

T34A CC: 516 D Wednesday 1530h**Plate Reorganization Events: Observations and Models II** (*joint with GP, S*)**Presiding:** S King, Purdue University; J Lowman, University of Leeds**T34A-01 1530h INVITED****Changing Plate Configurations in Models of Mantle Convection**

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In the Plate Tectonic model, continents are carried as passive rafts on lithospheric plates, eventually arriving at subduction zones where they accumulate, an idea first suggested by Vening-Meinez in 1962. A subsequent reorganization of plate motions is required to carry continental fragments away in new directions. Paleogeographic reconstructions of the changing locations of continents in the past can act as a proxy for the history of plate motions for the past several hundred My. This history is episodic and has repeatedly assembled large continental masses, or supercontinents. Convection models with buoyant continents can mimic this Wilson cycle type of activity, and internal heating in two- and three-dimensional models with plates can spontaneously reverse, or alter, spreading directions. Kinematic models can also be employed to examine the times required to assemble continents into a single supercontinent. The timescales for supercontinent assembly are found to depend most strongly on the total fraction of the Earth covered with continental material. For current continental masses, the typical assembly time is found to be approximately 400 My while for smaller amounts of continental material supercontinent assembly may require over 1,000 My.

T34A-02 1550h**Convection with Mobile Plates: Testing Plate Formulations with Complex, Time-Dependent Fluid Systems**Donald E. Koglin¹ (765-494-0268; dkoglin@purdue.edu)Scott D. King¹ (765-494-3696; sking@purdue.edu)¹Department of Earth and Atmospheric Sciences Purdue University, 550 Stadium Mall Drive, West Lafayette, IN 47907-2051, United States

Lowman et al. (2001) presented results of 2D convection with mobile plates where the plate velocities reverse due to the evolution of the flow in the fluid beneath them. Lowman et al. used a force balance method to implement mobile plates and we reproduce their results using a 'weak zone' based rheological plate method. For the unit aspect ratio domain with a stiff plate with a thickness of 0.05d, where d is the depth of the domain, we find linear relationships between the surface velocity and size of the weak zones and the surface heat flux and the size of the weak zones. To match the results of Lowman et al. requires square weak zones that are 0.09d in length/depth. The results are less sensitive to the viscosity contrast between the fluid and the weak zone. For the case where Lowman et al. find plate motions that reverse on a periodic time scale we also find periodic, reversing plate motions. Using a T-R periodogram (Scargle 1982; Benson et al. 2003), we find that the periods are extremely similar, with main peaks near periods of 0.02 and 0.05 diffusion time. However, our results show an apparently more complex behavior than those of Lowman et al. (2001), as demonstrated by the difference in periodicity between the two datasets, and the amplitude modulation in our results. There are additional low-amplitude, short-period phases in our time series that are not present in the Lowman et al. results. We suspect this is a result of small-scale flow differences due to the weak zones. Using these simple 2D systems, we systematically build toward a plate formulation with a temperature and stress dependent olivine rheology, then investigate the effects of damage and history. Lowman, J.P., S.D. King and C.W. Gable, The influence of tectonic plates on mantle convection patterns, temperature and heat flow, *Geophysical Journal International*, 146, 619-636, 2001. Scargle, J.D., *Studies in Astronomical Time Series Analysis II. Statistical Aspects of Spectral Analysis of Unevenly Spaced Data*, *Astrophysical Journal*, 263, 835-853, 1982. Benson, J.L., B.P. Bonev, P.B. James, K.J. Shan, B.A. Cantor, and M.A. Caplinger, The seasonal behavior of water ice clouds in the Tharsis and Valles Marineris Regions of Mars: Mars Orbiter Camera Observations, *Icarus*, 165, 34-52, 2003.

T34A-03 1605h**Evolving Tectonic Plates in Convection Models: Investigating the Feedback Between Sources of Deep Mantle Buoyancy and Plate Motion**Andrew Gait¹ (A.Gait@earth.leeds.ac.uk)Julian P Lowman¹ (44-113-343-5212; J.Lowman@earth.leeds.ac.uk)¹University of Leeds, School of Earth Sciences, Woodhouse Lane, Leeds LS2 9JT, United Kingdom

Understanding the feedback between the dynamically coupled systems of mantle convection and plate tectonics is an important geodynamical problem. In particular, how does the time-dependence associated with tectonic plate velocity and morphology affect other time-dependent features such as plume motion and longevity, surface heat flux and core-mantle boundary heat flux? Previous authors have specified plate-like behaviour in mantle convection models with evolving plate velocities but static plate geometries over time periods approximating billions of years. These studies have led to a greater understanding of the role of plates on mantle convection including flow patterns, mantle temperature and plate velocities, however, the extent to which the temporal evolution of the plate geometry affects such models remains poorly understood. We systematically explore the effect of dynamic migrating plate boundaries in mantle convection models featuring increasing complexity by using a numerical two-dimensional mantle convection model in a Cartesian geometry incorporating stiff tectonic plates, in which the plate velocities and plate boundaries evolve dynamically in response to the buoyancy distribution within the convecting system. We implement two simple migration rules: divergent plate boundaries migrate to simulate symmetric sea-floor spreading and convergent plate boundaries migrate to simulate the subduction of older plate by younger plate, thus modelling asymmetric subduction. We investigate the effects of plate size and number, mantle internal heating rate and mantle viscosity stratification on time-dependent features of our calculations such as the plate velocities, plate ages and plate sizes. We also investigate how plate boundary migration constrains parameters such as mean mantle temperature and surface heat flux. Study of these time-dependent features will help us to further answer questions about plate reorganization events and flow reversals, and to what extent deep mantle processes may be expressed in the history of plate motion.

T34A-04 1620h INVITED**Periodic Variations in Subduction Zone Configuration in Spherical Models of Mantle Convection With Plate Tectonics**Sandrine QUERE¹ (square@sca.uqam.ca)Alessandro Forte¹ (forte.alessandro@uqam.ca)¹QUERE, Centre GEOTOP, Université du Québec A Montreal, CP 8888, Succursale Centre Ville, Montreal, Qc H3C 3P8, Canada

Paleogeographic reconstructions indicate that several cycles of oceanic opening-closing and continental collision-break-up have occurred. A more detailed understanding of the physical processes responsible for these cycles requires a consideration of mantle dynamics and the associated surface subduction-zone distributions.

Here we present a 3-D spherical model of mantle convection which incorporates surface tectonic plates which are dynamically coupled to the buoyancy-driven mantle flow. The formalism used to take into account the plates is the same as the one used by Monnereau and Quéré (2001). These time-dependent convection models reveal a cyclical re-organization of the subduction zones, alternating between two stable configurations around the same barycenter. The three main ingredients we employ in the models are: the present-day plate geometry; a multi-layer, geophysically constrained viscosity profile; and a large amount of distributed internal heating in the mantle.

As we have used a fixed plate geometry, one might expect that it would only provide stable subduction zone configurations. As we discover, this geometry will enable subduction zones to move from one state to another. A geometry with fixed boundaries is not, therefore, a restricting factor for the movement of the surface subduction patterns. We have also incorporated a multi-layer viscosity profile inferred from simultaneous inversions of convection and glacial isostatic adjustment (GIA) data (Mittrovia and Forte, 2004). This viscosity profile possesses a strongly defined low-viscosity layer at 670 km depth. The last main input corresponds to the amount of internal heating, and we assume 21 TW of radiogenic heating, as estimated by Stacey (1992).

In these numerical convection simulations, the cycling between the two stable subduction zone configurations is characterized by a period between 500 and 700 Ma.

This periodic behaviour is manifested in a relatively restricted range of model parameter space. Several model simulations have allowed us to focus on the main parameters which are able to provide this cyclicity. In this presentation, we will specifically explore the use of both a complex plate geometry, a multi-layer viscosity profile with a low-viscosity channel, and a large amount of mantle internal heating.

T34A-05 1640h**Mantle Convection Models Including Continents and Self Consistent Plates**Cecile Grigne¹ (310-825-9296; grigne@ess.ucla.edu)Paul J Tackley¹ (310-206-9180; ptackley@ess.ucla.edu)¹Earth and Space Sciences UCLA, 595 Charles Young Drive East 3806 Geology Building Box 951567, Los Angeles, CA 90095-1567, United States

Estimates of mantle heat flux under stable continental shields are low, around one tenth of the mean oceanic heat flux, which indicates a strong insulating effect of continents on mantle heat loss. This thermal blanketing effect is studied using numerical models of convection. Rigid conductive lids are set on top of the mantle to represent continents. A previous study had been carried out using an isoviscous fluid for the mantle (Grigne, PhD Thesis, 2003). A scaling law for the mean heat flux, oceanic heat flux, and mantle heat flux underneath the continent, as a function of the Rayleigh number of the mantle and of the width and thickness of the continent was constructed. It was shown that the continental lid strongly modified the pattern of convection in the mantle, producing a large wavelength in the flow. A temperature-dependent viscosity is now introduced, combined with a viscoplastic yielding. This combination was shown to produce plate tectonic-like behavior (e.g. Tackley, 2000). Models thus include self-consistently generated oceanic lithospheric plates and more artificially imposed continents. The study focuses on the effect of continents, with variable geometries and insulating effects, on the heat transfer of the mantle, on the pattern of convection and on the localization of plate boundaries.

T41A CC: 220 C-E Thursday 0830h**Mineral Physics Perspectives on the Structure, Composition, and Dynamics of Earth's Deep Interior Posters** (*joint with S, V, MR, SEDI*)**Presiding:** J Badro, Institut de Physique du Globe, Université Paris VI; D Farber, Lawrence Livermore National Laboratory**T41A-01 0830h POSTER****Defective Grain Boundary Structures in MgSiO₃**Maria Alfreddson¹ (m.alfreddson@ucl.ac.uk)John P. Brodholt¹ (j.brodholt@ucl.ac.uk)David P. Dobson¹ (d.dobson@ucl.ac.uk)David G. Price¹ (d.price@ucl.ac.uk)¹Department of Earth Sciences, University College London Gower Street, London WC1E 6BT, United Kingdom

Grain boundary processes are central to a wide range of geological phenomena, including deformation process by diffusional creep. In this project we employ computational modelling to study surface and grain boundary processes at an atomistic level, knowledge that is vital for the progress of our understanding of the rheological processes in the lower mantle. In our study we have performed calculations on the perovskite structure of MgSiO₃, which is believed to comprise more than 70% of the lower mantle (Ringwood AE (1991) *Geochim. Cosmochim. Acta* 55: 2083-2110). By studying different types of grain boundary structures and domain wall motions in MgSiO₃, we calculate the activation energy for the domain wall motions to be between 1.4 and 2.0 eV for the grain boundary structures that are described as MgO-types, while for the SiO-terminated grain boundaries the activation energies are predicted to exceed 6 eV, due to the formation of stable ring and cage structures at the grain boundary. We have also performed calculations on the analogue perovskite structure of CaTiO₃, but for this compound we

find that both the CaO- and TiO-terminated boundaries show activation energies between 1.4-2.0 eV. Both our experimental and computational studies propose that Fe-ions segregate toward the grain boundary structures. The Fe-rich structures at the grain boundaries introduce structural reconstructions, suggesting that the deformation mechanisms of the slip planes, and diffusional creep in the lower mantle change in the presence of impurities. This is justified by our calculations, which suggest lower activation energies for domain wall motion of defective grain boundaries than for non-doped perovskite structures. In this study we also report predicted crystal morphologies in the presence of divalent cations, e.g. we find a more tabular morphology in the presence of Fe²⁺-ions than in non-doped perovskite structure of MgSiO₃. We also find that some of the more reactive surface structures are less-favoured in the presence of the Fe-ions, which will change the reactivity of the minerals. Such information is important if we want to study the effect of water and other impurities in lower mantle. Furthermore, the absence of the more reactive surfaces imply that a number of grain boundary structures are less-favoured.

T41A-02 0830h POSTER

High Pressure Elastic Anisotropy of α -PbO₂-Type SiO₂

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The athermal elastic constants and bulk and shear moduli of orthorhombic stishovite and α -PbO₂-type SiO₂ were calculated using plane wave density functional theory (DFT) within the generalized gradient approximation (GGA), for a pressure range of 0-120 GPa. The values are in very good agreement with available experimental data at zero pressure. The elastic constants of α -PbO₂-type SiO₂ were used to determine the seismic anisotropy of the material as a function of pressure. Both compressional and shear waves exhibit significant azimuthal anisotropy at zero pressure, which increases with pressure for the shear waves, but remains relatively constant for the compressional wave. It is postulated that paleosubducted slabs could introduce excess amounts of SiO₂ into the lower mantle, leading to the formation of α -PbO₂-type SiO₂. Subsequent alignment of the mineral by lattice preferred orientation could therefore explain part of the observed seismic anisotropy in the D'' region just above the core/mantle boundary.

URL: <http://www.es.ucl.ac.uk/research/desmond/>

T41A-03 0830h POSTER

Structural Behavior of Hydrous Ringwoodite at High Pressure and Estimated Maximum Hydrogen Contents for Ringwoodite and Forsterite

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Sets of X-ray diffraction intensities up to 7.9 GPa of a single crystal of 35x35x24 micron hydrous ringwoodite Mg_{1.97}SiH_{0.06}O₄, synthesized by Ohtani and Mizobata (1998) using a multi-anvil apparatus at conditions of 1680 C and 22 GPa were measured using synchrotron radiation at the beam line BL-10A, Photon Factory, High Energy Accelerator Research Organization, Tukuba, Japan. The modified Merrill-Bassett type diamond anvil pressure cell was used. The 4:1 fluid mixture of methanol and ethanol was used for pressure medium. The compressibility of the unit cell is close to the compressibility of the MO₆ octahedron. The mean Si-O distance stay almost constant up to 7.9 GPa. The compression of the crystal structure is governed by the compression of MO₆ octahedron. This is consistent to the fact that the bulk modulus is affected significantly by the substitution of Mg by 2H. The octahedral shared edges are compressed more than the unshared edges, keeping the edge lengths of SiO₄ tetrahedron almost constant. Based on the assumption that the vacant octahedral sites are separated each other

with equal distances, the maximum H₂O content was obtained from the configuration with minimum separation distances. The maximum H₂O contents were thus estimated to be 3.3 wt% for ringwoodite and 0.78 wt% for forsterite, the low pressure polymorph of ringwoodite.

T41A-04 0830h POSTER

Ab initio studies of phonon softening at high pressure in alpha-quartz SiO₂

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The silica polymorph quartz exhibits several interesting properties including pressure induced amorphization, high pressure phase transitions, anomalous elastic properties, negative Poisson ratio, and soft mode behavior. We used *ab initio* density functional calculations of quartz to understand the changes in phonon frequencies and elastic properties under bulk and uniaxial compression. Non-hydrostatic stresses are believed to play an important role in the pressure induced amorphization (Badro et al., Phys. Rev. Lett. (1996) 76, 772). We have undertaken density functional perturbation theory computations of quartz within the local density approximation (LDA) to compute the phonon frequencies at various points in the Brillouin zone as a function of pressure using the code ABINIT (<http://www.abinit.org>). The calculated phonon frequencies are found to be in good agreement with experimental data. A 466 cm⁻¹ Raman active A₁ mode shifts considerably under uniaxial compression along the c-axis as compared to bulk compression in agreement with reported Raman data. This mode involves symmetric bending of the Si-O-Si bond, and is believed to have a principal role in the compression mechanism of quartz. A zone boundary (1/3, 1/3, 0) K-point phonon mode becomes soft at high pressures as also seen from the bulk compression *ab initio* studies of Baroni and Giannozzi (Materials Research Society Proceedings, 499, 1997, p233 (Ed: R.M. Wentzcovitch et al.)). The mode softening is related to the high pressure amorphization and phase transitions of quartz and our studies suggest that the mean amorphization pressure can be lowered under non-hydrostatic conditions.

T41A-05 0830h POSTER

X-radiography, XRD and Ultrasonic Data Transfer Function Technique - Simultaneous Measurements Under Simulated Mantle Conditions in a Multi-Anvil Device

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The interpretation of seismic data from the Earth's deep interior requires measurements of the physical properties of Earth materials under experimental simulated mantle conditions. Elastic wave velocity measurement is an important tool for the determination of the elastic properties. Ultrasonic interferometry allows the highly precise travel time measurement at a sample enclosed in a high-pressure multi-anvil device. But the calculation of wave velocities requires the exact sample length under in situ conditions. There are two options - scanning the interfaces of the sample by XRD (Mueller et al., 2003) and X-radiography (Li et al., 2001). The multi-anvil apparatus MAX80 is equipped for both methods. Only the X-radiography is fast enough for transient measurements. Contrary to XRD measurements, imaging the sample by X-rays requires a beam diameter larger than the sample length. Therefore the fixed primary slits of Max80 were exchanged by 4-blade high precision slits of Advanced Design Consulting, Inc. A Ce-YAG-crystal converts the X-ray image to an optical one, redirected by a mirror and captured by a CCD-camera. To derive the sample length, the different brightness of sample, buffer rod and reflector at the electronic image is evaluated. Classical ultrasonic interferometry is very time consuming, because the ultrasonic waves of the frequency range under study are generated and detected one after another

with a given step rate. A 60 MHz frequency sweep with 100 kHz steps lasts for more than 30 minutes. This is a serious limitation for all transient measurements, but also limits the data collection at elevated temperatures to prevent the pressure transmitting boron epoxy cubes and the anvils from overheating. The ultrasonic transfer function technique (UTF), first described by Li et al. (2002), generates all the frequencies simultaneously. Related to the results and experiences of Li the UTF-technique was developed independently at GFZ. This version allows to consider the characteristics of the specific transducer-glu-anvil combination (Mueller et al., 2003). To collect the data for the following calculation of V_p and V_s requires just few seconds. The excitation function, applied to the transducer by an arbitrary waveform generator, is the result of the summation of all sinusoidal waves inside the frequency range. The response of the system - transducer - anvil - buffer rod - sample - reflector - for each of the frequencies can be reproduced by convoluting the resulting transfer function with these monochromatic waves step by step. Some recent results on the non-quenchable high-P - low-P clinoenstatite transition and to the quartz-coesite transition will be given to discuss the different interferometric techniques, including the XRD-data and X-radiography results, necessary to detect the phase transitions under in situ conditions and to measure the sample deformation. Li, B.; Vaughan, M.T.; Kung, J.; Weidner, D.J., NLSL Activity Report 2001, 2-103-106, (2001). Li, B.; Chen, K.; Kung, J.; Liebermann, R.C.; Weidner, D.J., J. Phys.: Condens. Matter 14, 11337-11342, (2002). Mueller, H.J.; Schilling, F.R.; Lauterjung, J.; Lathe, C., Eur. J. Mineral., 15, 865-873, (2003). Mueller, H.J.; Wunder, B.; Lathe, C.; Schilling, F.R.; Eur. J. Mineral., submitted, (2004).

T41A-06 0830h POSTER

Elasticity of intrinsically anisotropic rocks with orthotropic symmetry

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Seismic anisotropy of the upper mantle has been detected in various seismological observations. In addition, peridotites frequently exhibit an elastic anisotropy in ultrasonic laboratory measurements. Observed anisotropy might be produced by variety of *in situ* causes such as developed texture (LPO), structural layering and/or alignment of melt filled pockets. LPO is generally accepted to be the main cause of anisotropy in the upper mantle on the basis of laboratory investigations of deformed peridotites. Here, the intrinsic anisotropy of peridotites is modelled using the theory of elasticity of polycrystalline aggregates. The model accounts for the rock texture and the elasticity of constituent minerals as weighted by their volumetric presence. The novel approach of this study is the use of the Geometric mean averaging (GMA) method to refine the elastic constants of textured olivine aggregate of orthotropic symmetry. The GMA method is based on physically meaningful assumption of the invertibility of the elastic constants into the elastic compliances and yields unique set of elastic constants that are independent of the averaging domain. On the basis of this method, the anisotropies, particularly shear wave splitting, are defined for a range of orthotropic distribution functions. Whether these results can be extended with this formulation to higher symmetries (e.g. isotropic or TI) remains to be seen.