Elasticity of ferropericlase through the pressure-induced high-spin to low-spin transition

J. Michael Brown - *University of Washington*
Earth and Space Sciences, Seattle, WA, 98195-1310
(206) 616 6058
brown@ess.washington.edu

Jonathan Crowhurst- *Lawrence Livermore National Laboratory*
L-350, Livermore, CA 94551
crowhurst1@llnl.gov

Alex Goncharov- *Geophysical Laboratory*
5251 Broad Branch Rd., N.W., Washington, D.C. 20015-1305
goncharov@gl.ciw.edu

Steven Jacobsen- *Northwestern University*
Department of Geological Sciences, Evanston, IL, 60208
steven@earth.northwestern.edu

We determined the pressure dependence of the single crystal elastic constants of ferropericlase ($Mg_{0.944}Fe_{0.056}O$) to a static pressure of 60 GPa. The velocities of the quasi-longitudinal and interfacial elastic wave were measured in the (100) crystal plane using impulsive stimulated light scattering. We observed anomalies in measured velocities over the pressure range of 40 to 60 GPa and associated them with the high-spin to low-spin (HSLS) transition in the Fe cations of ferropericlase. We find that all three elastic elements (c_{11}, c_{12}, c_{44}) smoothly pass through minima with respect to an extrapolation of the pure high-spin state. This behavior is consistent with a macroscopic thermodynamic description for the HSLS transition that predicts no sharp changes in spin fractions and dependent physical properties. The associated enthalpy and volume changes scale correctly between these data and literature compression data obtained on a sample with higher iron concentration. A significant geophysical consequence of the observed

behavior is that in the spin transition pressure regime, normal temperature derivatives of elasticity are reduced. Within Earth, a minimum in the temperature derivatives caused by the HSLS transition is predicted to occur at a depth of 1500 km. This correlates well with the depth where seismic tomographic results show minimum structure and model power. Thus, the HSLS transition may serve to mask velocity anomalies associated with lateral temperature differences.

A Bound on Heat Flow Below a Double Crossing of the Perovskite-Postperovskite Phase Transition

Bruce A. Buffett, Department of Geophysical Sciences, University of Chicago,
5734 S Ellis Avenue, Chicago, IL 60637 (buffett@geosci.uchicago.edu)

A double crossing of the perovskite-postperovskite phase transition in $(Mg,Fe)SiO_3$ has been proposed to explain seismic reflections from structures near the base of the mantle. Estimates of temperature inferred from the phase transitions can be extrapolated to the core-mantle boundary (CMB) using a simple model for the thermal boundary layer. However, a complication arises when flow is driven by the (negative) buoyancy of the postperovskite phase. Both latent heat effects and advective heat transport increase the temperature gradient and heat flow below the region of postperovskite. We obtain a minimum bound on the temperature gradient at the CMB by noting that the temperature gradient at the base of the postperovskite region must be at least as steep as the transition temperature with depth. A minimum bound on the local heat flow is 160 m W m^{-2}, given the seismically inferred geometry of the postperovskite region and a thermal conductivity of k=7 W K^{-1} m^{-1}. Such steep temperature gradients below a postperovskite region may yield an unrealistically high temperature at the top of the core unless restrictions are imposed on the values of the model parameters.

Imaging of structure at and near the core-mantle boundary

M.V. de Hoop, R.D. van der Hilst, P. Wang, L. Tenorio
and P. Ma

We discuss how imaging of the CMB and D'' can be accomplished using precursors and coda waves associated with ScS and SKKS. The use of these waves combined significantly improves the illumination of D'', while interfaces with a wavespeed drop beneath interfaces with a wavespeed increase will be better resolved. Moreover, we expect that a joint inversion of broad-band (transverse component) ScS and (radial component) SKKS wavefields and their precursors and coda will provide further insight in the anisotropy in the lower mantle.

THE EFFECT OF HYDROGEN ON THE IONIC DIFFUSION IN MANTLE MINERALS

SYLVIE DEMOUCHY – *LUNAR AND PLANETARY INST./USRA and UMN*
3600 BAY AREA BLVD, HOUSTON, TX 77058
612-626-0572
demou005@umn.edu

DAVID L. KOHLSTEDT – *UNIVERSITY OF MINNESOTA*
310 PILLSBURY DRIVE SE, MINNEAPOLIS, MN 55455
612-626-1544
dlkohl@umn.edu

Hydrogen substantially modifies many physical properties of minerals in Earth's mantle. Recently, it has been demonstrated that ionic self-diffusion and interdiffusion in olivine as well as in ferropericlase are significantly faster in the presence of hydrogen than in the absence of hydrogen. We detail here the results of experimental investigations of Mg-Fe interdiffusion under hydrous conditions in olivine, the most abundant mineral of the upper mantle and in ferropericlase the second most abundant mineral in the lower mantle. Annealing experiments under hydrous conditions were performed using a gas-medium pressure vessel at a confining pressure of 300 MPa over a temperature range of 1000o to 1250oC. The diffusion couples consisted of two oriented single crystal plates of different compositions. Each diffusion couple was placed in a Ni can, which controls the oxygen fugacity at Ni-NiO, together with a mixture of MgO and brucite powders. The presence of hydrogen in the sample was confirmed using Fourier-transform infrared spectroscopy. The Mg and Fe diffusion profiles were obtained with an electron microprobe. The interdiffusion coefficient was calculated from the Fe concentration as a function of position in the sample using the Boltzmann-Matano analysis. Our results indicate that Fe-Mg interdiffusivities are in both cases enhanced under hydrous conditions relative to under anhydrous conditions for similar composition in Fe.

These enhanced rates of interdiffusion are attributed to the increased concentration of metal vacancies resulting from the incorporation of hydrogen impurities as point defects into the crystal lattice.

Boundary Layers in the Mantle

Adam M. Dziewonski
Department of Earth and Planetary Sciences
Harvard University

This year marks the 30th anniversary of publication of the first global tomographic study and 25th anniversary of the discovery of a large degree-2 signal in the transition zone. In the subsequent years, there has been great progress in imaging of the Earth's interior both on the regional and local scale. However, most of the tomographic studies employed data sets that had satisfactory resolution either in a limited radial or horizontal extent. For example, the studies using teleseismic travel times do not have resolution in the upper mantle, even though using matrix conditioning methods it is possible to derive a "model" of the upper mantle. Similarly, some studies using surface waves presented detailed "models" at depths far exceeding resolution of the data used.

A data set that fills in the gap created by the limitations of the surface wave dispersion and teleseismic travel times data consists of the higher modes. They can be used either as a waveform inversion of body waves (since they represent a superposition of higher modes) or, after the decomposition of the body wave waveforms (van Heijst and Woodhouse, 1997), the laterally varying local eigenfrequencies of the first few overtones. The resolution increase through the introduction of this type of data is particularly important in the vicinity of the transition zone.

Only three modeling groups use the combination of all data types and, therefore, can resolve the structure with a sufficient radial resolution to identify the properties just above, within and just below the transition zone. These three groups are Berkeley (non-linear asymptotic coupling theory; Li and Romanowicz, 1996) with the most recent model by Panning and Romanowicz (2006), Harvard (path average approximation; Woodhouse and Dziewonski, 1984) with the most recent model by Kustowski et al. (2006) and Caltech/Oxford (separation of overtones; van Heist and Woodhouse, 1997) as represented by a model of Ritsema et al. (1999). These global models have a nominal horizontal resolution of about 1,000 km and variable radial resolution, from about 50 km below the Moho, 100-150 km in the asthenosphere and transition zone, and about 250 km in the middle and lowermost mantle.

These models show that there are three boundary layers in the mantle. The one near the surface is dominated by spherical harmonics up to degree 8, with the peak at degree 5. It ends between 200 and 250 km depth, after which the power spectrum is low and tends to be white. The second boundary layer is in the transition zone, where overall power increases and is clearly dominated by degree 2. The spectrum changes abruptly at the top of lower mantle, where it decreases in amplitude and becomes white; this character of the spectrum continues to about 2000 km depth. The third boundary layer has the maximum power near the CMB, it is dominated by degrees 2 and 3. These great wavelength velocity anomalies are not limited to the lowermost mantle, but extend to about 1000 km above the CMB and, perhaps, with a significantly diminished amplitude all the way to the transition zone. Because of this large radial extent it cannot be associated with phenomena such as the perovskite to post-perovskite transition.

The truly new information is the distinct termination of the surface boundary layer at about 225 km depth and the distinct character of the transition zone, which precludes continuous flow of the material across the upper-lower mantle boundary. It does not exclude an episodic (avalanches) or localized transport of the material. Indeed, there are three localized high-velocity anomalies under Indonesia, Fiji-Tonga and Chile-Argentina.

Workflows, Visualization, Web Service Generation

Gordon Erlebacher – *Florida State University*
489 Dirac Science Library, Tallahassee, FL 32306
Tel. (850) 644-0186/ FAX: (850) 644-0098
erlebach@scs.fsu.edu

Evan Bollig – *Florida State University*
489 Dirac Science Library, Tallahassee, FL 32306
Tel: (850) 644-1010/ FAX: (850) 644-0098
bollig@scs.fsu.edu

The vision of VLab is to make available a framework that allows scientists to perform their work in a collaborative manner, interacting through one or more web portals, and providing them with a wide range of tools to help them submit, track, analyze, visualize, and share their results. In this talk, we present an overview of three topics.

First, we describe a workflow visualizer. As a first step to tracking the job submissions and complex workflows inherent in the development and analysis of materials, we have developed a workflow visualizer, which allows users to view previously executed workflows and workflows in progress. Features include querying, interactive manipulation, and metadata viewing.

Second, we present a new tool developed to plot the data output from the phonon code that is a part of the Espresso package. Coded in Java and implemented as a WebStart application, users of the VLab portal can query data generated by this code and examine its results graphically.

Third, we present a new web service generator capable of translating Tcl scripts into web services. The WATT (Web Automation and Translation Toolkit) compiler generates C++ code, linked with gSoap stubs. Each Tcl procedures has a corresponding WebService procedure, callable from the client. We apply Watt to the task of representing three-dimensional charge density plots.

Incorporating seemingly disparate high resolution seismic findings in the context of deep mantle dynamics and chemistry

Edward J. Garnero
School of Earth and Space Exploration
Arizona State University
Tempe, AZ 85287-1404
Email: garnero@asu.edu
Web: http://garnero.asu.edu

The term "high resolution seismology" applied to Earth's lower mantle typically refers to regional analyses aimed at resolution of elastic structure at short lateral scale lengths, such as 100's of km or less. This type of information supplements the much longer wavelength patterns (e.g., 3000+ km) seen in global heterogeneity maps derived from tomographic inversions. As increasingly larger high quality data sets become available, e.g., the NSF-funded EarthScope's USArray, method development and refinement for more confidently characterizing the seismic wavefield at short wavelengths have come within grasp. These include a number of data organization, stacking and migration algorithms that were not possible with the sparser data sets of a decade ago. As a result, in the last few years, a number of detailed structural phenomena have been put forth from high resolution seismic studies.

Seismic findings include: a first order discontinuous shear velocity increase some 200-300 km above the core-mantle boundary (CMB), the so-called D" discontinuity, which contains significant topography. Beneath the Cocos plate / Central America region, an apparent 100 km step in the discontinuity has been imaged. A more subtle increase has been imaged in the central Pacific, within the large low shear velocity province (LLSVP). This increase has been attributed to the phase transition from perovskite (*Pv*) to post-perovskite (*pPv*). An exit from the *pPv* phase back to *Pv* is expected at greater depth, and advocated in some studies, though significant ambiguities may be present. A growing number of studies have found evidence for a sharp boundary between the LLSVPs beneath the Pacific and Africa, and the surrounding mantle. Chemically distinct LLSVPs appear to be the most parsimonious explanation for vertical boundaries or "edges". A number of studies have now documented thin ultra-low velocity zone (ULVZ) layering, some 10's of km thick, right at the CMB. The global distribution of ULVZs, however, is poorly resolved at present. Where best resolved, ULVZ properties are consistent with an origin of partial melt, which may relate to plume genesis. Dynamical studies suggest the hottest CMB regions may be near (and within) chemically distinct LLSVP boundaries, and hence the most significant ULVZ structures may be found there. Seismic wave speed anisotropy has been detected in a number of deep mantle regions, and may relate to convective flow.

Important uncertainties exist in studies of these and other phenomena (e.g., D" scattering, attenuation, CMB topography, etc.). In some cases, information from geodynamics and mineral physics helps to narrow the often large uncertainties in solution model space. In this presentation I will review the seismic information, which often involves extremely detailed information in isolated regions, and incorporate it in a global lower mantle framework. For example, the seismic findings increasingly support the notion of whole mantle convection with chemically distinct LLSVPs at the base, where plumes originate near LLSVP edges. Strong lateral temperature and chemistry variations can result in depth and strength perturbations of the *Pv*-to-*pPv* boundary that are consistent with those assigned to the seismically observed D" discontinuity. Where possible, this framework will be tied to global deep mantle long wavelength structure, as well as relevant phenomena imaged at mid-mantle depths.

Numerical modelling of shell tectonics during terrestrial planetary accretion

T.V. Gerya (1), J.R. Lin (2,1), P.J. Tackley (1), A.D. Yuen (3)

(1) Geophysical Fluid Dynamics Group, Institute of Geophysics, Department of Geosciences, ETH-Zurich, Switzerland (taras.gerya@erdw.ethz.ch)

(1) Institute of Oceanography, National Taiwan University, Taiwan(linj@erdw.ethz.ch)

(3) University of Minnesota Supercomputing Institute and Department of Geology and Geophysics, University of Minnesota, Minneapolis, USA

The early stages of terrestrial planetary accretion and differentiation are largely enigmatic and require extensive realistic numerical modelling efforts especially in 2D and 3D geometries. One of the hypothesised processes is destabilization of the cold undifferentiated core that builds up during "cold" accretion, by a surrounding liquid iron layer that builds up through iron segregation in a magma ocean, or by the accumulation of 'blobs' sinking from local magma ponds. This destabilization breaks the spherical symmetry of the planet and, therefore, can not be addressed properly in existing 1D models of accretion. We have developed a 2D thermomechanical numerical model of primordial core destabilization including self-gravity, visco-elasto-plastic rheology of materials, a free planetary surface and feedback from shear heating. By varying the size of the planet and metal/silicate ratio we tested various cases corresponding to early stages of terrestrial planet growth. Primordial core destabilisation causes rapid planetary scale reshaping that we call "shell tectonics" as the units involved in rearrangements are planetary shells. The gravitational redistribution process lasts for less then 1 Myr (depending on the effective rheology), being fully dominated by shear heating and thermal advection. Internal gravitational redistribution processes result in planetary shape-changing revealing significant transient aspherical deviations from the original perfectly spherical geometry. During this stage the primordial core can become exposed at the planetary surface making possible its reworking during ongoing accretion processes. Most of the enormous amount of heat is produced during this very short time span associated with the core-formation and is then chaotically distributed throughout both the core and the mantle. Gravitational energy dissipation along the localized deformation zones dramatically increases rates of rearrangement and can potentially result in thermal runaway processes and sudden primordial core fragmentation. The magnitude of thermal perturbations can reach several thousand degrees, which cataclysmically raises the effective Rayleigh number for the planetary mantle to a very large number favouring onset of powerful mantle convection and possibly results in the formation of a magma ocean with the molten mantle rocks rising from the deep planetary interior. In future work, such instabilities will be considered in the context of ongoing planetary accretion in 2D or 3D rather than starting from the end state of a 1D accretion model.

Molecular Dynamics Studies of $MgSiO_3$ Liquid to 150 GPa: Thermodynamics and Transport Properties

Mark S. Ghiorso
OFM Research–West, 7336 24th Ave NE, Seattle, WA. 98115

Dean Nevins, Frank J. Spera
Department of Earth Science, UC Santa Barbara, CA. 93106

Equilibrium Molecular Dynamics (MD) simulations are applied to molten $MgSiO_3$ using a Coulomb-Born-Mayer-van der Waals pair potential form and parameters from Oganov (2000) and Matsui (1994) to compute the thermodynamic and transport properties of this archetypical mantle silicate liquid. Experiments were performed using 8000 atoms and a 1 fs time step, with simulation durations of 50 ps for EOS development and analysis of atomic coordination statistics and 10 ns for calculation of shear viscosity. State points along isochores were computed every 500 K over a temperature range of 2500 – 5000 K to yield a grid of simulations spanning the pressure range 0 - 150 GPa. Atomic coordination statistics are determined by counting nearest neighbor configurations up to a cutoff distance defined by the first minima of the pair correlation function. The average coordination number (CN) of O about Si increases from IV at zero pressure to about VII in the highest-pressure simulations, while that of Mg increases over the same range from IV to VIII. Si[V] achieves maximal abundance at about 10 GPa. The CN of O about O varies congruently with the coordination environment of the cations up to pressures on the order of 70 GPa at which point the average O-O CN changes from XV to XI over a narrow pressure-temperature interval. The CNs of the Mg and Si vary smoothly and systematically over this interval and do not mimic the O-O nearest neighbor reconfiguration. Computed values of the internal energy and density are utilized to derive a thermodynamic model, following the method of Saika-Voivod et al. (2000), employing the equations of Rosenfeld and Tarazona (1998) and Vinet er al. (1986). The results of the Voivod-analysis indicate a liquid-liquid phase transition in the deeply supercooled region with a critical temperature close to 1050 K and critical pressure of about 1.5 GPa. Tracer diffusivity of Mg, Si and O have been fit to Arrhenian forms with pressure-dependant activation volumes reflecting profound changes in short range order as a function of pressure. The variation of shear viscosity with pressure along a mantle adiabat has been calculated.

Structural and spin transitions in Fe_2O_3

Dipta Bhanu Ghosh
DEMOCRITOS National Simulation Center
Via Beirut 2-4; Trieste 34014, Italy
Phone: +39 040 3787 477
Fax: +39 040 3787 528
Email: ghosh@sissa.it

Stefano de Gironcoli
SISSA - Scuola Internazionale Superiore di Studi Avanzati
& DEMOCRITOS National Simulation Center
Via Beirut 2-4; Trieste 34014, Italy
Phone: +39 040 3787 433
Fax: +39 040 3787 528
Email: degironc@sissa.it

Fe_2O_3 is a fascinating material displaying a number of structural phase transitions along with high spin to low spin transitions. The few theoretical studies reported so far shed light mainly on the α-Fe_2O_3 (corundum structure) phase which is the low pressure phase. The experimentally found high pressure phases and the high spin to low spin transition are yet to be addressed theoretically. In order to address and understand the underlying physics of these issues we have performed detailed calculations of the different possible candidate structures that might be stable at the relevant conditions. Results at the GGA level shed light on the sequence of the structural phase transitions. However, GGA is not sufficient to describe the other intricacies of Fe_2O_3. The GGA+U treatment is essential to properly describe the iso-structural spin transition, more realistic valence edge along with a sizable fundamental band gap.

THERMAL CONDUCTIVITY OF LOWER MANTLE MINERALS

ALEXANDER F. GONCHAROV, PIERRE BECK, BENJAMIN D. HAUGEN *,
VIKTOR V. STRUZHKIN, BURKHARD MILITZER
Geophysical Laboratory, Carnegie Institution of Washington,
5251 Broad Branch Rd., N.W., Washington, D.C. 20015-1305, USA
202-478-8900/8901, goncharov@gl.ciw.edu
*) *Department of Geological Sciences, University of Colorado*,
Boulder, Colorado 80302, USA (benjamin.haugen@colorado.edu)

STEVEN D. JACOBSEN,
Department of Earth and Planetary Sciences, Northwestern University,
Evanston, Illinois 60208, USA (steven@earth.northwestern.edu)

Optical absorption spectra have been measured at pressures up to 133 GPa for the lower-mantle oxide, (Mg,Fe)O and iron-bearing magnesium silicate perovskite, (Mg,Fe)SiO_3. Unlike (Mg,Fe)O, which shows a strong pressure dependence of absorption below and upon the high-spin (HS) to low-spin (LS) transition of Fe^{2+} (*Goncharov et al., 2006*), the pressure dependence of optical absorption in (Mg,Fe)SiO_3 is relatively weak. We observe a slight overall increase of the absorption coefficient in (Mg,Fe)SiO_3 in visible and infrared spectral range due to an increased and lower-energy shifted absorption in ultraviolet. Concomitantly, the crystal-field transitions of Fe^{2+} become weaker with pressure and disappear above 50 GPa as a result of the HS-LS transformation in (Mg,Fe)SiO_3, while the intervalence charge-transfer transition shifts to higher energies. The estimated total pressure dependent radiative conductivity is lower than expected from the pressure extrapolation of the ambient and low-pressure data (*Hofmeister, 2000*). Preliminary measurements of (Mg,Fe)O at high *P, T* conditions to 65 GPa and 800 K show a very weak temperature dependence of the optical absorption. Measurements of the thermal diffusivity of the mantle materials using time-resolved radiometry combined with a pulsed IR source (*Beck et al. submitted*) are in progress.

Goncharov, A. F., Struzhkin, V.V., and Jacobsen, S. D. (2006): Reduced radiative conductivity of low-spin (Mg,Fe)O in the lower mantle. *Science,* 312, 1205-1208.

Hofmeister, A. M. (2000): Mantle Values of Thermal Conductivity and the Geotherm from Phonon Lifetimes. *Science,* 283, 1699-1706.

Beck, P., A. F. Goncharov, V. Struzhkin, B. Militzer, H.-K. Mao, and R. J. Hemley (submitted): Flash heating high-pressure measurement of thermal diffusivity of materials in diamond cells.

PREDICTING A GLOBAL PEROVSKITE AND POST-PEROVSKITE PHASE BOUNDARY

Don Helmberger[1], Daoyuan Sun[1] Xiaodong Song[2], and Stephen P. Grand[3]
[1]Seismological Laboratory, California Institute of Technology
[2]Department of Geology, University of Illinois at Urbana-Champaign
[3]Department of Geological Sciences, University of Texas at Austin

Abstract

A lower mantle S-wave triplication with a S_{cd} branch occurring between S and ScS has been recognized for many years with a variety of explanations. It is particularly strong when sampling regions beneath the circum-Pacific lower mantle fast velocity belt seen in global tomographic models where it has been modeled with a 2-3% jump in S-velocity. General properties are; (1) it tends to arrive earlier beneath the fastest anomalies and (2) its rapid changes in strength and timing relative to S. The recently discovered Perovskite (Pv) to Post-perovskite (PPv) phase transition [*Murakami et al.*, 2004] is expected to show this change in timing assuming a positive Clapeyron slope (γ) between 3 to 9 MPa/K, however, the predicted velocity jump is about half of the above 1D modeling results. Here, we model the phase boundary height by mapping S-wave tomography into temperature assuming uniform chemistry, or a Mono-Phase-Transition (MPT), and a more complex mapping procedure involving possible changes in Chemistry (CPT). A few adjustable parameters involving reference phase boundary height and velocity jump are determined from comparing synthetic seismogram predictions with densely sampled observations. Particularly strong S_{cd} data are explained by focusing effects caused by small zones of enhanced velocities (slab buckling) seen in some tomographic models. These sharp features in S-wave tomography are confirmed by the behavior of differential PKP (AB-DF) which shows 4 s changes over a distance of 300 km correlating well with the corresponding S-wave models beneath Central America.

Hydrous partial melting of the upper mantle as judged from mineral/melt partition coefficients.

Marc. M. Hirschmann, Cyril Abaud, Tony Withers Dept. of Geology and Geophysics, University of Minnesota, Minneapolis, MN

It has been known for more than 10 years that nominally anhydrous minerals may incite small amounts of melting in Earth's mantle. In recent years, there has been a great increase in experimental data on the H_2O storage capacity of nominally anhydrous minerals. Yet, disagreement among models for the locus of dehydration melting in the upper mantle is growing rather than narrowing. Models span the gamut from requiring small amounts of hydrous melt throughout the upper mantle, to hydrous melting in a global low velocity zone layer at depths of ~80-200 km, to melting only beneath ridges and oceanic island in a restricted interval a few 10s of km beneath the locus of dry melting. These disagreements persist because direct experimental investigations of the influence of small amounts of H_2O on mantle melting are not feasible, and consequently understanding comes from parameterization of indirect experimental constraints.

One key constraint on the possible locus of hydrous melting in the upper mantle is the range of feasible concentrations of H_2O in near-solidus hydrous melts. For a mantle with a fixed amount of H_2O, $C_{\mathrm{H2O}}^{\mathrm{mantle}}$, the maximum H_2O concentration of an incipient partial melt is given by $C_{\mathrm{H2O}}^{\mathrm{mantle}} / D_{\mathrm{H2O}}^{\mathrm{peridotite/melt}}$, where $D_{\mathrm{H2O}}^{\mathrm{peridotite/melt}}$ is the equilibrium bulk partition coefficient between the peridotite mineral residue and the partial melt. Experimental determinations of $D_{\mathrm{H2O}}^{\mathrm{mineral/melt}}$ for upper mantle minerals have been made feasible by new low-blank ion probe measurements. Although thermodynamic calculations of $D_{\mathrm{H2O}}^{\mathrm{olivine/melt}}$ predict that it should depend on both pressure and H_2O concentration, such dependences are not apparent in the experimental data. Values for $D_{\mathrm{H2O}}^{\mathrm{garnet/melt}}$ span a wide range, and are apparently controlled by the concentration of minor elements in garnet, notably TiO_2. Finally, values for $D_{\mathrm{H2O}}^{\mathrm{pyroxene/melt}}$ depend strongly on the concentration of Al in pyroxene, and in particular on the abundance of tetrahedral Al in pyroxene.

Combining experimental constraints on $D_{\mathrm{H2O}}^{\mathrm{peridotite/melt}}$ with the modal proportions and compositions of minerals near the peridotite solidus, it is possible to estimate the H_2O concentration of incipient partial melts. For mantle with 100 ppm H_2O, such partial melts have 1.2 wt. % H_2O at 3 GPa and 2.3 wt.% at 7 GPa. Such modest concentrations of H_2O provide only small stabilization of melt relative to a dry peridotite system, thereby supporting the inference that dehydration partial melting of normal mantle is feasible only near where the dry peridotite solidus is approached, meaning immediately below the locus of dry melting beneath ridges and mantle plumes.

Measurements and Models of Thermal Transport Properties

Anne M. Hofmeister – *Dept. EPSc, Washington University*
1 Brookings Dr., St. Louis, MO 63130 USA
314-935-7440, fax 935-7361
hofmeist@wustl.edu

This report discusses new measurements and theory for various mechanisms of heat transport in the mantle. Misconceptions connected with decades of problematic data and historical development are discussed. Key parameters controlling heat flow in the Earth are emphasized and directions needed for effective progress are pointed out.

The vibrational component of heat transport in minerals is difficult to measure because they are transparent to near-IR light and are hard. Technology transfer of accurate (±2%), contact-free, laser-flash analysis (LFA) for measuring thermal diffusivity (*D*) from materials science and engineering to Earth science has revealed that previous geomaterials measurements of *D* contain substantial and systematic errors, and likewise for thermal conductivity (k=□$C_P D$). At 298 K, *D* is underestimated on average by 10% per thermal contact (e.g., sample with thermocouples). This error is offset as temperature (*T*) increases to spurious, direct radiative transfer. In LFA, using coatings and Mehling et al's. (1998) model removes unwanted radiative transfer. These opposing errors sum to provide erratic values in contact methods, but in general *D* is under-estimated at 298 K by up to 50% and overestimated by 800 K. In correcting contact data, formula for diffusive radiation were misapplied, adding prejudice. These problems exist in high pressure experiments, and are compounded by deformation and compression of pore space. Also, anisotropy is underestimated due to use of long cylinders in many contact measurements. True values of *D* and *k* from LFA data on minerals, glasses and melts show that these are effective conductors of heat. Theory has been benchmarked against bad data and the misconception that this anharmonic process can be represented by thermodynamic properties, which are mostly harmonic. Progress has been impeded by calculation of *k*, which involves convolution with C_P, rather than the simpler, more direct measure of transport, *D*, and by unsupported emphasis of acoustic modes, traceable to Debye.

Diffusive radiative transport ($k_{rad,dif}$), as occurs in the mantle, is not constrained by laboratory experiments, and is therefore calculated from spectroscopy. All models of diffusion by radiation are phenomenological because physical scattering limits the mean free path of the photons, i.e, $k_{rad,dif}$ is not a bulk material property. The most commonly applied formula $k_{rad,dif} \sim T^3$ is invalid for the mantle as it as it requires partial and uniform transparency over frequencies from 0 to ∞ (i.e., like graphite) and neglects physical scattering. The latest model accounts for scattering, back reflection, grain-size, and emissivity on . Spectral data of mantle materials needed for model input are inadequate, so results for olivine are generalized to other mantle phases at the expense of accuracy. For all phases, $k_{rad,dif}$ depends non-linearly on *T*, grain-size, and Fe content. Different regimes exist: for example radiative transfer is low for small grain-size and low for large Fe contents.

.

Determination of the hyperfine parameters of iron in aluminous $(Mg,Fe)SiO_3$ perovskite

Jennifer M. Jackson - *Caltech*
1200 E. California Blvd., M/C 252-21
626-395-6780
jackson@gps.caltech.edu

Knowledge of iron valences and spin states in silicate perovskite is relevant to our understanding of the physical and chemical properties ofEarth's lower mantle such as transport properties, mechanical behavior, and element partitioning. We will discuss recent experimental results on the hyperfine parameters of the iron component of an aluminous Fe-bearing silicate perovskite sample using synchrotron Moessbauer spectroscopy and laser heated diamond anvil cells at beamline 3-ID of the Advanced Photon Source. Evaluation of the spectra provide the isomer shift and the quadrupole splitting of the iron component in silicate perovskite, which gives information on valence and spin states under lower mantle conditions.

Thermoelastic Properties of Magnesiowüstite at Earth's Lower Mantle Conditions

C. R. S. da Silva[(1)], J. F. Justo[(1,2)], Z. Wu[(2)], T. Tsuchiya[(3)], and R. M. Wentzcovitch[(1,2)]

(1) Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455

(2) *Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455*

(3) *Geodynamics Research Center, Ehime University, Matsuyama, Ehime, 7908577, Japan*

Abstract

The thermoelastic properties of magnesiowüstite $(Mg_{1-x} Fe_x)O$ (x = 0.19), across the iron high to low spin transition, have been investigated by first principles calculations at the Earth's lower mantle conditions. The spin transition leads to dramatic effects on bulk and shear moduli. However, such transition occurs smoothly along a typical geotherm, spreading across most of the lower mantle. Additionally, the transition causes important variations in the seismic parameters, the ratios of bulk velocity ($R_{\phi/s}$) and density ($R_{\rho/s}$) anomalies. The results suggest that the spin transition in magnesiowüstite, and possibly in ferrosilicate perovskite, can explain the anticorrelation between bulk and shear wave velocities in the middle of the lower mantle.

GEODYNAMIC SIGNIFICANCE OF SEISMIC ANISOTROPY OF THE UPPER MANTLE: NEW INSIGHTS FROM LABORATORY STUDIES

SHUN-ICHIRO KARATO – *YALE UNIVERSITY*
DEPARTMENT OF GEOLOGY & GEOPHYSICS, NEW HAVEN, CT 06520
203-432-3147 (PHONE), 203-432-3134 (FAX)
shun-ichiro.karato@yale.edu

Seismic anisotropy is caused mainly by the lattice-preferred orientation of anisotropic minerals. Major breakthroughs have occurred in the study of lattice-preferred orientation (LPO) in olivine during the last ~10 years through large-strain, shear deformation experiments at high pressures. The role of water as well as stress, temperature, pressure and partial melting has been addressed. After reviewing published results, I conclude that the intrinsic effect of pressure on olivine LPO has not been demonstrated, so is the intrinsic effect of partial melting. However, the influence of water is well established: It is large and new results require major modifications to the geodynamic interpretation of seismic anisotropy in tectonically active regions such as subduction zones, asthenosphere and plumes. The main effect of partial melting on deformation fabrics is through the redistribution of water, not through any change in deformation geometry. A combination of new experimental results with seismological observations provides new insights into the distribution of water associated with plume-asthenosphere interaction, formation of oceanic lithosphere and subduction. In particular, anomalously strong V_{SH}/V_{SV} anisotropy together with the anomalously low electrical conductivity in the central Pacific suggests that the asthenosphere in this region contains unusually low water content. A plausible explanation is that hot and *wet* plume supply *dry* materials to the asthenosphere due to deep melting.

A Visualization Framework for Earth Materials Studies

Bijaya B Karki – *Louisiana State University*
Department of Computer Science, Department of Geology and Geophysics
225-5783197/225-5781465
karki@csc.lsu.edu

Ever larger amounts of data related to the structural, electronic and mechanical properties of Earth materials (in their solid and liquid phases) are routinely produced by massively parallel computer simulations. Such simulations are based on approaches ranging from the empirical molecular dynamics (MD) methods to the sophisticated first-principles molecular dynamics (FPMD) methods based on density functional theory (DFT). The simulated data, which are time-dependent and three-dimensional in the nature, are not illuminating by themselves; gaining insight into them is, however, a non-trivial task. In order to take advantage of maximal information contained in various data related to modeling of materials including those of direct geophysical relevance, we have been developing a scalable and adaptive visualization framework. Our approach aims to fulfill domain-specific needs thereby justifying the effectiveness of visualization for fundamental interdisciplinary science. The current activities include: 1) Interactive atomistic visualization at space-time multiresolution with on-the-fly extraction and rendering of a variety of data needed for a complex analysis. 2) Multiple datasets visualization (simultaneous rendering of more than one datasets to examine cross-correlations among them) based on isosurface extraction and hardware-assisted texture mapping/clipping methods. 3) Remote visualization with on-line reposition of multivariate elasticity data within the client-server paradigm. These visualization techniques are being integrated within the V-Lab computational framework.

Refactoring Finite Element Codes

Matthew G. Knepley - *Argonne National Laboratory*
9700 S Cass Ave., Chicago, IL 60439
630-252-1870
knepley@mcs.anl.gov

Historically, finite element codes were monolithic, single author applications which were slowly adapted over time. However, this prevented experimentation with novel elements, as well as comparison of the performance of different elements, since each new element had to be essentially written from scratch. The discretization could not be disentangled from mesh handling, and sometimes even the algebraic solver. This resembles the situation with Krylov solvers in the late 1980s. Eventually, a linear algebraic interface was adopted, independent of the underlying data structures, and different Krylov methods became interchangeable. We will present an interface inspired by the theory of fiber bundles on manifolds which allows finite element methods to be used interchangeably. An initial implementation is available as part of the PETSc libraries from ANL.

SEISMOLOGICAL TESTS OF POST-PEROVSKITE PRESENCE

THORNE LAY – *UC SANTA CRUZ*
EARTH AND PLANETARY SCIENCES DEPARTMENT
831-459-3164/3074(FAX)
thorne@pmc.ucsc.edu

The discovery of post-perovskite (pPv), the high pressure polymorph of $(Mg_x,Fe_{1-x})SiO_3$ perovskite (Pv), may have profound implications for the thermal, chemical and dynamical structure of the deep Earth, *if* it can be demonstrated that pPv currently exists in the lower mantle. The requisite basis for such a demonstration is seismological observation of elastic velocity and density structures diagnostic of or at least compatible with the expected properties of pPv occurrence in a realistic lower mantle chemical and thermal environment. A critical assessment of seismological observations versus predictions for a lower mantle model with pPv is undertaken, with the limitations and robust attributes of the seismological data being summarized. The existence of a seismic velocity discontinuity several hundred kilometers above the core-mantle boundary is a primary line of evidence for the presence of a Pv-pPv phase change. However, some attributes of the discontinuity, such as localized *P* wave reflections from a large *P* velocity increase and the sharpness of observed *P* and *S* velocity increases, reveal inconsistencies with expected properties of a Pv-pPv phase transition. Lateral variations in temperature can produce complex phase boundary structure that explains variable *S* wave observations, but such elastic heterogeneity intrinsically complicates testing the pPv hypothesis. The combination of rapidly expanding seismological data sets and new high resolution data analysis procedures reveal multiple seismic discontinuities near the base of the mantle; in some cases these may be consistent with forward and reverse Pv-pPv transformations, bounding a pPv layer or lens in D" above the CMB. Other phase changes or compositional contrasts could also be involved. At present, existence of pPv in the deep Earth is quite plausible, but not yet conclusively demonstrated. Future seismological and mineral physics research directions for further testing the hypothesis that pPv is present in the lower mantle are suggested.

Constraints on Mantle Composition from 1D Earth Models

Baosheng Li
Stony Brook University

Comparison of seismic 1D velocity-depth profiles with plausible compositional models can place constraints on the mineralogical composition of the Earth's mantle. In the upper mantle and transitions, one often infers olivine content is by matching the size and amplitude of 410- and 660-km discontinuities observed in regional or globally averaged seismic data (e.g., PREM, or AK135). With the advancement of acoustic techniques at high pressure and high temperature (e.g., Brillouin scattering and ultrasonic interferometry), bulk and shear properties at conditions relevant to upper mantle and transition-zone have become available for many mantle phases, including olivine and its polymorphs, pyroxenes (orthopyroxen and high-P clinopyroxene), majoritic garnet, CaSiO3 perovskite, magnesiowustite and MgSiO3 perovskite With these new data, we have compared the velocity and density profiles for two mantle compositional models, pyrolite and piclogite. We find that P and S wave velocities for pyrolite model along 1600K adiabatic geotherm provide an adequate explanation of the discontinuities and gradient, while piclogite provides a poor match at 400-500km depth. Based on the comparisons in the current study, a whole mantle convection model is favored than layered convection with chemical boundaries at 660 km depth.

Geophysical Implications of the Spin Transition in the Earth's Lower Mantle

Jung-Fu Lin – *Lawrence Livermore National Laboratory*
7000 East Avenue, Livermore, CA 94550
Tel: (925) 4244157
Fax: (925) 422-6594
afu@llnl.gov

Electronic spin-pairing transitions of iron and associated effects on the physical properties of host phases have been recently reported in lower-mantle minerals including ferropericlase, silicate perovskite, and possibly in post-perovskite at lower-mantle pressures. Geophysical relevance of the electronic spin transition is its effects on the physical and chemical properties of the lower-mantle phases. Here I will evaluate current understanding of the spin and valence states of iron in the lower-mantle phases, emphasizing the effects of the spin transitions on the density, sound velocities, and transport properties of the lower-mantle phases, mainly in ferropericlase. The spin transition of iron results in enhanced density, incompressibility, and sound velocities, and reduced radiative thermal conductivity in the low-spin ferropericlase, which should be considered in future geophysical and geodynamic modeling of the Earth's lower mantle. Evaluation of the experimental and theoretical pressure-volume results shows that the spin transition of iron results in a few percent increase in density in ferropericlase, thus allowing direct comparison to pressure, temperature, and compositional effects in the lower mantle. Along the lower-mantle geotherm, the spin crossover in ferropericlase and perhaps in perovskite would lead to an increasingly steeper than normal density and sound velocity gradients as compared to that without the spin crossover. The emerging picture of the Earth's deeper mantle indicates that previous models of lower-mantle from mineral physics data using high-spin ferropericlase and silicate perovskite are insufficient to correctly model the geophysical behavior in the lower mantle. This work was performed under the auspices of the U.S. DOE by UC\LLNL under Contract W-7405-Eng-48. UCRL-ABS-224133

IRON-RICH POST-PEROVSKITE SILICATE AT THE CORE-MANTLE BOUNDARY

WENDY MAO- *STANFORD UNIVERSITY*
450 SERRA MALL, BRAUN HALL BLDG 320, STANFORD, CA 94305
202-320-2025
WMAO@STANFORD.EDU

The Earth's D" layer, the lowermost 130 to 300 km of the silicate mantle, is a region with a complex seismic signature. One particularly enigmatic feature are areas of ultralow seismic velocities that have been observed at the base of D" where this boundary layer comes in contact with the liquid, iron-rich outer core. In a series of laser-heated diamond anvil cell experiments simulating the ultrahigh pressure-temperature conditions of the core-mantle boundary, we observed that a large amount of iron can be incorporated into the recently discovered post-perovskite (ppv) silicate phase, and that this significantly changes its properties relative to the pure $MgSiO_3$ endmember. We determined the aggregate compressional and shear wave velocities of this iron-rich silicate at high pressure and found that ppv with up to 40 mol% $FeSiO_3$ may be able to explain the properties seismically observed in ultra-low velocity zones.

Single-crystal elasticity of hydrous wadsleyite and implication for the Earth's transition zone

Zhu Mao[1], Steven D. Jacobsen[2], Fuming Jiang[1], Joseph R. Smyth[3], Christopher M. Holl[3], Daniel J. Frost[4], Thomas S. Duffy[1]

[1]Princeton University, Department of Geosciences, Princeton, NJ, 08540
[2]Northwestern University, Department of Geological Sciences, Evanston, IL 60208
[3]University of Colorado, Department of Geological Sciences, Boulder, CO 80309
[4]Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany

As a high-pressure polymorph of olivine, Wadsleyite (β-Mg_2SiO_4) is expected to be a dominant mineral in the transition zone from 410 km to 520 km depth in the mantle. Previous studies show wadsleyite can incorporate variable amounts of water up to greater than 3 wt% of water (Kohlstedt et al. 1996; Inoue et al. 1995; Smyth et al. 1987, 1994). Small amounts of water could strongly influence a number of physical properties of wadsleyite. The effects of water on the elasticity of wadsleyite are poorly known. We measured the single-crystal elastic constants of wadsleyites with 0.37 wt%, 0.84 wt% and 1.66 wt% H_2O at ambient conditions by Brillouin spectroscopy. By computing the aggregate elastic properties, we find that the bulk (K_{S0}) and shear modulus (G_0) of hydrous wadsleyite decrease linearly with water content according to the following relations: K_{S0}=170.3-12.4X_W; G=111.8-7.9X_W; where X_W is the water H_2O weight percent. Compared with anhydrous wadsleyite, 1 wt% of water will lead to 7.3% decrease in bulk modulus, 7.1% decrease in shear modulus. Water has a greater or comparable effect on the elastic moduli of wadsleyite as that of olivine or ringwoodite. To quantify the effect of pressure on the elasticity of hydrous wadsleyite, we also carried out Brillouin measurements for samples containing 0.84 wt% H_2O to 12 GPa. Pressure derivatives of bulk and shear moduli of hydrous wadsleyite are similar to the anhydrous phase: K_S'=4.2(1), G'=1.4(1). To evaluate the effect of H_2O on the 410-km discontinuity, we calculate the velocity contrast at 13.7 GPa along a 1400°C adiabatic. 10 mol% iron is assumed. We assume the pressure and temperature derivatives of aggregate elastic moduli of hydrous olivine are the same as anhydrous phase. The H_2O partition coefficient between olivine and wadsleyite is taken to be 2 (Frost and Dolejš 2007). Compared with a dry transition zone, 0.9 wt% H_2O in wadsleyite decreases the velocity contrast between wadsleyite and olivine from 10.4% to 8.5% for P wave velocity and from 11.9% to 9.3% for S wave velocity. Thus, 0.9 wt% H_2O in wadsleyite could decrease the velocity contrast by ~20%. For a pyrolite upper mantle (60 vol% olivine), 1.3 wt% (or 1.5 wt% determined by S wave) H_2O in wadsleyite is required to match the velocity contrast given by seismic model AK135. On the other hand, if the transition zone is considered to be water saturated which corresponds to 0.9 wt% H_2O in wadsleyite, 45-49 vol% olivine is needed to explain the magnitude of the 410-km discontinuity.

INTERMEDIATE-SPIN FERROUS IRON IN LOWER MANTLE PEROVSKITE

C. McCAMMON, I. KANTOR, O. NARYGINA, J. ROUQUETTE, L. DUBROVINSKY
BAYERISCHES GEOINSTTUT
UNIVERSITAET BAYREUTH, D-95440 BAYREUTH, GERMANY
TEL: +49-(0)921-553709; FAX: +49-(0)921-553769
catherine.mccammon@uni-bayreuth.de

U. PONKRATZ, I. SERGUEEV, M. MEZOUAR
EUROPEAN SYNCHROTRON RADIATION FACILITY
BP 220, F-38043 GRENOBLE CEDEX, FRANCE

V. PRAKAPENKA
CENTER FOR ADVANCED RADIATION SOURCES
UNIVERSITY OF CHICAGO, CHICAGO, IL 60637, USA

The lower mantle is dominated by iron-containing magnesium silicate perovskite, where the ability of iron to adopt multiple valence and spin states can affect a broad spectrum of physical and chemical properties. Conflicting results have been reported of iron spin transitions in silicate perovskite, but no interpretation has been found that is consistent with all of the data. We have conducted *in situ* high-pressure high-temperature Mössbauer and nuclear forward scattering (NFS) studies of $Mg_{0.88}Fe_{0.12}SiO_3$ and $Mg_{0.86}Fe_{0.14}Si_{0.98}Al_{0.02}O_3$ perovskite combined with high-resolution X-ray diffraction experiments that reconcile the controversy and show all existing data to be consistent with a high- to intermediate-spin transition of Fe^{2+} starting at approximately 30 GPa. High-temperature data show that elevated temperatures stabilise the intermediate-spin state; hence Fe^{2+} in silicate perovskite is inferred to be predominantly in the intermediate-spin state throughout most of the lower mantle.

Topology of the Post-Perovskite Phase Transition and Mantle Dynamics

Marc Monnereau – *University of Toulouse*
OMP, 14 avenue E. Belin, 31400 Toulouse, France
+33 561 332 968/+33 561 332 900
marc.monnereau@dtp.obs-mip.fr

Dave A. Yuen – *University of Minnesota*
Department of Geology and Geophysics,UMN, Minneapolis, MN 55455-0219, USA
daveyuen@gmail.com

The D" layer is a seismic structure whose complexity has remained puzzling for a long time. Interpreted in terms of post-perovskite boundary undulations, it would offer the chance to provide an absolute constraint on the temperature within the thermal boundary layer of the mantle. This would have great impact on our understanding of the dynamical state and thermal history of the earth. Concerted efforts recently have been devoted to sharpening the seismic imaging of D", but results remain interpreted in the framework of 1D thermal models. For instance, the recent seismological discovery of a possible double crossing is a strong indication that the core-mantle boundary (CMB) temperature would be higher than the temperature intercept T_{int}, which is the temperature of the post-perovskite phase change at the CMB pressure. This double crossing has also been used to constrain the temperature gradient at the base of the mantle, but numerical models of mantle convection show that the thickness of a thermal boundary layer greatly varies from one place, so that various different geotherms can account for this seismic observation.
The purpose of this study is to investigate through simple 3D spherical experiment of mantle convection how it is possible to draw any constraint on the thermal state of the deep mantle, as the core heat flux, from the topology of the post-perovskite. We have found a great sensitivity of the shape of the ppv surface from variations of different parameters such as the amount of internal heating, the Clapeyron slope, but also the temperature intercept. Three-dimensionnal spherical models of mantle convection that can satisfy the seismological constraints depend on the Clapeyron slope. At moderate value, 8MPa/K, the best fit is found with a core heat flow amounting 40% of the total heat budget (~15TW), whereas for 10 MPa/K the agreement is for a lower core heat flow (20%~7.5TW). In all cases these solutions correspond to temperature intercept 200K lower than the core-mantle boundary temperature. These models have holes of perovskite adjacent to post-perovskite in regions of hot upwellings.

First-Principles Study of Fe Spin Crossover in the Lower Mantle

Dane Morgan - University of Wisconsin, Madison
244 MSE, 1509 University Ave, Madison, WI 53706
608-265-5879, ddmorgan@wisc.edu

Amelia Bengtson - University of Wisconsin, Madison
137 MSE, 1509 University Ave, Madison, WI 53706
608-890-0968, akberta@wisc.edu

The lower mantle makes up approximately half the volume of the Earth and its material properties play a fundamental role in planetary dynamics. The lower mantle is known to be composed primarily of $(Mg,Fe,Al)(Si,Al)O_3$ perovskite and (Mg,Fe)O ferropericlase. The properties of these phases, particularly the Fe partitioning between them, may be strongly affected by recent discovery of a crossover from high- to low-spin Fe under lower mantle conditions. We use first-principles methods to study the spin crossover as a function of Fe composition in these two phases. We find a significant reduction in the effective volume of Fe upon the spin transition and that this plays a dominant role in the crossover. We also find a strong dependence of the spin crossover on composition and structure, including opposite compositional trends for perovskite compared to ferropericlase.

Deep Earth Viscosity: A New Test Based Upon the Impact of Variations in Earth's Rotational State Upon Holocene Relative Sea Level Histories

W. Richard Peltier, Department of Physics, University of Toronto, Canada

Analyses of the Earth's rotational response to the glaciation and deglaciation process of the Late Pleistocene ice-age have demonstrated that both the non-tidal acceleration of rotation and true polar wander components of this response are well explained as consequences of this ice-age influence. What has remained unclear until very recently is the fact that the latter of these impacts upon Earth rotation has a significant influence upon relative sea level history. The form of this feedback is characterized by a spatial pattern defined by a spherical harmonic of degree 2 and order 1. As I will show, this provides us with a means of testing whether or not the same radial viscosity structure that is required to fit the rotational observables themselves is able to properly predict the anomalies in relative sea level history recorded on radio-carbon dated relative sea level histories that are associated with the influence of "rotational feedback". As it happens the available data base of such measurements that has been assembled in Toronto contains a sufficient number of distinct time series from within each of the extrema of the degree 2 and order 1 pattern as to make possible an unambiguous identification of this influence. The fact that there exists no significant error in the predictions of the model that includes this feedback, across the 4 extrema of this pattern, provides direct evidence that the lateral heterogeneity of viscosity on such large spatial scales is negligible.

Open grid computing environments collaboration

Marlon Pierce
Community Grids Laboratory
Indiana University

The VLAB portal is based on the portlet component model that has been adopted by many scientific portal developers, including many participants in the TeraGrid Science Gateway program. One of the shortcomings of this model is that portlets, while reusable and sharable between development groups, provide a coarse component model that limits reusability. We thus need to complement this model with a finer grained component model that will enable us to build portlets out of reusable parts. To address this issue, we present our work developing Grid Tag Libraries and Beans (GTLaB), a set of software libraries that encapsulate common Grid client operations as XML tags. These are designed to enable portlet developers to more rapidly develop portlets and standalone web applications. We describe our work and provide a case study example of wrapping a simple science application workflow that can be encoded as a directed acyclic graph.

The transition zone and mid-mantle in regions of subduction

Justin Revenaugh - *University of Minnesota*
Geology and Geophysics
310 Pillsbury Dr. SE.
Minneapolis, MN 55455
612-624-7553
justinr@umn.edu

Anna Courtier - *University of Minnesota*
Geology and Geophysics
310 Pillsbury Dr. SE.
Minneapolis, MN 55455
612-624-7553
cour0090@umn.edu

We examine multiple *ScS* reverberation records of reflections from the transition zone and mid-mantle in three regions of active or recent subduction. In addition to the ubiquitous 410 and 660-km discontinuities, we find occasional evidence of a reflector near 520 km depth, a moderate-thickness low-velocity layer atop the 410-km discontinuity and a consistent set of mid-mantle reflectors. The latter appear restricted to subduction affected regions, and have estimated impedance increases on the order of 2 to 8 percent and median depths of ~900 and ~1150 km. Mantle water offers a consistent framework to interpret many of our observations, including coupled variability in the reflectivity of the 410 and 520 km discontinuities, possible melt just above the transition zone, and mid-mantle reflectors perhaps produced by lower-mantle slab dewatering accompanying the breakdown of superhydrous B and phase D. If the last inference is correct, slabs may deliver a non-trivial amount of water to the uppermost lower mantle.

Enabling Science with Grid Technology

JAMIE M. RINTELMAN – *STFC - DARESBURY LABORATORY*
KECKWICK LANE, DARESUBURY, WARRINGTON WA4 4AD GREAT BRITAIN
+44(0)1925-603 102
j.m.rintelman@dl.ac.uk

Kerstin Kleese – Van Dam - *STFC - DARESBURY LABORATORY*
KECKWICK LANE, DARESUBURY, WARRINGTON WA4 4AD GREAT BRITAIN
+44(0)1925-603 832
k.kleese-van-dam@stfc.ac.uk

As Grid technology matures it becomes more and more easy to adopt and more useful to a wider range of scientific applications. This talk will describe some of the approaches to job submission and data management developed at the Science and Technology Facilities Council eScience Centre. Particular emphasis will be placed on the scientific projects that have been performed with the aide of this technology. These include computational chemistry study of catalyst design, band theory studies of high T_c materials, and several applications of computational materials science.

Monte Carlo Simulations of Water Speciation in Hydrated Silica

J. Ilja Siepmann - *University of Minnesota*
Depts. of Chemistry and of Chem. Eng. & Mats. Sci., Minneapolis, MN 55455-0431
Phone: +1-612-624-1844
siepmann@chem.umn.edu

Kelly E. Anderson and Lorna C. Grauvilardell - *University of Minnesota*
Depts. of Chemistry and of Chem. Eng. & Mats. Sci., Minneapolis, MN 55455-0431
Phone: +1-612-624-7666
kanderson@chem.umn.edu and grauv002@umn.edu

Marc M. Hirschmann – *University of Minnesota*
Dept. of Geology and Geophysics
Phone: +1-612-625-6698
hirsc022@umn.edu

Understanding the phase behavior and properties of hydrated liquid silica under extreme conditions is of interest for gaining insight into Earth materials. The high melting temperature of silica, though, makes it difficult to study this phase, particularly at high pressure. Using Monte Carlo simulations and reactive potentials, we determine an equation of state for hydrated silica (with water mole fractions up to 0.4) at extreme conditions (up to 9000 K and 10 GPa) and examine the structure and chemical speciation in this system.

Correlation and Scaling of P and S Anomalies in D" Beneath Central America

Xiaodong Song – University of Illinois at Urbana-Champaign
Department of Geology, University of Illinois, Urbana, IL 61801
Phone: 217-333-1841, email: xsong@uiuc.edu

Global seismic tomography has produced consistent images of very large-scaled seismic structure of Earth's mantle over the last decade. However, details of smaller-scaled structure, such as slabs and plumes, differ. Most studies of the lowermost mantle region have focused on shear-wave structure, with the availability of differential S phases (S, ScS, and SKS). Because of different sensitivity of bulk and shear moduli to temperature and chemical composition, understanding the relative behavior of P and S velocities in the mantle is important to infer mantle properties in the lowermost mantle. We have recently examined a large collection of PKP data from earthquakes in S. America recorded at new broadband digital stations in China. The data provide dense samples of the lowermost mantle region beneath the Central America, where S structure has been intensively investigated over the decades, offering a rare opportunity to examine P and S anomalies of the lowermost mantle simultaneously. Observed PKP anomalies vary rapidly (by 2-4 s) over a narrow azimuthal range sampling the Central America. The general trends of PKP residuals correlate well with the predictions for Grand's S tomographic model. The good correlation makes it possible to use the 3D tomographic model as a reference model to map further finer structures. Our modeling reveals a sharp lateral boundary separating broad slow and fast anomalies. The result suggests evidence of subducted slabs reaching the deepest mantle. The slow anomalies may be the result of thermal chemical upwelling induced by the subducted slabs or the manifestation of the Pacific superplume at its edge. To obtain the scaling of P and S anomalies, we compare our PKP data with S tomographic predictions as well as dense raw S data directly. The ratio $R = d\ln V_s / d\ln V_p$ is estimated about 1.9. This value is not anomalous, comparable to values for mid-mantle and significantly less than estimated global average of 2.5 or larger for the lowermost mantle.

INVESTIGATING WATER IN THE DEEP EARTH BY DENSITY FUNCTIONAL THEORY

LARS STIXRUDE – *UNIVERSITY OF MICHIGAN*
Department of Geological Sciences, Ann Arbor, MI 48104
734-647-9071
stixrude@umich.edu

The amount of water contained in Earth's mantle and core may substantially exceed that in the surface oceans as suggested by observations of natural mantle samples, raising fundamental questions regarding the origin and evolution of Earth's hydrosphere. A crucial question is where deep water might be stored. Possible sites include hydrous phases, such as phyllosilicates and dense hydrous magnesian silicates, nominally anhydrous phases, such as olivine and its high-pressure polymorphs that can accommodate ~0.1 % H_2O by mass, and silicate melts. We have explored via first principles calculations all of these potential storage sites. Examples to be discussed include stishovite, in which Si may be replaced by Al+H up to several weight percent H_2O, $MgSiO_3$:Al+H perovskite, in which water solubility appears to be severely limited, the 10 Å phase, a hydrous phyllosilicate, which fills a crucial gap in pressure-temperature space allowing water to be transported in subducting slabs to greater depths, and hydrous silicate melt, which may be neutrally buoyant at the base of the upper mantle and the base of the lower mantle.

ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES IN IRON COMPOUNDS: SPIN-CROSSOVER EFFECTS.

VIKTOR V. STRUZHKIN
Geophysical Laboratory, Carnegie Institution of Washington,
5251 Broad Branch Rd., N.W., Washington, D.C. 20015-1305, USA
202-478-8900/8901, struzhkin@gl.ciw.edu

The active topic of current research in systems with strong electron correlations is high-pressure-induced insulator-metal transition (I-M), which is accompanied by the collapse of the magnetic moments. The oxides of transition metals present a very large class of materials, which are important for both fundamental science and practical applications. In these materials, the strong electron correlations play a crucial role in the formation of a variety of electronic and magnetic properties of the transition metal oxides. A qualitative picture of the electronic structure in several Fe^{2+} and Fe^{3+} materials at the spin-crossover transition will be presented, with the emphasis on novel physics emerging close to the insulator-metal transition regime. With all the progress in the experimental and theoretical developments, one of the simplest oxides, iron monoxide (FeO) remains one of the least understood materials. The high pressure behavior of FeO has been probed with advanced synchrotron techniques combined with four-probe transport measurements up to 200 GPa in a diamond anvil cells. The results of synchrotron Mössbauer spectroscopy (nuclear forward scattering -NFS), and electro-resistivity measurements suggest a complicated scenario of magnetic interactions governed by band-broadening effects.

PHONON DENSITY OF STATES AT THE SPIN CROSSOVER IN ($Mg_{0.75}Fe_{0.25}$)O FERROPERICLASE

WOLFGANG STURHAHN - *ARGONNE NATION LABORATORY*
9700 SOUTH CASS AVE, ARGONNE, IL 60439, USA
PHONE: (630) 252 0163
EMAIL: STURHAHN@ANL.GOV

Iron-bearing minerals of the Earth's lower mantle like ferropericlase and silicate perovskite have recently been studied to evaluate the presence of pressure-dependent crossovers between the high-spin and the low-spin state of iron. Such a crossover was clearly observed in ferropericlase using x-ray emission spectroscopy [1,2], conventional Mössbauer spectroscopy [3], and synchrotron Mössbauer spectroscopy [4]. In the case of silicate perovskite, the electronic state of the iron has been studied with x-ray emission spectroscopy [5,6] and synchrotron Mössbauer spectroscopy [7] but the situation remains unclear.

We applied nuclear resonant inelastic x-ray scattering to determine the vibrational density of states (VDOS) of Fe in ($Mg_{0.75}Fe_{0.25}$)O ferropericlase up to 110 GPa and observed a significant effect of the spin crossover on its elasticity and sound velocities that can be derived from the vibrational density of states [8]. Here we report Grüneisen parameters that are derived from the volume dependence of the VDOS and show a dramatic change when crossing over into the low-spin region.

This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357 and by NSF through COMPRES.

[1] Badro J. et al. (2003) Science 300, 789
[2] Lin J.-F. et al. (2005) Nature 436, 377
[3] Speziale S. et al. (2005) PNAS 102, 17918
[4] Lin J.-F. et al. (2006) Phys.Rev. B 73, 113107
[5] Li J. et al. (2004) PNAS 101, 14027
[6] Badro J. et al. (2004) Science 305, 383
[7] Jackson J.M. et al. (2005) American Mineral. 90, 199
[8] Lin J.-F. et al. (2006) Geophys.Res.Lett. 32, L22304

Infrared Reflectance of Ferropericlase ($Mg_{1-x}Fe_xO$): Experiment and Theory

Tao Sun - *SUNY at Stony Brook*
Dept. of Physics & Astronomy, Stony Brook, NY, 11794
631-632-4071
tsun@grad.physics.sunysb.edu

Philip B. Allen – *SUNY at Stony Brook*
Dept. of Physics & Astronomy, Stony Brook, NY, 11794

David G. Stahnke – *UC San Diego*
Dept. of Physics, La Jolla, CA 92093

Steven D. Jacobsen – *Northwestern University*
Dept. of Earth and Planetary Sciences, Evanston, IL, 60208

Christopher C. Homes – *Brookhaven National Laboratory*
Condensed Matter Physics & Materials Science Department, Upton, NY, 11973

The temperature dependence of the reflectance spectra of magnesium oxide (MgO) and ferropericlase ($Mg_{1-x}Fe_xO$, for x = 0.06 and x = 0.27) have been measured over a wide frequency range (≈ 50 to 32 000 cm^{-1}) at 295 and 6 K. The complex dielectric function has been determined from a Kramers-Kronig analysis of the reflectance. The spectra of the doped materials resemble pure MgO in the infrared region, but with much broader resonances. We use a shell model to calculate the dielectric function of ferropericlase, including both anharmonic phonon-phonon interactions and disorder scattering. These data are relevant to understanding the heat conductivity of ferropericlase in the earth's lower mantle.

DYNAMICAL IMPLICATIONS OF THE POST-PEROVSKITE PHASE TRANSITION

PAUL J. TACKLEY - ETH ZÜRICH
INSTITUTE FOR GEOPHYSICS, ETH HÖNGGERBERG HPP L13, 8093 ZÜRICH, SWITZERLAND
+41 446332758
PTACKLEY@ETHZ.CH

TAKASHI NAKAGAWA -KYUSHU UNIVERSITY
DEPARTMENT OF EARTH AND PLANETARY SCIENCES, KYUSHU UNIVERSITY, FUKUOKA, JAPAN
TEL: +81-92-642-2313; FAX: +81-92-642-2684
TAKASHI@GEO.KYUSHU-U.AC.JP

Since the discovery of the post-perovskite (PPV) phase transition, several researchers have investigated its possible implications for dynamics in the CMB region and its influence on the mantle above. The first thermal convection models to include it (Nakagawa and Tackley, GRL 2004; Matyska and Yuen, EPSL 2005) indicated a small dynamical effect in slightly destabilizing the lower thermal boundary layer, thereby increasing plume vigor and slightly increasing mantle temperature. As it has long been thought that seismic heterogeneities in the D" region might be caused partly by chemical variations, dynamical issues associated with a mixed thermal-chemical-phase boundary layer are reviewed here. If recent mineral physics data on the density of MORB are correct, a significant fraction of subducted MORB segregates into a layer above the CMB. A layer formed in this way is very heterogeneous and lacks a sharp, clean boundary, unlike layers inserted a priori into calculations. A layer may be global or in the form of intermittent 'piles' and has a large effect on both the mean value and the lateral variation of core heat flux. The post-perovskite transition has a destabilizing influence due to its positive Clapeyron slope, although this is partly offset by latent heat effects. Post-perovskite may occur in localized patches, or in a global, strongly undulating layer, depending on whether the CMB temperature is hot enough to be in the perovskite stability field. Post-perovskite regions may have near-vertical sharp edges, perhaps accounting for some seismic observations. Lateral variations in the occurrence of post-perovskite can cause seismic velocity variations larger than those caused by thermal or chemical variations. If the phase transition pressure is independent of composition, then regions containing a thick layer of post-perovskite are anticorrelated with regions containing thick accumulations of chemically-dense material, but if the PPV transition occurs at lower pressures in the dense material then it can also occur in ‘piles’. Heat flux across the CMB, as well as lateral variations in this heat flux, are strongly influenced by the presence of global or local chemical layering, but only mildly influenced by post-perovskite, and can be constrained by seismological observations of the post-perovskite boundary. Coupled models of core-mantle evolution taking into account these effects predict that radioactive potassium is needed in the core, in order to simultaneously allow the extraction of enough heat to drive the geodynamo while not growing the inner core to larger than its observed size.

Spin transition in Ferrous iron in $MgSiO_3$ Perovskite under Pressure

Koichiro Umemoto – *Minnesota Supercomputing Institute and Department of Chemical Engineering and Materials Science*, *University of Minnesota*
421 Washington Ave SE, Minneapolis, MN 55455, USA

umemoto@cems.umn.edu

We present a density functional study of the pressure induced spin transition in ferrous iron in $MgSiO_3$ perosvskite. We address the influence of iron concentration and configuration (structural and magnetic), as well as technical issues such as the nature of the exchange correlation (XC) functional (CA-LDA versus PBE-GGA) on the spin transition pressure. Supercells containing up to 160 atoms were adopted to tackle these issues. We show that there are preferred configurations for high-spin and low-spin iron and that the spin transition pressure depends strongly on iron concentration and XC functionals. We also address a structural change around Fe atoms accompanying the spin transition.

Research supported by NSF/EAR 013533, 0230319, and NSF/ITR 0428774 (VLab). Computations were performed at the Minnesota Supercomputing Institute and Indiana University's BigRed system.

Convection modeling of the postperovskite transition and Constraints on thermal conditions near the core mantle boundary

Arie van den Berg – Utrecht University, Dept.Earth Sciences
Inst.Earth Sciences, Budapestlaan 4, 3584 CD Utrecht, The Netherlands
(+31) 30 253 5072
berg@geo.uu.nl

David Yuen – University of Minnesota, Dept. Geology and Geophysics and
Minnesota Supercomputing Institute
Minneapolis, MN 55455-0219, United States
612 6249801
daveyuen@gmail.com

Recent seismological evidence links the irregular structure of the bottom D" zone of the Earth's mantle to the postperovskite phase transition. The possibility of delineating the phase boundary seismologically has made it possible to obtain temperature estimates at very close range from the Earth's core. Combined with an estimated temperature of the core-mantle boundary (cmb) this provides direct evidence for the structure of the bottom thermal boundary layer of the mantle, independent from estimates based on data from the transition zone interpolated across the depth of the lower mantle.

We have conducted mantle convection experiments with an extended Boussinesq model including the postperovskite phase transition. The experiments were focused on the structure of the phase boundary, in particular under conditions where the intercept temperature at the cmb is several hundred Kelvin below the cmb temperature, resulting in multiple crossings of the geotherm with the phase boundary.

Our convection results include regions with a thin bottom layer of perovskite underlying a thicker postperovskite layer where the phase transition is inside the thermal boundary layer at the cmb.

The modeling results clearly indicate the feasibility of estimating the local thermal gradient at the cmb from seismologically determined mapping of the bottom phase boundary. This opens the perspective of stronger constraints of the local heatflow from the Earth's core.

Earth's Deep Water Cycle

Suzan van der Lee
Northwestern University
Dept. Earth and Planetary Sciences
1850 Campus Dr.
Evanston IL 60208
1 847 491 8183
suzan@earth.northwestern.edu

Major minerals in the deep upper mantle and particularly in the transition zone can hold considerable quantities of hydrogen from water. Exactly how much there is and how this hydrogen affects the mineral's physical properties is a topic of current research. Observed seismic waves indeed show evidence of lateral variations in the depth, thickness, and jumps in seismic velocity of transition zone phase transitions in these minerals. Observed seismic waves also show clear evidence for regions of anomalous seismic velocity. Both types of evidence can be a result of spatial variations in hydrogen content; how much hydrogen is needed to explain the observations and how to discriminate the effects of hydrogen from those of heat are also topics of current research. I will discuss some of this recent and ongoing research on detecting water in the mantle and then focus on a seismic anomaly beneath the eastern margin of the US. This anomaly is a region of weakly reduced shear-wave velocity that stretches laterally in a direction parallel to the eastern margin and stretches vertically from the top of the lower mantle to lithospheric depths. In the lower mantle, this low S-velocity anomaly sits adjacent to and above an east-dipping high S-velocity region, which likely represents subducted lithosphere from the Farallon Plate. The least unlikely explanation for the low-velocity anomaly is that it is relatively hydrous, with up to 1 wt % of water above average. If this hydrous region is slightly buoyant, it could well up and hydrate the strong lithosphere at the currently passive margin between the North-American continent and Atlantic Ocean. If the lithosphere is sufficiently weakened by hydration it might give way to typical forces from ridge push and sediment loads to develop a new subduction zone. I will discuss implications of such a scenario for the evolution of plate tectonics.

Hydrogen bonding in minerals

Bjoern Winkler – *Johann Wolfgang Goethe Universitaet Frankfurt*
Geowissenschaften, FE Mineralogie / Kristallographie
+49 69 798 40107
b.winkler@kristall.uni-frankfurt.de

The influence of hydrogen bonding on structural and physical properties of hydrous and nominally anhydrous minerals is well established [1]. However, little is known about the pressure-induced changes of hydrogen bonds. The main problem is that even for hydrous minerals the determination of the positions of hydrogen atoms at high pressures is experimentally challenging, and hence often structure-property correlations established at ambient pressure are employed for the interpretation of spectroscopic measurements.

In the presentation, I will discuss our recent experimental and theoretical studies on hydrogen-bearing systems at high pressures. For diaspore, we have refined the structure at 50 GPa, and can correlate these findings with spectroscopic data and with lattice dynamical calculations. For zoisite and orthozoisite, the pressure-induced shifts of the OH-valence vibration are very different and this difference can be explained using density functional theory calculations. These results imply that a straight-forward application of structure-property correlations established at ambient pressures cannot be employed to infer the atomic arrangement of hydrogen bonds at high pressures. Also, our calculations on brucite indicate that to obtain realistic models of the hydrogen dynamics, conventional MD simulations may be inappropriate and instead alternatives such as path integral methods have to be used. Finally, I'll discuss the use of density functional theory calculations for the interpretation of resonant ultrasound spectra and discuss elasticity data for some hydrous and anhydrous minerals.

[1] Keppler, H and Smyth, JR (eds) (2006) Water in nominally anhydrous minerals. Rev. Min. Geochem., 62

SEISMIC WAVE ATTENUATION AND WATER IN THE LOWER MANTLE

MICHAEL WYSESSION – *WASHINGTON UNIVERSITY*
DEPT EARTH AND PLANETARY SCIENCES, CAMPUS BOX 1169,
ST. LOUIS, MO 63130
314-935-5625/314-935-7361
MICHAEL@SEISMO.WUSTL.EDU

JESSE FISHER LAWRENCE – *UCSD*
IGPP 0225, 9500 GILMAN DRIVE, LA JOLLA, CA 92093
858-822-5979/858-534-5332
JLAWRENCE@UCSD.EDU

We use seismic attenuation tomography to identify a region at the top of the lower mantle that displays very high attenuation consistent with an elevated water content. Tomography inversions with >80,000 differential travel-time and attenuation measurements yield 3D whole-mantle models of shear velocity (V_S) and shear quality factor (Q_μ). The global attenuation pattern is dominated by the location of subducting lithosphere. The lowest Q_μ anomaly in the whole mantle is observed at the top of the lower mantle (660-1400 km depth) beneath eastern Asia. The anomaly occupies a large region overlying the high-Q_μ sheet-like features interpreted as subducted oceanic lithosphere. Seismic velocities decrease only slightly in this region, suggesting that water content best explains the anomaly. The subducting of Pacific oceanic lithosphere beneath the eastern Asia likely remains cold enough to transport stable dense hydrous mineral phase D well into the lower mantle. We propose that the eventual decomposition of phase D due to increased temperature or pressure within the lower mantle floods the mantle with water, yielding a large low-Q_μ anomaly.

3-D Interactive Visualization with Mantle Convection

Dave A. Yuen(1), Megan Damon(1), Erik O.D. Sevre (1), Mike Knox(2) David H. Porter (2)
M. Charley Kameyama (3)

1. Dept. of Geology and Geophysics and Minnesota Supercomputing Institute, Univ. of Minnesota, Minneapolis, MN
2. Laboratory of Computational Sciences and Engineering, Univ. of Minnesota, Minneapolis, MN
3. Geodynamics Research Center, Ehime University, Matsuyama, Japan

Researchers at the University of Minnesota and from Japan have implemented a system capable of interactive exploration of large numerical simulated data sets which are volumetrically rendered in near real time. These 3-D data sets are computed over hundreds of processors on a Linux cluster and are sent over a local Infiniband network to the Laboratory of Computational Sciences and Engineering Laboratory (LCSE) on a short-term periodic basis for visualization and rendered on an extremely high definition display device, called the PowerWall, which has over 13 million pixels. We describe the technical details involved in designing such as system and describe the specific application to the 3-D mantle convection parallel MPI code, ACuTEMan. by M.C. Kameyama.