Investments in computational infrastructure must parallel other areas of infrastructure development. Advances in computational hardware and software continue at a fast pace, presenting our community with great opportunities for addressing new problems with greater accuracy. Challenging issues in this area include incorporating the effects of chemical environment, such as oxygen fugacity, on the solubility of elements in iron, and calculating transport properties such as diffusion rates and thermal conductivity. As computational technology advances, accurate calculations of these properties will be possible via simulations with large number of atoms and the proper treatment of interatomic forces.
Much of the fundamental research in high-pressure mineral physics is supported by the National Science Foundation Division of Earth Sciences. The Earth and planetary sciences communities make observations round the clock, 365 days per year. Seismometers are monitoring ground motion and earthquake activity, while space probes, satellites, and telescopes are constantly recording diverse sets of data on planetary bodies. Interpreting these vast quantities of information to form a physical picture of what Earth (or other planetary body) is like inside requires input from high-pressure scientists doing experiments in their laboratories or on their computers. Information on the properties of Earth and planetary materials at high pressures and temperatures is indeed the key that allows us to see inside planetary bodies, to understand what deep interiors are made of, and to decipher how they work. In addition, many industrial or other processes of practical importance involve high pressures. Therefore, very natural connections exist between the activities of high-pressure researchers and other scientific programs or agencies. Several examples of such relationships are given in the following columns.

EarthScope is an integrated geological, geophysical, and geochemical investigation of the North American continent. One of the three EarthScope components is USArray, a dense network of permanent and portable seismometers that will provide images of Earth’s interior with unprecedented clarity. USArray will be a major breakthrough in our ability to precisely define Earth structure at depth: its composition, thermal structure, and dynamic state. This is a key element of understanding the forces that drive plate tectonics, the depths from which magmas are derived, and the evolution of North America. Knowledge of mineral properties under the high pressures and temperatures of Earth’s interior will be required to make such interpretations from USArray data. In particular, studies of seismic velocities of minerals under the full range of pressure-temperature conditions inside Earth will be necessary. There is a natural synergy between EarthScope’s goals and those of the high-pressure Earth and planetary sciences community.

The National Aeronautics and Space Administration (NASA) missions to various parts of our solar system return diverse geophysical, chemical, spectroscopic, and photographic data sets on planetary bodies. As soon as one tries to infer what the interiors of these bodies are like, using primarily remote-sensing data obtained from planetary surfaces and atmospheres, input from the high-pressure materials properties community is needed. Everything from determining the size of rocky or metallic cores of planets, to understanding the surface fractures and topography on giant ice bodies, to understanding the origin of sulfurous volcanism on Io depends on knowing the properties of planetary materials at high pressure. Understanding the conditions under which life forms might be hidden below the surface, perhaps even thriving at high pressures, is another question that high-pressure experimentalists will address in the next decade.
A major goal of the Integrated Ocean Drilling Program (IODP) is to understand the nature of the seafloor and crust beneath the oceans. Among their specific goals is characterizing the distribution and nature of clathrates within ocean sediments because these compounds are a vast potential energy resource and they likely play a role in climate change. Sampling clathrates is a difficult task because they are only stable at high pressure and they quickly decompose when drilling cores are recovered to the surface. Designing drilling experiments and analyzing the results will depend on knowledge of the pressure-temperature conditions under which clathrates are stable. Measurements of the seismic velocity properties of clathrates will likely play a large role in future attempts to prospect for clathrates using seismic techniques. Other areas of interface include measurements of the thermal conductivity of materials at high pressures, which are needed to interpret heat-flow measurements at the ocean floor.

The Department of Energy (DOE) operates the synchrotron and neutron facilities that are at the heart of much of the research done by the high-pressure materials properties community. The high-pressure community has worked with DOE to develop a number of beamlines for state-of-the-art high-pressure studies. These facilities are used not only by researchers in the Earth and planetary sciences, but also for fundamental research in physics, chemistry, and materials sciences. In addition to a number of synchrotron beamlines dedicated to high-pressure research, a new high-pressure beamline for neutron scattering studies is being developed at the Spallation Neutron Source currently under construction at Oak Ridge National Laboratory.

Research on the equations of state and properties of materials at high pressures and temperatures is central to the mission of the Department of Defense (DOD). Many of the issues that arise in designing materials suitable for specialized military applications and in predicting the performance of hardware involves the behavior of matter under extremely high pressures and temperatures. The experimental techniques developed by the Earth and planetary sciences community and the training that it provides to young scientists are of direct relevance to DOD research.
Appendix One

Attendees of the March 22-23, 2003 Workshop

A Vision for High Pressure Earth and Planetary Sciences Research:
The Planets from Surface to Center

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
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<tbody>
<tr>
<td>Rob Abbott</td>
<td>Sandia National Laboratory</td>
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<td>Ross Angel</td>
<td>Virginia Polytechnic Institute and State University</td>
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<td>Jay Bass</td>
<td>University of Illinois, Urbana-Champaign</td>
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<td>Bruce Buffett</td>
<td>University of British Columbia</td>
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<td>Pamela Burnley</td>
<td>Georgia State University</td>
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<td>Jiuhua Chen</td>
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<td>Hyunchae Cynn</td>
<td>Lawrence Livermore National Laboratory</td>
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<td>Przemek Dera</td>
<td>Carnegie Institution of Washington</td>
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<td>Robert Downs</td>
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<td>Michael Drake</td>
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<td>Thomas Duffy</td>
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<td>William Durham</td>
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<td>Michael Furnish</td>
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<td>Ivan Getting</td>
<td>University of Colorado, Boulder</td>
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<td>Harry Green</td>
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<td>Russell Hemley</td>
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<td>Donald Isaak</td>
<td>University of California, Los Angeles</td>
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<tr>
<td>Chi-Chang Kao</td>
<td>Brookhaven National Laboratory</td>
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<td>Shun Karato</td>
<td>Yale University</td>
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<tr>
<td>Abby Kavner</td>
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<td>David Lambert</td>
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<td>Kurt Leinenweber</td>
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<td>Baosheng Li</td>
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<td>Ho-kwang Mao</td>
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<td>Guy Masters</td>
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<td>Li-chung Ming</td>
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<td>Richard O'Connell</td>
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<td>Eiji Ohtani</td>
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<td>Dean Presnall</td>
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<td>Jianzhong Zhang</td>
<td>Los Alamos National Laboratory</td>
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<tr>
<td>Yusheng Zhao</td>
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Suggested Reading


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