

iron under high pressures and temperatures are still lacking. We have built a double-sided YLF laser heating system to study iron with nuclear resonant inelastic x-ray scattering technique under simultaneously high pressures and high temperatures. Sound velocities of iron have been directly measured up to 58 GPa and 1700 K in a laser-heated diamond cell. The "detailed balance" principle applied to the inelastic X-ray scattering spectra provides absolute temperatures of the laser-heated sample. These temperatures are in very good agreement with values determined from the thermal radiation spectra fitted to the Planck radiation function. This independent temperature measurement of the laser-heated sample confirms the validity of temperatures determined from Planck radiation law in the laser-heated diamond anvil cell experiments. We found that temperature has a strong effect on the sound velocities; the compressional (V_P) and shear wave velocities (V_S) of hcp-Fe decrease significantly with increasing temperature under high pressures. V_P and V_S are only linearly related to the density for a given, constant temperature, while the bulk sound velocity (V_ϕ) follows Birch's law, i.e., V_ϕ is linearly related to the density and mean atomic weight. The linear sound velocity-density line should be corrected to lower velocities in extrapolations to inner core conditions. Our results have important implications for understanding the sound velocities of the Earth's inner core as well as the fundamental physical properties of iron under extreme pressures and temperatures.

T32A-02 1045h

Bulk Properties of FeO under Zero and High Pressure Conditions

Maria Alfredsson¹ (m.alfredsson@ucl.ac.uk)

David G. Price¹ (d.price@ucl.ac.uk)

John P. Brodholt¹ (j.brodholt@ucl.ac.uk)

¹Department of Earth Sciences, University College London Gower Street, London WC1E 6BT, United Kingdom

Determining the effect of Fe on the chemical and physical properties of lower mantle minerals is fundamental to interpreting lower mantle seismic data. While ab initio computational modelling has proven to be an invaluable tool for Fe-free systems, there are serious problems with these techniques when applied to transition metal oxides (ref to Cohen). For example, Density Functional Calculations (DFT) predict FeO to be metallic when in fact it is a wide band-gap insulator. In this study we use different hybrid functionals between Hartree-Fock and DFT as an alternative to the traditional approaches of LDA+U and Self-configuration interactions (SIC) calculations. We determine the geometrical structures and bulk properties of different magnetic and crystallographic structures of FeO and find that the different functionals predict quite different elastic properties. By comparing with available electronic and structural experimental data, we suggest an optimum range of mixing between HF and DFT. Using this we find that the antiferromagnetic (AFM) NaCl-structure (B1) is the energetically most stable structure at zero temperature and pressure, and we also obtain a lattice parameter (4.36 Å) and bulk modulus (185 GPa) in good agreement with experimental values (4.34 Å and 179 GPa). Moreover, we also predict a wide band gap. We have also calculated the pressure at which stoichiometric FeO undergoes a phase transition from the distorted B1 to B8 (NiAs-type) structure. This ranges from 75 to 183 GPa, depending on which method we use. Our preferred mixing predicts a phase transition of ca. 90 GPa. This phase transition is associated with a high spin (tg3, eg2, tg1) to low spin (tg3, tg3) transition of the Fe²⁺ ions. Experimentally the reported observations disagree with each other. Mossbauer measurements report a high spin to low spin transition between 90-140 GPa (Pasternak MP et al. (1997) PR Letters. 79: 5047-5049), while X-ray emission spectroscopy suggest a preserved high spin state up to 143 GPa (Badro J et al. (1999) PR. Lett. 83: 4101-4104). Our calculations, using our preferred mixing, are, thus, in favour of the observations from Mossbauer spectroscopy.

T32A-03 1100h INVITED

Post-Perovskite Phase Transition in MgSiO₃

Kei Hirose¹ (+81-3-5734-2618; kei@geo.titech.ac.jp)

Motohiko Murakami¹ (mmurakam@geo.titech.ac.jp)

Katsuyuki Kawamura¹ (kats@geo.titech.ac.jp)

¹Dept. Earth & Planetary Sciences, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro, Tokyo 152-8551, Japan

MgSiO₃-perovskite is believed to be a principal mineral at least in the upper part of the lower mantle, but its stability and possible phase transition at

greater depths remain uncertain. Since seismic observations have shown unexplained features in the lowermost mantle, solid-solid phase transitions that could occur in this region are under debate. We performed in-situ X-ray diffraction measurements of MgSiO₃ at high pressure and high temperature at BL10XU of SPring-8. Experiments were made in a laser-heated diamond anvil cell (LHDAC) up to 134 GPa and 2600 K corresponding to the conditions of core-mantle boundary region. MgSiO₃ gel mixed with platinum powder was used as starting material. Results demonstrate that MgSiO₃-perovskite transforms to a new high-pressure form with stacked SiO₆ octahedral sheet structure above 125 GPa and 2500 K (2700-km depth near the base of the mantle) with an increase in density by 1.0-1.2 %. The transition pressure coincides with the depth of the D'' seismic discontinuity, and its origin may be attributed to this post-MgSiO₃-perovskite phase transition. The new phase is likely to have strong single-crystal elastic anisotropy and develop shape preferred orientation with a platy crystal habit in the shear flow. This can cause seismically detectable anisotropy below the D'' discontinuity. We observed similar phase transition in MgGeO₃ above 70 GPa. The post-perovskite phase of MgGeO₃ transformed to a different form upon decompression at room temperature.

T32A-04 1115h

Elasticity of Polycrystalline Py50Mj50 to 9 GPa and 1000K by Ultrasonic Interferometry with Synchrotron X-radiation.

Gabriel Gwanmesia¹ ((302) 857 6653; ggwanmes@desu.edu); Jennifer Kung^{2,3}; Liping Wang^{2,3}; Baosheng Li^{2,3}; Michael Vaughan^{2,3}; Robert C Liebermann^{2,3}

¹Department of Physics and Pre-Engineering, Delaware State University, Dover, DE 19901, United States

²Mineral Physics Institute, Stony Brook University, Stony Brook, NY 11794-2100, United States

³Department of Geosciences, Stony Brook University, Stony Brook, NY 11794-2100, United States

Compressional (P) and shear (S) wave velocities have been measured on dense (99.5% of theoretical density), elastically isotropic polycrystalline Py50Mj50 to 9 GPa and 1000K using ultrasonic interferometry, in conjunction with in-situ synchrotron x-ray diffraction and imaging techniques. Fine-grained polycrystalline specimens of Py50Mj50 were fabricated in a 2000-ton uniaxial split-sphere apparatus at 16 GPa and 1500aC for 4 hrs, from a homogeneous glass starting material. The physical properties of the recovered specimens have been characterized with density measurements and x-ray diffraction. Elastic compressional and shear wave velocities determined at room temperature and pressure are in excellent agreement with the Hashin-Shtrikman averages calculated from single-crystal elastic moduli. Travel times of acoustic P and S waves were measured to 9 GPa and 1000K in a DIA-type cubic anvil high-pressure apparatus (SAM-85) interfaced with synchrotron x-radiation and x-ray imaging. We will present results of the pressure and temperature derivatives of the elastic moduli and equation state of Py50Mj50 and discuss implications of the new results on velocity gradient in the transition zone of the Earth's mantle.

T32A-05 1130h

First-principles determination of element partitioning in multi-component systems

Taku Tsuchiya¹ (612 6258597; takut@cems.umn.edu)

Jun Tsuchiya¹ (612 3772855; junt@cems.umn.edu)

Renata M Wentzcovitch¹ (wentzcov@cems.umn.edu)

Koichiro Umemoto¹ (umemoto@cems.umn.edu)

Razvan Caracas¹ (caracas@cems.umn.edu)

¹Dept of Chemical Engineering and Materials Science, Supercomputing Institute, University of Minnesota, 151 Amundson Hall, 421 Washington Ave. SE, Minneapolis, MN 55455, United States

Element partitioning of low concentration solutes in multi-phase systems is an important problem in high-pressure high-temperature mineral physics. Theoretical prediction of partitioning coefficients is especially important because precise thermodynamic equilibrium is not easily realizable in high-pressure experiments. To our knowledge, this problem has not been addressed by first principles yet. In this study we develop the general formulation for calculating partitioning coefficients and calculate it for a system of utmost importance in geophysics: partitioning of Fe²⁺ between (Mg_{1-x}Fe_x)SiO₃-perovskite and (Mg_{1-y}Fe_y)O, the

dominant aggregate in the Earth's lower mantle. In this first principles pseudopotential study thermodynamic properties have been obtained from free energy computations using the quasiharmonic approximation in conjunction with vibrational densities of states obtained from linear response calculations of phonon frequencies. The method, its applicability to actual systems, and the nature of the predictions will be discussed in the context of various experiments. Research supported by NSF/EAR, COMRPES, and JSPS

T32A-06 1145h

Insights on the thermochemical state of the lower mantle

Renata Wentzcovitch¹ (wentzcov@cems.umn.edu)

Taku Tsuchiya¹ (takut@cems.umn.edu)

Jun Tsuchiya¹ (junt@cems.umn.edu)

Koichiro Umemoto¹ (umemoto@cems.umn.edu)

Razvan Caracas¹ (caracas@cems.umn.edu)

¹Dept of Chemical Engineering and Materials Science, Supercomputing Institute, University of Minnesota, 151 Amundson Hall, 421 Washington Ave. SE, Minneapolis, MN 55455, United States

The thermochemical state of the lower mantle is still a underdetermined problem. The increasing availability of first principles results on partitioning coefficients and thermoelastic properties is helping to reduce the number of independent unknowns and to improve the accuracy of predicted aggregate properties at pertinent conditions. In a first step, the information contained in seismic models should be interpreted in light of mineral physics results. In a second step, the outcome should be tested against constrained inferences and observables. We report here some steps taken in this direction. The procedure is based on a comparison between results from 1D seismic models and calculated thermoelastic properties of multi-component systems in thermal equilibrium. Presently the analysis is restricted primarily to systems with three components and two phases only ((Mg,Fe)O and (Mg,Fe)SiO₃-perovskite) for which detailed first principles thermoelastic properties are available. Research supported by NSF/EAR, COMRPES, and JSPS

T32B CC: 516 D Wednesday 1030h

The Structure and Formation of Atlantic Rifted Margins: Observations and Numerical Models II (joint with GP, S, V, NS)

Presiding: K E Loudon, Dalhousie University; S Dehler, Geological Survey of Canada

T32B-01 1030h INVITED

Structural And Depositional Style Of The Syn-Rift Systems Of The West African And Brazilian Continental Margins: Regional Subsidence Independent Of Brittle Deformation

Garry D Karner (845 365 8355; garry@ideo.columbia.edu)

Lamont-Doherty Earth Observatory, P.O. Box 1000, Palisades, NY 10964, United States

The West African and Brazilian passive continental margins are characterized by the regional distribution of syn-rift and post-rift sediment assemblages that are inconsistent with the minor amounts of brittle deformation interpreted from seismic sections across the margin or from field mapping of exposed rift systems. Fundamentally, the rift phase of West Africa and Brazil consists of a series of stacked sag basins. Ostracod data from the West African margin indicate that the distal syn-rift sag basins, where dated, are Neocomian to Aptian in age and are contemporaneous with proximal syn-rift deposits developed inboard of a major hinge zone, the Atlantic Hinge zone. Despite being syn-rift deposits (by virtue of their age), the sag basins exhibit none of the diagnostic characteristics of brittle deformation, such as the existence of normal faults, the rotation of crustal blocks, the existence of prominent rift onset unconformities (onlap surfaces), and the generation of sediment wedges. Seismic sections across the Camamu-Almada margin of Brazil indicate that the regional generation of space is essentially independent of faulting, as indicated by an absence of stratigraphic growth across normal faults and a regional seaward dip of the entire syn-rift stratigraphic package. The

late syn-rift history of the West African and Brazilian margins is dominated by the creation of regional but shallow depositional environments that allowed the accumulation of the Loeme and Ezanga evaporites of West Africa and the Iburra, Taipus Mirim, and Mariruc evaporites of Brazil. Following break-up, the margins underwent significant post-rift subsidence allowing the deposition of the late Cretaceous, Paleogene and Neogene sedimentary packages. The development of significant post-rift accommodation in the same region characterized by minor syn-rift faulting and shallow depositional environments is the crucial observation requiring an explanation in terms of extensional strain partitioning through the lithosphere, lower crustal flow, major dyking of the lower crust during the extension process, and the thermal effects of mantle plumes. This presentation will show seismic and drilling data for the West African and Brazilian margins that clearly demonstrates the structural and depositional style of syn-rift systems: the stacking of syn-rift sag sequences showing subtle stratal relationships rather than the more familiar (and expected) characteristics of brittle deformation. Driscoll and Karner (1998) have suggested that the formation of syn-rift sag basins requires partitioning of extension across a mid-crustal decoupling zone separating upper crust (the upper plate) from a ductile-deforming lower crust and lithospheric mantle (the lower plate). The obvious problem with this hypothesis is that extension within the upper and lower plate needs to be laterally balanced. The exact form and location of the counterbalancing upper plate extension presumably exists in the vicinity of the ocean-continent transition zone where the extensional balance through the upper crust probably occurs by a combination of thinned and "rafted" crustal blocks and exposed continental mantle. Nevertheless, it remains to be shown that this strain balance actually exists in addition to exploring alternative mechanisms that can augment syn-rift and post-rift subsidence without upper crustal brittle deformation.

T32B-02 1055h

Modelling Sea-floor Spreading Initiation and Rifted Continental Margin Formation: Does Depth Dependent Stretching Occur Pre- or Syn-breakup?

Nick J Kusznir¹ (+44-151-794-5182; sr11@liverpool.ac.uk)

Garry D Karner² (845-365-8355; garry@ldeo.columbia.edu)

¹Department of Earth and Ocean Sciences, University of Liverpool, Liverpool L69 3BX, United Kingdom

²Lamont-Doherty Earth Observatory, 61 Route 9W, Palisades, NY 10964, United States

Depth dependent stretching, in which upper continental crustal extension is much less than that of the lower crust and lithospheric mantle, is a characteristic of both non-volcanic and volcanic rifted margins. A key question is whether depth dependent stretching of rifted margin lithosphere occurs during the initiation of sea-floor spreading or during pre-breakup rifting. A kinematic fluid-flow model of sea-floor spreading initiation has been developed to determine the concomitant distribution and amplitude of rifted continental margin lithosphere thinning and thermal evolution. The ocean-ridge initiation model uses an iso-viscous corner-flow stream-function solution (Batchelor 1967) to predict the divergent lithospheric and asthenospheric fluid-flow field of the extending continental margin lithosphere. The thinning of the continental margin lithosphere is calculated by material advection in the newly initiated ocean ridge fluid-flow field. The ocean-ridge initiation model predicts depth dependent stretching of continental lithosphere. Rifted continental margin lithosphere thinning and thermal evolution are dependent on ocean-ridge spreading rate (V_x), the mantle upwelling velocity beneath the ridge axis (V_z), and the pre-breakup lithosphere beta stretching factor. The sea-floor spreading initiation model predicts that the distribution and magnitude of depth dependent stretching of continental margin lithosphere is highly sensitive to the ratio of V_z/V_x . For volcanic margins V_z/V_x may be > 5 during sea-floor spreading initiation, reducing to $V_z/V_x \sim 1$ after a few Myr (Nielsen & Hopper 2002), while for non-volcanic margins, lower values of V_z/V_x (~ 1) are expected during sea-floor spreading initiation. For $V_z/V_x \sim 1$ the sea-floor spreading initiation model predicts that lower continental crust and continental lithospheric mantle adjacent to the margin are advected oceanward and result in rifted margin depth dependent stretching and continental mantle exhumation. For $V_z/V_x \gg 1$ lower continental crust and lithospheric mantle near the margin are advected continentward and mantle exhumation is not predicted to occur. The consequences of pre-breakup stretching of continental lithosphere on lithosphere thinning and thermal evolution are also included in the margin formation model using 2D depth independent pure-shear stretching (McKenzie 1978). The combined lithosphere thinning and thermal response to pre-breakup stretching and sea-floor spreading initiation are used to determine the resulting margin bathymetry and subsidence

history, top basement heat-flow and gravity anomaly, which are dependent on V_x and V_z during sea-floor spreading initiation and pre-breakup lithosphere beta stretching factor. The magnitude and timing of pre- and post-breakup extension and subsidence predicted by the new model are compared with observations for the Exmouth Plateau margin, the Norwegian Voering and Lofoton margins, and the Woodlark Basin with the aim of determining whether depth dependent stretching of rifted continental margin lithosphere occurs pre- or syn-breakup.

T32B-03 1115h

Asymmetric Lithosphere Extension: Factors Controlling Rift Mode Selection.

Ritske S. Huismans¹ (Ritske.Huismans@dal.ca)

Susanne JH Buitter¹

Christopher Beaumont¹

¹Geodynamics Group, Department of Oceanography, Dalhousie University, Oxfordst, Halifax, NS B3H 4J1, Canada

We use thermo-mechanical models of the lithosphere and upper mantle to study lithosphere extension and passive margin formation. We focus on factors controlling the asymmetry of lithosphere extension. We simulate lithosphere and upper mantle deformation in a 2D 1200 x 600 km domain. Initially the crust and lithosphere are 35 km and 120 km thick respectively. Extension rates vary between 0.1 cm/yr (slow) and 10 cm/yr (fast). The model is thermally coupled and has a free surface. The rheology is frictional-plastic or viscous and depends on temperature, pressure, strain-rate and composition. Frictional-plastic strain softening, which leads to strong localization and asymmetric deformation, is considered in cases where the crust is either strongly or weakly coupled to the mantle lithosphere. The model results predict lithosphere asymmetry for low to moderate extension velocities and for cases where the crust is entirely frictional-plastic. The fundamental asymmetry is suppressed at high rifting velocities and in cases where thermally activated creep occurs in the lower crust. We compare the fully thermo-mechanic models of extension with simple two-layer models with a frictional plastic strain-softening layer overlying a uniform viscous layer. We use estimates of the rate of energy dissipation in the simple two layer system to derive criteria that control mode selection by comparing the respective rate of dissipation for each rifting mode. The mode with the least dissipation is favored. The primary controls are the relative rates of dissipation in the frictional-plastic and viscous layers. The dissipation in the plastic layer is determined by the yield strength and its strain dependence, both of which are independent of velocity. The dissipation in the viscous layer is partly determined by the viscosity and the strain rate, and is, therefore, dependent on the rifting velocity. The remaining control is the traction coupling between the layers. The dissipation analysis predicts that at low viscous stresses, arising from low viscosities and/or low extension velocities, the fundamental asymmetry promoted by the strain softening frictional-plastic layer is fully expressed and rifting of the lithosphere may be asymmetric. At higher viscous stresses this tendency is suppressed and symmetric or pure shear lithosphere extension is predicted. The results from the forward mechanical models are in well agreement with the dissipation analysis.

URL: <http://is.dal.ca/~huismans/jgr-animations.html>

T32B-04 1130h

The Seismic Characteristics of the Ocean-Continent Transition (OCT) Across the Eastern Grand Banks Margin

Ka Wai Helen Lau¹ (kwhlau@dal.ca); Keith E Loudon¹ (Keith.Loudon@dal.ca); Jeremy Hall² (jeremyh@mum.ca); Sharon Deemer² (ecsot@waves.esd.mun.ca); Brian E Tucholke³ (btucholke@whoi.edu); W. Steven Holbrook⁴ (steveh@uwyo.edu); Hans Christian Larsen⁵ (hcl@dlc.ku.dk); Thomas Funck⁵ (tf@dlc.ku.dk); John R Hopper⁵

¹Department of Oceanography, Dalhousie University, Halifax, NS B3H 4J1, Canada

²Department of Earth Science, Memorial University of Newfoundland, St. John's, NF A1B 3X5, Canada

³Department of Geology and Geophysics, Woods Hole Oceanographic Institution, Woods Hole, MA 02543, United States

⁴Department of Geology and Geophysics, University of Wyoming, Laramie, WY 82071, United States

⁵Danish Lithosphere Center, Øster Voldgade 10, Copenhagen K DK-1350, Denmark

Coincident 2D multi-channel seismic (MCS) and wide-angle reflection/refraction seismic data were collected across the Eastern Grand Banks, the Flemish Cap and the Newfoundland Basin. The southernmost profile, Line 3, transects the full thickness continental crust beneath the shelf, the Jeanne d'Arc Basin, the Carson Basin, the Salar Basin, and it extends into the Newfoundland Basin north of the Newfoundland Seamounts. Our results show that the continental crust beneath the shelf, of ~ 35 km thick, is comprised of 3 layers - upper (velocity = 5.8-6.2 km/s), middle (6.3-6.5 km/s) and lower crust (6.8-6.9 km/s). Crustal thinning that led to continental breakup was initially abrupt beneath the Carson Basin and then more gradual seaward beneath the Salar Basin and the Newfoundland Basin. This formed a wide zone (~ 100 km) of very thin (< 8 km) continental crust sitting on a layer of serpentinized mantle (7.5-8.0km/s). Only the upper crust exists across the seaward most 50 km of this zone and may be a result of a westward dipping detachment fault. The crust-mantle boundary at the landward end of the serpentinized mantle layer coincides with a prominent landward dipping reflector, similar to the "L-reflector" previously observed on Lithoprobe profile 85-2 across the SE Grand Banks. Beyond where the tilted fault blocks cease to exist, an ocean-continent transition (OCT) zone ~ 75 km wide consists of extremely thin (~ 5 km) and unreflective basement layer with high velocity gradient (4.5-7.7 km/s). Such properties are consistent with either exhumed mantle or ultra-slow spreading oceanic crust. The serpentinized mantle layer that underlain the thin continental crust extends seaward beneath this basement layer, making a total width of ~ 200 km and a lower boundary depth of ~ 15 km. The serpentinized mantle layer pinches out seaward where seafloor spreading formed normal oceanic crust. Similar mantle layers of different widths were observed across the E. Flemish Cap margin and the SE Grand Banks. Although the widths and detailed structures of crustal zones vary along the eastern Grand Banks margin, serpentinized mantle exists across the OCT and might have been exhumed, as was suggested by recent ODP drilling results north of Line 3 (Leg 210) and in the conjugated Iberia margin (Leg 149 and 173).

T32B-05 1145h

Southeast Newfoundland Continental Slope: SCREECH Lines 401 and 403

Krista Solvason¹ (k19kls@mum.ca); Jeremy Hall¹; Sharon Deemer¹; Keith Loudon²; Helen K.W.H. Lau²; Steven Holbrook³; Brian Tucholke³; John Hopper⁵; Hans Christian Larsen⁶

¹Memorial University, Earth Science Dept., St. John's, NL A1B 3X5, Canada

²Dalhousie University, Dept. of Oceanography, Halifax, NS B3H 4J1, Canada

³Woods Hole Oceanographic Institution, Dept. of Geology and Geophysics, Woods Hole, MA 02543-1541, United States

⁴University of Wyoming, Dept. of Geology and Geophysics, Laramie, WY 82071, United States

⁵IFM-GEOMAR, Wischhofstrasse 1-3, Kiel D-24148, Germany

⁶Danish Lithosphere Center, Øster Voldgade 10, Copenhagen DK1350, Denmark

Multichannel seismic reflection data were collected by a cooperative international group in the summer of 2000 along 3 transects across the southeast Newfoundland margin. These transects extend from the continental shelf across the continental slope and rise, and they provide seismic data on the Newfoundland side needed to study rifting across the Newfoundland-Iberia non-volcanic conjugate passive margins. SCREECH lines 401 and 403 are contained within transect 3, which is the southernmost transect. Lines 401 and 403 image the continental shelf east of the southern Jeanne d'Arc basin, and they extend past the shelf break and onto the continental slope. Both lines clearly show the Carson basin located on the continent side of the shelf break, and a ridge located below the slope. Seismic profiles running parallel to the SCREECH lines were provided by WesternGeco. These lines enhance the interpretation of the basement ridge, which is shown to shallow towards the north and may extend as far as the Flemish Pass basin. The top of the ridge is well defined in the profiles and is strongly reflective. The ridge was modelled using gravity data recorded on the SCREECH cruise. Based on resulting models it was determined that the ridge is mainly composed of crustal basement material with minor amounts of salt present in localized areas. Strong lower crustal reflections near the shelf break are imaged on SCREECH profiles 401, 3MCS and 403 as well as two WesternGeco lines. Lower crustal reflections are not imaged beneath the Carson basin most likely due to masking by multiples from the overlying sedimentary sections. Line 403 shows the best example of lower crustal reflections that are strong and continuous. These lower crustal reflections are shown to be deeper in the north and shallow to the south. An interpretation which incorporates the shallow basement block and the lower crustal structure will be given.