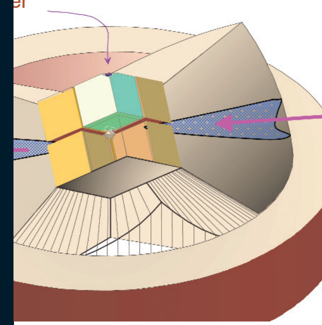

# Elastic Properties of Minerals: A Key for Understanding the Composition and Temperature of Earth's Interior

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**Seismological studies give us a high-definition 3-D picture of the Earth's interior in terms of seismic velocity and density. Near the surface, observations of these properties can be compared with rock samples. As we go deeper into the Earth, interpretation of seismic data is more difficult. Laboratory measurements of velocities and other elastic properties of minerals are the key to understanding this seismic information, allowing us to translate it into quantities such as chemical composition, mineralogy, temperature, and preferred orientation of minerals. Here we present a description of modern techniques for measuring elastic properties at high pressures and temperatures, emphasizing those most relevant to understanding the interior of the Earth and other planets.**

KEYWORDS: elastic properties, mineral physics, Earth's mantle

## INTRODUCTION

Seismology provides a means of imaging the interior of the Earth. The pictures provided by seismologists give us important clues as to what the interior is made of and what conditions are like at depth. Seismological investigations are unique in their ability to isolate the properties of the Earth at specific depths with high resolution, which is essential for understanding the otherwise inaccessible interior of our planet. However, there is a caveat: we need an additional ingredient to translate this information into quantities of interest, such as temperature, mineralogy, and chemical composition. As described in the seminal paper by Birch (1952), this essential ingredient is knowledge of the elastic properties of minerals, especially at high pressures and high temperatures.

Elastic properties describe the instantaneous but temporary volume and shape changes that occur when stresses are applied to a material. An elastic material returns to its original volume and shape when stress is released, just as an elastic band returns to its original length after you stop pulling on it. Field geologists are familiar with permanent deformations such as folds, boudinage, faults, etc. These deformations are not elastic; rather, they are termed anelastic because they remain after rocks are exhumed and freed of stress. In contrast, you cannot see elastic deformation in the field. Among the reasons that make elastic properties so important is that they are related to (1) the velocities of seismic waves and (2) the change in density that occurs when minerals are under pressure. Thus, knowledge of the elastic properties of minerals is essential for interpreting the seismic properties of the Earth and for calculating the density distribution and mass of a planetary body.

When an earthquake occurs, two types of seismic waves travel through the body of the Earth: fast primary (P) or longitudinal waves, which vibrate material parallel to the direction in which the wave propagates, and slower secondary (S) or shear waves, which vibrate material perpendicular to the propagation direction. Seismic waves are sound waves, also known as elastic waves, and they travel with speeds $V_P$ and $V_S$, respectively. Your vocal chords excite a longitudinal sound wave in the air, and this wave travels with the velocity $V_P$ for air. Shear waves do not propagate in fluids like air or water, but they are transmitted by solid rocks. In early studies on rocks and minerals, it was not possible to measure the velocities $V_P$ and $V_S$ in the laboratory, although this would have been optimal. Rather, the change in volume, $dV$, resulting from a change in pressure was measured (note: the volume per unit mass is equal to the inverse of density, $1/\rho$). These pressure and volume changes define the isothermal incompressibility, $K_T$, expressed more formally as

$$K_T = -V\left(\frac{dP}{dV}\right)_T = \rho\left(\frac{dP}{d\rho}\right)_T$$

The incompressibility is more commonly known as the bulk modulus. The more difficult to compress (or "stiffer") a material is, the higher the value of $K_T$. By measuring the volume or density of a sample at several known pressures, we get $K_T$. Note that, by definition, $K_T$ gives the variation of density with pressure, making it essential for determining the density and pressure distribution in the Earth.

Measurement of the bulk modulus continues to be an active area of research because it is related to seismic velocities $V_P$ and $V_S$ through the following relationships:

$$V_P = \sqrt{\frac{K_S + (4/3)\mu}{\rho}} \qquad V_S = \sqrt{\frac{\mu}{\rho}}$$

$$K_S = \rho\left(V_P^2 - \tfrac{4}{3}V_S^2\right) \qquad \mu = \rho V_S^2$$

where $\mu$ is the shear modulus (a measure of the rigidity of a material), $\rho$ is the density, and $K_S$ is the adiabatic bulk modulus. $K_T$ and $K_S$ usually differ only by about 1%, and we

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ignore this difference in the following discussion. The important point is that if one knows the moduli $K$ and $\mu$, and the density, the velocities are then known, and vice versa. Both the velocities and moduli are elastic properties. In fact, many elasticity techniques involve measurements of $V_P$ and $V_S$, so it is fair to ask why we need to worry about the elastic moduli at all. The answer is that to calculate elastic properties at high temperatures and/or pressures, or to use measurements on minerals to infer the properties of rocks, these calculations are usually cast in terms of moduli, not velocities. Moreover, the bulk modulus is readily measured experimentally or calculated.

The density of a mineral sample is often measured by X-ray diffraction. When a mineral is compressed hydrostatically, the atoms get closer together. We can measure the distance, $d$, between the compressed atomic lattice planes using Bragg's law, $n\lambda = 2\, d \sin\theta$, where $\lambda$ is the X-ray wavelength, $n$ is an integer, and $\theta$ is the diffraction angle. By measuring several $d$-spacings in a high-pressure experiment, the atomic unit-cell volume is known. The density of a sample can then be calculated from its chemical composition and this volume.

In many experiments the samples are single crystals, as opposed to rocks or polycrystalline aggregates. Most single crystals are elastically anisotropic, meaning that sound velocities are not the same in different crystallographic directions. The situation is analogous to the propagation of light in optically biaxial and uniaxial crystals, except that with elasticity there is velocity anisotropy for both P- and S-waves. We can obtain information on velocity anisotropy from single crystals, and this can be used to understand the sources of seismic anisotropy in the Earth. Velocity anisotropy in rocks can indicate preferred orientations of minerals (similar to foliated metamorphic rocks), perhaps induced by solid-state flow. Further information on elasticity theory is found in numerous textbooks (e.g. Musgrave 1970; Nye 1985), whereas the elastic properties for many minerals are summarized by Bass (1995) and Knittle (1995).

## EXPERIMENTAL TECHNIQUES

Because the pressures (P) and temperatures (T) in the Earth are extreme, reaching over ~3.6 million atmospheres (3.6 Mbar, or 360 GPa) and ~4000–7000 kelvins, respectively, at the Earth's center, we are concerned with techniques that can be used at the highest P–T conditions possible. Geoscientists have thus played a prominent role in the development of new high-pressure techniques. Many modern techniques for measuring elastic properties are based on light scattering. The light sources may be lasers with visible wavelengths or X-rays produced by synchrotrons. In particular, the availability of intense synchrotron X-rays has led to the development of new techniques that were not even considered possible just a decade ago (Sutton et al. 2006). Further details are given in a review by Bass (2007).

### *Static Compression Measurements of the Bulk Modulus*

The most direct and oldest method of measuring an elastic property is by exerting a sustained pressure on a sample (static compression) and measuring the volume change. In this way the bulk modulus $K$ is determined from the definition above. The simplest experiment would be to put a sample in a hole or cylinder and to compress it with a tight-fitting piston. This is the basis of the piston-cylinder apparatus, which was developed long ago for measuring the bulk modulus. Although the piston-cylinder is important historically, and is still in use commercially for the production of synthetic diamond, it has been surpassed by the diamond anvil cell and the multi-anvil apparatuses discussed below.

### *Diamond Anvil Cell*

The diamond anvil cell (DAC) is probably the most commonly used instrument in high-pressure research. This device produces the highest pressures of any static-compression device, reaching pressures of the Earth's core (Mao et al. 1990) or greater. The DAC is versatile due to its simplicity and the transparency of diamond. Pressure is generated by compressing samples between small, flat "culet" surfaces at the tips of two gem-quality diamonds (FIG. 1). Because the diamond culets are small (0.1–1 mm) and pressure = force/area, a moderate force on the diamonds produces very high pressure (see Jayaraman 1983).

To produce near-hydrostatic conditions, the diamonds usually compress the sample in a sample chamber consisting of a hole in a thin metal foil, and pressure is transmitted to the sample via a soft medium such as He, Ne, or NaCl. The fluorescence wavelengths of ruby are strongly pressure dependent, and this property can be used to determine pressure in the sample chamber. Alternatively, one can use the lattice parameters of an inert standard material, such as MgO or Au.

By focusing an infrared laser on the sample, it can be heated to several thousand kelvins while under pressure (Meng et al. 2006). This makes it possible to simulate the actual P–T conditions in the mantle. The versatility of the diamond anvil cell for use in many types of elasticity measurements is illustrated in some of the following sections.

### *Multi-Anvil Devices*

Sometimes called "large-volume presses," multi-anvil presses (MAPs) are far bulkier than the DAC but hold much larger samples, on the order of 1 $mm^3$ or larger. This has great advantage in many experiments. Cube-anvil presses with six anvils have been used to pressures of about 10–15 GPa and at high temperatures (Wang et al. 1996). Higher pressures and temperatures are obtained using a "two-stage" MAP (Kawai and Endo 1970), in which eight inner tungsten carbide or sintered-diamond anvils compress the sample (FIG. 2; also see Bass and Parise 2008 this issue). Synchrotron X-rays are introduced via gaps between the anvils for X-ray diffraction measurements of the sample volume. Measurements of the P–V–T relations (hence, $K$) and sound

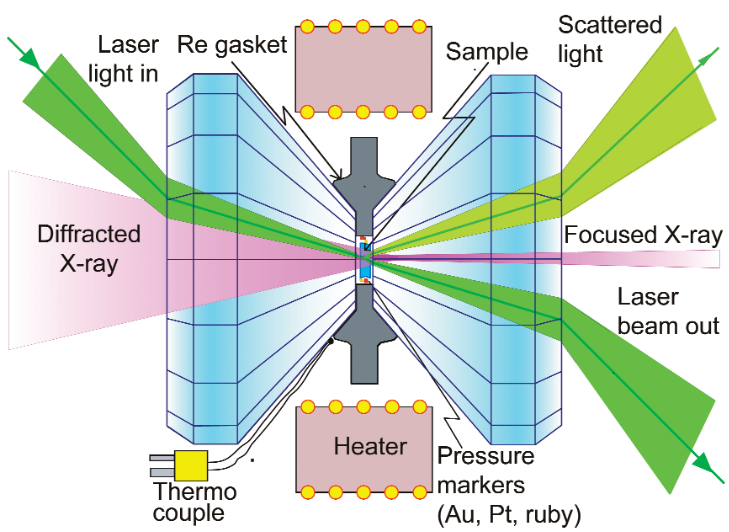


**FIGURE 1** Schematic of a diamond anvil cell. The sample is between the diamonds, within a hole in the gasket (sample chamber). Synchrotron X-rays coming from the right are diffracted by the sample, and the diffracted X-rays are used for determining the sample volume and density. A green laser beam for a light-scattering experiment enters from the left and passes through the transparent diamonds. A wire resistance heater is shown for high-T–P measurements. A laser beam for heating the sample could be used as well. AFTER SINOGEIKIN ET AL. (2006)

velocity measurements can be performed on minerals pressurized by a MAP. It has also been one of the main tools for determining the phase relations of possible mantle assemblages as well as phase transitions (Frost 2008 this issue).

## Ultrasonic methods

With most ultrasonic methods, sound waves propagate through the sample and their speeds are measured, giving $V_P$ and $V_S$ for the sample directly. With its adaptation for use with smaller samples and multi-anvil presses, ultrasonics has become one of the primary techniques for measuring elasticity at high pressure and temperature. An alternative approach is to vibrate a sample at its resonant frequencies, like a tuning fork, using the technique of resonant ultrasound spectroscopy (RUS). RUS has been especially fruitful in measuring high-temperature elasticity (Anderson and Isaak 1995).

### *Wave-Transmission Techniques*

The basic idea in ultrasonic transmission is to measure the travel time of a sound wave through a sample. Knowing the length of the sample and the travel time, the velocity of the ultrasonic wave is defined. In practice, one often measures the time it takes for a sound wave to make several round trips through the sample by reflecting from either end (Fig. 3). The sound wave is generated by a device called a transducer, which will be familiar to those who have used vinyl records and turntables. The needle cartridge in a turntable converts the mechanical wiggles in a vinyl record into an electrical signal that can be amplified and sent to loudspeakers. In the same way, the transducer in an ultrasonic experiment takes an electrical pulse and turns it into a vibration that propagates as a sound wave in a sample.

For studies of Earth's interior, the adaptation of ultrasonics for the measurement of elastic properties at high pressure has been a major advance. The highest pressures (>20 GPa) can be reached with a MAP (Li et al. 2004), with simultaneous temperatures up to ~1600°C, i.e. P–T conditions comparable to those in the transition zone.

## Light-Scattering Techniques

By light scattering, we mean any of a class of experiments in which light interacts with a sample and is changed. The light photons exchange energy and momentum with a material, either exciting new lattice vibrations (phonons) or picking up energy from existing lattice vibrations. As a result, part of the scattered light has a different frequency from the incident light. By measuring these changes, we obtain information on the atomic vibrations. In fact, many interactions take place, and many different frequency shifts occur. Some lattice vibrations correspond to the atomic motions that occur when a sound wave or seismic wave propagates through a material; these are acoustic phonons. Light scattered from these acoustic modes of vibration contains information on the velocity of sound. The frequency changes of light are small and were difficult to detect before relatively recent advances in technology.

The main requirements for the input light are that it be highly monochromatic and intense. Either laser light or X-rays are used. Because X-rays are simply light of short wavelengths, we can group X-ray and light-scattering techniques together; the concepts behind the experiments are the same. A big advantage of light-scattering methods is that they can be used with very small samples. Many materials of interest for deep-Earth studies cannot be synthesized as large single crystals, making light scattering one of the only ways to determine their elastic properties.

### *Brillouin Scattering*

Over the past few decades, Brillouin scattering has been used to measure the sound velocities for a wide range of materials of geophysical interest. Of particular importance are phases that are stable only at high pressures.

In a Brillouin scattering experiment, laser light is focused on a sample and the scattered light is analyzed (Fig. 4). Some of the scattered light is Doppler shifted in frequency (the Brillouin shift) by acoustic phonons in the sample, and this frequency shift gives the sound velocity. The sound waves change the incident light in the same way that the pitch of the sound of a train varies with its velocity (the Doppler shift). Thus, by measuring the Brillouin frequency shift, the velocity of the sound wave can be determined.

Brillouin scattering was applied to small single crystals of geological importance by Weidner et al. (1975). Subsequently, high-pressure Brillouin experiments have been performed using a DAC on a number of mantle minerals (e.g. Duffy et

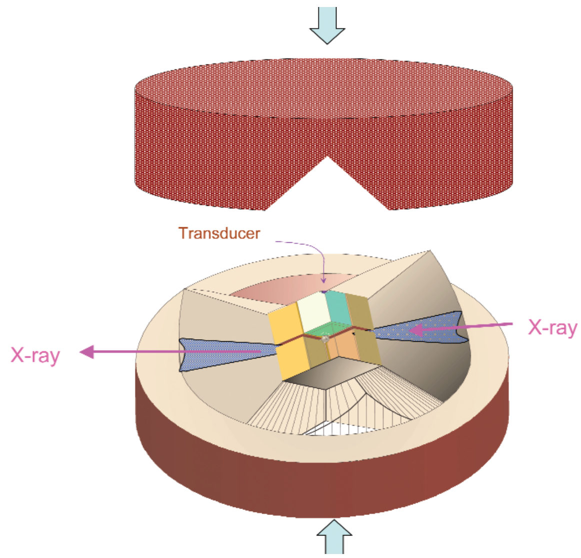


**Figure 2** Schematic diagram of a two-stage Kawai-type multi-anvil apparatus. The eight inner cubes are anvils that compress an octahedron-shaped sample assembly. The transducer produces an ultrasonic signal that is transmitted to the sample and detects the return signal.

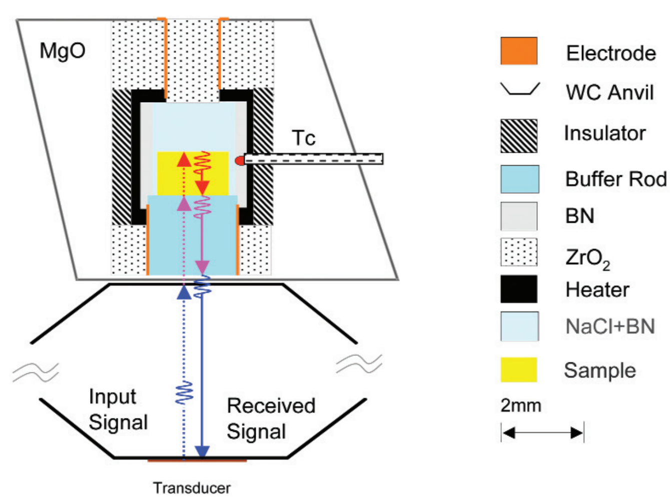


**Figure 3** Ultrasonic pulses in a modern high-presssure experiment. The transducer is mounted on a pressure-generating anvil. A buffer rod simply connects the transducer to the sample, which is embedded in a pressurized medium. WC = tungsten carbide; BN = boron nitride; Tc = thermocouple

include most of the materials in Earth's core and mantle. In NRIXS, nuclear resonances are excited by interaction of X-rays with the $^{57}Fe$ isotope. The measured spectrum of vibrational states, called the density of states, is sensitive to the shear velocity. If $K$ and the density of the sample are known from X-ray diffraction, then $V_S$ and $V_P$ can be obtained. Measurement of the velocity of Fe at high pressure and temperature using a laser-heated DAC (Lin et al. 2005) provides a basis for assessing the light elements in Earth's core. Mao et al (2006) have used NRIXS measurements on the post-perovskite phase to explain ultralow-velocity zones in the D" layer.

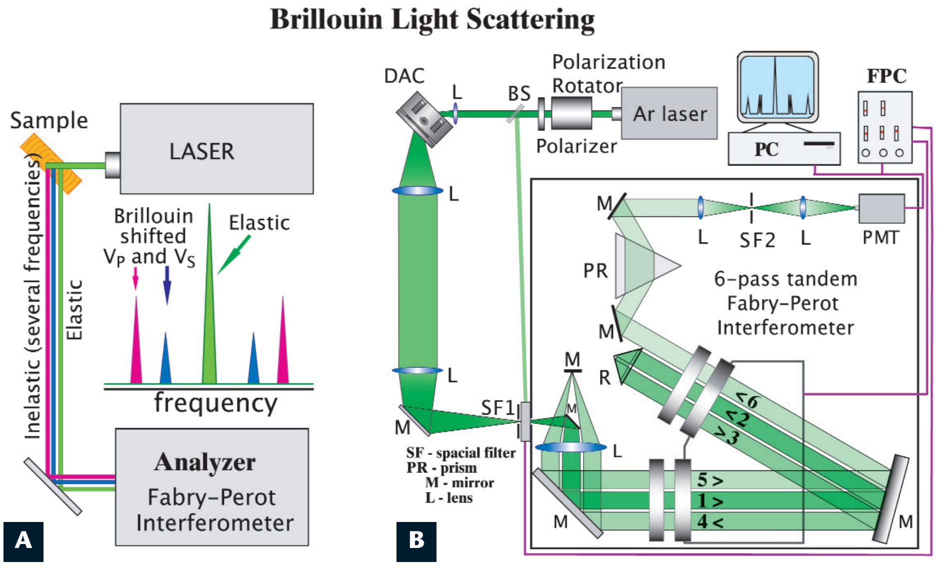


**FIGURE 4** (**A**) General schematic for most light-scattering experiments. Laser light hits the sample and the scattered light is analyzed. (**B**) A more complete diagram of a Brillouin-scattering experiment using a sample at high pressure in a DAC. PC = personal computer; PMT = photomultiplier tube; FPC = Fabry-Perot controller; BS = beam splitter.

al. 1995). It is now possible to measure sound velocities to pressures greater than those at the core–mantle boundary, as in the work on the perovskite and higher-pressure form of $MgSiO_3$ (Murakami et al. 2007; Hirose and Lay 2008 this issue). High-temperature measurements can be performed using laser heating to T > 2500 K (Sinogeikin et al. 2004). A recent advance has been the interfacing of Brillouin scattering with synchrotron radiation for simultaneous measurements of velocity and density at GSECARS of the Advanced Photon Source (Sinogeikin et al. 2006).

### *Impulsive Stimulated Scattering*

Impulsive stimulated scattering (ISS) is another laser-based technique for measuring elastic properties at high pressure with a DAC. Unlike the Brillouin- and inelastic X-ray-scattering techniques (see below), this method scatters light from sound waves that are artificially stimulated in the sample. Two laser beams are focused on the same spot in a sample and optically interfere where they meet. This launches sound waves in opposing directions. The scattering of a third light beam from these stimulated sound waves allows the velocity to be measured. The application of ISS for measuring sound velocities in geologic materials, including possible core-forming metals and alloys, is described by Abramson et al. (1999). Recently, ISS has been used to measure how a change in the electronic structure of iron at high pressure (from a high-spin to a low-spin state) affects the velocity of sound in the lower-mantle mineral ferropericlase, (Fe,Mg)O (Crowhurst et al. 2007).

## *Inelastic X-ray Scattering*

Intense third-generation synchrotron X-ray sources make it possible to measure sound velocities by inelastic X-ray scattering (IXS) (Burkel 2000). These emerging techniques will likely play a prominent role in future studies of Earth materials under extreme conditions.

### *Nuclear Resonant Inelastic X-ray Scattering (NRIXS)*

This synchrotron-based X-ray technique is increasingly being used in mineral-physics research. It is particularly useful for iron and iron-bearing compounds (Sturhahn 2004), which

### *Inelastic X-ray Scattering from Phonons*

Inelastic X-ray scattering (IXS) from phonons is analogous to Brillouin scattering, but with X-rays instead of visible light, because it measures the frequency shift of X-ray photons scattered by thermally generated phonons. The applications of IXS from phonons to geophysical research are described by Fiquet et al. (2004). An advantage of IXS from phonons over visible-light-scattering methods is that X-rays penetrate all materials. This makes it possible to determine the velocities $V_P$ and $V_S$ in opaque materials of relevance to Earth's core (Fiquet et al. 2004).

## *Other Techniques*

Before DACs could attain multi-megabar pressures, **shock waves** were the only way to explore the P–T range of Earth's lower mantle and core. In a shock-wave experiment, a projectile impacts a sample at high velocity, up to ~7 km/s (over 25,000 km/h!). Upon impact, a high-pressure and high-temperature state (the shock wave) propagates through the sample. In a shock compression experiment, the pressure and density are determined (Ahrens and Johnson 1995). In particular, the pressure is known with relatively high accuracy, making shock experiments important in the determination of pressure scales for high-pressure research. The results of shock-wave equation-of-state experiments have been critical to our understanding of Earth's interior. Experiments on Fe alloys provide compelling evidence that the density of the outer core is too low for it to be composed of pure Fe and, therefore, that it contains lighter elements.

**Inelastic neutron scattering** is arguably the optimal way to investigate elastic properties (Shirane 1974). Its application to deep-Earth studies has thus far been limited because neutron scattering requires large samples, which are not generally available for high-pressure phases. However, more-intense neutron sources, such as the new Spallation Neutron Source in Oak Ridge, Tennessee (USA), will greatly reduce the sample size needed, making high-pressure research possible.

**Radial X-ray diffraction** in the diamond anvil cell is another technique that has been used to provide constraints on the strength and elasticity of materials (e.g. Merkel et al. 2002; Speziale et al. 2006). This experimental method utilizes the fact that samples in the DAC are usually not under hydrostatic pressure. By using X-rays to measure the difference in strain in a sample in different directions, a measure of the elastic moduli can be obtained.

## APPLICATIONS TO THE DEEP EARTH

We can get some idea of what minerals might exist at depth from the compositions of mantle xenoliths, meteorites, high-pressure phase equilibrium experiments, and other lines of petrologic, geochemical, and geophysical evidence. Elasticity measurements on minerals then allow us to test different mineralogical models by comparison with seismic results for the Earth. Some of the main results of elasticity measurements on minerals and other high-pressure phases can be summarized by curves that show how velocity changes with depth (or pressure). A set of such velocity–depth curves for important mantle minerals is shown in FIGURE 5. These curves take into account the increase in temperature that occurs along an adiabatic temperature gradient. Knowing these "adiabats" for minerals, we can in principle find the right combination of phases to match the velocities in any given part of the mantle, thereby defining a satisfactory composition.

### Lower Mantle

To illustrate the implications of these adiabats, we look at the lower mantle. The adiabats for the lower-mantle phases perovskite (Pv) and ferropericlase [also known as magnesiowüstite = Mw, (Mg,Fe)O] straddle the $V_P$ and $V_S$ curves for the lower mantle given by the PREM seismic model, with perovskite being faster than PREM and (Mg,Fe)O being much slower (FIG. 5). This indicates that a mixture of perovskite and ferropericlase yields velocities matching the PREM seismic velocities for the lower mantle. It is not certain, however, whether the mixture that gives the closest match to PREM represents a chemical composition that would also fit the upper mantle (Fiquet et al. 2008 this issue). Comparing the velocity–depth curves for mineral assemblages that satisfy the upper and lower mantle seismic velocity profiles is perhaps the most promising way of telling whether the mantle is chemically layered.

### Transition Zone

The seismic discontinuities at depths of ~410 km and ~660 km, and the high seismic velocity gradients in between, are diagnostic of the chemical composition in the transition zone. Looking at the adiabats for olivine (Ol) and wadsleyite (Wd) in FIGURE 5, we see that the phase transformation from olivine to wadsleyite—which we are fairly certain occurs at ~410 km depth—produces an increase in velocity that is as much as several times the size of the PREM 410 km discontinuity. Therefore the upper mantle cannot be composed only of olivine, but must be diluted with other minerals such as garnet and pyroxenes. It is also evident that seismic gradients, or slopes of the PREM velocities, are much steeper than the mineral adiabats in the transition zone. It is generally agreed that the pyroxene–majorite transition could contribute to high seismic velocity gradients between 300 and 450 km depth. Some authors claim that a mantle with a high olivine content, such as pyrolite, produces too large a velocity jump at 410 km and seismic gradients that are too low to match seismic models (Bass and Anderson 1984). Others contend that a uniform pyrolite mantle is acceptable within the uncertainties of the data (Li and Liebermann 2007; Frost 2008). It is a matter of current debate whether a change in composition occurs at 410 km depth, or whether the upper mantle to 660 km depth is, on average, of uniform composition. Elasticity measurements at high pressures and temperatures, as well as refinements in seismic models, will be required to resolve these issues.

### Uppermost Mantle

For several decades it has been known that seismic velocities appear to decrease in the shallow mantle between ~70 km depth and about 200 km depth, forming a low-velocity zone (LVZ; FIG. 6). The LVZ has been associated with a very deformable asthenosphere that is highly attenuating and absorbs seismic energy, possibly due to partial melting or the presence of hydrous minerals (Karato and Jung 1998). Using newly available elasticity data for upper mantle minerals, Stixrude and Lithgow-Bertelloni (2005) investigated the nature of the LVZ by calculating velocity–depth curves for various mineral assemblages (FIG. 6). The resulting curves are not adiabats, but they correspond to the high geothermal gradient in the upper few hundred kilometers of the Earth. Their results show that for olivine-rich compositions like pyrolite or harzburgite, the LVZ is a natural result of rapidly increasing temperatures within and immediately below the lithosphere. Attenuation and partial melting could lower the velocities further but are unlikely to be the primary cause of the LVZ.

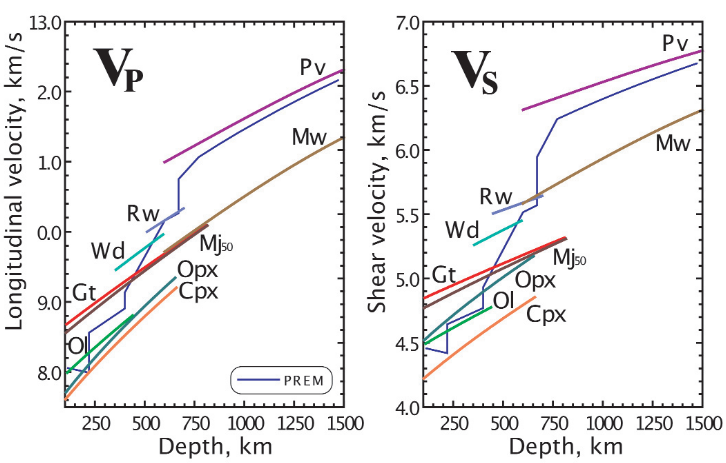


FIGURE 5 The variation in sound velocity with depth for various key mantle minerals: olivine (Ol), diopside (Cpx), enstatite (Opx), garnet (Gt), majorite-garnet solid solution ($Mj_{50}$), wadsleyite (Wd), ringwoodite (Rw), magnesiowüstite (Mw), Mg-silicate perovskite (Pv). Increases in temperature for an adiabatic gradient are taken into account. The reference model PREM (Dziewonski and Anderson 1981) is shown for reference. The length of an adiabat indicates approximately the maximum pressure stability of any given phase.

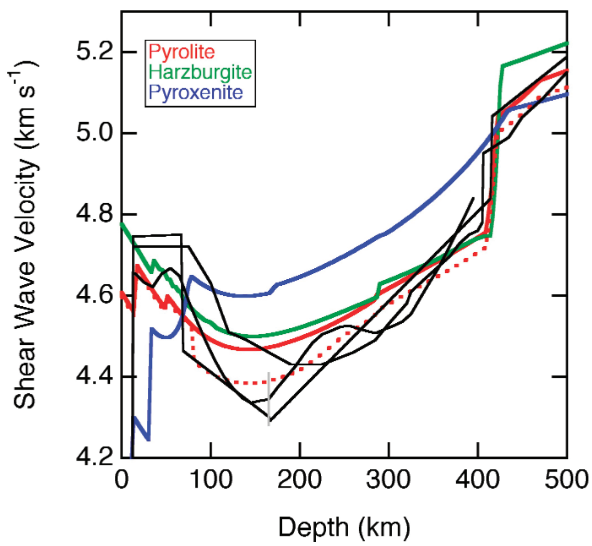


FIGURE 6 Shear-wave velocity in the elastic (infinite frequency) limit for three model mantle compositions: pyroxenite (blue solid line), harzburgite (green solid line), and pyrolite (red solid line), and shear-wave velocity at seismic frequencies for pyrolite (red dashed line), computed along a 100 Ma oceanic geotherm, compared with several seismological models of 100 Ma Pacific Ocean upper mantle (black solid lines). The grey bar indicates the seismologically constrained magnitude of shear anisotropy. AFTER STIXRUDE AND LITHGOW-BERTELLONI (2005)

## CONCLUSIONS

Advances in the technology of elasticity measurements now make it possible to quantitatively address many fundamental questions about the Earth's interior that previously were in the realm of speculation. New questions have emerged, such as how electronic transitions in Fe affect the elastic properties of lower-mantle phases, and many critical measurements remain to be made. Among the most important are measurements of the elastic properties of key mantle minerals under the actual P–T conditions of the mantle and core. This goal is now within reach using several techniques. The results of such studies will likely change our view of Earth's interior and will be essential for improving our understanding of the composition, thermal structure, and evolution of the mantle and core.

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