ppv@10

A meeting to celebrate the tenth anniversary of the discovery of ***post-perovskite***

25–27 June 2014

School of Earth Sciences,
University of Bristol

www1.gly.bris.ac.uk/ppv

Image courtesy Paul Statham
www.paulstathamphotography.co.uk

Support

ppv@10 gratefully acknowledges financial support from:

The Mineral Physics Group of the
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The British Geophysical Association
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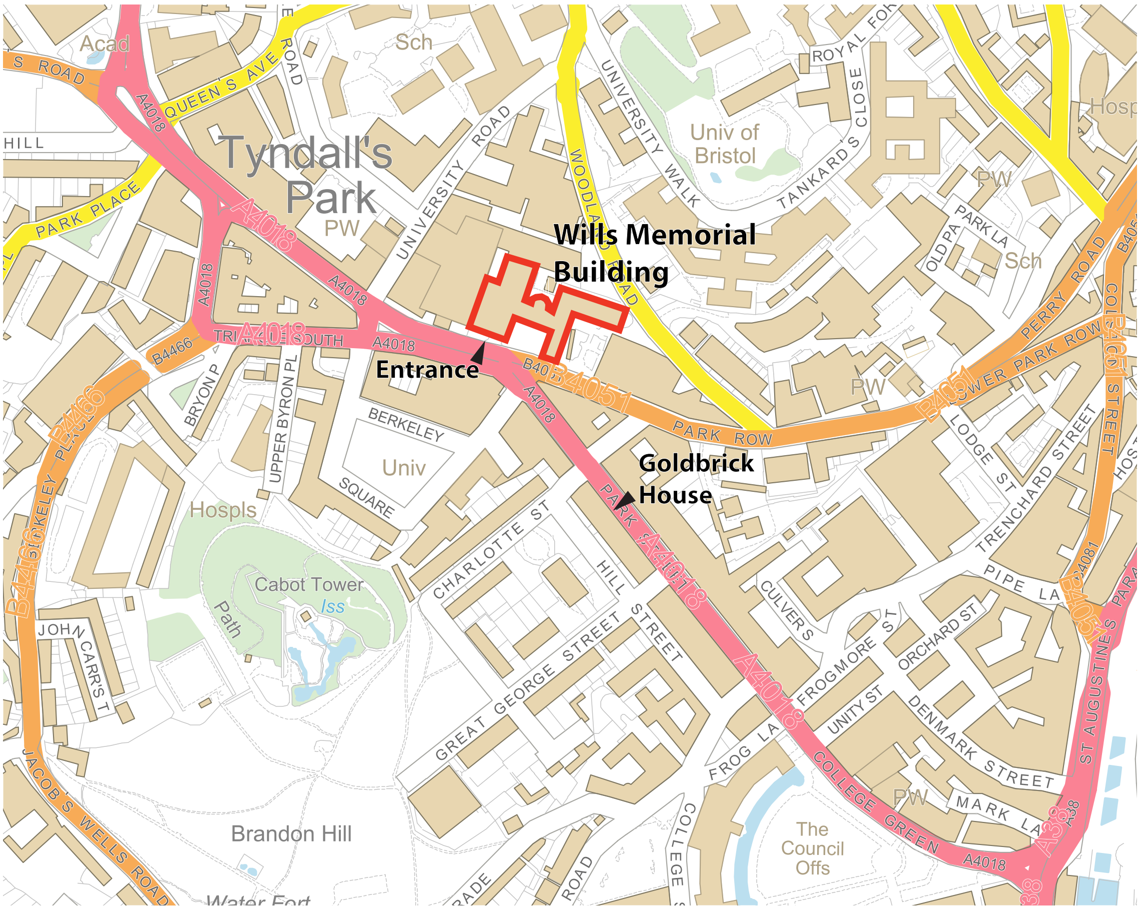
CoMITAC – Core-Mantle Interface: Thermodynamics
And Chemistry (ERC Stg Grant 2009: 240473)

BUMPs – Bristol University Microseismicity ProjectS

Information and programme

Directions and location

The oral and poster sessions, as well as the icebreaker, will be held in the School of Earth Sciences, University of Bristol, in the Wills Memorial Building:



Mapping from OS

Talks will be given the the Reynolds Lecture Theatre, and poster sessions and refreshments will be in G27. Ample wayfinding (i.e., signs) will be present to help you find these places.

Registration

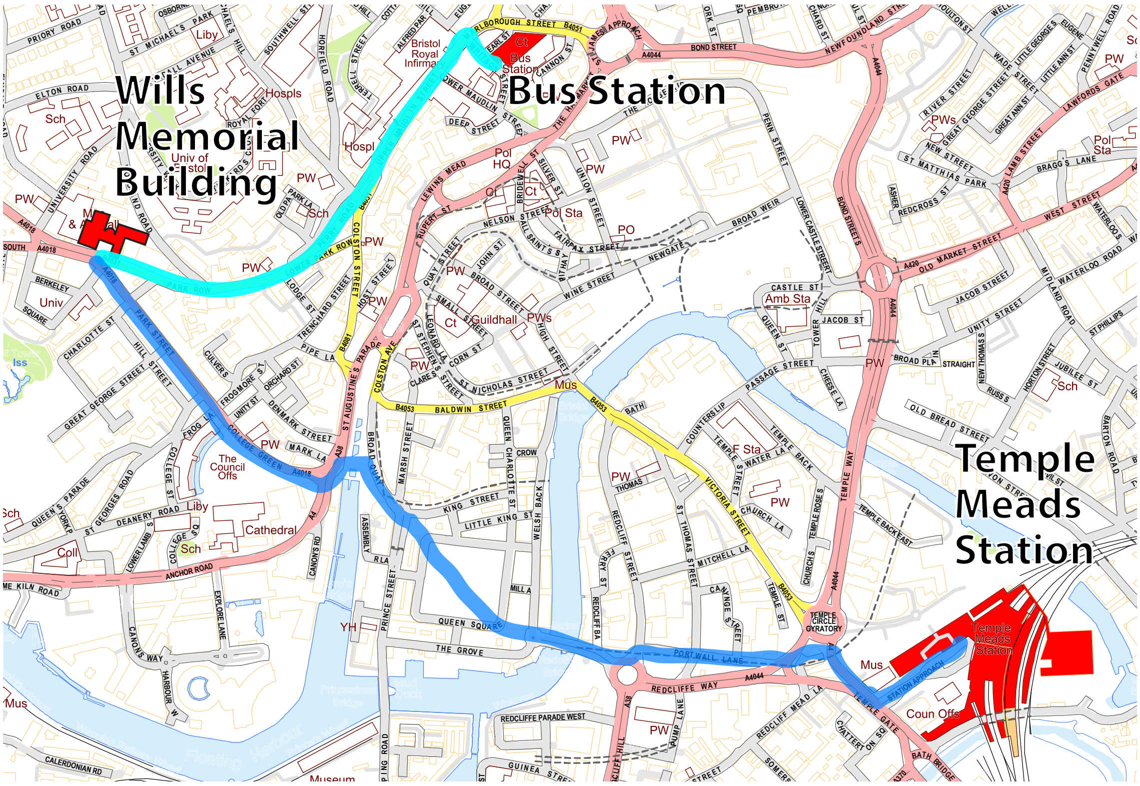
You may register your attendance and pick up your name badge between 16:00 and 18:00 (before or during the icebreaker) in G27, or between 09:30 and 10:00 on Thursday morning. If you arrive later, please get in touch with the committee.

Finding the School of Earth Sciences

The School of Earth Sciences on the ground floor of the Wills Memorial Building, Queen's Road, BS8 1RJ. Those familiar with Bristol may know the Wills Memorial Building as the large neo-gothic tower that dominates the University precinct and hosts Great George, the large bell that can be heard striking each hour. Please use the main entrance to the

Wills Memorial Building underneath the Wills Tower on Queen's Road (opposite the top of Park Street and adjacent to the end of the Triangle). Once inside you should find abundant signage pointing the way to registration for the meeting.

Those not familiar with Bristol may find the following map and instructions useful.



Mapping from OS

If you arrive at the coach station the Wills Memorial Building is a 15 minute walk. In general the best advice is to keep going uphill on Queen's Road in front of the Bristol General Infirmary, then find the Wills Memorial Building on your right just past the junction with Park Street.

The walk from Bristol Temple Meads is longer (about 30 minutes) and requires the safe navigation of some of the city's historic docks. The best walking route involves diagonally crossing Queen's Square at the half way point then climbing Park Street with the Wills tower clearly visible at the top of the hill. Alternatively, a bus (service 8 or 9) or taxi will take you directly to the Wills Memorial Building.

Further travel advice can be found on the University website (`www.bristol.ac.uk`).

Conference dinner

The conference dinner will be at 19:00 on Thursday evening at Goldbrick House, 69 Park Street (see map above). The restaurant is a few minutes' walk (downhill) from the School.

Wireless internet access

Eduroam

Most attendees will be able to access the internet using eduroam, if they are from organisations which are part of the eduroam federation. For details of how to connect, please check your home institution's instructions.

VisitorNet

Attendees who cannot access eduroam can use the University of Bristol's VisitorNet (`wireless.bristol.ac.uk`). Connect to the `Bristol-VisitorNet` wireless network and use the username and password provided on the reverse of your name badge.

Schedule

Wednesday 25

16:00 – 17:00	Registration
17:00 – 18:00	Ice breaker (registration continues)

Thursday 26

09:30 – 10:00	Registration
10:00 – 12:20	**Session 1: The discovery of post-perovskite and implictions for geophysics** *Convenor: John Brodholt*
10:00 – 10:05	Introductory remarks
10:05 – 10:45	Kei Hirose: *The discovery of post-perovskite and its unique physical property*
10:45 – 11:15	Coffee
11:15 – 11:40	Dan Shim: *The post-perovskite transition and deep mantle structures*
11:40 – 12:05	Stephen Stackhouse *Post-perovskite at ten years: theoretical insights into its physical properties*
12:05 – 12:20	*Discussion*
12:20 – 13:30	Lunch
13:30 – 15:00	**Session 2: Composition, structure and dynamics of the lowermost mantle** *Convenor: James Wookey*
13:30 – 13:55	Saskia Goes: *The deep mantle large low shear-velocity provinces – largely thermal features?*
13:55 – 14:20	Ron Cohen: *Is PPV the last mantle phase transition?*
14:20 – 14:35	*Discussion*
14:45 – 17:00	**Poster session 1**
(16:00 – 17:00)	*(School of Earth Sciences Seminar: Joanna Morgan (Imperial): High-resolution seismic imaging using 3D full-waveform inversion)* ppv@10 delegates are welcome to attend the School Seminar
15:00 – 15:30	Tea
17:00 – 17:30	Tour of the tower of the Wills Memorial Building
19:00	Conference dinner: Goldbrick House, Park Street

Friday 27

09:00 – 10:40	**Session 3: Seismology of the lowermost mantle**
	Convenor: Andy Nowacki
09:00 – 09:40	Thorne Lay: *Deep mantle seismic structure related to post-perovskite*
09:40 – 10:05	Sanne Cottaar: *The rôle of post-perovskite in explaining observations of seismic anisotropy*
10:05 – 10:30	Christine Thomas: *Are seismic structures in the lower mantle due to post-perovskite?*
10:30 – 10:40	*Discussion*
10:40 – 11:10	Coffee
10:40 – 12:20	**Poster session 2**
12:30 – 13:30	Lunch
13:30 – 15:00	**Session 4: The physical properties of post-perovskite**
	Convenor: Andrew Walker
13:30 – 13:55	David Dobson: *What can analogue studies tell us about post-perovskite?*
13:55 – 14:20	Sébastien Merkel: *Anisotropy, textures, and slip systems in post-perovskite: experimental approach*
14:20 – 14:45	Patrick Cordier: *Modelling dislocations and plasticity in high-pressure polymorphs of* $MgSiO_3$
14:45 – 15:00	*Discussion*
15:00 – 15:30	Tea
15:30 – 17:00	**Session 5: Implications and unresolved questions**
	Convenor: Geoff Bromiley
15:30 – 15:55	Arwen Deuss: *What do normal modes tell us about the lowermost mantle and post-perovskite?*
15:55 – 16:20	James Wookey: *Linking the dynamics of the lowermost mantle to observations of seismic anisotropy*
16:20 – 16:45	John Hernlund: *Post-perovskite: Past, present, future*
16:45 – 17:00	*Discussion*

Invited oral abstracts

The discovery of post-perovskite and its unique physical property

Kei Hirose (Earth-Life Science Institute (ELSI), Tokyo Institute of Technology; kei@elsi.jp)

Silicate perovskite was first synthesized at 30 GPa based on laser-heated DAC technique by Liu (1974 GRL). Since then, $MgSiO_3$-rich perovskite is known to be a primary constituent in the lower mantle, but a number of seismic anomalies observed in the lowermost mantle are not reconciled with the property of such perovskite phase. Sidorin et al. (1999 Science) suggested a solid-solid phase transition with a positive Clapeyron slope in the lowermost mantle from the correlation between temperature estimated from velocity anomalies and elevation of the observed D″ discontinuity. It was speculative but their proposal of an unknown phase transition in the deep lower mantle has encouraged the development of in-situ XRD measurements in a DAC at relevant high P-T conditions. Indeed, such in-situ measurement was crucially important for the discovery of post-perovskite because it converts into amorphous during decompression and thus cannot be identified at ambient pressure. The phase transition from perovskite to post-perovskite was discovered above 120 GPa by the in-situ XRD measurements using intense synchrotron X-rays and first reported by Murakami et al. (2004 Science), thirty years after the discovery of silicate perovskite. Soon after the discovery of post-perovskite, many people from related fields, not only mineral physics but also seismology and geodynamics, have started to work on post-perovskite and the deep lower mantle. These efforts revealed that the D″ region is an unique layer because of the distinctive property of post-perovskite that is very different from that of perovskite. The high positive Clapeyron slope of the post-perovskite phase transition was first estimated by theoretical calculations (Tsuchiya et al., 2004 EPSL; Oganov and Ono, 2004 Nature), suggesting that it promotes the mantle convection remarkably. Post-perovskite is likely much weaker than perovskite (Hunt et al., 2009 NatureGeo; Ammann et al., 2010 Nature), which further enhances the dynamical activity of the lowermost mantle. The strong lattice preferred orientation is developed in post-perovskite much more easily than in perovskite (Niwa et al., 2007 PCM), which explains the strong seismic anisotropy observed in the D″ region (Miyagi et al., 2010 Science). Experiments also demonstrated that post-perovskite exhibits electrical and thermal conductivity much higher than that of perovskite (Ohta et al., 2008 Science, 2012 EPSL; Hunt et al., 2012 EPSL). On the other hand, inconsistency is often found among DAC experiments performed at deeep lower mantle P-T conditions. The accuracy of pressure determination above $\sim$100 GPa has been always a matter of debate, in particular for high-temperature experiments. Another source of discrepancy is the Soret diffusion during laser heating. The long heating duration in laser-heated DAC experiments does not necessarily attain chemical equilibrium (sample grain size is usually limited only to 100 nm and thus long heating duration is not required for equilibrium) but often causes depletion in iron at the hot spot, in particular when the sample is mixed with a metal powder of laser absorber (Sinmyo and Hirose, 2010 PEPI). The electrical and thermal conductivity is strongly dependent on temperature, but most of the previous DAC measurements of such transport property were limited to room-temperature. We still need more efforts to better understand the unique property of post-perovskite and the lowermost mantle.

The post-perovskite transition and deep mantle structures

S.-H. Dan Shim (Arizona State University; shdshim@asu.edu)
Yu Ye (ASU), Brent Grocholski (Smithsonian)

The discovery of the post-perovskite transition in 2004 has made profound impacts on our views about how the deep mantle works. One of the most important questions addressed by the post-perovskite transition is the relationship between the phase boundary and the D'' seismic discontinuity. However, there remain important questions. Due to the uncertainties in pressure and temperature measurements in the laser-heated diamond-anvil cell, the uncertainty in the depth of the phase transition remains large (∼200 km). Redox conditions in the laser-heated diamond-anvil cell may have large effects on the measured depth of the post-perovskite boundary, but the conditions are poorly constrained. Existing results on how Fe and Al alter the depth and thickness of the post-perovskite transition are inconsistent with each other. The situation is much more complicated when the strong compositional variations (from primordial to recycled compositions) expected for the core-mantle boundary (CMB) region is considered. Mid-oceanic ridge basalt (MORB) transported to the CMB may contain a large amount of free SiO_2 (∼30%) that has a phase transition near the depth of the post-perovskite transition. Furthermore, the high temperature of the CMB region may allow MORB to react with pyrolite (or even primordial materials) to produce distinct chemical heterogeneities. I will report data on the effects of compositional variations and chemical reactions on the post-perovskite boundary, and the uncertainties in the depth and thickness of the post-perovskite boundary.

Post-perovskite at ten years: theoretical insights into its physical properties

Stephen Stackhouse (University of Leeds; s.stackhouse@leeds.ac.uk)
Michael Ammann (UCL), John Brodholt (UCL), David Dobson (UCL), Alessandro M. Forte (Université de Québec à Montréal), J.-Michael Kendall (U. Bristol), G. David Price (UCL), Andrew M. Walker (U. Leeds), James Wookey (U. Bristol)

The discovery in 2004 of the perovskite to post-perovskite phase transition in $MgSiO_3$ provided an explanation for many of the usual seismic features observed at the base of the lower mantle: the frequent detection of a discontinuity a few hundred kilometres above the core-mantle boundary, seismic anisotropy and the anti-correlation of bulk and shear velocity anomalies. The full impact of the phase transition has enfolded over subsequent years, as experimental and theoretical studies have provided information on the physical properties of the perovskite and post-perovskite phases. These have aided the interpretation of seismic observations and provided input for dynamical models. Here we review progress in determining the properties of the perovskite and post-perovskite phases at lower mantle conditions, with particular attention given to the results of theoretical mineral physics studies. Our focus will be on the phase boundary, elastic properties and transport properties. The influence of impurities will also be considered. Implications for the structure, composition and dynamics of the mantle will be discussed in each case.

The deep mantle large low shear-velocity provinces: largely thermal features?

Saskia Goes (Imperial College London; s.goes@imperial.ac.uk)
D. Rhodri Davies (ANU)

The two large low shear-wave velocity provinces (LLSVPs) that dominate lower-mantle structure may hold key information on Earth's thermal and chemical evolution. It is generally accepted that these provinces are hotter than background mantle and are likely the main source of mantle plumes. Increasingly, it is also proposed that they hold a dense (primitive and/or recycled) compositional component. The principle evidence that LLSVPs may represent thermo-chemical 'piles' comes from seismic constraints. To test these constraints, we compare imaged seismic structures with synthetic seismic structures from a set of thermal and thermo-chemical mantle convection models that are constrained by $\sim$ 300 Myr of plate motion histories. Modelled physical structure is converted into seismic velocities via a thermodynamic approach that accounts for elastic, anelastic and phase contributions and, subsequently, a tomographic resolution filter is applied to account for the damping and geographic bias inherent to seismic imaging. We find that anomaly shapes, amplitudes and gradients, (relative) variation of shear, compressional and bulk-sound speeds, and a relation between LLSVPs and the distribution intraplate volcanism can be equally well explained with thermal and thermo-chemical models. Only an anti-correlation between shear-wave velocity anomalies and density, found by some studies but questioned by others, would provide unambiguous evidence for chemical heterogeneity. In any case, imaged distributions of lower-mantle shear-velocity anomalies allow at most very low-volume piles of dense chemical heterogeneity in the deep mantle. Such heterogeneity, although geochemically significant, would exert little control on large scale geophysical structure and mantle dynamics.

Is PPV the last mantle phase transition?

Ronald E. Cohen (UCL, Carnegie Institution; ronald.cohen@ucl.ac.uk)
Yangzheng Lin (Carnegie Institution)

We report results of structure searching for a new iron-rich post-perovskite phase. A new phase was reported from experiments by Zhang et al., Science, 2014. We report a new $FeSiO_3$ phase found with DFT+U computations using the XTALOPT evolutionary structure searching code.

Deep mantle seismic structure related to post-perovskite

Thorne Lay (University of California Santa Cruz; `tlay@es.uscs.edu`)

Seismological characterization of the lowermost mantle structure as inhomogeneous dates back to the work of Bullen, and even earlier workers (such as Dahm) who were developing first-generation radial velocity models for the interior. In the 1970s array methods that had developed for resolving upper mantle triplications were applied to detect evidence of rapid velocity increases that produce P wave triplication arrivals, and S wave triplications were documented in the early 1980s. Large-scale structures began to be mapped in the 1990s, including large low shear velocity provinces (LLSVP) and ultra low velocity zones (ULVZ) based on travel time and waveform analyses of expanding global seismic recordings. The interpretation of these structures was very constrained by the limited sensitivity of seismic waves to temperature and composition, and while speculations about possible effects of thermal structure, boundary layer flow structures, compositional stratification and conjectured phase transitions were advanced, this effort was not grounded in a specific hypothesis-testing context until the discovery in 2004 of a candidate phase change affecting the dominant mineral of the lower mantle, magnesium silicate perovskite. With experimental and theoretical exploration of P-T-X sensitivity of elastic properties of the new post-perovskite phase along with its transport properties, there was a large expansion of interdisciplinary research on the lower mantle structure and dynamics. After ten years, the advances in understanding are substantial, but challenges remain regarding confidence of interpretations. For example, seismically-detected velocity increases and decreases are not fully reconciled with expectations of a phase change, although there are interesting consistencies. The apparent sharpness of reflectors, the relative strengths of P and S wave reflectors, the multiplicity of reflectors in certain regions, the relative magnitude of P and S velocity reductions in ULVZ and LLSVP regions, and the characteristics of anisotropy in D'' structures all exhibit variations that require strong thermal and compositional heterogeneity at least, and given this, there is attendant uncertainty in the role, if any, actually played by post-perovskite in the actual mantle of Earth. Thus, much work remains to be done.

The role of post-perovskite in explaining observations of seismic anisotropy

Sanne Cottaar (University of Cambridge; sc845@cam.ac.uk)
Mingming Li (ASU), Allen K. McNamara (ASU), Barbara Romanowicz (UC Berkeley), Hans-Rudolf Wenk (UC Berkeley)

More and more observations of strong seismic anisotropy in the D″ emerge from different seismic phases. To explain the observations of seismic anisotropy in terms of flow, we need to understand what patterns of seismic anisotropy result from different geodynamical and mineralogical assumptions. In this multi-disciplinary forward modelling approach we test seismic anisotropy resulting from deformation of a subducting slab onto the core-mantle boundary for the presence and deformation mechanisms of post-perovskite. Tracers in a 3D geodynamical model with a subducting slab track the velocity gradient tensor along the slab. This information is fed into a viscoplastic polycrystal plascticity model. We test models of perovskite and post-perovskite, assuming different dominant slip systems. The different mineralogical models are evaluated against published seismic observations by analysing different anisotropic components: the radial anisotropy; the splitting for (sub-)vertical phases (i.e. azimuthal anisotropy); and the splitting for sub-horizontal phases. The patterns in radial anisotropy and splitting in sub-horizontal phases are only consistent with our model of post-perovskite with (001)-slip, confirming our earlier results in 2D. The strongest radial anisotropy in this model localises where the slab impinges on the core-mantle boundary. The azimuthal anisotropy pattern shows fast axis directions at the edges of the slab (sub-)parallel to flow directions, suggesting horizontal flows may be mapped out in the lowermost mantle using seismic observations.

Are seismic structures in the lower mantle due to post-perovskite?

Christine Thomas (University of Münster; tine@earth.uni-muenster.de)

Seismology has provided information about the deep Earth's mantle with structures that span a large range of length scales. Large slow-velocity regions, seismic reflectors, small-scale scatterers, ultra-low velocity zones, and anisotropy can be found in this complex region a few hundred kilometres above the core-mantle boundary. Especially the seismic reflectors in the D'' region can provide information on the dynamics of the Earth's mantle and mineralogy near the core-mantle boundary. Using array seismology and reflected waves from the D'' region, including information on travel times, amplitudes and polarities of the seismic waves it is perhaps possible to discriminate between different mechanisms that cause these reflectors. In recent years the mineral phase transition from perovskite to post-perovskite has provided a possible cause for several of the observed structures including the seismic reflectors. Here we test several regions in the lowermost mantle, sampling high- and low-velocity areas and extracting as much information as possible from the seismic waves to test the hypothesis that post-perovskite could be the cause of the observed structures. Especially in high-velocity regions, i.e. possible places of past subduction, the observations are variable and do not agree with the simple phase transformation hypothesis. In these cases anisotropy may help to explain these observations but also a change in mineralogy. Seismic modelling of the observed structures gives another constraint on the reliability of the seismically observed structures and with that we may have to rethink some of the interpretations. While the phase transition from perovskite to post-perovskite is still a likely candidate for D'' structures, other possibilities cannot be ruled out completely and we will review evidence for and against a phase transition as cause for structures in the D'' region.

What can analogue studies tell us about post-perovskite?

David Dobson (UCL; d.dobson@ucl.ac.uk)

The high stabilisation pressure of post-perovskite precludes the measurements of many important physical properties and makes any measurements very challenging. There has therefore been a concerted effort to perform analogue studies which use chemical systems which crystallise in the post-perovskite structure experimentally tractable conditions. Indeed, the structure-type material is $CaIrO_3$ which is 'post-perovskite' structured under ambient conditions. Among other things $CaIrO_3$ has been used to study structural, rheological, chemical and thermal transport properties of post-perovskite. Unfortunately, no analogue materials perfectly mimic the properties of $MgSiO_3$ perovskite – if they did then their pressures of stabilisation would also be prohibitively high – so we must develop a range of analogue systems which will show a range of behaviours. We can then, hopefully, develop an understanding of post-perovskite behaviour as a function of crystal-chemistry and other properties which are measurable in $MgSiO_3$-post-perovskite, allowing us to predict the behaviour of $MgSiO_3$-post-perovskite for the properties which we cannot measure. Combining these analogue studies with ab initio simulations can secure our understanding of the processes involved and provide an independent test of the simulations results. As a consequence, many analogues have been developed. Among the oxides, most are only stable at pressures above 30 GPa, not very useful for analogues, but $CaIrO_3$, $CaPtO_3$, $CaRhO_3$ are all stable at atmospheric pressure. The fluoride post-perovskite can be synthesised in the multi-anvil pressure range (typically 12-20 GPa) and are being developed for a range of physical property measurements. Some properties (relative thermal conductivity between perovskite and post-perovskite; relative strength) are remarkably consistent between different analogues and agree well with simulation results on the $MgSiO_3$ system, whereas others (texture generation, compression and expansion mechanisms) are very different between the different analogues. Even these 'bad analogue' properties can add confidence to simulations results if the simulations can reproduce the results across a range of analogues. Here I review the range of available oxide and fluoride analogue systems and their usefulness in predicting $MgSiO_3$ properties and briefly survey the likelihood of finding new, better, analogue materials.

Anisotropy, textures, and slip systems in post-perovskite: experimental approach

Sébastien Merkel (Université Lille 1; sebastien.merkel@univ-lille1.fr)

Seismic anisotropy in the D$''$ region has been studied since the late 1980's. At the time, this observation was hard to model based on preferred mineral alignment. In particular, the transition from weak to strong anisotropy between the lower mantle and D$''$ was rather enigmatic. The discovery of the perovskite to post-perovskite transformation in $MgSiO_3$ therefore triggered an intense interest in understanding how such transformation would allow for modelling D$''$ anisotropy based on post-perovskite textures. Diamond anvil cells allow plasticity experiments at the pressures of the D$''$ region and efforts are still under way for reaching combined conditions of pressures and temperatures relevant for D$''$ and suitable for measuring plastic properties. Over the last 10 years, we have learned that post-perovskite could develop various types of textures and anisotropy, depending on synthesis and deformation conditions. In this presentation, will summarise the advances in high pressure experimental methods, from radial x-ray diffraction at ambient temperature, combined radial x-ray diffraction and heating techniques, and the newly developed 3D x-ray diffraction. I will highlight the results that were obtained regarding post-perovskite plasticity at D$''$ conditions and how the work could be pursued in the future.

Modelling dislocations and plasticity in high-pressure polymorphs of $MgSiO_3$

Patrick Cordier (University of Lille 1; `Patrick.Cordier@univ-lille1.fr`)
Alexandra Goryaeva (Lille 1), Philippe Carrez (Lille 1)

Magnesium silicate perovskite and post-perovskite phases represent the most important phases of the lower mantle down to the core-mantle boundary. Their rheological properties play a key role in constraining the viscosity and hence dynamics of the mantle. The extreme pressure, temperature and timescale conditions that are relevant for deformation of materials involved in convection of the deep mantle extremely challenging experimental approaches. In the ERC founded RheoMan project we propose, as a complementary approach to develop multiscale modelling of dislocations and plasticity of these phases. Generalized stacking faults (GSF) are calculated at the atomic scale to provide a first constrain on the dislocation Burgers and slip systems. They are used as an input in a generalized Peierls-Nabarro model to model the dislocation core of pure edge and pure screw dislocations which are compared to full-atomistic models. The mobility of these defects are then modelled in the framework of the kink-pair model. In this presentation, we present the first results obtained on the perovskite and post-perovskite phases of $MgSiO_3$.

What do normal modes tell us about the lowermost mantle and post-perovskite

Arwen Deuss (University of Cambridge; afd28@cam.ac.uk)
Paula Koelemeijer (U. Cambridge), Jeroen Ritsema (UMich)

The core mantle boundary region (CMB) is the largest density and compositional interface in the Earth; it is a thermal boundary layer at the base of the mantle. The seismic structures found in the D$''$ regions just above the CMB, including ultra low velocity zones, large low shear velocity provinces, anisotropy and discontinuities, rival the structures found in the lithosphere, the mantle's top thermal boundary layer. The majority of these structures have been found using short seismic body wave observations, while long period free oscillation observations, or normal modes, have been lacking. The advantage of normal modes is that they are sensitive to variations in density in addition to velocity, while body waves are only sensitive to velocity variations.

Ideally, we would like to confirm all the observed body wave features in D$''$ with normal mode data. As a first step towards this goal, we have been measuring splitting functions for long period CMB Stoneley modes, which are uniquely sensitive to the lowermost mantle and D$''$ region. We use the new Stoneley mode observations in combination with existing normal mode splitting functions, P and S body wave and surface wave data in a tomographic inversion for mantle P and S-wave structure. Our aim is to answer questions about the ratio between the P- and S-velocity variations, which provides information about the thermal or compositional origin of the observed heterogeneity. We compare our results with predictions for thermal and thermochemical convection models with and without post-perovskite to draw constraints on its existence in the lower most mantle. We also run tests to find the most likely density structure in the lowermost mantle, with a particular focus on the LLSVP's.

Linking the dynamics of the lowermost mantle to observations of seismic anisotropy

James Wookey (University of Bristol; j.wookey@bristol.ac.uk)
Andy Nowacki (U. Bristol), Jack Walpole (U. Bristol), Andrew M. Walker (U. Leeds), Alessando M. Forte (GEOTOP, UQÀM), T. Guy Masters (IGPP, UCSD) and J.-Michael Kendall (U. Bristol)

At the core-mantle boundary (CMB), the largest change in physical properties occurs within the Earth. Furthermore, up to a few hundred kilometres above the CMB – the region known as D'' – the largest lateral variations in seismic wave speed are observed outside the upper mantle. Work over the last decade strongly suggests that the presence of a post-perovksite phase of $MgSiO_3$ can explain many of the anomalous seismic features of this region.

Observations of shear wave splitting in D'' shows that the lateral velocity heterogeneity is dependent not only on position, but also wave propagation direction and polarisation; that is, strong seismic anisotropy is a pervasive feature of D'', just as in the upper mantle (UM). Similarly to the UM, it is frequently argued that alignment of anisotropic minerals (such as post-perovskite) due to flow is the cause of this. Were this the case, this anisotropy could be used to retrieve the recent strain history of the lowermost mantle.

We review recent modelling of mineral alignment in D'', which has shown that quite simple models of mantle flow do not produce simple anisotropy. Global inversion for radial anisotropy permits complete coverage of the CMB but so far has relied on core-diffracted waves (Sdiff) which are challenging to accurately interpret. Studies of shear wave splitting in body wave phases which transit D" do not impose any assumed type of anisotropy but have been traditionally limited in their geographical scope.

We present the results of a consistent analysis of core-reflected shear waves (ScS) for shear wave splitting, producing broad scale coverage of D''. Over 12,000 individual measurements are made, from ∼470 events. Along well-studied paths such as beneath the Caribbean, our results agree excellently with previous work. Elsewhere, a full range of fast orientations are observed, indicating that simple SV-SH comparisons may not accurately reflect the elasticity present.

We compare these results to candidate models of D'' anisotropy assuming a simple flow model derived from geophysical observables. A number of different mechanisms (different slip systems causing alignment of $MgSiO_3$-perovskite, -post-perovskite or MgO) are possible, hence we compute the expected seismic response for several. To accurately reproduce the wave field we make use of the spectral element method. This suite of results allows us to contemplate the challenges to be faced in recovering dynamics from measurements of seismic anisotropy in the lowermost mantle. Many such remain, including resolving many outstanding mineralogical questions and properly accounting for a dynamical evolving strain field.

Post-perovskite: Past, present, future

John Hernlund (Earth-Life Science Institute, Tokyo Institute of Technology; hernlund@gmail.com)

Years before a phase transition in $MgSiO_3$ from perovskite (Pv) to post-perovskite (PPv) at conditions of the deep mantle was discovered, Sidorin and co-workers had already predicted that the D'' discontinuity was best explained by some kind of phase transition exhibiting a relatively large Clapeyron slope (>6 MPa/K). Such an explanation was the only plausible way to explain elevation of this relatively sharp discontinuity in seismically fast (presumably cold and downwelling) regions of the deep mantle, a feature that cannot be easily explained by thermal gradients or chemical layers. Thus the framework for understanding how PPv could help explain the D'' discontinuity was already in place when experimental evidence compatible with the predictions was published in 2004. Presently we have moved beyond some first-order debates regarding PPv, and the range of uncertainties has narrowed. The active slip system in line defect-modulated PPv-deformation, and the role of deformation fabric vs. transformation fabric, is better resolved. Diamond-anvil cell experiments suggest that harzburgite-like bulk composition is the best candidate for producing a sharp Pv–PPv transition, which is compatible with the expectation of subducted depleted lithospheric slabs in cold regions where PPv would be stable, particularly in the circum-Pacific where seismic evidence for many proposed PPv features appears to be most consistent (especially beneath the Caribbean region). However, there is still much disagreement and debate regarding precise P–T conditions, elemental partitioning, and other important topics. Different research groups continue to exhibit their results using different pressure standards, yielding enormous variations in reported P–T conditions relevant to Pv/PPv stability, perhaps highlighting the need for more inter-laboratory cooperation in establishing a consistent pressure standard. Important effects such as elemental partitioning are claimed to be well-handled by each group, but when confronted with different results from another research group they invariably ascribe the other groups' approaches to be susceptible to Soret and/or other non-equilibrium effects. In any case, laser-heated diamond anvil cell experiments are invariably conducted under conditions far from thermal equilibrium, and nobody in this field has worked to establish any theoretical confidence in any particular technique. There are also many geodynamical and seismological aspects related to the Pv–PPv phase change and D'' discontinuities that need better explication and integration. The combined role of anisotropic fabric transitions and variations in phase proportions needs to be worked out more thoroughly, at best our present models are simply cartoons. The coupled dynamical role of a decreased shear viscosity and/or enhanced thermal conductivity also needs to be further integrated into a robust framework yielding specific hypothesis tests for seismologists. In seismology, more work to constrain the detailed structure of the D'' discontinuity in various settings, relative changes in SH vs. SV, and combined P vs. S behaviour could likely provide more complete tests of higher-order models. Finally, the stable phase at the CMB P–T carries important implications for interpreting temperature and heat flux variations, topics that are important for understanding the thermal evolution of Earth.

Poster abstracts

Paleozoic plate motion history and the longevity of deep mantle heterogeneities

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Numerical studies of mantle convection have attempted to explain tomographic observations that reveal a lower mantle dominated by broad regional areas of lower-than-average shear-wave speeds beneath Africa and the Central Pacific. The anomalous regions—termed LLSVPs ("large low shear velocity provinces")—are inferred to be thermochemical structures encircled by regions of higher-than-average shear-wave speeds associated with Mesozoic and Cenozoic subduction zones. The origin and long-term evolution of the LLSVPs remains enigmatic. It has been proposed that the LLSVP beneath Africa was not present before 200 Ma (i.e. before and during most of the life-time of Pangea), prior to which time the lower mantle was dominated by a degree-1 convection pattern with a major upwelling centred close to the present-day Pacific LLSVP and subduction concentrated mainly in the antipodal hemisphere. The African LLSVP would thus have formed during the time-frame of the supercontinent Pangea as a result of return flow in the mantle due to circum-Pacific subduction. An opposing hypothesis, which propounds a more long-term stability for both the African and Pacific LLSVPs, is suggested by recent palaeomagnetic plate motion models that propose a geographic correlation between the surface eruption sites of Phanerozoic kimberlites, major hotspots and Large Igneous Provinces to deep regions of the mantle termed "Plume Generation Zones" (PGZs), which lie at the margins of the LLSVPs. If the surface volcanism was sourced from the PGZs, such a link would suggest that both LLSVPs may have remained stationary for at least the age of the volcanics, i.e., 540 Myr. To investigate these competing hypotheses for the evolution of LLSVPs in Earth's mantle, we integrate plate tectonic histories and numerical models of mantle dynamics and perform a series of 3D spherical thermochemical convection calculations with Earth-like boundary conditions. We improve upon previous studies by employing a new global plate motion model to impose surface velocity boundary conditions for a time interval that spans the amalgamation and subsequent break-up of Pangea. Our results are distinct from those of previous studies in several important ways: our plate model explicitly includes (i) absolute longitudinal reconstructions and (ii) TPW-correction, and (iii) our model extends back to the mid-Paleozoic (410 Ma). We find that, were only the Pacific LLSVP to exist prior to the formation of Pangea, the African LLSVP would not have been created within the lifetime of the supercontinent. We also find that, were the mantle to be dominated by two antipodal LLSVP-like structures prior to the formation of Pangea, the structures would remain relatively unchanged to the present day and would be insensitive to the formation and break-up of the supercontinent. Our results suggest that both the African and Pacific LLSVPs have remained close to their present-day positions for at least the past 410 Myr.

Testing thermal versus compositional mantle convection hypotheses

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Mantle convection is considered by many to be thermally driven but recent models have incorporated dynamically significant chemical heterogeneity at the base of the mantle. These new models have been motivated by the two large low shear-wave velocity provinces (LLSVPs) which have been interpreted by many as thermo-chemical 'piles'. For example, it has been argued that low relative velocities of hotspots requires them to be compositionally anchored. We find that thermal models can also have low relative hot-spot velocities. The strongest arguments regarding the LLSVPs compositional heritage arguably come from seismology. We have tested them quantitatively.

There will be an oral presentation by Dr. Goes presenting these tests together with further work. This poster presentation will emphasise the geodynamic models and a subset of the seismic tests. The tests are based on thermal and thermo-compositional mantle circulation models, constrained by $\sim$ 300 Myr of plate motion history. The models are compressible and have a depth and temperature dependent viscosity. The model has mixed heating with a core-mantle temperature of 4000K and a close to chondritic rate of internal heating 5.5×10^{-12} W/kg. The models also incorporate an endothermic 660 km and an exothermic 410 km depth discontinuities. The resulting present day structure (temperature, composition) is converted into seismic velocities using a thermodynamic model, incorporating anelasticity and limited seismic resolution. For the thermo-compositional model we have considered two possibilities: a primitive iron-rich composition, and a recycled basaltic composition.

Both the thermal and thermo-compositional models reproduce features reminiscent of LLSVPs. One test concerns the LLSVPs sharp sides, i.e. high seismic gradients at the anomaly edges. It was argued that thermal anomalies would diffuse and so only compositional anomalies could produce such high gradients. Steep seismic gradients similar to ones observed are in fact just as easily reproduced in thermal models which is not surprising once one realises they are advection dominated. In contrast the anti-correlation between shear and bulk sound velocity is not well reproduced in either the thermal or thermo-compositional models. In fact the post-Perovskite phase change produces an anti-correlation. We will also present considerations of the amplitude of the anomaly, and the variation of the shear and compressional speeds and density.

In summary the thermal model predictions fit the observations as well as the thermo-compositional models. Occam's razor would make the thermally driven engine the leading mantle dynamics paradigm. Challenges for the thermally driven mantle convection model includes predicting observations such as chemically heterogeneous magmas and the recycling of oceanic plates inherent in plate tectonics.

Stratification at the top of the outer core: constraints from SmKS and PmKP phases

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Convection in the Earth's outer core is responsible for the generation of the planet's magnetic field and is strongly dependent on interactions between the mantle and inner core. However, despite undergoing vigorous convection, the outer core is not necessarily a single uniform, homogeneous layer of the Earth. Recent seismic and geomagnetic studies suggest that the uppermost outer core is comprised of a chemically distinct layer of stably stratified material. This layer is likely enriched in light elements, which may either be accumulating due to the release of light elements during the solidification of the inner core, or due to a flux of material across the core mantle boundary. Here we compile a new dataset of SmKS and PmKP differential travel time data to investigate the vertical and geographical extent of stratification in the uppermost outer core. By jointly considering SmKS and PmKP phases, carefully correcting for known mantle structures, exploring the effect of CMB topography, and considering changes in the core over recent time, we are able to place new constraints on this stably stratified layer at the top of the outer core.

Seismic anisotropy in D$''$ beneath western North America from discrepant splitting of SKS and SKKS pairs

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Propagation of shear waves through an anisotropic medium can lead to shear wave splitting, in which an initially linearly polarised shear wave is split into fast and slow components. Discrepant splitting of SKS and SKKS arrivals for the same earthquake-seismometer pair indicates the presence of anisotropy in D$''$, as the two phases sample the same region of the upper mantle but different areas of D$''$. I observe discrepant splitting of SKS and SKKS arrivals from earthquakes in south-east Asia recorded by the Transportable Array of seismometers in North America, indicating anisotropic structure in D$''$ beneath western North America. Due to inadequate characterisation of upper mantle anisotropy beneath North America it is not possible to obtain the fast axis orientations in D$''$ and relate the splitting directly to processes, such as mantle flow, which may be responsible for the anisotropy.

Atomistic modelling of dislocations with [100] Burgers vector in $MgSiO_3$ post-perovskite

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The recently discovered $MgSiO_3$ post-perovskite phase (*Cmcm*) is only stable at high pressure and temperature conditions corresponding to the lowermost ∼150 km of the mantle (the D″ layer). The unusual for the high-pressure phases layer-like structure of the post-perovskite may be responsible for the observed seismic anisotropy of the D″ layer. However, mechanical properties, information about dislocations and their behaviour under stress are not well known still. This work represents a theoretical study of the post-perovskite within the semi-empirical approach using the Buckingham interatomic potential parameters previously derived by [3].

To describe the energy cost incurred as a result of a shift and to deduce the most favourable slip systems, the GSF excess energies are calculated at 120 GPa. The lowest energy barrier as well as the smallest values of the ideal shear stress (ISS), are related to the slip systems with the smallest [100] Burgers vector ($b = 2.521$ Å) and to the slip system [001](010) with the glide plane cutting only Mg–O bonds. Good agreement with the *ab-initio* results [4] verifies the accuracy of the chosen interatomic potential model [3].

The *C*-lattice of the post-perovskite results in four potential Burgers vectors: [100], [010], [001] and [011]. Taking into account the results of GSF calculations, the [100] Burgers vector was chosen as the most promising to test first. After structural relaxation, two possible locations of the stable [100] screw dislocation were revealed. Both dislocations have pure screw cores spreading in {011}. The spreading of the dislocation cores is limited by Si-layers. The observed geometry of the dislocation core spreading suggests the [100](010) slip system as the most probable. Indeed, the evaluated peierls stress for the [100](001) slip system is more than ten times bigger than for [100](010).

Modelling of [100] edge dislocations is in progress.

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Analytical parameterization of self-consistent polycrystal mechanics

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Progressive deformation of upper mantle rocks via dislocation creep causes their constituent crystals to take on a non-random orientation distribution ('crystal preferred orientation' or CPO) whose observable signatures include shear-wave splitting and azimuthal dependence of surface wave speeds. Simulation of the development of CPO in models of mantle deformation, and comparison of this with seismic observations of the Earth, allow mantle dynamics to be unraveled on global and regional scales. However, these simulations are computationally challenging when performed for time varying models of mantle convection. We describe here an accurate but computationally efficient alternative to existing methods for the simulation of CPO development in the upper mantle. We have developed a new analytical model that gives predictions indistinguishable from the second-order (SO) model of Ponte-Casteneda (2002), at a fraction ($\sim$0.0001) of the cost. We illustrate the approach for pure olivine polycrystals subject to different types of deformation (e.g. uniaxial compression, pure shear, simple shear, etc.).

Rate of texture development in post-perovskite

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The D″ layer of the mantle exhibits significant seismic anisotropy which contrasts with the rest of the lower mantle which is seismically isotropic. This, otherwise anomalous anisotropy, was explained 10 years ago with the discovery of a new post-perovskite phase of $MgSiO_3$ at pressures and temperatures in excess of 135 GPa and 3500 K. The post-perovskite phases exhibits large elastic anisotropy and with the correct lattice preferred orientation can at least partially explain the seismic observations.

However, in order to generate the required anisotropy the deformation of the post-perovskite has to be accommodated by a dislocation glide mechanism. Due to the extreme conditions under which MgSiO3 post-perovskite is stable determining its deformation mechanism is extremely difficult and so analogue materials have been used to investigate the deformation mechanism. The results of these studies show a range of dislocation glide mechanisms, only some of which can explain the lower mantle anisotropy (e.g. Wookey et al. 2005). Attempts to model the generation of seismic anisotropy via the development of a deformation induced lattice preferred orientation (LPO) are made difficult by a shortage of data on the relative activity of the various slip systems and a lack of information on the rate of its development with strain (Walker et al. 2011). Indeed, the speed at which the LPO develops is critical to determining the dynamics of the D″. For example, rapid development of LPO following the perovskite post-perovskite transition will give a larger degree of shear wave splitting than a slowly developed LPO, for the same post-perovskite path length. On the other hand, tardy development of LPO will make the boundary at the edges of the post-perovskite fields in D″ significantly less distinct.

To investigate the rate of LPO generation and the slip system activities in post-perovskite, we undertook simple shear deformation experiments of $CaIrO_3$, the low-pressure analogue of $MgSiO_3$ post-perovskite, at 400 °C and 1 GPa. The experiments were performed in the deformation-DIA, at the NSLS on beam line X17B2. During deformation, we recorded diffraction patterns from the sample using the 10-element energy dispersive detector (Weidner et al. 2010). Nine of the detectors are arranged in a semi-circle, which gives good coverage of the Debye rings in the sample. From the position of the peaks in these diffraction patterns, the evolution of elastic strain and the stresses in the sample can be observed as a function of bulk sample shear strain (γ). The distribution of the elements is such that pole figures can be recovered from the diffraction intensities. The change in the pole figures with time allows the development of LPO in the sample to be tracked.

The LPO calculated here shows slip on the experiment performed here shows the dominant deformation mechanism in $CaIrO_3$ is [100]{010}, which is consistent with EBSD measurements of our sample and previous studies. The LPO develops quickly with strain; the majority of the intensity in the LPO develops before $\gamma = 0.5$ and subsequent increases in LPO appear to be slight.

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Presence of post-perovskite implied by tomographic-geodynamic model comparisons

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Large-low-shear velocity provinces (LLSVPs) dominate shear wave velocity (V_S) models of the deep mantle. Furthermore, tomographic models find an increase in the ratio of shear wave to compressional wave velocity (V_P) variations, accompanied by a significant anti-correlation between shear wave and bulk sound velocity (V_C) variations. These characteristics have been interpreted in terms of chemical variations but could potentially also be explained by the presence of post-perovskite (pPv). Accurate seismic characterisation of the long wavelength velocity and density structure of the lower mantle is required to investigate the possible presence of chemical heterogeneity and/or post-perovskite and to assess the nature of the LLSVPs.

Earth's normal modes provide an invaluable tool for probing the Earth's deep interior since they are global in character and affected by density variations in addition to velocity. In particular, Stoneley modes, confined to solid-liquid interfaces such as the core-mantle boundary (CMB), are primarily sensitive to structures in the D$''$ region. Observations of these modes increase the depth resolution and provide unique constraints on long wavelength structures in the deep mantle.

We make use of a recent normal mode splitting function data set of 143 modes including 33 modes sensitive to V_P and 9 CMB Stoneley modes. We combine these data with independent constraints from body waves and surface waves and invert jointly for lateral V_S and V_P variations in Earth's mantle. We compare the obtained tomographic model SP12RTS to thermal and thermochemical models of mantle convection with and without pPv and/or chemical variations. In addition, we perform hypothesis tests for possible density structures in the lowermost mantle.

SP12RTS shows an increase in the V_S/V_P ratio up to 2500 km depth followed by a decrease towards the CMB as well as an anti-correlation between V_S and V_C variations in the lowermost mantle. Our tomographic-geodynamic model comparison implies that these characteristics can be explained by the presence of post-perovskite but allows no discrimination between isochemical and thermochemical models of mantle convection. Our density hypothesis tests indicate that previous studies, which suggested dense LLSVPs, can be reproduced using normal mode data available at the time, whereas current normal mode data are best explained by density models containing light LLSVPs.

First principle studies on elasticity and thermal conductivity of aluminous phase minerals under LLSVP conditions

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The large low shear velocity provinces (LLSVPs) cover almost half of the outer core surface and connect the lowermost mantel and outer core. Although there are lots of reports about the image of LLSVPs but the composition of them are still unclear because of the inaccessibility of direct observation and limit of the experimental technique at extreme values of pressure and temperature. Theoretical studies can help us to explain the experimental phenomenon and predict some unknown properties of minerals. Firstly, First principle calculation will be carried out to study the elastic properties of aluminous phase minerals of LLSVPs under high temperature and pressure. The relations between the elastic properties and seismic velocity will be used to connect mineralogy and seismology, and then we will predict the composition of the LLSVPs. Secondly, we will implement the linear scaling DFT code SIESTA with non-equilibrium molecular dynamics method to calculate thermal conductivity to describe the heat transfer from core to mantle. Elasticity and thermal conductivity can be used to understand the composition and other important properties of LLSVP under such extreme condition near core-mantle boundary as the first step to understand the evolution of the earth interior.

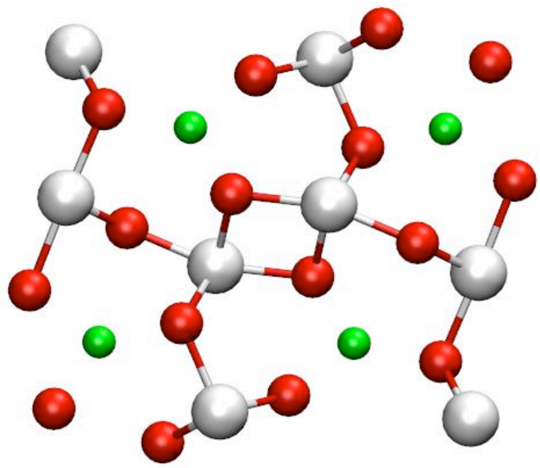

Figure : The structure of CF-$MgAl_2O_4$ under 136 GPa and 0 K. Oxygen in red, magnesium in green, and aluminium in grey.

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Partitioning of $FeSiO_3$ and $FeAlO_3$ between $MgSiO_3$-based perovskite and post-perovskite

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The phase transition of Mg-perovskite (pv) to post-perovskite (ppv) at pressure-temperature conditions of the lowermost mantle (D$''$ zone) has a large positive Clapeyron slope. Large thermal gradients above the core-mantle boundary may re-stabilise pv in the lowermost 50-100 km of the mantle. The D$''$ includes two antipodal Large Low Shear-wave Velocity Provinces (LLSVPs) under Africa and the Pacific separated by a high-V_S, circumpolar belt under east Asia, Australia and the Americas. Seismic discontinuities delineate 200–300 km thick ppv-layers, especially within the high-V_S belt and tentatively within portions of the LLSVPs. The mostly 300–500 km thick LLSVPs appear to have sharp boundaries and long-term stability and must therefore contain hot and dense material, of either basaltic or Fe-rich peridotitic composition.

Pv and ppv are ABO_3-componds with large, 8-coordinated A-sites filled by Mg, Fe^{2+}, and Fe^{3+} and smaller octahedral B-sites with Si and Al. In pv octahedral Al is dominantly charge-balanced by A-site incorporation of ferric iron. Our Monte Carlo simulations with DFT in the grand canonical ensemble (GGA +U method) to investigate solid solutions in the binary systems $MgSiO_3$–$FeSiO_3$ (MS–FS) and $MgSiO_3$–$FeAlO_3$ (MS–FA). We focused on the pv–ppv transition and the partitioning of the FS and FA components between pv and ppv under pressures and temperatures corresponding to the D$''$ zone.

The Clapeyron slope of the transition for MS is 9.6 MPa/K, decreasing to 8.4 and 8.1 MPa/K at 6.3 and 12.5 mol% FS and to 8.2 and 7.3 MPa/K at 6.3 and 12.5 mol% FA. The FS and FA components partition in opposite directions, towards ppv and pv, respectively. The contrasting partitioning of ferrous iron and ferric iron coupled to octahedral Al is broadly consistent with most of the experimental partitioning studies, that previously seemed partly conflicting. In Al- poor and Fe-rich peridotite compositions, the simple pv to ppv partitioning of divalent Fe will lead to increased Mg/Fe-ratio of the coexisting ferropericlase (fp). The exchange partition coefficient $K_D^{\mathrm{pv/fp}}$(Fe/Mg) and $K_D^{\mathrm{ppv/fp}}$(Fe/Mg) will therefore decrease from pv-bearing to ppv-bearing lithologies, according to the reaction:

$MgSiO_3$ *(pv) + FeO (fp) =* $FeSiO_3$ *(ppv) + MgO (fp)*

A net chemical reaction from FA-rich pv coexisting with reduced Fe-metal to form FS-rich ppv produces additional Al_2O_3 and MgO:

$2\ FeAlO_3 + 3\ MgSiO_3 + Fe = 3\ FeSiO_3 + Al_2O_3 + 3\ MgO$

The host phases for the excess Al_2O_3 and MgO will vary with lithological environment. In peridotite, MgO will increase the proportion and Mg-number of ferropericlase, and some Al_2O_3 may dissolve as an additional component in ppv and/or coexisting pv. Separate Ca-ferrite- (CF-) or Ca-titanite- (CT-) structured phases containing the $MgAl_2O_4$ component might form if the solubility of Al_2O_3 in ppv is exceeded. In basaltic and komatiitic rocks the $MgAl_2O_4$ component can dissolve in preexisting CF-CT-phases, with excess MgO reacting with SiO_2 from the silica-dominated phases to increase the MS-component of ppv.

Double seismic discontinuities within the D$''$ zone, observed mainly in regions with high S-wave velocities, but possibly also in the northeastern part of the Pacific LLSVP, have been ascribed to the upper and lower boundaries of ppv- dominated lenses. Recent experiments, indicating very high pressure for the ppv-transition in $FeAlO_3$-rich compositions, have made the interpretation of ppv-lenses within hot, and presumably Fe-rich, LLSVPs questionable. Our results, however, may explain the presence of ppv-lenses within the hot LLSVPs, provided that they contain pv and ppv that are poor in aluminum, but rich in ferrous iron. Iron-rich magma ocean cumulates may have such compositions.

Elasticity of solid solutions with $FeSiO_3$ and $FeAlO_3$ in Mg-perovskite and post-perovskite

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In spite of broadly similar stoichiometry and major element compositions, perovskite (pv) and post-perovskite (ppv) have markedly different crystal structures and elastic properties. The large positive Clapeyron slope of the pv-ppv transition and the large thermal gradient over the lowermost 200–400 km above the core-mantle boundary (CMB) lead to thick lenses of ppv-dominated material in the circumpolar belt of high S-wave velocities between the two antipodal and equatorial Large Low S-wave Velocity Provinces (LLSVPs) under the Pacific and Africa. The indications that the LLSVPs have sharp margins and long-term stability imply hot and dense materials. Although double seismic discontinuities within the range of 100–350 km above the CMB in the northeast part of the Pacific LLSVP have also been ascribed to the the ppv-in and ppv-out reactions, this interpretation is still open to discussion and dependent on the composition of the LLSVP-material.

An ongoing Monte Carlo simulations with density functional theory in the grand canonical ensemble (GGA +U method) in the systems $MgSiO_3$–$FeSiO_3$ and $MgSiO_3$–$FeAlO_3$ (MS–FS and MS–FA) have demonstrated that the $FeSiO_3$ and $FeAlO_3$ components partition in opposite directions, into ppv and pv, respectively. Therefore, the tentative allocation of paired seismic discontinuities within the Pacific LLSVP to the ppv-in and ppv-out transitions may require peridotitic cumulate or solidified melt material which is Al-poor and Fe^{2+}- rich.

Our DFT results show that any isochemical pv to ppv transition within the investigated solid solution range (up to 20–25 mol% FS and FA) would be accompanied by decreasing bulk and increasing shear modulus. At a reference pressure of 100 GPa, the bulk modulus for pv and ppv increases by 1.4% and 1.0%, respectively, from MS_{100} to MS-$FS_{12.5}$ and decreases by 0.4% and 0.2%, respectively, from MS_{100} to MS-$FA_{12.5}$ (subscripts indicate mol%). The shear modulus decreases for both pv and ppv along both of the solid solution series from the pure MS composition, with the largest decrese along the FA-join. For pv and ppv the shear modulus decreases with 2.4% and 1.3%, respectively from MS_{100} to MS–$FS_{12.5}$ and with 4.4% and 3.0%, respectively, from MS_{100} to MS–$FA_{12.5}$.

The results for the MS–FS join are in general agreement with previous DFT-studies (Caracas & Cohen, 2005, GRL; Stackhouse et al. 2006, GRL; Stackhouse & Brodholt 2008, PEPI). Boffa Ballaran et al. (2012, EPSL), however, found a decrease in the bulk modulus for pv on the MS-FS join relative to pure MS. Our DFT results indicating slightly decreasing bulk modulus along the MS-FA join agrees with Boffa Ballaran et al. (2012, EPSL).

If the LLSVPs consist largely of iron-rich peridotitic cumulates from magma ocean crystallization with FS as the dominant Fe-component, the indications of sharp and steep margins (e.g. Garnero & McNamara, 2008, Science) may be readily explained by an elevated bulk modulus. The overall decrease in shear modulus with increasing proportion of the two iron components in both pv and ppv will likely contribute to the low V_S in the LLSVPs. Further thermophysical data, including thermal expansivity and thermal conductivity, are critically important to resolve the seismic structures of the D$''$ region and improve our insights in the core-mantle heat flow and convective dynamics near the CMB. It is also important to clarify the iron partitioning involving a possible "H-phase"

(Zhang et al., 2014, Science) and its thermoelastic properties.

Approximate vs. purely numerical approaches for full waveform modelling of global Earth structure.

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The quality of 3-D tomographic Earth models strongly depends on the forward modelling scheme used in their construction. Purely numerical methods such as the Spectral Element Method (SEM) are available for the accurate simulation of seismic wave propagation in laterally varying 3-D Earth models, but their computational cost is still prohibitive for global tomography applications, which typically involve inversions of hundreds of thousands of waveforms.

In this study we test for the first time whether two complementary approximate forward modelling schemes can be useful for waveform tomography. We here calculate teleseismic synthetic surface waveforms using the Born approximation and Full Ray Theory for different realistic 3-D Earth mantle models and compare them to SEM solutions. Our tests aim at exploring quantitatively the validity domains of these two approximations in order to find an optimal forward modelling scheme for global tomography.

Comparison of P-, SV, and SH-wave velocity models below Japan and North-East China

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The recent deployment of the NECESSArray seismic network in North-East China has allowed new insights on the velocity structure of this formerly poorly resolved area. This experiment has brought new data to debate about the geodynamical context in this region (stagnant slab, origin of intraplate volcanoes, ...).

We use a more efficient method for the measurement of traveltime residuals by cross-correlating observed and synthetic waveforms. Synthetic seismograms are convolved with high-frequency source-time functions inverted along with focal depths, following a simulated annealing approach. Thus, resulting modelled waveforms take more accurately account for the source effects. The method is used to perform measurements on direct P, SV and SH phases extracted from, respectively, vertical, radial and transverse band-pass-filtered records from NECESSArray and F-NET seismological networks.

We finally invert the resulting datasets in order to obtain P-, SV, and SH-wave velocity models. To do so, we use a fast and efficient inversion method using ray theory. Observed structures in the three tomographic models show a very good geographical coherency. Nevertheless, some differences are observed below Songliao basin and Changbaishan volcanoes between the three models, that are highlighted through $V_\mathrm{P}/V_\mathrm{S}$ and $V_\mathrm{SH}/V_\mathrm{SV}$ perturbation ratios.

P- and S-wave boundaries of the African Large Low Shear Velocity Province

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Tomographic images of Earth's lowermost mantle are dominated by two nearly antipodal regions of reduced seismic velocities. These areas are now dubbed Large Low Shear Velocity Provinces (LLSVPs) and are proposed to be thermochemical piles of unknown origin, although purely thermal models are also being discussed. The purpose of this study is to determine the location of the boundaries of African LLSVP, specifically along its north-western margin. Although LLSVP boundaries are usually constrained by a specific drop in seismic velocities in tomographic models it remains unclear which velocity reduction is indicative for LLSVP existence. Here we aim to define the north-western boundary of the Africa LLSVP from direct seismic observations.

The African LLSVP is a ridge-like structure that extends from the Indian Ocean through Central Africa along to the Atlantic where it turns northwards and runs towards Iceland. Using a combination of data from European and African seismic stations we aim to better constrain the north western boundary of the African LLSVP and especially determine its extent towards Iceland and a possible connection to the Icelandic hotspot. Our dataset will allow the largest lateral extent of the north-western margin to be examined to date. The vertical extent of the LLSVP could potentially be examined as well in this region through traveltime and waveform analysis providing further insight into the origin of the African LLSVP.

This study will combine three main strands of investigation: firstly travel-time anomalies, secondly wave-form complexities and thirdly anisotropy changes across the LLSVP boundary. We are using traveltime anomalies for a variety of seismic phases including P, PcP, P_{diff}, S and SKS and across different frequencies and therefore will be able to determine the boundary for P and S waves. The combined P- and S- wave study will help to elucidate any chemical contributions to the velocity anomalies. Ultra-Low Velocity Zones will be investigated along the newly defined boundaries using travel-time delays. Wave-form complexities will also be used in conjunction with 3D waveform modelling to determine the sharpness of the boundaries detected. Using anisotropy, this study, will look at how mantle flow is altered at the LLSVP boundary potentially increasing anisotropy at the LLSVP boundary. Combining constraints from all three methods will provide evidence for the location of the north-western boundary African LLSVP and its origin. It will also provide an insight into how the surrounding mantle is affected by the African LLSVP.

Global ultra-low velocity zone geometries and distribution resolved by multi-dimensional waveform modelling of SP_dKS/SKP_dS

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Ultra-low velocity zones (ULVZs) are thin patches of strongly reduced seismic velocities and likely increased density at the core-mantle boundary (CMB). A common phase to detect ULVZs is SP_dKS (SKP_dS), an SKS wave with a short diffracted P leg along the CMB. The characterisation of ULVZ properties typically uses waveform modelling through wave propagation through 1D (radial) Earth models. Here we apply 2.5D modelling using the finite difference algorithm PSVaxi for rotationally symmetric velocity models for a suite of ULVZ models to better characterise the location and properties of ULVZs at the CMB. We use 80 deep focus events between 2005 and 2011 recorded on ∼2400 global stations to detect ULVZ structures using the SP_dKS waveform. The data is compared to a library of approximately 1400 2.5D SP_dKS waveforms including variations in ULVZ shape (boxcar, Gaussian, and trapezoid), height (10 km or 20 km), location, size, and limited velocity and density variations. To detect ULVZs a combination of visual examination of the data and multiple statistical tests including a paired difference t–test are applied to compare the data to potential ULVZ model candidates. The results indicate preferred characteristics including a tendency for ULVZs sensitive to SP_dKS likely be steep sided as indicated by the dominance boxcar ULVZ model detections and a percent drop in V_P to percent drop in V_S ratio of ∼1/3. The modelling yields additional constraints as the combination of geometry and seismic properties permits a rough calculation of ULVZ viscosity and potential melt fraction. This calculation, however, is limited by ill-constrained material properties of the lowermost mantle.

Modelling the tectonics of the lowermost mantle

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The discovery of the perovskite to post-perovskite phase transition in (Mg,Fe)SiO_3 explains many of the seismic observations of the lowermost mantle including the presence of significant seismic anisotropy. However, the explanations of many detailed features remain elusive. We have extended our previous work linking models of flow in the lowermost mantle with simulations of texture development and predictions of seismic anisotropy [1] in order to account for the topotaxy between perovskite and post-perovskite predicted by experiments on analogue materials [2]. In particular, we compare four cases: (1) As in [1], anisotropy is only generated in post-perovskite by dislocation mediated deformation dominated by one of a number of slip systems, phase transitions destroy texture and ferropericlase and perovskite dominated rocks are isotropic. (2) Although phase transitions destroy texture, ferropericlase and/or perovskite deform by dislocation motion permitting the generation of seismic anisotropy in warmer regions of the mantle where post-perovskite is unstable. We account for the possibility of the inversion of slip-system activities in ferropericlase at high pressure as suggested by models of dislocation motion based on atomic scale simulations [3]. (3) Allow texture development by dislocation motion in perovskite and post-perovskite and texture inheritance through phase transitions by the mechanism described in [1]. However, we assume that the bulk of the lower mantle deforms by a mechanism that does not lead to the development of texture and so begin the simulation from a random distribution of crystal orientations the first time the post-perovskite stability field is encountered for downward migrating packages of mantle material. (4) Allow the bulk of the lower mantle to deform by dislocation creep such that material entering the lowermost mantle for the first time is already textured, allow this texture to be inherited and further modified by strain and phase transitions. These calculations show clear differences in global and local scale elastic anisotropy in the lowermost mantle between cases where texture is allowed to persist through the phase transitions and those where it is not. On a global scale and when radial anisotropy is imposed the inclusion of topotaxy results in a dramatic decrease in the strength of the degree two signal and better agreement between observations and the model for post-perovskite deformation where dislocations moving on (001) dominate.

References:
[1] Walker et al. 2011 Geochem. Geophys. Geosys. 12:Q10006
[2] Dobson et al. 2013 Nature Geosci. 6:575578
[3] Cordier et al. 2012 Nature 481:177-180

Post-perovskite deformation in the lowermost mantle: constraints from seismic anisotropy

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The lowermost 250 km of mantle acts as the lower boundary layer to mantle convection. The region is rich in anomalous features, as evidenced by seismic scatterers, reflections, anisotropy, and travel time anomalies. These features remain mysterious, although the perovskite to post-perovskite phase transition in the $MgSiO_3$ system which is expected to be present at these depths could help to explain some of them. Simmons et al. (2009) invert geophysical data for flow in the mantle, producing a smooth model, with horizontal flow in the lowermost mantle directed from areas of downwelling towards regions of upwelling. Here we focus on the seismic anisotropy, which provides a direct constraint on the flow patterns. We make hundreds of good quality shear wave splitting measurements on ScS arrivals that traverse the lowermost mantle at multiple locations across the globe. The data are corrected for anisotropy in the upper mantle, therefore any residual splitting is very likely due to anisotropy in the lowermost mantle alone. The splitting data reveal a complex pattern of anisotropy in the lowermost mantle. We test the ability of the flow model TX2008 (Simmons et al., 2009) to fit the observations. This is achieved by modelling the development of a lattice preferred orientation texture of a post-perovskite layer subject to the TX2008 flow field using a visco-plastic self consistent theory (Walker et al., 2011). Due to uncertainty in the slip system of post-perovskite three candidate slip systems are trialled: (100)/{110}, (010), and (001). The seismic anisotropy of these model layers is then probed using the finite frequency full wave field simulation code SPECFEM3D_GLOBE (Tromp et al., 2008). Using these synthetic seismograms we assess the ability of flow model TX2008 (assuming a post-perovskite lowermost mantle) to explain our observations, and determine which of the candidate slip systems fit the data best.

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