Opening up the Earth

Physicists detail the structures and transformations of minerals in regions deep inside the planet

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Going to the Moon, which is almost 400,000 kilometers away, or sending satellites to explore other planets may seem harder than investigating the Earth's interior. Earth is only 12,000 km in diameter, but boreholes have only reached 12 km deep, hardly penetrating the crust, the outer layer of the Earth just beneath the surface. Because scientists cannot directly examine the interior of the planet, they are using computer simulations to understand how minerals behave and transform in the deepest layers of the Earth, where pressures and temperatures are much higher than those on the surface. Computations have identified minerals formed thousands of kilometers below the surface, and there may be a volume of water larger than an ocean dispersed in the thick mass of rocks under our feet.

Brazilian physicist Renata Wentzcovitch, a professor at the University of Minnesota in the United States, is responsible for fundamental discoveries about the interior of the planet. Since 1990, she has been developing analytical and computational methods to model deep-Earth structure and processes, especially in the lower mantle, the largest layer of the Earth. The lower mantle is a 2,200 km thick layer and much less understood than the other layers of the mantle (*see infographics below on the layers of the Earth's interior*). In 1993, she shed light on the atomic structure of perovskite at high pressures. Perovskite is the most abundant mineral in the lower mantle (~75% vol) and its properties are essentially responsible for the properties of this large layer still not well understood.

In 2004, Wentzcovitch and her team identified post-perovskite, a mineral that results from the transformation of perovskite under pressures thousands of times greater than those on the surface. Their results helped explain the speed of seismic waves throughout the deepest part of the mantle. Seismic wave speeds depend on the density and elastic properties of rocks they travel through and three dimensional velocity maps are widely-used for investigating the nature of Earth's interior. New studies by Wentzcovitch and her team have now indicated that post-perovskite tends to break down into elementary oxides, such as magnesium oxide and silicon oxide when pressure and temperature increase way beyond those reached in the Earth's interior, as those found in the interior of giant planets Jupiter, Saturn, Uranus, and Neptune.

"We have powerful computational tools for discovering the mineralogical make up of planetary interiors", she says. According to Wentzcovitch, the techniques she pioneered can forecast the behavior of complex crystalline structures, such as those of silicate perovskite with 20 atoms per unit cell. "The crystalline structure of minerals change with depth in the Earth's mantle but its chemical composition seems to be uniform, except perhaps in the deepest regions of the mantle above the core mantle boundary."

This kind of research helps us to understand how minerals deep in the Earth become denser and harder. Pressure and temperature increase with depth, so we expect the greatest density in the Earth's center. Research has shown the Earth's core is a layered mass of iron, the outer part being liquid while the inner is solid. Temperatures in the core are close to 6,000°C and density there is almost 13 grams per cubic centimeter, twice greater than the density of iron on the surface.

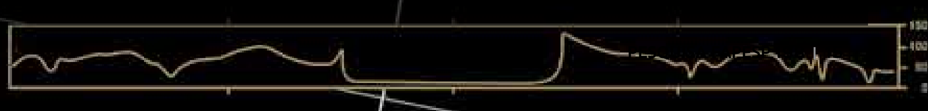
Without resorting to fiction, physicists, geophysicists, and geochemists are opening up the planet and expanding our knowledge about the compacted, rocky region below 600 km. Laboratory experiments have helped us understand the upper layers, the upper mantle, down to 410 km depth, and the transition zone, from 410 km to ~ 660 km. However, much less is known about the Earth below the transition region. Scientists are now making extensive use of computer simulations of rock properties, seismic wave propagation, and geodynamic flow in the Earth in addition to laboratory experiments and geological surveys to understand Earth's interior structure and processes and perhaps one day predict surface processes such as earthquakes and tsunamis.

SUBMERGED OCEANS

New facts are emerging that are calling into question the image of the interior of the planet as a sequence of regular, onion-like layers. In 2003, detailed global surveys began to show irregularities in the thickness of the crust. It varies between 20 and 68 km, leaving the thinner regions more subject to earthquakes and the thicker ones to collapse.

"We began to see the interaction of the crust and the region of the mantle closer to the surface," commented geophysicist Walter Mooney of the United States Geological Survey (USGS) at the "Frontiers in Earth Science" meeting that was held in June at the University of São Paulo (USP). Geophysicists are reexamining the possible consequences of two phenomena that occur within the crust. The first is the diving of tectonic plates (movable and rigid pieces of the lithosphere, the surface layer that includes the outermost region of the mantle) into deeper regions of the mantle, increasing the risk of earth tremors in the regions where they occur. The data confirm the conclusions of a recent study coordinated by Marcelo Assumpção, a professor at the Institute of Astronomy, Geophysics and Atmospheric Sciences (IAG) at USP. Assumpção, in collaboration with researchers from the University of Brasília, found that earth tremors in Brazil occur most frequently in regions where the crust and the lithosphere are thinner and, therefore, more fragile.

The entry of water into the lithosphere, below the crust, is another phenomenon being detailed. This phenome-



non is intriguing: water cannot be stored in the lower crust because the pressure caused by the layers of rock and the temperature (almost 205°C) would cause the water to quickly evaporate. In fact, what is present in the Earth's interior is not exactly water but the components of the water molecule—hydrogen and oxygen—linked to the crystalline structure of minerals in the form of H_2O or OH.

Mooney and his team detected an intense aquatic intromission in regions of the Andes, where the crust is as much as 65 km thick, but they were unable to explain why. Speaking to colleagues from various countries at USP, Mooney asked, "Where is this water stored? What is the volume of the water? Perhaps," he noted, "the water comes from tectonic plates that sink or separate." The specialists have determined that the lithosphere without water is geologically older, whereas the hydrated lithosphere is more recent, indicating that hydration may contribute to the formation or transformation of the outer layers or even of the deeper mantle, closer to the core.

Water molecules are important because, "even in minute proportions, such as 0.1%, they can change the viscosity of materials and therefore the view of the circulation of matter and energy in the interior of the Earth," comments physicist João Francisco Justo Filho, a professor at USP's Polytechnic School who has been working with Renata Wentzcovitch since 2007. "A great amount of water may be hidden in the lower mantle in minerals," says geochemist Francis Albarède, from the Lyon *École Normale Superieure*, in France. "Perhaps the equivalent of a whole ocean," he adds. Or "perhaps several oceans" ponders Wentzcovitch. Using computational methods, she began to examine the possibilities of two atoms of hydrogen substituting for the magnesium linked to oxygen and forming units of H_2O. "The more we looked, the more we found defects in the crystalline structures, where the hydrogen could enter," she says. The problem is that it is not known how much hydrogen may be stored in the mantle.

Lower down, the uncertainties increase, given the impossibility of accurately measuring what happens at depths of 6,000 km. Little is known about the composition of the Earth's core, which is so dense as to concentrate

The interior of the Earth may house a volume of water equivalent to several oceans that is present in the form of H_2O molecules and OH ions dispersed in the midst of the mass of rocks

30% of the planet's mass in two regions: one external, which is molten, and the other internal, which is solid and where the temperature may exceed 6,000°C. A team from University College London used the same conceptual approach as the group from Minnesota, density functional theory, to estimate the intensity of the heat flow that comes from the boundary region between the core and the mantle, based on the amount of iron, oxygen, sulfur and silicon as suggested by the speed of the seismic waves that cross the core and by the flow of heat from the lower mantle. The results, published in May in *Nature*, indicate that the heat flow that emanates from the core must be two or three times greater than previously estimated. Where this energy goes, no one can yet say.

MINERAL DECOMPOSITION

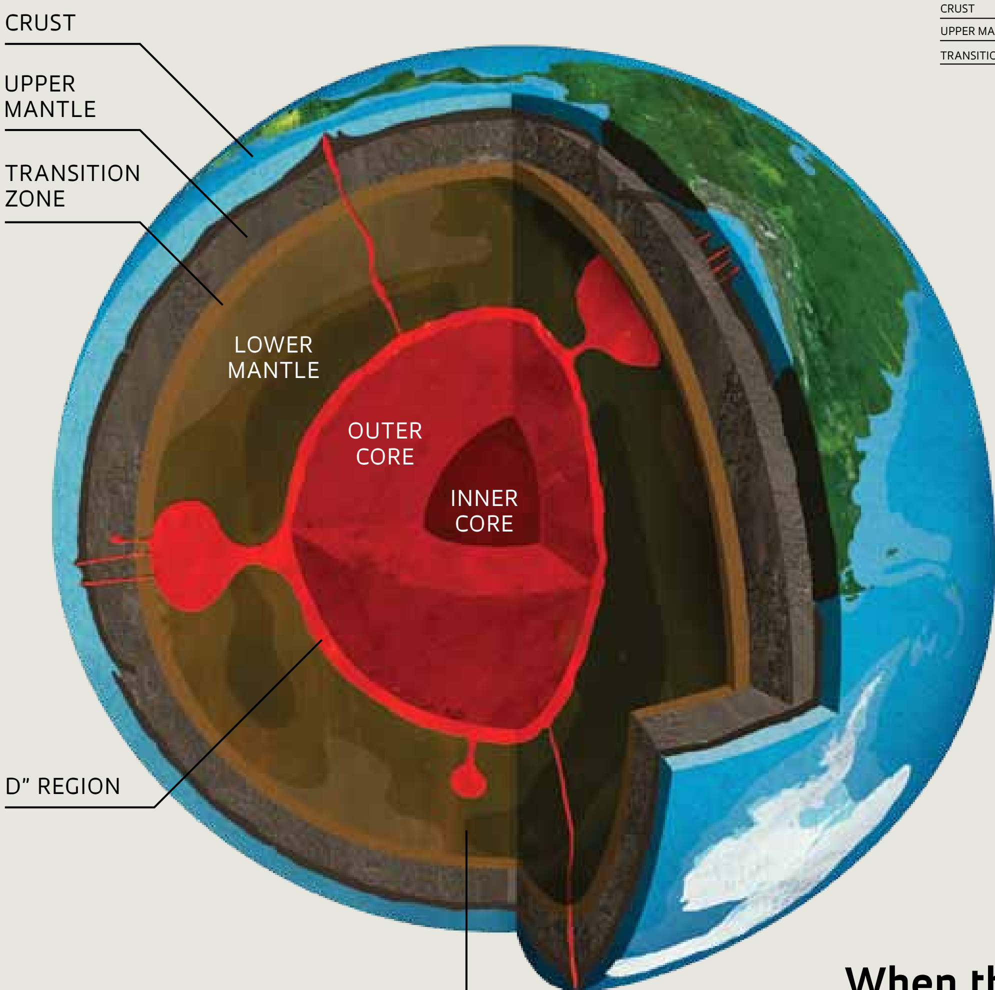
Many ongoing studies are concentrating on the mantle, a thick, solid, slightly flexible layer that deforms very slowly, like pitch. Only rarely, when magma emerges from volcanoes, bringing material from the mantle, are studies carried out indirectly, by monitoring the speed of the seismic waves, because it is difficult to directly study what happens in the mantle. The Japanese want to beat the current 12 km drilling record and reach the mantle by using a ship with a drill similar to an oil drill. The mission, announced in July in *New Scientist*, will not be easy: the material for the drill bits to be used for drilling through the crust and reaching the mantle has to resist pressures 2,000 times greater than on the surface, as well as temperatures close to 900°C, a task similar to the plan to extract oil from the pre-salt layer off the coast of São Paulo.

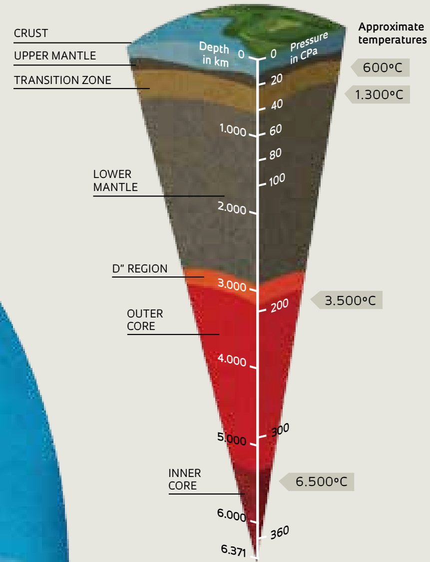
"I cook rocks to understand how they were formed," says geologist Guilherme Mallmann, a researcher from the Institute of Geosciences at USP, who has adopted another method for getting to know the interior of the planet better. He submits the chemical components that constitute the minerals to high pressures and temperatures in the laboratory. Furnaces and presses like the ones he uses, however, only allow him to reproduce phenomena that take place up to 150 km down, the region of the upper mantle in which the magma that sometimes emerges via volcanoes is formed. The pressure conditions at a greater depth in the Earth's interior may also be achieved experimentally, according to Mallmann, but it is far more difficult. Because pressure is the result of the force on an area, the volume of material analyzed would have to be greatly reduced to achieve these extremely high pressures. "Producing greater pressures is often unfeasible."

Perovskite, named in honor of Russian mineralogist Lev Perovski, is formed in environments under high pressures and temperatures, which in the lower mantle may vary from 23 to 135 gigapascals (1 gigapascal is approximately 10,000 times greater than the pressure on the Earth's surface) and 2,000°C to 4,000°C, respectively. Wentzcovitch presented the crystalline structure of this mineral (a silicate of magnesium and iron) in 1993 in *Physical Review Letters* using green and yellow rhombuses reminiscent of the Brazilian flag. The reason was simple: "I miss the country," says the researcher, who lives in the twin cities of Minneapolis-Saint Paul, which have 2.5 million inhabitants and are close to the border with Canada, where the temperatures in winter can remain at - 20°C for weeks at a time.

A press under our feet

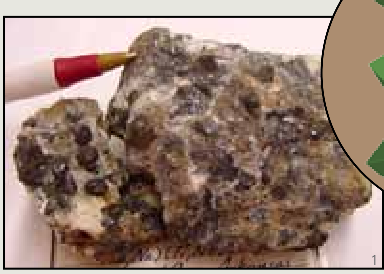
Minerals in the interior of the planet lose their elasticity and become denser as the pressure and temperature increase

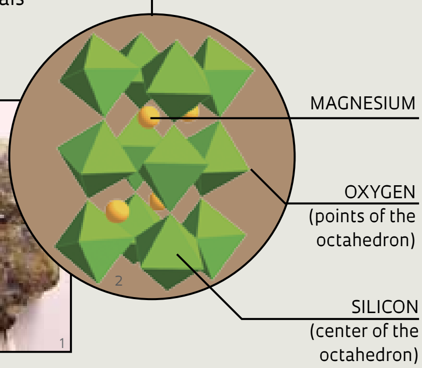




Perovskite in transformation

High pressures and temperatures modify the most abundant minerals in the lower mantle

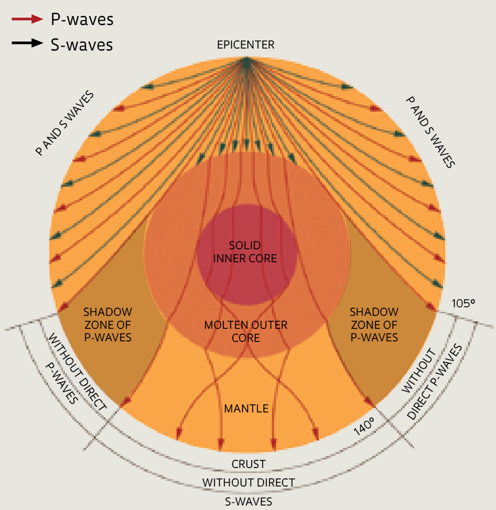




Perovskite is transformed into post-perovskite in the Earth's interior and eventually decomposes into simple oxides in the regions closest to the core of giant planets in the Solar System

When the Earth shakes

Earthquakes generate two types of waves, P and S. P-waves cross the entire Earth, whereas S-waves die when they reach the outer core. The path of the wave depends on the properties of the materials it crosses



INFOGRAPHICS DRUM IMAGES 1 ANDREW SILVER / USGS 2 RENATA WENTZCOWITCH SOURCE UNIVERSITY OF YORK

In collaboration with physicists from Italy and Brazil, Wentzcovitch found that the iron atoms of a mineral called ferropericlase, the second most abundant mineral in the lower mantle, lose one of their magnetism, thus explaining a phenomenon that has been observed in the laboratory. In 2007, João Justo worked in Minnesota with Wentzcovitch and developed a series of equations that establish the change in elastic properties and seismic speeds during the loss of magnetism in ferropericlase.

"The size of the iron atom decreases when it loses the magnetic moment, and this is what makes the ferropericlase denser. Furthermore, minerals with iron soften during the slow densification process, as has already been observed in the laboratory, but has not yet been explained," says Justo. This is a surprising phenomenon because the material normally becomes harder as it becomes denser.

The results that he and Wentzcovitch obtained were published in 2009 in the journal *PNAS*. Their results explained the loss of magnetism under pressures and temperatures equivalent to those in the lower mantle, which James Badro, from the Universities of Paris 6 and 7, had detected in the laboratory and reported in *Science* in 2003 and 2004. Experimental verification of this phenomenon, one of the great discoveries of geophysics in the last few years, indicated that the proportion of non-magnetic iron may increase with depth. What is more, the deeper layers of the lower mantle may be even denser than the shallower layers.

Views of the Earth

ATHANASIUS KIRCHER
1665

HANS KRAMER
1902

Under very high pressures, iron atoms lose one of their remarkable characteristics, their magnetism, and become more compact

THE JOURNEY

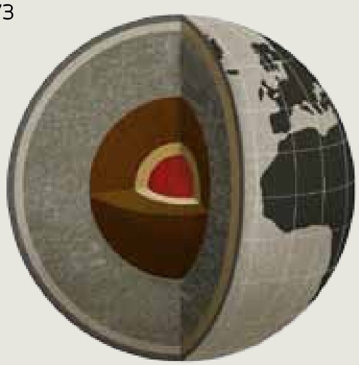
As a child, Renata Wentzcovitch enjoyed the math tests that her grandfather, Adolfo Foffano, used to give her every day when they were together during her end-of-year vacations in Sumaré, in the State of São Paulo. She studied physics at the University of São Paulo and then began studying at the University of California at Berkeley in the United States in 1983, on the recommendation of José Roberto Leite and Cylon Gonçalves da Silva.

Wentzcovitch's journey included a stay in Cambridge, in the UK, and London from 1990 until 1992 after she had broadened the applicability of her material simulation techniques. Her new techniques were so general that they served to study the atomic movement and transformations of crystalline structures at high pressures and temperatures. To do this, she used so-called first-principles calculations, based on the density functional theory, whose essence is simple: the total energy of a group of electrons in their state of equilibrium depends on the total electron density.

Her hard work eventually paid off. "In less than a month, using my techniques, I'd solved the structure of magnesium silicate at high pressure, which researchers at Cambridge had been working on for two years," she says. Solving a structure, she explains, "means identifying the position of equilibrium and the degrees of freedom of a crystalline structure with a certain symmetry that minimize the internal energy." Until then, it was only possible to easily determine structures such as that of diamond, which is formed by two atoms at the base and has a degree of freedom that is reflected in the distance between the carbon atoms. The structure of perovskite has 20 silicon, magnesium and oxygen atoms and 10 degrees of freedom. "It is much more complex than the structure of semiconductors, and that's why its behavior at high pressures was unknown until then," she says.

In the beginning, one of her problems was that she was unable to check her theoretical forecasts experimentally. However, in 2003, while working with researchers from the Tokyo Institute of Technology, Wentzcovitch and her team from Minnesota analyzed the spectrum of X-rays, which differed greatly from what was expected at very high pressures. They concluded that a phase transformation had occurred (or a change in the crystalline structure) to an unknown structure. "At first I didn't believe it," she says, "because perovskite seemed so stable!" The following year,

BRUCE BOLT
1973



ADAM DZIEWONSKI
1990

an article in *Science* presented the new crystalline structure, christened post-perovskite. Today, post-perovskite is recognized as the most abundant material in the region of the mantle known as D”, which is in contact with the outermost layer of the Earth’s core. “Post-perovskite explains many geophysical characteristics of this region of the Earth,” observed Mallmann, from USP.

Post-perovskite has a layered structure, through which seismic waves travel at speeds that depend on their initial direction. This work reinforced the conclusion of other studies that had indicated that this mineral could be formed at different depths in the lower mantle.

In a report published in *Science* on March 24, 2004, physicist Surendra Saxena, from the International University of Florida, challenged the conclusions and said that he still believed that perovskite decomposes only in those regions of the mantle closest to the core, and he reiterated that the theory was still not perfect. Subsequent studies on the propagation of seismic waves, however, seem to confirm the presence of post-perovskite in region D”. “We’ve been very lucky,” Wentzcovitch commented. “The results of the computational calculations of speeds in post-perovskite are surprising because they reproduce many seismological observations of D” inexplicable until then. It can’t be mere coincidence.”

It was also in 2004, when this work began to circulate, that Wentzcovitch received funding of US$ 3 million from the National Science Foundation of the United States to assemble the Virtual Laboratory of Planetary and Earth Materials (VLab) at the Supercomputing Institute of the University of Minnesota. The VLab brought together chemists, physicists, computational scientists, geophysicists and mathematicians who, motivated by the possible existence of post-perovskite on other planets, began to look at the probable transformations that minerals could undergo at even higher pressures and temperatures inside the giant planets in the solar system (Jupiter, Saturn, Uranus and Neptune), which have masses at least 10 times greater than that of the Earth.

The results of her group, like those detailed in *Science* in 2006, presenting the probable transformations of magnesium silicate in the giant planets closest to Earth, indicated that these calculation techniques might be useful for studying the evolution of planets. “The behavior patterns of minerals on different planets cannot be just a coincidence,” she commented to an audience that listened attentively to her during the seminar at USP.

Simulations of the behavior of materials at great depths and experimental studies, principally when they coincide, help clarify phenomena in the interior of the Earth. In July, French researchers announced that they had managed to re-create the environmental conditions at the limit of the outer core and lower mantle in the laboratory. They showed, by means of X-ray analyses, that partially molten rocks, when submitted to high temperatures and pressures, may move toward the surface of the Earth, giving rise to volcanic islands, such as those of Hawaii.

A MORE REAL EARTH

The new information about the interior of the planet is being used in the work of Brazilian research groups in basic geophysics at São Paulo, Rio de Janeiro, Rio Grande do Norte and the Federal District who are focusing on examining the Earth on a large scale. More broadly, this information is useful to the applied geophysics teams that are working with oil, mining and underground water in Bahia, Pará, Rio, São Paulo, Rio Grande do Norte, the Federal District and Rio Grande do Sul.

Taken together, the results help construct a more solid picture of the Earth, which has been represented in many ways over the past few centuries. Knowledge of the structure of the Earth’s interior has greatly advanced since 1912, when German geophysicist Alfred Wegener concluded that the Earth is likely formed of rigid plates that move, and our understanding is moving increasingly farther away from the poetic images of *Journey to the Center of the Earth*, the magnificent work by French writer Jules Verne, published in 1864. “Today, we know that the center of the Earth, unlike the version described by Jules Verne,” Justo guarantees, “is absolutely mysterious and certainly uninhabitable.” “But that’s no reason for our planet to be any less fascinating,” says Assumpção. ■

The Project

Simulation and modeling of minerals at high pressures no. 09/14082-3 **Modality** Thematic Project **Coordinator** João Francisco Justo Filho – USP **Investment** R$ 184,378.73

Scientific articles

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