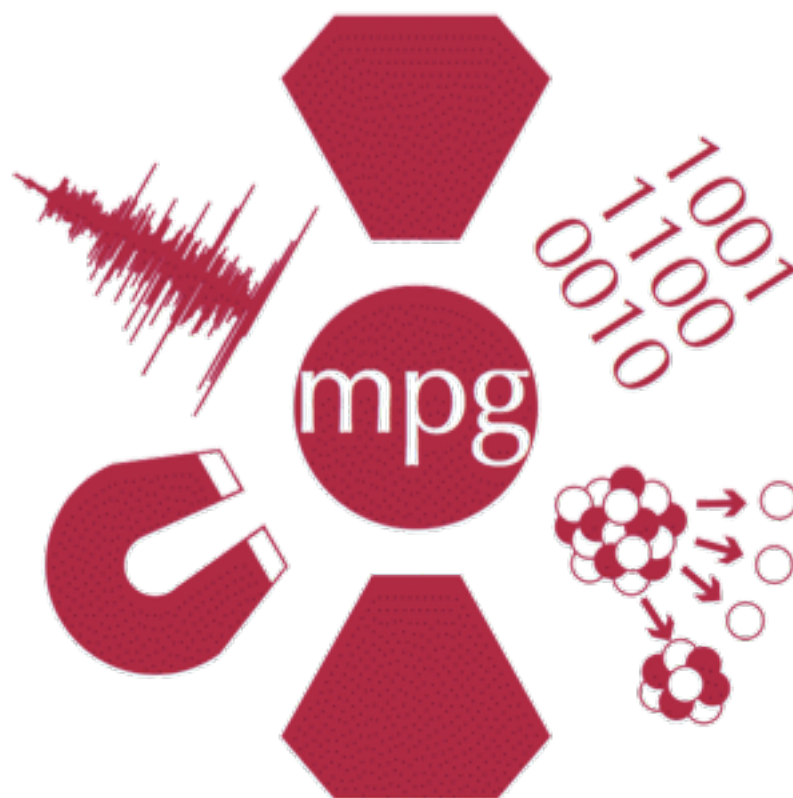


Mineral Physics Group

Research in Progress Meeting

Abstracts



**1st and 2nd November 2017 at the
University of Leeds**

Talks – November 1st

The formation of metallic cores in terrestrial planets: novel, time-resolved, in-situ observation of percolation under extreme conditions

G.D. Bromiley (University of Edinburgh), Madeleine Berg (University of Edinburgh), Yann Le Godec (Universite Pierre et Marie Curie), Mohammed Mesouar (European Synchrotron Radiation Facility), Jean-Philippe Perrillat (Universite Claude Bernard Lyon), Ian Butler (University of Edinburgh), Nicci Potts (University of Edinburgh)

Core formation represents one of the most significant events in the formation and evolution of the rocky (terrestrial) planets, large asteroids and moons of the inner solar system. Percolation, or the separation of Fe-rich liquids from solid silicate, has been invoked numerous times as a low-temperature mechanism for core formation under certain limiting conditions. Although this mechanism can explain various geochemical signatures of differentiation, the efficiency of percolation-driven core formation has yet to be demonstrated. Here, we describe the results of novel X-ray tomographic imaging experiments which provide time-resolved, micron-resolution 3-D imaging of core-formation processes under the extreme pressure-temperature conditions of planetary interiors. For the first time, we are able to directly extract data on melt migration velocities under extreme conditions. Experiments in various analogue systems demonstrate that percolation is a highly episodic, yet efficient mechanism for physically separating metallic melts, compatible with observed geochemical timescales for core-formation. As such, it is likely that core-formation in the inner solar system was a complex, multi-stage process which resulted in partial chemical disequilibrium between metallic cores and silicate mantles.

Sound velocities of fcc-Fe at lunar core conditions: result from ab initio calculations

M. C. Wood (University College London), L. Vočadlo (University College London), I. G. Wood (University College London)

Studies, such as the reanalysis of the Apollo lunar seismograms [1], have shown that the Moon has undergone differentiation and possesses a small core. The composition of the lunar core is not well constrained, and many compositional models have been suggested including combinations of iron, nickel, and light elements such as sulphur and carbon [e.g. 1, 2, 3, 4], and other more exotic compositions [5]. Additional constraints are crucial to our understanding of the Moon, including its formation, the dynamics of its interior, and a lunar dynamo.

We use ab initio molecular dynamics simulations to calculate elastic constants of face-centred cubic (fcc) iron and iron alloys and hence sound velocities at lunar core conditions, at ~5-6 GPa and ~1,300-1,900 K [3]. The results from these simulations will then be compared with the data from the Apollo seismograms and experimental data to help form a description of the lunar interior.

[1] Weber et al. (2011) *Science* 331, 309-312. [2] Dasgupta et al. (2009) *Geochim. Cosmochim. Acta* 73, 6678-6692. [3] Antonangeli et al. (2015) *Proc. Natl. Acad. Sci. U.S.A.* 112, 3916-3919. [4] Righter et al. (2017) *Earth Planet. Sci. Lett.* 463, 323-332. [5] Wicczorek & Zuber (2002) *Lunar Planet. Sci.* 33, abstract 1384.

Thermochemical solution properties of silicate liquids at extreme conditions and implications for the magma ocean.

Alfred Wilson (UCL)

All planetary bodies are evolved from a history of accretionary impacts, delivering mass and energy to an otherwise geologically closed system. These impacts generate melting proportional to impactor size. In the case of our moon formation, despite uncertainties regarding the nature of impact and subsequent satellite formation, widespread melting would have been unavoidable. Gaining a better understanding of the properties of a molten mantle system may allow us to contemporarily identify remnants of the magma ocean, in addition to learning how the present-day system evolved. However, the process by which the magma ocean crystallized is still uncertain, including the temperature of liquidus and solidus, crystallization sequence, and compositions of crystallizing phases. Here we take a novel approach towards constraining multi-component freezing equilibria via first principles molecular dynamics simulations. Our initial focus has been on computation of the entropy of silicate liquids. The entropy is inaccessible to standard molecular dynamics methods and is therefore a crucial missing ingredient in the first principles computation of phase equilibria. We have investigated methods of computing the two-body configurational entropy deficit, initially focusing on the MgSiO_3 - CaSiO_3 join. We show results for the absolute entropy and the entropy of mixing across the mantle pressure-temperature regime.

The lunar interior as a window into the early Earth.

N. J. Potts and G. D. Bromiley (The University of Edinburgh)

Olivine, and its high-pressure polymorphs, are thought to be the largest reservoirs of volatile material, including water and fluorine, on Earth. Cycling of volatiles between the Earth's interior and surface throughout geological time, however, has overprinted any primordial volatile signatures. As the Moon has no plate tectonics, it is expected that any volatile material present in the deep lunar interior would have been inherited during accretion and differentiation. Furthermore, it is now widely accepted that the Moon is mostly formed of proto-Earth material, or at the very least is geochemically indistinct from the Earth, making the Moon an appropriate analogue for the early Earth. Incorporation of trace elements into major minerals varies as a function of temperature, pressure, $f\text{O}_2$, and bulk composition. Experiments were, therefore, performed in a primitive lunar mantle composition, intended to replicate the initial stages of LMO solidification with some combination of olivine, pyroxene, and melt present, and run at relevant temperatures, pressures, and $f\text{O}_2$ (below the IW buffer). Mineral-melt partition coefficients (D_x) derived for volatile (F, Cl, S, H_2O) incorporation into olivine varies significantly compared to terrestrial studies. Preliminary results suggest that an order of magnitude more H_2O can partition into the lunar mantle compared to the terrestrial upper mantle. While an inverse trend between DF and DOH hints towards de-coupled substitution mechanisms between H and F under low- $f\text{O}_2$ /lunar bulk composition. These results suggest that if volatile material was present in the lunar magma ocean a significant proportion could be partitioned into the lower lunar mantle. The implications of this are not only important for understanding the delivery and behaviour of volatiles during planetary differentiation but would impact any future seismic study of the Moon.

The rheology of bridgmanite analogues: implications for the strength of the lower mantle

E. Mariani (University of Liverpool), P. Kaercher (University of Liverpool), J. Mecklenburgh (University of Manchester), M. Allen (University of Liverpool) and J. Wheeler (University of Liverpool)

The rheology of lower mantle minerals has direct influence on mantle viscosity and therefore affects a number of geophysical processes such as mantle mixing, formation of mantle plumes and hotspots, slab subduction and stagnation, and plate motion. Knowing which deformation mechanism(s) are most active in the lower mantle may help answer a number of outstanding questions such as: i) why slabs descend to different depths; ii) why the lower mantle is mostly isotropic despite the large strains predicted by convection models, iii) how can we refine our predictions of lower mantle viscosity. Experimental flow laws that describe the rheology of lower mantle minerals quantitatively should be used to underpin and better constrain current geophysical models. However, major limitations are: the challenges we are presented with when running deformation experiments at P-T conditions realistic for the lower mantle, and the lack of natural lower mantle samples exposed at the Earth's surface that could be studied to infer deformation history from microstructures.

As a valuable alternative we have synthesized and deformed neighborite (NaMgF_3), a low pressure analog of bridgmanite (MgSiO_3), the most abundant mineral in the lower mantle and the Earth. Neighborite was deformed at 200 MPa confining pressure and temperatures between 500-700°C in compression, using a Nimonic-type deformation apparatus, where strain rate and stress can be controlled and measured accurately, and flow laws determined reliably. In addition we have recovered samples and examined deformation microstructures in a scanning electron microscope, using electron backscatter diffraction. Mechanical results show a switch from linear-viscous deformation at lower stress (<50 MPa) to power law creep accommodated by grain boundary sliding at higher stress (>50 MPa). We also see strain weakening. Microstructures of samples deformed at a range of stresses show grain boundary migration recrystallization (likely from lower stress) and crystallographic preferred orientation with poles to (100) planes parallel to the compression direction (likely from higher stress). Further work is in progress to assess the role of grain size in the switch from power-law creep to linear-viscous flow. We compare our results to those of other bridgmanite analogs and bridgmanite itself and extrapolate to the slower, natural strain rates of Earth's mantle.

Rheology of olivine and ringwoodite/spinel structures in Co_2SiO_4 and Ni_2SiO_4

S.A. Hunt (UCL), A.R. Thomson (UCL), M.G. Pamato (UCL), I.S. Ezad (UCL), J. Van Driel (UCL), R. Wang (China University of Geosciences)

The polymorphs of $(\text{Fe,Mg})_2\text{SiO}_4$ (olivine, wadsleyite and ringwoodite) form ~60% of the Earth's mantle to ~660 km depth. The rheology of these three phases plays a significant role in controlling the dynamics of the Earth's mantle and has implications for the origins of deep focus Earthquakes. Each of the three polymorphs has a different crystal structure and therefore different physical properties, including rheology.

The importance of olivine rheology is reflected in the large body of work investigating it over multiple decades. The rheology of wadsleyite and ringwoodite, while equally important, has not been so comprehensively studied because of the historic difficulty of performing controlled strain-rate deformation experiments under the stability conditions of the higher pressure phases. Recent studies investigating the rheology

of wadsleyite and ringwoodite [e.g. 1,2] do not directly compare their strengths to that of olivine. To date there is only one study directly comparing the strengths of the $(\text{Fe,Mg})_2\text{SiO}_4$ polymorphs [3], which demonstrated that at low temperatures ($\leq 800^\circ\text{C}$) olivine is significantly weaker than its higher pressure polymorphs. However, these experiments were stress-relaxation experiments.

To investigate the strength of the transition-zone, we have deformed olivine and spinel structured Ni_2SiO_4 and Co_2SiO_4 against MgO. Each sample and the MgO are deformed simultaneously in a single experiment and the ratio of their strains gives the relative strength. We have done this both with synchrotron data (Co_2SiO_4) and by recovery (Ni_2SiO_4). We find that the spinel structure is stronger than olivine in both cases.

1: Hustoft et al., 2012, Earth Planet. Sci. Lett. 361, 7

2: Kawazoe et al., 2010, J. Earth Sci. 21, 517

3: Chen et al., 1998, Geophys. Res. Lett., 25, 575

Water, viscosity and mantle convection: the effects of weakening and mixing

K. Chotalia (UCL), C. Lithgow-Bertelloni (UCL), Neil Cagney (UCL), John Brodholt (UCL)

The effect of water on mantle minerals and their viscosity is complex. Experimental work such as that by Mei & Kohlstedt (2000) has shown significant rheological weakening with the addition of a few hundred ppm water contributing up to several orders of magnitude reduction in viscosity. The impact on thermal evolution and water cycling has been investigated in parametrised and two-dimensional models e.g. Crowley et al., (2011) and Nakagawa et al., (2015). However, the impact of different viscosity laws is often overlooked.

We examine mantle evolution arising from the implementation of viscosity laws with varying sensitivities to water content. The model, based on Crowley et al., (2011), solves for the conservation of energy and mass across the mantle and a surface ocean. Parametrised models also assume that subducted material is instantaneously incorporated into the mantle. We investigate the role of a time delay due to mixing, a process not readily implemented into these models.

Preliminary results show greater present day temperatures due to degassing. Degassing increases viscosity and the stiff mantle convects slowly allowing periods of heating. This increases temperature and reduces viscosity cooling the mantle $\sim 500^\circ\text{C}$ from 1 to 4.6 Gyrs. A water independent viscosity law loses 600°C , a value greater than the upper limit of 500°C from petrology and geochemistry (Grove & Parman 2004; Condie et al. 2016). This suggests that a water dependent viscosity law is required to obtain mantle temperature changes between the expected 200°C and 500°C .

Talks – November 2nd

Magnetic microscopy of metallic meteorites: probing the magnetic state of the early solar system

R.J. Harrison (University of Cambridge)

Meteorites are fragments of asteroids. They represent the oldest and most primitive materials in the solar system – rubble left over after the planets formed over four and half billion years ago. Information about the magnetic state of asteroids during the early solar system can, in principle, be recovered from meteorites. The paleomagnetic potential of meteoritic metal has been overlooked in the past, due to the fact that they are mostly comprised of kamacite (a soft magnet that makes a notoriously poor paleomagnetic recorder). Recent research, however, has uncovered regions buried within the Widmanstätten pattern that can capture reliable records of magnetic activity on asteroid bodies. This discovery, combined with the advent of high-resolution magnetic imaging methods, has allowed us to decipher the magnetic signals encoded within meteoritic metal for the very first time. Our attention has focussed on the ‘cloudy zone’: a region just a few microns wide lying next to the kamacite lamellae that define the Widmanstätten pattern. The cloudy zone consists of a tightly packed array of nanoscale islands of tetrataenite, an ordered Fe_{0.5}Ni_{0.5} phase that forms by the diffusive rearrangement of Fe and Ni atoms into alternating layers during slow cooling. The high intrinsic coercivity (> 2 Tesla) of tetrataenite makes it an excellent permanent magnet. Each island is ~100 nm or less in diameter, and is uniformly magnetised in one of six crystallographically defined directions. The proportions of islands magnetised in each direction are biased by interaction with the magnetic field of the asteroid. This bias is detected using X-ray photo-emission electron microscopy (XPEEM). Magnetic contrast is obtained using circularly polarised X-rays incident at a glancing angle to the surface, exploiting the resulting X-ray magnetic circular dichroism (XMCD) signal to reveal intricate nanoscale domains within the cloudy zone. Combined with extensive image simulations, quantitative information about the magnetic state of the asteroid can be extracted from the data.

Grain growth kinetics of ringwoodite and majorite garnet mixtures and implications for the rheology of the transition zone.

I. S. Ezad (University College London), D. P. Dobson (University College London), J. P. Brodholt (University College London), S. A. Hunt (University College London), A. R. Thomson (University College London)

The grain size of the mantle is a poorly known but important geophysical parameter. Among others, the grain size may control the rheology, seismic attenuation and radiative thermal conductivity of the mantle. However, the grain size of the transition zone minerals ringwoodite (Mg,Fe)₂SiO₄ and majorite garnet MgSiO₃ under appropriate zone conditions is currently unknown and there are very few experiments with which to constrain it. In order to determine the grain size of the transition zone, the grain growth kinetics must be determined for a range of mantle compositions. We have, therefore, experimentally determined the grain growth kinetics of the lowermost transition zone minerals through multi anvil experiments at University College London (UCL). This is achieved through a comprehensive set of time series experiments at pressures of 21 GPa and temperatures relevant to the transition

zone. We also determined the effect of varying water content, oxygen fugacity, iron content and aluminium content (Dobson and Mariani, 2014). Our initial grain growth experiments conducted at 1200°C and 1400°C at 18 GPa show extremely slow grain growth kinetics; time series experiments extended to 105.8 seconds are unable to produce grains larger than 100 nm. This suggests that fine-grained material at the base of the transition zone will persist on geological timescales. Such small grains size suggests that diffusion creep might be the dominant deformation mechanism in this region.

Dobson, D.P., Mariani, E., 2014. The kinetics of the reaction of majorite plus ferropicrinite to ringwoodite: Implications for mantle upwellings crossing the 660 km discontinuity. *Earth Planet. Sci. Lett.* 408, 110–118. doi:10.1016/j.epsl.2014.10.009

Making and Breaking of Minerals, Rocks and Planets: A Textural Perspective

Sandra Piazzolo (University of Leeds), Patrick Trimby (Oxford Instruments)

In the geosciences, textures along with spatially controlled crystallographic orientation analysis is mainly used for deformation studies in the crystal-plastic field. In these studies, the main interest lies either in deciphering the underlying processes of strain localization or in the geophysical expression of textures. However, in other research areas, orientation relationships can be just as important. In the field of biomineralization, textural analysis shows that there is a distinct interplay between crystal growth regulated by the organism itself and subsequent growth governed by the physics of crystal growth alone. The product is of exceptional strength and toughness.

Geological materials are commonly polymineralic and through in-flux of hydrous fluid, melt or gas reactions occur at variable temperature and pressure conditions. In many cases, the sequence of reactions and their progression is pivotal to our understanding in Earths' or Planetary Evolution.

The possibility to combine textural analysis with chemical analysis at a similar scale allows for new exciting avenues of research. For example, the replacement reaction of a mineral (e.g. KBr) by another similarly structured mineral (e.g. KCl) results in textural relationships that can be easily misinterpreted as microstructures originating from crystal plastic deformation unless the orientation relationships are studied in detail (1). Similarly, if a feldspar, the most common mineral in the lower crust of the Earth, reacts with a fluid, it will form complicated reaction and inclusion textures, which if analyzed in detail can be used to determine the relative sequence of events (2).

The advent of Transmission Kikuchi Diffraction enabling orientation and chemical analysis at the nanometer scale (3) opens up new research fields, promising to transform our understanding of geological processes at a fundamental level. Details of inter- and intragrain crystallographic orientation relationships can help to determine if the enigmatic diamond aggregate "carbonado" has an extraterrestrial or terrestrial origin (4). Furthermore, in-depth analysis of nanoscale reaction rims open up new avenues to understanding deep mantle processes. Magnetite growth at the interface between pyrrhotite and diamond, allows for the first time to pinpoint the details of the carbon cycle deep within the mantle (5). In fault zones nanoscale deformation structures are common deciphering their origin and rheological consequence is essential for hazard management. Preliminary data on experimental carbonate rich fault rocks show that during subseismic slip twin formation and dislocation accumulation at grain boundaries along with brittle failure result in the production of a weak texture and nanoscale particles. Further deformation results in

mechanically dissociation producing amorphous carbon. However, different to common believe, little rheological weakening occurs with these processes.

- [1] Spruzeniece et al. (2017) Nat Comms 8.
- [2] Spruzeniece et al. (in press) Journal of Metamorphic Petrology
- [3] Trimby (2012) Ultramicroscopy, 120, 16
- [4] Piazzolo et al. (2016) Lithos, 265, 244
- [5] Jacob et al. (2016) Nat. Comms. 7.

Effect of pressure on shear coupled grain boundary migration

J. van Driel and J. Brodholt (University College London)

Grain boundary sliding has been proposed as a possible mechanism for both attenuation and anelasticity within the earths interior [1]. We simulate shear coupled grain boundary motion, which involves a displacement both parallel and perpendicular to the grain boundary. Although we shall primarily focus on grain boundary sliding achieved by the parallel motion of the two adjacent grains, migration perpendicular to the surface also has implications of grain boundary mobility and grain growth. We use the climbing image nudge elastic band to calculate the migration energy (MEB) barrier [2] for a range of pressures from 0 - 120 GPa on three separate MgO twin grain boundaries, 210/[001], 310/[001] and 410/[001]. We find the that effects of pressure and orientation on MgO grain boundary MEBs are non-linear, containing peaks at finite pressures.

- [1] Grain-size-sensitive seismic wave attenuation in polycrystalline olivine, Jackson et al, 2002
- [2] Migration energy barriers of symmetric tilt grain boundaries in body-centered cubic metal Fe, Wu et al, 2015

Stress and mineral transformation

J. Wheeler

How stress affects chemical process - the fundamental thermodynamic basis

The potential for mineralogical mapping through machine learning

Joshua .F. Einsle, R.J. Harrison, B. Martineau, I. Buisman¹, A.M. Piotrowski, S.M. Collins, Z. Saghi, D. Johnstone, A. Eggeman and P.A. Midgley

Modern electron microscopes offer a variety of techniques for mapping chemical and crystallographic information in geological samples from micrometre to nanometre scales in both two and three dimensions. A typical data set comprises hundreds of thousands of spectra acquired pixel by pixel as the electron beam scans over the specimen. Routine analysis procedures include background subtraction, peak identification and quantification. This work highlights the application and benefits of machine learning to identify and extract the essential features that describe the mineralogical system being examined. Application of data decomposition techniques (similar to principal component analysis, PCA) to multidimensional data sets reveals key and often overlooked features. This presentation presents several different

geological systems, which provide unique analytical challenges, which are directly addressed through the use of machine learning.

In the first example, scanning electron microscope energy dispersive spectroscopic (SEM-EDS) maps of a symplectite texture from the Bushveld large igneous province demonstrates both the power of machine learning to pull out mineral phases, but also the limitations of EDS as technique for mineralogical classification. The decomposition method of non-negative matrix factorisation (NMF) identifies four unique mineral phases. Due to the compositional similarity of many minerals, EDS characterisation does not fully describe a mineral system, as spectrographic data does not include any crystallographic information. Crystal structure is the other key bit of information to uniquely identify a mineral phase. This highlights the need for combining composition information with crystallographic data.

For the second part of the presentation, I address the limitations of EDS only characterization, by presenting a comparative studies of the cloudy zone in the Tazewell IIICD iron meteorite to produces a complete chemical and crystallographic characterisation of this nanoscale intergrowth. Three-dimensional physical features found in the cloudy zone combine with decomposition of the EDS spectra to produce quantification of the constituent mineral phases that are within 2 % of atom probe tomography results. Cluster analysis of the scanning precession electron diffraction maps enables identification of a Fe_7Ni structure in the matrix phase of the cloudy zone. This combination of EDS with diffraction information demonstrates the potential to combine analytical modalities for the complete mineralogical characterisation of a sample. These studies demonstrate the potential for multi-scale and multi-dimensional mineralogical characterisation using machine learning and electron microscopy.

Solubility of water in Ca-rich perovskite under lower mantle conditions

B. J. Heinen (University of Bristol), O. T. Lord (University of Bristol), M. J. Walter (University of Bristol)

The nature of the deep Earth water cycle has an important impact on physical and chemical geodynamics. Water in the mantle can exist in small degree melts, as hydrous phases or stored within the crystal structures of nominally anhydrous minerals (NAMs). The mass of the lower mantle is so great that the presence of even a few hundred ppm of H_2O results in a huge bulk reservoir. Determining the solubility of water in lower mantle NAMs provides constraints on the bulk water storage capacity of the deep Earth. Perovskite structured phases are important in both peridotitic and mafic lithologies throughout the lower mantle. Here we consider calcium-rich perovskite, which constitutes up to 30% of subducted oceanic crust and ~7% of peridotitic lower-mantle. CaSiO_3 perovskite is unstable at ambient conditions and so we use CaTiO_3 perovskite as a structural analogue. CaTiO_3 perovskites were synthesised from bulk compositions with 0–10000 ppm H_2O at 50 GPa and ~1800 K in the laser-heated diamond anvil cell. Run products were quenched to ambient conditions and analysed by synchrotron micro-X-Ray diffraction at beamline I15 of the Diamond Light Source, UK. An increase in unit cell volume is observed with the addition of water, and the location of a plateau constrains water solubility to ~0.5 wt.% H_2O . If CaSiO_3 perovskite can dissolve similar amounts of water, these early results suggest calcium perovskite may comprise over 85% of the lower mantle hydrogen reservoir.

Ab initio calculations on and iron alloys at inner core conditions

L.Vocadlo, Y.Li, B.Martorell, J.Brodholt, I.Wood

Although one third of the mass of our planet resides in its metallic core, fundamental properties such as its chemical composition and internal structure remain poorly known. While it is well established that the inner core consists of iron with some alloying lighter element(s), the crystal structure of the iron and the nature and concentrations of the light element(s) involved remain controversial. To date, no candidate composition for the inner core has been able to match both the density and seismic wave velocities observed by seismology. In particular, seismically observed shear waves show unexpectedly low propagation velocities through the inner core. Unfortunately, the extreme conditions of pressure (up to 360 GPa) and temperature (up to 6000 K) required make results from laboratory experiments tricky. An alternative and complementary approach is computational mineral physics, which uses computer simulations of materials at inner core conditions. We find that while binary alloys do not match the observations, there are a range of ternary and quaternary alloys that do match the seismology. Interestingly, carbon is always a necessary component of these alloys, since C has the greatest effect on the elastic moduli. This is the first time that V_P , V_s and the density of the inner core have been matched directly with an hcp-Fe alloy.

Posters – November 1st

The Structure of Naturally Hydrated Ferrihydrite

H. F. Chappell (University of Leeds) and W. Thom (University of Cambridge)

Ferrihydrite is an amorphous iron oxide, ubiquitous in the environment and important in the metabolism and regulation of iron in humans, animals, plants and bacteria. In this study, first principles modelling and neutron diffraction are used together to generate a model of naturally hydrated nanoparticulate ferrihydrite. We show that a single-phase model can account for all the analytical data without breaking any of the rules of coordination chemistry. Previously, a more complex three-phase model was proposed to account for anomalies, now resolved, in the best single-phase model.

Novel microstructural analysis of slip systems in olivine and orthopyroxene

C. Gregson (University of Bristol) and J. Wheeler (University of Liverpool)

Active slip-systems of dislocations in upper mantle minerals have a fundamental control on intracrystalline plastic deformation driven by dislocation creep processes. This deformation is a key factor in understanding upper mantle rheology that controls large scale geodynamic processes such as plate tectonics. Deduction of slip-systems in mantle minerals is significant yet the techniques to quantify dislocation densities, distribution and types are limited. This has proved difficult in determining active slip-systems. The recent development of the Weighted Burgers Vector method, a mathematical analysis that utilises electron backscatter diffraction patterns to quantitatively examine dislocations densities in crystalline material, can help resolve this issue. This new approach can aid in the determination of active slip-systems by providing information on the slip direction vector of dislocation densities in subgrain wall in distorted grains, in particular olivine and orthopyroxene.

The effect of water on the postspinel transition

Joshua Muir (UCL) and John Brodholt (UCL)

The transition of ringwoodite to bridgmanite and periclase is a geologically important transition generally considered responsible for the '660' seismic discontinuity. Recent experimental investigations, however, have shown that this transition would likely occur at a depth that is too shallow and that the Clapeyron slope of the transition is too shallow to explain seismically observed variation in the discontinuity depth. The presence of water has been shown to have large effects on the rheology and phase stability of upper mantle minerals and thus it is a candidate to explain the discrepancies in the 660 discontinuity. There is, however, a lack of experimental evidence for its effect on lower mantle minerals due to the high temperatures and pressures required to investigate these structures.

In this study, therefore, we use DFT methods to calculate the transition of ringwoodite to bridgmanite and periclase under both dry and hydrated conditions and at the conditions of the 660 discontinuity. We find agreement with those who find a fairly shallow Clapeyron slope for the dry condition (~0.7 MPa/K). We also find that while water has a large effect on the phase diagram and causes significant broadening and deepening of the transition these effects are unlikely to be large enough to fully explain seismic variations seen in the mantle.

Deforming salt bodies and seismic anisotropy

Philipp Prasse (University of Bristol), James Wookey (University of Bristol), Michael Kendall (University of Bristol) and Martin Dutko (Rockfield Software Ltd)

The physical properties of salt make it to an important player in a number of industrial applications. Due to its low permeability, density and viscosity salt can often form hydrocarbon traps. The crystalline structure and texture of salt changes during this process, which can lead to effective seismic anisotropy. This study links the deformation of salt with seismic anisotropy. Numerical texture simulations of halite single crystals deformed in simple deformation regimes using the visco-plastic self-consistent approach (VPSC) show that high anisotropy can arise. In a next step this method were applied to a complex high-resolution salt diapir model, provided by our industrial partner Rockfield. High strain areas show high amount of seismic anisotropy. The results demonstrate that a significant degree of seismic anisotropy can be generated, validating the view that this should be accounted for in the treatment of seismic data in, for example, salt diapir settings.

Simulating the thermal conductivity of lower mantle bridgmanite as a function of temperature, pressure, and composition.

Ben Todd, Stephen Stackhouse, Andrew Walker, Jon Mound (University of Leeds)

Thermal conductivity is a key parameter for Earth models involving heat flow across the core-mantle boundary. It is not currently possible to experimentally measure the thermal conductivity of minerals at lower mantle temperatures, meaning that lower temperature values must be extrapolated, introducing considerable uncertainty. Furthermore, the effect of impurities, such as Fe, is poorly constrained.

In view of this, we use theoretical methods to determine the lattice thermal conductivity of (Fe,Mg)SiO₃ bridgmanite, with varying concentration of Fe impurities. We utilise the “direct method” (non-equilibrium molecular dynamics), which allows thermal conductivity to be calculated via Fourier’s law from the ratio of an imposed heat-flux and induced thermal gradient.

We find the thermal conductivity follows the expected trends, decreasing then saturating with increasing temperature and a linear increase with pressure. At low temperatures (1000 K) the conductivity results forma “trough” as a function of Fe impurities. At high temperatures (4000 K) adding any amount of Fe causes an abrupt decrease and subsequently saturation in the conductivity result.

This work aims to create a model of lower mantle thermal conductivity across all relevant conditions, with the goal of determining the heat flux from the Earth’s core to mantle.

Storage of hydrogen in ringwoodite

Andrew Thomson, Ross Piltz, Wilson Crichton, Valerio Cerantola, David Dobson, John Brodholt

The transition zone, between 410 km & 660 km depth, is believed to be the primary destination of subducted water [1], with the main transition zone minerals (wadsleyite and ringwoodite) capable of holding 1 - 3 wt.% H₂O in their crystal structures’. Geophysical observations of high attenuation and elevated conductivity suggest some areas of the transition zone are hydrated [2,3], whilst material rising and sinking out of the region appears to undergo dehydration melting [4,5]. Combined

with the observation of ~ 1.4 wt% H₂O in a diamond-hosted ringwoodite inclusion [6], it is probable that the transition zone is at least regionally, if not globally, “wet”.

Understanding the water concentration in the transition zone is critical, because water can induce partial melting, alter chemical partitioning and drastically change the creep strength/viscosity of rocks. The detailed effect of water’s presence will strongly depend on the hydrogen incorporation mechanism, i.e. whether it is exchange with Si⁴⁺, Mg²⁺, Fe²⁺ cations or whether it is coupled to Fe³⁺ cations in the crystal structure. However, due to a lack of suitable techniques it has not yet been possible to determine the crystallographic position of hydrogen in small samples recovered from high-pressure experiments. Recent developments in neutron single-crystal Laue diffraction now allow such measurements on crystals smaller than 0.1 mm³ [7]. Here we quantitatively study the incorporation of hydrogen in a synthetic iron-bearing ringwoodite. A multi-technique approach, with independent determination of chemistry, ferric iron content, water content and structure via x-ray and neutron diffraction, allows a detailed study of the hydrous ringwoodite structure and the incorporation mechanism of water throughout Earth’s transition zone.

- (1) Bercovici, & Karato, *Nature*. 425, 39–44 (2003).
- (2) Zhu et al., *EPSL*. 381, 1–11 (2013).
- (3) Kelbert et al., *Nature*. 460, 1003–1006 (2009).
- (4) Schmandt et al., *Science*. 344, 1265–1268 (2014)
- (5) Vinnik, & Farra, *EPSL*. 262, 398–412 (2007).
- (6) Pearson et al., *Nature*. 507, 221–224(2014).
- (7) Purevjav et al., *Sci. Rep.* 6, 34988 (2016).

Towards mineralogical models to constrain temperature variation in the lowermost mantle

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Three dimensional temperature variation in the lowermost mantle is diagnostic of the pattern of mantle convection and controls the extraction of heat from the outer core. Direct measurement of mantle temperature is impossible and the temperature in the lowermost mantle is poorly constrained. However, changing temperature indirectly, via modification to the density and elasticity, changes many geophysical observables and it is possible to determine how changing temperature alters these if mantle composition and the physical properties of mantle minerals is known.

Here we describe a scheme that allows seismic, geodynamic, and thermal properties of the core and mantle to be calculated given an assumed temperature (T) and mineralogy (X) of the mantle while making use of a self consistent parameterisation of the thermoelastic properties of mantle minerals. For a given T and X, this scheme allows us to determine the misfit between our model and observations for the long-wavelength surface geoid, core-mantle boundary topography, inner-core radius, total surface heat-flux and p- and s-wave tomography. The comparison is quick, taking much less than a second, and can accommodate uncertainty in the mineralogical parameterisation. This makes the scheme well-suited to use in a Bayesian approach to the determination of the long-wavelength temperature and composition of the lowermost mantle. We present some initial results from our model, which include the robust generation of a thermal boundary layer in the one-dimensional thermal structure.