INTERVIEW

Earth science gets to the core

Some 20 years ago, Prof. G David Price was one of the first to establish the now major field of computational mineral physics. He combines experiment, theory and modelling to tackle major deep Earth science problems. He is vice-provost for research and professor of mineral physics at UCL. David Smith quizzed him on behalf of *Physics Education*.


David Price, vice-provost for research at UCL.

DS: How did you become an Earth scientist?

GDP: I did natural sciences at Cambridge and I still think that a natural-sciences-type degree is the best kind that you can do because it makes you look beyond traditional A-level training. I'm afraid that I decided that I didn't want to be a physicist (because I knew that I wasn't actually good enough to do physics) so I did chemistry, with an option in crystalline materials, and geology.

What really began to fascinate me was condensed-matter physics. I tried to pursue that through chemistry, mineralogy and crystallography but in those days Cambridge was renowned for being 'wet and windy'—in other words, gases and liquids were as far as you went. It was before the days of Sir John Meurig Thomas, who really established solid-state chemistry there, so I ended up doing my final-year courses in mineralogy and petrology. I then did my PhD in what would now be called nanotechnology, on the microstructure of iron titanium oxides.

Why iron titanium oxides?

They are interesting from an Earth sciences point of view because they carry the remnant magnetic signal that gives rise to the magnetic striping of the ocean floor, on which plate tectonics is based. I was looking at what happens to these things in slowly cooled environments. They have a phase separation and you get this beautiful microstructure that you can only see with transmission electron microscopy (TEM) because it's suboptical.

Halfway through my PhD, one of my undergraduate lecturers went to a meeting in which it was claimed that a mineral called ringwoodite (a material that we now know makes up the Earth at a depth of about 550–670 km) had been discovered in a meteorite. Some PhD student in Harvard—a brilliant chap called Ray Jeanloz who's since become a major national adviser to the US government—tried to discredit this. So that was what started me looking at high-pressure minerals, because ringwoodite is only formed at pressures of more than 12 GPa, such as in a shocked meteorite that crashed into another body in space.

How did this lead to computational mineral physics?

What drove me to that was discovering what happens to these materials at high pressures and temperatures. When I was doing the TEM work on ringwoodite, I discovered a mineral called wadsleyite (which we now know makes up the Earth at a depth of 400–550 km). It turns out that these two minerals are polytypes, which is to say that they're the same basic structure but they have slightly different stacking sequences of their structural units.

You can map a lot of these crystal stuctures onto Ising spin models so that, for instance, ringwoodite can be mapped onto a spin-up-spin-down antiferromagnetic structure, whereas wadsleyite maps onto a two-spins-up-two-spins-down structure.

I wondered what it is that determines which sequence is stable under high pressure and temperature conditions. I started getting interested in what it is about atomic structures that determines the free energies of materials in pressure and temperature space, and the only way of making the link between the atomic and the thermodynamic is through interatomic interactions. Today we use quantum mechanics, but in the 1980s we would describe the factors that determined the crystal structure in terms of electrostatics and repulsion, and they were amenable to computer simulation, though a calculation that would take 50 min using the whole mainframe computer back then can be completed in 0.5 s on my laptop today.

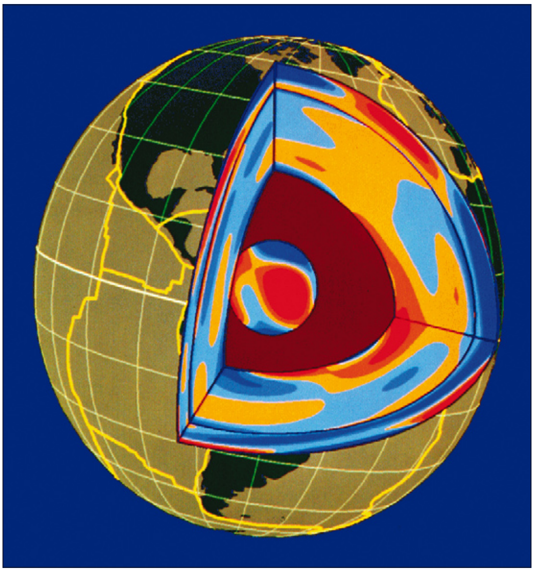
I find it intriguing that quantum mechanics can be applied to the Earth

Well, Kohn and Pople got the Nobel Prize a few years ago for their innovation in density functional theory, which enables you to solve Schrödinger's equation to arbitrary levels of precision by saying that the energy of the system depends on the effective electron density distribution in it. Density functional theory is really the key now to most condensed-matter physics calculations, the other important thing being the entropy or temperature dependence. You get that by calculating the vibrational modes of a lattice—which depends on the curvature of the potential energy well and its depth—and the first derivative of the potential energy defines the density. So if you have the potential energy as a function of geometry, you get all of the parameters that you need to determine the free energy of a system, and if you can determine that, you can produce a phase diagram.

The only information we have about the interior of the Earth comes from seismology, and the speed of sound waves depends on two things: the density and the bulk modulus. The latter also depends on the curvature of the potential energy well, while the former depends on the first derivative. So once you've got the potential energy function you've got the physical properties that seismology measures.

It must be quite frustrating not to have more ways of testing your ideas

You can in the movies; remember *The Core*? The deepest drill hole on Earth is about 15 km but we sample material from deeper than that from volcanic inclusions that are brought to the surface. So we have a pretty good idea of what the chemistry of the Earth is down to depths of 200–300 km.



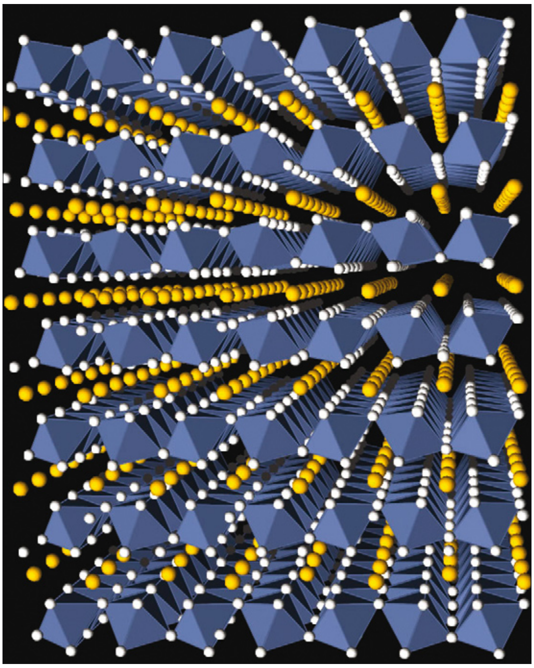
Tomographic image of the Earth's interior, showing in red the seismically slow (relatively hotter) and in blue the seismically fast (relatively colder) regions of the mantle and inner core.

Since the beginning of the 20th century we've had quite a clear understanding of the seismic structure of the Earth's interior, in other words the density, elastic moduli and pressure. The two things that are less well constrained are the temperature structure and the atomic arrangements, and this is where experiment and observation move hand in hand. In the laboratory it's now possible to reach pressures above 1 million atmospheres routinely, with diamond anvil cells, for example.

What sort of pressures do you need to recreate?

The pressure in the centre of the Earth is 3.6 million atmospheres. We can reach those sorts of pressures, though not routinely, by firing hypersonic missiles at targets. We are now able to recognize, through a series of experiments, that there are phase transformations inside the Earth that are associated with observed discontinuities in the sound-wave velocity.

There are three divisions in the outer part of the



The crustal structure of the 'post-perovskite phase', recently discovered and now thought to make up the deepest part of the Earth's mantle, at a depth of ~2600 km beneath the surface [1].

Earth: the upper mantle, which goes down to a depth of 400 km; the transition zone, which goes from 400 km to 670 km, where the wadsleyite and ringwoodite phases exist; and then beyond about 670 km is what's called the lower mantle, which is a two-phase assembly of a magnesium silicate perovskite structure plus magnesium oxide. We've been able to make some of these things and measure their physical properties approximately. The trouble is that magnesium silicate perovskite requires something like 0.25 million atmospheres to become stable. You can investigate materials under those conditions, but only a pinhead's worth, and that makes measuring its physical properties exactly quite challenging.

The role of computational mineral physics now, therefore, is to ground-truth our observations and then use quantum mechanics to go beyond the realms of experiment. Using HPCx, which is the national supercomputer, it might require 12 hours using 256 nodes to simulate a picosecond of real time. But thermodynamics is a very, very forgiving thing and you can get good statistical averages quite effectively, so after just three days of supercomputer time you can get a data point.

This procedure enables us to work out what the physical properties of the Earth's materials are at pressures and temperatures that are beyond experiment, but with the confidence that we can do it with the same uncertainty as we have under ambient or experimental conditions.

Are there any big outstanding questions?

The really big question about the Earth is its thermal structure, because that would tell us something about the evolution of our planet, in terms of knowing how much energy was in there to start with and how it has evolved over 4.5 billion years. Kelvin, if you remember, proved quite effectively—and quite devastatingly to Earth scientists—that the Earth couldn't be any more than 100–120 million years old, by solving the heat-flow equation for a crystallizing liquid. That was a huge challenge to Darwinian thinking until Rutherford gave his discourse at the Royal Institution, where he very cleverly gave Kelvin the credit for anticipating the errors in his own calculation by saying: 'unless another heat source is identified…'. Understanding the thermal structure of the Earth is vital if you want to develop models for the Earth's magnetic field, mantle convection or tectonic processes.

Another big question is about the details of the Earth's structure. Imagine trying to make sense of an antenatal ultrasound scan if you didn't know what the internal structure of the human body was. That's how seismology is and it's why it's such an exciting subject. I've got a friend who works in the City who says that they prefer to employ Earth scientists over physicists or chemists because Earth scientists are trained to make decisions based on inadequate data. You have to use your knowledge to synthesize things much more and that's why I'm very happy to be a geophysicist and not a particle physicist.

Can you get any clues about the Earth's structure from the rest of the solar system?

The fascinating thing about the Earth is that it's the one and only of its kind. Plate tectonics turns out to be unique. So the real question is: 'Why is the Earth so different from the other planets?' Which leads to the interesting question: 'What is the role of free water on the surface of the Earth?' It probably plays some vital part in changing the mechanical properties of rocks, which perhaps enables plate-tectonic processes to occur.

You can push that further back and ask: ‘Why do we have water on Earth?’ The answer is: ‘Because we have life on Earth.’ So you end up with this fascinating conjecture that the entire mechanical evolution of the Earth is determined by the fact that life formed early enough to stabilize the hydrosphere, which enables plate tectonics to occur.

Work I’ve done with colleagues also shows that plate tectonics is essential for having determined the rate of extraction of energy out of the Earth to maintain its magnetic field. So the Earth’s strong magnetic field, which again is unique in the inner solar system, is there because of life, which is quite interesting. We often think that the Earth evolved in a gaiaesque fashion and that life is passively responding to it, but maybe life has been actively involved in the physical evolution of the planet. We might have a very rare planet indeed and there may not be a plethora of Earth-like systems out there.

Should we, then, be looking for magnetic fields as a sign of possible life on other planets?

Yes, I think so. Exobiology, or exoplanet studies, is very important and I really look forward to the time when astronomy will be able to resolve terrestrial as opposed to Jupiter-like planets. However, there is this very strong argument that you won’t find the combination of circumstances that we have on Earth anywhere else. We are in a ‘habitable zone’ but we also have orbital stability because of the Moon and we have Jupiter riding shotgun for the outer solar system, soaking up the Shoemaker–Levy-like impacts. We’ve got the right balance between a stable environment that will enable evolution to occur over periods of millions of years, plus punctuated catastrophes. I mean if you didn’t have the mass extinctions that we had in the Ordovician period, at the end of the PermoTriassic period and at the end of the Cretaceous period, then you wouldn’t have had the slight resetting of the evolutionary clock that eventually led to the mammals.

There’s a very good book by Simon Conway Morris called *Life’s Solution: Inevitable Humans in a Lonely Universe*, in which he showed that, because of convergence in evolution, there are certain things that are inevitable. But to get mammals you had to have the extinction of the dinosaurs, and to get dinosaurs you had to have the extinction of the tetrapods, and that wouldn’t have happened without something that took out top competitors.

Are we clear what that was?

Well, there are up to five schools of thought, so the answer is: ‘Maybe.’ The classical geological view has always blamed climate change, but the cretaceous/tertiary boundary seems to be quite closely related to an impact, and that’s the classic Chicxulub case. Then there are other events called large igneous provinces that correlate with extinction events very well, plus at the same time as the impact off the Yucatan there was in India a volcanic eruption that gave rise to the Deccan Traps, which covered an area from north India through to Burma in volcanic eruptives that included something of the order of 10 million cubic kilometres of basalt in less than a million years. At the moment the rate of eruption over the entire planet is a fraction of that, so to have that all in one place produced vast outpourings of CO_2 and SO_2 and major climatic changes.

My own view is that a lot of extinction events were caused by cataclysmic volcanic eruptions. In fact there is a school of thought that suggests that those were triggered by massive impacts. The Siberian Traps in central Russia date to 251 million years ago, which is exactly the date of the end of the Permian period, famously described as ‘the day the Earth nearly died’ because more than 95% of species became extinct.

You mentioned ‘magnetic striping’ at the start of the interview. I seem to recall you once said that another ‘flip’ was around the corner.

Prove me wrong! There’s no evidence to suggest that advanced cellular bodies require a stable magnetic field, and we have periodically had hundreds of reversals or near-reversals in the last 500 or 600 million years. Most animals would be damaged by the flux of the solar wind, but that’s a relatively long-integrated experience relative to their lifespan. Humans could live through a reversal period, but one’s life expectancy might be reduced to, say, 25 years because of the triggering of skin cancer.

One interesting idea is that magnetic field reversals are correlated to periods of speciation because genetic damage, which would be stimulated by exposure to the solar wind, could give rise to mutations that could be both beneficial and detrimental. It remains to be shown whether it is significant or otherwise that the development of large cranial capacity hominids, dated to the best of our ability to 780 000 years ago, corresponds to the last significant magnetic field reversal.

Do we understand why the reversals take place?

It’s a chaotic process. Magnetohydrodynamics is quite a challenging branch of mathematics. I think Einstein is quoted as saying that it’s the most challenging problem in physics, so he moved on to a grand unified theory because he thought that was relatively easy! It’s a problem because you have to solve simultaneously something like 15 coupled partial differential equations. To model climate at all accurately you need to divide 10 km of atmosphere and 2 km of ocean across the Earth’s surface into 1 km voxels, but the outer core of the Earth (where convective flow takes place) is 2000 km deep—a calculation that is just beyond the realms of computing today and probably still will be in 20 years’ time. The outer core has a viscosity similar to that of water, but we can only treat it like cold bitumen.

If you were to discover a new mineral, what would it be called?

Well, I did that and it was called wadsleyite. Ted Ringwood, a very famous Australian experimental petrologist, created a new form of magnesium silicate in the 1960s, but the convention in mineralogy is that you can’t give anything a name until it’s found in nature—and then somebody else found it in a meteorite, so it was called ringwoodite. He had also made a phase called the beta phase and he wrote in a paper that, should anybody find it, it would be nice to call it wadsleyite because his colleague Alan Wadsley was the crystallographer who worked with him. I was the person who found it in nature and I called it wadsleyite.

There is a mineral called priceite that I saw in the Smithsonian museum in Washington. I believe it’s described on the label as ‘an amorphous globular mass’, which I think is an appropriate description of me as well. It’s a borate I think.

Reference

[1] Tsuchiya T, Tsuchiya J, Umemoto K and Wentzcovitch R M 2004 Earth planet *Sci. Lett.* **224** 241