Deep Earth and Recent Developments in Mineral Physics

Jay D. Bass¹ and John B. Parise²

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Very few rocks on the Earth’s surface come from below the crust. In fact, most of Earth’s interior is unsampled, at least in the sense that we do not have rock samples from it. So how do we know what is down there? Part of the answer comes from laboratory and computer experiments that try to recreate the enormous pressure–temperature conditions in the deep Earth and to measure the properties of minerals under these conditions. This is the realm of high-pressure mineral physics and chemistry. By comparing mineral properties at high pressures and temperatures with geophysical observations of seismic velocities and density at depth, we get insight into the mineralogy, composition, temperature, and deformation within Earth’s interior, from the top of the mantle to the center of the planet.

Keywords: Earth’s interior, mineral physics, mantle, core, high pressure

INTRODUCTION

As far as we can tell from recorded history, there has always been interest and curiosity about the interior of the Earth. Very early on, religion gave us the notion of a fiery, superheated hell at depth, a view that in fact may not be too far from the truth. Various science fiction accounts, such as Jules Verne’s Journey to the Center of the Earth and the recent movie The Core, show, if nothing else, our fascination for what lies below our feet. If one lives close to a volcano or in a seismically active area, concerns about the deep Earth take on a real and practical significance. Due to the difficulty of understanding such natural phenomena, it is perhaps not surprising that people often turned to religion or folklore to explain their observations and calm their fears.

Since the formulation of plate tectonic theory, it has become increasingly clear that nearly all geologic activity at the surface, e.g. mountain building, earthquakes, volcanism, and even the composition of the atmosphere, is intimately related to processes that occur at depth. Indeed, the motion of lithospheric plates—the central element of plate tectonic theory— involves the density difference between cold, dense lithospheric slabs and hotter mantle beneath, as well as the ease with which mantle material flows. Thus, there has been increasing interest in understanding the state of the Earth’s interior, its dynamics, and its evolution through time. In short, in order to understand how the Earth system works, we need to understand the mantle and core. What are they made of? What are their thermal structures? What is the nature of heat and mass transfer within and between them?

These are obviously difficult questions, because most of the Earth is inaccessible by drilling or other direct means. However, it turns out that a great deal of relevant information has been accumulating over the past several hundred years. By 1800, the density of the Earth was known to be about 5.5 g/cm³, very close to the currently accepted value of 5.52 g/cm³. Because this density is greater than the value for surface rocks (~2.6 g/cm³), we can immediately conclude that the bulk of Earth’s interior is much denser than rocks at the surface and, therefore, different from what we see around us. In the early part of the 20th century, it was clear from the Earth’s moment of inertia (which tells us how the internal mass is distributed) that mass is concentrated toward the center. From these facts, a good case was made in the late 19th century for an Earth model with a very dense metallic core surrounded by a mantle of less dense rocks. Thus, we can arrive at some profound conclusions knowing just two numbers about the Earth and without having a sample from the interior to guide us.

The major limitation to using just the mass and moment of inertia of the Earth is that no unique solution for the internal structure can be derived from this information. Far more data are now at our disposal, in particular from the field of seismology, and a more detailed picture of Earth’s interior has emerged (Fig. 1). Earthquakes generate two types of sound waves, which pass through the body of the Earth to distant locations: primary, or compressional, P-waves (which are faster and arrive first at a distant seismometer), and secondary, or shear, S-waves (which are slower and arrive after the P-waves). Seismological studies of when these waves arrive at different places on the globe reveal the velocity variation of P-waves and S-waves with depth. That is, seismology is one of the few ways we can “see” the interior of the Earth (another way is through gravity, which gives density at depth, but with relatively low depth resolution). Because the seismic velocity is well determined in any depth interval, we say that seismology has high spatial resolution, and this is a powerful source of information. This greatly reduces the ambiguity in Earth structure. But in order to interpret the information from seismology in terms of parameters like composition, temperature, flow, etc., we need additional information on the properties of Earth materials at high temperatures and pressures, through either laboratory experiments or computer simulations. The field of high-pressure mineral physics provides this information.

¹ Geology Department, University of Illinois at Urbana-Champaign
1301 West Green Street, Urbana, IL 61801, USA
E-mail: jaybass@uiuc.edu

² Department of Geosciences and Chemistry Department
Mineral Physics Institute, Stony Brook University
Stony Brook, NY 11794-2100, USA
E-mail: jparise@notes.cc.sunysb.edu
This issue focuses on experiments at high pressure and temperature and what they tell us about Earth's deep interior, when combined with seismology data. In such experiments, the physical and chemical properties of materials are measured at extreme pressure–temperature conditions that are as close as possible to those inside the Earth (Fig. 2). As noted throughout this issue, there is a natural and intimate connection between the disciplines of mineral physics and seismology. Part of this connection comes through the elastic properties of minerals, which determine the velocities of seismic waves throughout the Earth. One of the very earliest efforts to exploit this relationship was by Williamson and Adams (1923), who used the available seismic data and elasticity measurements on rocks and minerals to calculate a density distribution for the Earth. They also proposed a compositional model for the interior that bears a remarkable similarity to present-day models.

Sources of information on the Earth’s interior include geochemical and petrological studies of meteorites, basalts, and mantle rocks, as well as results from the fields of geodesy, geodynamics, and cosmochemistry, to name a few. In the limited space of this issue, it would be impossible to cover all of these topics. Even our attempt to focus the issue on results provided by high-pressure mineral-physics data and seismology is necessarily just an introduction. Space does not allow a comprehensive discussion of all techniques and interpretations arising from the increasingly rich datasets these interconnected disciplines provide. Indeed, an important part of the field of mineral physics is the theoretical calculation of mineral properties, often under pressure–temperature conditions that cannot be attained experimentally. Theoretical advances and the ever-increasing speed of computers make computational mineral physics indispensable for studying planetary interiors. We regret that this issue of *Elements* lacks an article on this topic, and we hope one will appear in a later issue. However, several recent theoretical results related to the D” layer of the mantle are referred to in the article by Hirose and Lay (2008 this issue).

**GENERAL STRUCTURE OF THE EARTH**

The major divisions of the Earth—crust, mantle, and core—are defined seismologically (Fig. 1). At shallow depths from about 6 km beneath ocean basins and 30–50 km beneath continents (with a maximum of ~70 km beneath Tibet), the speeds of P-waves and S-waves jump dramatically at the Mohorovičić seismic discontinuity (the Moho), which separates the crust and mantle. Beneath the mantle is the liquid outer core, a low-velocity zone where wave speeds drop suddenly (going to zero for S-waves) at the core–mantle boundary. At the boundary with the solid inner core, seismic velocities rise again. This is all that's needed to infer Earth's basic layered structure. Far more observations go into the 1-dimensional whole-Earth models, like the preliminary reference Earth model, PREM (Dziewonski and Anderson 1981) shown in Figure 1, and a slightly more complex Earth structure is suggested. We can describe the stratigraphy of the mantle as follows:

1. An upper mantle, down to ~660 km depth. This includes a “transition zone,” where velocities increase extremely rapidly with depth (that is, velocity gradients are high). The
transition zone is now often taken as the shell between the major seismic discontinuities at 410 km and 660 km depth, with the upper mantle ending at 660 km (although slightly high seismic velocity gradients persist to ~900 km).

(2) A lower mantle with the defining characteristic of smoothly and slowly varying velocities, which appear to be consistent with the compression of a uniform material. The lower mantle is usually taken as starting at the 660 km discontinuity. In early models, the lower mantle was referred to as layer D, at the bottom of which is a thin layer of anomalous seismic structure, labeled the D'' layer in Figure 1B.

**Minerals and Other Phases Present at Depth**

One of the few mantle rocks found at the surface is kimberlite, which contains abundant olivine and, in some cases, xenoliths of peridotite and eclogite. The presence of diamonds and other high-pressure indicator minerals has led to the general view that kimberlites tap upper mantle sources to about 200 km depth (a very few of them may tap deeper sources). These rocks suggest an olivine-rich uppermost mantle, at least under cratons, with lesser amounts of eclogite. Thus, early studies of mantle mineralogy focused on the mineral olivine, (Mg,Fe)2SiO4. Among the more important studies were those by Katsura and Ito (1989) and Akaogi et al. (1989), who showed that magnesium-rich olivine transforms into a high-pressure phase called wadsleyite (β-phase), at a pressure that corresponds well to the seismic discontinuity at 410 km depth. We therefore infer that this olivine to wadsleyite phase transformation is responsible, at least in part, for the jump in velocity at 410 km depth. At a pressure corresponding to ~520 km depth, β-phase transforms into ringwoodite, or γ-(Mg,Fe)2SiO4, with a cubic structure related to the mineral spinel, MgAl2O4. However, olivine-composition minerals cannot be the only minerals present in mantle rocks if they are to produce mid-ocean ridge basalts (MORB) by partial melting. Accompanying (Mg,Fe)2SiO4 in the upper mantle are a Ca-poor pyroxene (enstatite), a Ca-rich pyroxene (diopside or augite), and an aluminous phase (garnet) (note that spinel, MgAl2O4, is the aluminous phase at shallower depth). Figure 1A shows the major minerals that are likely present at different depths in the mantle. The pyroxenes and garnet react with each other as pressure increases, and by about 450–500 km depth, they form a single solid solution with the garnet structure (majorite-garnet solid solution). The lower mantle is almost certainly dominated by (Mg,Fe)2SiO4 with the perovskite crystal structure, (Mg,Fe)O, and CaSiO3 perovskite. Aluminum in the lower mantle would reside primarily in the (Mg,Fe)SiO3 perovskite phase. Ironically, although the lower mantle is dominated by perovskite-structured (Mg,Fe)SiO3, it is more abundant in the Earth, it is not a mineral because it has not been found in nature. The phase transformations producing (Mg,Fe)SiO3 perovskite and (Mg,Fe)O are widely thought to contribute to the 660 km discontinuity. Just above the core-mantle boundary, in the D'' layer, (Mg,Fe)SiO3 perovskite transforms into the recently discovered "post-perovskite" phase, which may explain many of the seismic features of this region. The liquid outer core is likely an Fe-Ni alloy with ~10% of some unknown lighter alloying elements. The solid inner core is likely composed of a nearly pure metallic phase, with smaller amounts of light elements than in the outer core.

Thus the Earth is chemically layered, with a silicic crust, a mafic mantle, and a metallic core. A fundamental but more difficult question is whether seismic discontinuities within the mantle, for example at 410 km and 660 km depth, represent chemical layering on a finer scale, as well as transformations of individual phases into higher-pressure forms. Does the mantle, on average, have a single composition because it is well stirred by whole-mantle convection, or is it divided into separate partially isolated layers of different composition? At present, this question is hotly debated and cannot be answered. More detailed and accurate information, from both mineral physics and seismology, will be critical in determining the answer.

**Seismic Tomography**

An exciting development in Earth science over the past couple of decades has been seismic tomography: mapping out the lateral variability in seismic wave speeds throughout the globe (Fig. 3). For example, the cold oceanic lithosphere subducted into the upper mantle is seen as a high-velocity layer, primarily because low temperature causes seismic waves to travel faster. These high velocities and, presumably, the subducting slabs can in some places be tracked for over 1000 km into the mantle (Grand et al. 1997). In this case, seismic results provide information on tectonics, the exchange of material between the surface and the interior, and large-scale mantle flow. However, as we go deeper into the lower mantle, or away from plate boundaries, seismic features do not necessarily have a clear-cut relationship to surface tectonics, and their interpretation is not as intuitive. For example, it is now well established that seismic heterogeneity exists throughout the lower mantle (e.g. Woodhouse and Dziewonski 1989). That is, the velocities at a given depth are different in different parts of the globe. It was thought at first that these differences in velocity were due to differences in temperature only, by analogy with assumptions about upper-mantle heterogeneity. It was enticing to think of seismically slow material as being hot and buoyant, thus driving mantle flow. However, mineral-physics data have shown that the temperatures required to explain lower-mantle seismic heterogeneity may be unreasonably high. It is more likely that this heterogeneity is due to a combination of chemical, thermal, and phase-change effects (Trampert et al. 2004). This example illustrates how the results of lab-
Laboratory high-pressure experiments are needed to interpret the available seismic information. The assumption of seismically fast material being cold (or of slow material being hot) probably does not strictly hold in any part of the mantle. When one considers the extreme seismic heterogeneity of the upper mantle (Fig. 3), showing many small regional (that is, not global) boundaries on a variety of length scales, perhaps the concept of a single average composition for the upper mantle is not at all appropriate.

HIGH-PRESSURE MINERAL ELASTICITY AND SYNCHROTRON-BASED STUDIES

One of the keys to refining our understanding of Earth’s interior and narrowing the range of acceptable compositional and thermal models is the acquisition of elasticity and phase equilibrium data under conditions closely simulating those in the mantle and core (Fig. 2). This lofty experimental goal is now within reach. Scientists in the discipline of high-pressure mineral physics studying the Earth’s deep interior have recently made an unprecedented number of breakthroughs, some of which are described by Bass, Sinogeikin, and Li (2008 this issue). Many of the experimental studies described in this issue were inconceivable only a decade ago, mainly because of technical limitations. Developments in the area of diamond anvil cells (DAC), coupled with ever-brighter synchrotron X-radiation, now permit the acquisition of X-ray diffraction data at P–T conditions prevailing throughout the planet (Fig. 4). Developments in large-volume high-pressure apparatuses are allowing precise measurements of phase stability, strength, texture, and flow at transition zone and lower-mantle pressures for the first time (Fig. 5). Other non-synchrotron-based techniques, particularly in the area of mineral elasticity, have seen similar advances (Fig. 6) and are even being combined with synchrotron radiation for simultaneous measurement of several physical properties on tiny samples at high pressures (see Elements vol. 2, no. 1: “User Research Facilities in Earth Sciences”).

The fruits of these laboratory-based studies are numerous. A growing database of crystal structures, elastic properties, and rheologic properties (both theoretically and experimentally derived) can be compared with physical measurements of the planet. Just as importantly, groups from different disciplines are being drawn together in an effort to integrate their data. Finally, the technical developments in high-P–T research, initially aimed at understanding the operation of Earth’s deep interior, are applicable to a broad range of materials research at extreme conditions, including investigations in the seemingly disparate fields of planetary science, materials chemistry, and condensed-matter physics.

Developments at synchrotron sources have proceeded apace due in no small measure to gains in brightness at the European Synchrotron Radiation Facility (ESRF), at the 8 GeV Super Proton ring (Spring-8) in Japan, and at the Advanced Photon Source (APS) in the United States. Study of the Earth’s interior necessarily requires high pressure, and as the pressure of an experiment increases, the size of the sample must be smaller. Sample volumes of 1 nanoliter held at a million bars of pressure (1 Mbar = 100 GPa) can be heated to several thousand degrees and examined using synchrotron radiation (Fig. 4). Innovations in high-pressure research have made this field a focus in the planning and development of new synchrotron sources.

MODELS OF THE UPPER MANTLE

The mineralogical composition of much of the upper 200 km of the mantle has long been thought to be equivalent to garnet lherzolite, which is composed of olivine, Ca-poor and Ca-rich pyroxenes, and pyrope-almandine garnet (Fig. 1). In the “pyrolite” mantle model, the olivine component of this lherzolite is about 55–60% (Ringwood 1975). As a working definition, pyrolite is an olivine-rich rock that,
upon equilibrium partial melting, yields the great volumes of basalt that underlie the world’s ocean basins. The composition of pyrolite is similar to the most fertile (i.e. the most garnet- and Ca-pyroxene-rich) olivine-rich mantle xenoliths found in kimberlites.

Frost (2008 this issue) examines the applicability of the pyrolite model to the upper mantle, including the transition zone. Key observations that must be explained by the model include the magnitude of the seismic velocity jumps at 410 and 660 km depth, the high seismic velocity gradients in the transition zone, and the sharpness of these discontinuities. Phase transformations in olivine clearly play a role in the 410 km and 660 km discontinuities. Frost also points to studies indicating that given the uncertainties in the elastic and thermal properties of the relevant phases, a homogeneous lherzolite model for the entire upper mantle is viable (Cammarano et al. 2005). However, we would emphasize, as Frost points out, that the transition zone is likely a complex heterogeneous region. In some places, subducting slabs lie on top of the 660 km discontinuity (FIG. 3), at least temporarily, and in other places they penetrate readily into the lower mantle. Although penetrating slabs are often taken as suggestive of large-scale whole-mantle mixing and homogenization (e.g. Grand et al. 1997), in our view it is possible that no single compositional model can adequately explain this complex transition zone. As Birch (1952) stated in his classic paper on the Earth’s interior, “The transitional layer appears to hold the key to a number of major geophysical problems.” Finding the key is not easy. Increasing the quality and global coverage of seismological datasets and combining them with mineral-physics data are clearly the way forward.

Eclogite in the Upper Mantle?

Eclogite is composed mainly of Ca-rich pyroxene and garnet. Some eclogites are the high-pressure equivalent of basalt. The occurrence of eclogite in kimberlites suggests its presence in the mantle, although the amount is uncertain. Eclogite has two notable properties compared with olivine-rich lherzolites: a higher density (at depths less than 400 km) and a lower melting point. The high density may play a key role in the subduction of cold, dense oceanic plates through the surrounding mantle and provide part of a gravitational driving force for slab-driven mantle convection. Moreover, in some compositional models of the upper mantle, the 410 km discontinuity represents a change in composition as well as phase changes, with the transition zone depleted in olivine relative to the pyrolite model and enriched in an eclogitic (garnet + pyroxene) component. This is reminiscent of early proposals by Birch (1952). Such models may provide a better explanation for the velocity jumps at 410 km depth and the gradients in the transition zone (Bass and Anderson 1984; Duffy et al. 1995). The low melting point of eclogite may play a role in some basaltic volcanism. Aspects of this issue are reviewed by Anderson (2007) and Foulger et al. (2005).
Lower Mantle and Core

In their article on the lower mantle and core, Fiquet et al. (2008 this issue) review in broad strokes our current understanding of this part of the planet. As they point out, the mantle and core should be considered together as a coupled system comprising the vast majority of Earth’s mass. To constrain the composition of this system, one can consider the bulk composition of the Earth to be similar to the composition of volatile-rich chondritic meteorites, which presumably have not been extensively melted or differentiated. These authors discuss different models for the core and mantle, including a homogeneous lherzolite mantle and a relatively SiO2-rich lower mantle that would yield a Mg/Si ratio for the bulk Earth that is closer to that implied by meteorites (Matas et al. 2007). Models for the formation and composition of the core and lower mantle are presented, along with unresolved questions and key mineral-physics experiments that still need to be done to improve our understanding. Critical studies for the future include phase-equilibrium experiments to determine which elements dissolve into the core and which might give it a density matching that in Earth models such as PREM. Fiquet et al. (2008) also describe a new class of experiments (inelastic X-ray scattering, in which sound velocities at high pressures are measured using synchrotron radiation) that may be used to study M. Karato and D. Bass.

Studies of the D” Layer

The D” layer is one of the most complex and seismically puzzling regions in the Earth’s interior. High-resolution seismology is providing increasingly detailed pictures of shear wave splitting (two S-waves traveling at different speeds) and anisotropy, a highly variable D” discontinuity with a jump in velocities, ultralow velocity zones, and a variable Vp/Vs ratio (e.g., Garnero et al. 2004). One can easily imagine the core-mantle boundary as a zone of chemical reactions between the metallic core and the silicate mantle, with perhaps partial melting above the interface. Either of these mechanisms would cause a pronounced change (most likely a decrease) in seismic velocities. A third possible cause for the D” discontinuity is a phase transformation from (Mg,Fe)SiO3 perovskite to a “post-perovskite” (PPv) phase. Hirose and Lay (2008 this issue) present some historical context for the discovery of this phase transformation, which had long been anticipated on the basis of seismology, and discuss its implications. The transformation of perovskite to a post-perovskite structure was first discovered in experiments using a DAC (FIG. 4) on MgSiO3 at a pressure of 120 GPa and a temperature of ~2500 K. Subsequent experimental work on more-complex and more-realistic chemical compositions demonstrated that this transformation should occur a couple of hundred kilometers above the core-mantle boundary. Theoretical and experimental studies further showed that the PV-PPV transformation pressure is temperature dependent (that is, it has a positive Clapeyron slope). Thus, the depth of the PV-PPV phase transformation has the potential to define the temperature just above the core-mantle boundary. Aside from explaining many of the observed seismic features of the D” layer, the PV-PPV phase transformation is one of the few available means by which the thermal structure of the deepest mantle can be determined.

RHEOLOGY

Studies of the dynamics or flow of material within the Earth require knowledge of the strength and rheological properties of candidate mantle minerals. Despite the vast differences in timescales, or strain rates, between the flow of rocks in the Earth and in the laboratory, the understanding of the fundamental mechanisms that operate during flow and the judicious application of laboratory-based observations are opening windows on the way the mantle conveys. Karato and Weidner (2008 this issue) review early studies of rock deformation and mention the exciting prospects for future developments using different types of high-pressure devices. The outlook for rheological measurements mirrors earlier developments in phase diagrams and elasticity. The advent of high-energy synchrotron X-ray sources facilitates new in situ observations that go beyond early work, which was mainly on olivine at lower-crustal pressures. The power of high-energy X-rays to penetrate stress-generating apparatus allows simultaneous measurements of diffraction and direct imaging of the sample to define stress and strain. The ability to “dial in” stress states and then watch temporal variation of stress and strain at different temperatures provides information on the rate of plastic deformation. Coupling these observations with post-mortem TEM investigation of the deformed samples provides constraints on the rheological properties of mantle minerals, at least to the pressures of the transition zone. Karato and Weidner (2008) also examine the prospects for extending existing approaches to the lower mantle, with an eye to all-important rheological measurements on MgSiO3 perovskite under the appropriate P-T conditions.

CONCLUSIONS

The science and technology of high-pressure mineral-physics research are advancing at an astonishing pace. Measurements of a wide variety of properties, only some of which are described in this issue, are possible under the actual P-T conditions that exist in the deepest parts of the Earth, and even at more extreme conditions. Mineral physics has led the way in understanding the properties of matter under extreme conditions, and the results of this
research have had a significant impact in fields such as condensed matter physics and materials science. Our understanding of how the entire Earth system works is progressing rapidly, through the integration of results from mineral physics and seismology, petrology, geochemistry, and other disciplines in Earth science.

We hope that this issue conveys some of the excitement in the field of high-pressure mineral physics. We are now at a time when novel techniques and combinations of techniques using multiple in situ probes are coming online, and where collaborations between observational seismology and mineral physics are expanding, thus opening up unprecedented opportunities for understanding the deep Earth.

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REFERENCES


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