We have undertaken density functional LDA calculations of quartz using extended norm conserving pseudopotentials to compute the phonon frequencies at various points in the Brillouin zone as a function of pressure. The calculated equation of state and phonon frequencies are found to be in good agreement with experimental data. A 466 cm^{-1} Raman active A_1 mode shifts considerably under uniaxial pressure along the c-axis as compared to bulk compression in agreement with reported Raman data. This mode involving symmetric bending of the Si-O-Si bond 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. The mode softening is related to the high pressure amorphization and phase transitions of quartz and these studies suggest that the mean amorphization pressure can be lowered under non-hydrostatic conditions.

V21E-06 1135h INVITED

Solid state magnetic resonance from first principles: applications to silicates

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I will describe a recently developed technique for the prediction of magnetic resonance properties (NMR and EPR/ESR) of the solid state. The method is implemented within density functional theory, and periodic boundary conditions, and uses the efficient plane-wave basis and pseudopotential combination. I will demonstrate the method by reference to applications to the silicates: the assignment of the NMR spectra of the zeolite Ferrierite, and EPR g-tensor measurements of defects in quartz.

V21E-07 1150h

Theoretical study on structural factors correlated with ^{23}Na NMR parameters

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Ab initio NMR calculations at the HF/6-311+G(2df,p) GIAO level are performed on many Na-centered clusters with different O-ligands. Several aspects of the relationship between local structure and ^{23}Na NMR parameters have been carefully investigated. The accuracy of ^{23}Na NMR calculation is checked by calculating ^{23}Na NMR shieldings for similar crystalline materials with known experimental shieldings. The largest Na-O distance which can still contribute to the Na shielding is found to be about 3.5 Å. Quantitative contributions to the Na shielding from different individual O-ligands are emphasized in this paper. These contributions are carefully calculated and compared to establish the order of decreasing deshielding as: OH, NBO(Al)>Al-O-Si>NBO(Si)>Al-OH >H2O>Si-O-Si>Si-OH Na-clustering effects from other cations nearby are also found to tremendously increase the shielding of Na. Finally, the relationship between local structure and the Na NMR has been used to explain the Na NMR data for hydrous albite glasses.

V21E-08 1205h INVITED

Mineral Surfaces From First principles: Structure, Adsorption and Hydration

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Atomic scale phenomena occurring at the interface of minerals and water are, on one hand, very important in Earth and Environmental Sciences, and, on the other, extremely difficult to address, either from experiments or from simulations. The altered chemical bonds at surfaces demand quantum-mechanical first-principles simulation tools, while the complexity of the mineral surfaces and of water itself demand large simulation cell sizes and long simulation times, respectively. We approach the problem from two opposite starting points: (i) from the dry side: studying the effect of the first water layers on mineral surfaces, and (ii) from the wet side: studying liquid water and its response to the presence of ions and surfaces. This double route is justified by the very different characteristic time scales in the wet surface problem: some water molecules bind to the surface for very long times as compared to typical simulation times (picoseconds), while other molecules diffuse quite freely in the liquid. After a brief description of the methodology we use, based on linear-scaling density-functional theory, results will be presented for (i) the adsorption of pollutants onto dry clay surfaces and how the adsorption characteristics are modified by water molecules;(ii) the adsorption of water on calcite surfaces; and (iii) the characteristics of liquid water as described by our method.

V21F MCC: 3001-3003 Tuesday 1020h

The Origins of Hot Spots, LIPs, Seamount Chains, and Volcanic Ridges III *(joint with OS, T)*

Presiding: **D Forsyth,** Brown University; **D Naar,** University of South Florida

V21F-01 1020h

Shear-wave splitting as a diagnostic tool for resolving plume-related mantle flow around hotspots

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The plate tectonics hypothesis successfully explains most of Earth's geological and geophysical features. However, mantle hotspots, regions often associated with large magmatic provinces, linear age progressions of volcanism, and/or large topographic swells, do not fit into a simple plate-tectonic model. Most hotspots are explained by a simple plume model, i.e. a conduit of hot buoyant upwelling material that originates from a deeper thermal boundary layer, the origin of which is often assumed to be in the lower mantle. Past global seismic tomography has had little success in resolving plume-like structures due to resolution limitations. Recent regional teleseismic imaging above hotspots has had limited success in imaging plume-like conduits down to depths of ~400 km. Receiver function and SS precursor studies have also had limited success in detecting the thinning of the transition zone beneath hotspots, which is expected on physical grounds due to the penetration of hot plume material from below. It has been proposed recently that some of these features associated with hotspots can be explained by more complicated plate tectonic models, leading to significant debate. We analyze shear-wave splitting of upward propagating shear waves through the seismically anisotropic upper mantle around the Hawaii and Eifel hotspots, and southwest of Yellowstone along the hotspot axis. If plumes exist beneath these hotspots, these data may resolve the geometry and magnitude of upper-mantle flow and anisotropy associated with the interaction between the moving plate and upwelling plume material. Each of the hotspots we investigate is in a unique geophysical setting. For each study region, we observe an approximately parabolic pattern in map view of the splitting fast directions that is predicted by a simple kinematic plume model. The common pattern we observe, along with inferences about the location of anisotropy, suggests that plume conduits exist in at least the upper mantle beneath Hawaii, Eifel, and eastern Nevada. The best plume model for Hawaii fits the few observations well, but more data are needed to critically test it. The optimum Eifel plume model predicts the splitting fast directions fairly well, with complexity observed between nearby stations that suggests contributions from lithospheric and/or shallow asthenospheric sources. Fast directions from six stations in Idaho, in addition to splitting data collected across eastern Idaho, western Utah, and Nevada are predicted well by a plume model centered in eastern Nevada, but not beneath Yellowstone. We show that shear-wave splitting may be resolving plume-related mantle flow around some hotspots, and therefore if enough splitting data are collected, they could be used as a diagnostic tool to help resolve between plume and non-plume sources for other hotspots. A helpful complement to such future splitting investigations are regional surface-wave anisotropy investigations to better determine the depth extent of azimuthal anisotropy, and the development of better tools that more accurately predict fast directions and delay times from numerical mantle flow models.

V21F-02 1040h

Joint inversion of short- and long-period P traveltimes reveals a variety of plumes in the mantle.

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Diffraction theory predicts that traveltimes of finite-frequency waves are affected by heterogeneities within a narrow region around the ray-theoretical path, called Fresnel zone. Because of wavefront healing, heterogeneities whose scale-length is smaller then the size of the Fresnel zone do not significantly affect the traveltimes. Dahlen et al. (GJI, Vol 141, 157, 2000) show how to correct for wavefront healing effects with a method we refer to as finite-frequency modeling. We perform a global tomographic study by using the finite-frequency modeling, which allows to combine data of different dominant frequencies. To enhance the resolution, we combine long- and short-period data, and we introduce an irregular model parameterization. Our new tomographic model shows a strong correlation between low velocity anomalies and the location of a large number of known hotspots. To test the reliability of these anomalies, an extensive resolution analysis was performed. As result, we can confidently say that deep mantle plumes are located beneath Ascension, Azores, Canary, Easter, Hawaii, Samoa and Tahiti. Other plumes, among which is Iceland, originate at much shallower depth. Newly discovered plumes-like features are located beneath the Mid-Atlantic Ridge, the Southeast Indian Ridge, beneath the Seychelles and the Coral Sea.

V21F-03 1100h

The Upper Mantle Under the South Pacific Super-Swell from Multimode Surface Waveform Tomography

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The South Pacific contains a swarm of volcanic island chains superimposed on a broad bathymetric high known as the South Pacific Superswell. The islands and swell are thought to be the surface manifestation of a "superplume" beneath the the region. We present a Sv-wave speed tomographic model for the South Pacific derived from multi-mode waveform inversion of more than 17,000 vertical component seismograms. Most of the data are from the Global Digital Seismic Network but we include important data from ten broadband seismographs deployed in French Polynesia as part of the PLUME experiment (Polynesia Lithosphere and Upper

V

Mantle Experiment). We use preferentially short propagation paths ($\Delta < 54^{\circ}$) to minimize off great circle path propagation, but increase the path length in areas of insufficient coverage. We resolve the subduction zones bounding the South Pacific to the east and west with a width compatible with the smoothing used in the tomographic inversion. The slow wave speed structure associated with the East Pacific Rise is offset to the west as has previously been noted in more detailed local studies. There seems to be no pervasive low wave speed feature in the upper mantle beneath the South Pacific. However, low wave speed structures extend from shallow depth to the transition zone beneath the Society hotspot, the Austral hotspot and Easter Island. The presence of similar structures beneath other Pacific hotspots is currently masked by lack of resolution.

V21F-04 1115h

The 'Plate-Like' Subsidence of the East Pacific Rise - South Pacific Superswell System

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The separation of small-scale features from the regional seafloor depth is an important problem in the geosciences, especially as it impacts our understanding of mid-plate topographic swells and subsidence away from mid-ocean ridges. In the south Pacific ocean, for example, the removal of these features from the bathymetry using modal techniques has revealed a large and unusually shallow region of the seafloor, which at ~3000 km wide and up to 1 km high has been dubbed a "Superswell". Modal analysis, however, does not completely isolate and remove small-scale features such as oceanic islands, seamounts, oceanic plateaus and localised hot-spot swells from the regional bathymetry. This is because these features are superimposed upon the unperturbed ridge-generated regional bathymetry, accordingly a technique is required that underlines topographic constructs rather than passing through them as is the tendency of any average (mean, median or mode). We have therefore developed an algorithm that reproducibly simulates manual interpretation (**MiMIC**), thereby removing the superimposed features and revealing larger scale trends. Application of **MiMIC** to grids of bathymetric data in the region 12-26°S, 200-243°E shows that seafloor of all ages (0.5-112Ma) deepens slowly (initially ~218 $mMa^{-1/2}$) and in essence monotonically from the East Pacific Rise (EPR). Although initially deep (-2712m) with respect to a standard plate model (-2500m, 125km, 1350°C), the low subsidence rate reduces the negative depth anomaly with time until it becomes a positive anomaly west of ~234°E (~20-25Ma) that increases to a maximum of 712±66m at 98Ma, not 1300m at ~65Ma as previously observed. Most significantly though, the Superswell appears to be part of a larger scale, monotonic and 'plate-like' subsidence trend that extends to the EPR, not an isolated shallowing that reverses subsidence and causes uplift between 40-80Ma. The continuous nature of the EPR-Superswell subsidence trend suggests to us a common causal mechanism that links processes acting at the Superswell with those at the EPR. Previous studies at the EPR show asymmetry in seafloor subsidence and other observables such as seismic velocity and electrical conductivity which have been interpreted in terms of an across-axis temperature gradient, possibly sustained by a flow of hotter material from the west. Thus, a lateral temperature gradient may exist across the entire EPR-Superswell system. We have tested this hypothesis using a model in which the isostatic and thermal effects of a lateral sub-lithospheric temperature gradient are allowed to perturb the subsidence of a standard plate. Our preferred model has a depth of isostatic compensation of 320km and a linear temperature gradient of only 0.014°C/km. Such a model better explains the regional seafloor depths of the EPR-Superswell system than published cooling plate models and is in accord with constraints from elastic thickness, heat flow, seismic tomographic and long-wavelength gravity anomalies.

URL: http://www.earth.ox.ac.uk/~johnh/AGU2003.html

V21F-05 1130h

Reconstruction of Pacific-Nazca Plates, Nazca Ridge, and Easter Seamount Chain

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Relative plate motion history since 30 Ma between the Pacific and Nazca (Farallon) plates has been constrained by available seafloor magnetic anomaly data and a two-minute grid of predicted bathymetry. These data are used to create a new plate reconstruction based on finite and stage poles of rotation and radiometric ages along the Easter-Salas y Gomez-Nazca Ridge volcanic lineament. An iterative process of anomaly identifications, pole calculations and anomaly rotations was used to test for self-consistency in the interpretation. The new identified magnetic isochrons (10y, 7y, 6c, 5d, 5b, 5aa, 5o, 4a, and 3a) and the predicted tectonic history provide an improved understanding between chrons 7y (24.73 Ma) and 3 (4.18 Ma). However, the finite poles for 6c and 5d are poorly constrained. Eleven stage poles were calculated using the nine finite poles and two published instantaneous Euler vectors for the 1o and 2a isochrons. The stage poles indicate full-spreading rates increased from about 175 mm/yr to about 205 mm/yr after the break-up of the Farallon plate, and then have slowed to about 145 mm/yr. The tectonic reconstruction indicates two major southward propagating events, the first starting by 28 Ma and terminating by 18 Ma. The second starting in association with breakup of the Farallon plate around 24 Ma and terminating by about 11 Ma. Lithosphere was transferred from Nazca to Pacific during the first event and in the opposite sense during the second. Development of the Mendoza microplate east of the second propagator occurred at about 20 Ma and this dual spreading process appears to have lasted until about 15 Ma. Radiometric ages, geochemical data, relative and absolute motion models presented at the Nice AGU meeting by Duncan et al., Ray et al., Wilder et al., and Harada et al. indicate that since 30 Ma: 1) a hotspot located near Salas y Gomez Island does not require significant motion of the hotspot with respect to the Hawaiian hotspot; 2) that this hotspot has generated similar proportions of OIB vs. MORB endmember compositions in most samples collected east of Salas y Gomez; and 3) that the change of plate motion velocity was primarily accommodated by the combination of propagating rifts and microplate formation, including a rapid clockwise rotation of spreading direction and rapid increase in spreading rate, followed by a subsequent decline until present.

URL: http://imina.soest.hawaii.edu/wessel/drft06rr/

V21F-06 1145h

Revised Estimate of the Cenozoic Motion Between the Tristan da Cunha Hotspot and Pacific Hotspots

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We present a new method for objectively estimating the uncertainties of finite rotations of plates relative to hotspots. The input for our analysis are coeval dated locations along two or more ancient hotspot tracks, as well as the present locations of the hotspots. The output is a covariance matrix that can be used for testing hypotheses and for constructing confidence regions. Unlike prior methods, our method incorporates the uncertainties in all 3 degrees of freedom of a finite rotation. We apply our method to the Hawaiian and Louisville tracks on the Pacific plate and used the results to predict the track (and uncertainties) of the Tristan da Cunha hotspot on the Nubian plate. The Tristan da Cunha track provides a critical test for the fixed hotspot hypothesis because it has a fairly continuous track and has remained beneath the Nubian plate for the past 70 Myr and thus has not (in that time interval) greatly interacted with a mid-ocean ridge, which can severely complicate the track. In contrast to the results of prior studies, the predicted and observed Tristan da Cunha tracks have no significant differences for the past 48 Myr, which includes reconstructions for 11 Ma (chron 5), 20 Ma (chron 6), 33 Ma (chron 13), and 39 Ma (chron 18). For example, the predicted location of the Tristan hotspot at 48 Ma (chron 21) is about 100 km (± 250 km) from the nearest point on the Walvis Ridge, corresponding to motion between hotspots of 2 mm/yr ± 5 mm/yr. Numerical experiments indicate that the improvement to the fit to the fixed hotspot assumption for reconstructions over the past 48 Myr come from many sources including improvements to the geomagnetic reversal time scale, improvements in relative plate reconstructions, improvements in Pacific-hotspot rotation parameters, and improvements to age dates along the Hawaiian-Emperor chain. Unlike the reconstructions for the past 48 Myr, reconstructions for 56 Ma (chron 25) and 68 Ma (chron 31) have huge misfits between predicted and observed tracks. For example, the misfit between the predicted and observed point at 68 Ma (chron 31) is 1000 ± 250 km. A possible, but unlikely, explanation is that from 68 to 48 Ma, the Tristan da Cunha hotspot moved relative to the Pacific hotspots at a rate of 50 ± 12 mm/yr. An alternative explanation is that the misfit is largely accommodated by a "missing" plate boundary in the early Tertiary and Late Cretaceous global plate motion circuit, as is independently indicated by global paleomagnetic data [Acton & Gordon, 1994].

V21F-07 1205h

Revised Indo-Atlantic absolute plate rotations and their uncertainties based on moving hotspots

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Inconsistencies between the paleomagnetic and hotspot reference frames have been ascribed to the effects of hotspot motion and true polar wander (TPW). While revised models based on moving hotspots have been shown to improve a measure of fit; namely the difference between the predicted and observed hotspot tracks, the real uncertainties in such models can be quite large. We present a method for constraining the uncertainties in absolute plate motion models using a modified version of the Hellinger criterion. We use the dated tracks of four of the best studied hotspots in the Indo-Atlantic hemisphere; namely, Kerguelen, Reunion, Tristan de Cunha and the New England hotspots, together with their present positions to obtain finite rotations for the African plate. We also use models of hotspot motion to obtain analogous rotations for a moving hotspot' reference frame. The motion is consistent with available paleomagnetic constraints, and results in a significantly improved fit to the hotspot tracks. The uncertainty regions are less for the moving hotspot model due to the improved fit, and the covariance matrices obtained are equivalent to published relative plate rotation covariance matrices, and allow a combination of these uncertainties.

V22A MCC: Level 1 Tuesday 1330h

Rift Zones on Volcanic Islands: Structure, Evolution, and Magmatic Processes II Posters *(joint with S, T)*

Presiding: **T R Walter,** Rosenstiel School of Marine and Atmospheric Science, University of Miami**; A KLGEL,** University of Bremen

V22A-0561 1330h POSTER

Subsidence of Askja Volcano, North Iceland: InSAR Observations and Different Modeling Approaches

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