V21A-06 0915h

New Non-local Density Functionals for More Accurate First-principles Calculations

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Although the density functional theory based on local density approximation (LDA) and (general gradient approximation) GGA are extraordinarily successful, they fail to predict certain properties accurately. The weighted density approximation (WDA), which incorporates nonlocal information through a model exchange-correlation (xc) hole, was proposed to fix the drawbacks of LDA and GGA. We used a uniform xc G function to calculate ground-state properties of some common perovskite ferroelectric materials. The WDA yields much better equilibrium volumes than LDA for the cubic structure. The WDA also gives correct description of ferroelectric instability. However, For the relaxed structure of tetragonal PbTiO$_3$, WDA predicts a strain and volume bigger than experiment. We also presented WDA for rare-earth trihydrites, YH$_3$ and LaH$_3$. The LDA predicts YH$_3$ and LaH$_3$ as semi-metals. We investigate some commonly used pair-distribution functions G. These calculations show that the WDA can predict a substantial insulating gap while at the same time retaining structural properties in accord with experimental data. Our WDA band structures agree with those of GW approximation very well, but the calculated band gaps are still 1.0-2.0 eV smaller than experimental findings. This work is Supported by ONR.

V21A-07 0930h

Low $<->$ high density transformations in ice

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We have investigated through first principles computations the pressure induced behavior of ice XI and ice VIII. They are respectively low and high density hydrogen-ordered forms of ice that amorphize under pressure inside each other' stability field. We have found that: 1) low-to-high density transformations between ordered structures consisting of one and two hydrogen-bond-networks should happen continuously and preserve the style of electric dipole ordering. 2) In this process we have synthesized computationally two metastable phases, antiferroelectric ice XI-like and ferroelectric VIII-like. Higher energy barriers for structural transitions involving dipole reordering leads to large metastability fields. 3) Entire acoustic branches destabilize before the low$<->$high density transformations occur. The multitude of metastable structures produced by these intervening instabilities compete and conspire to produce the amorphous. In simple Landau terms, ice XI and VIII are located in deep basins of the free-energy landscape separated from each other by a few intermedieate rugged basins associated with amorphous states.

V21A-08 0945h

A determination of the melting slope of MgO from first principles

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Using a combination of density functional theory (DFT) and molecular dynamics simulations we have calculated the low pressure melting slope of MgO. Our molecular dynamics simulations are performed on both the DFT potential energy surface and a potential energy surface calculated with a new class of highly accurate classical potentials which closely reproduce the DFT results. With these tools we have reduced the error in our evaluation of the melting slope to that intrinsic to the DFT energy functionals that we use. Our results suggest that the melting temperature of MgO increases much more rapidly with pressure than has been found by diamond-anvil cell experiments[1]. Previous theoretical determinations of the melting slope using empirical potentials have also disagreed strongly with experimental results. However, by testing different DFT energy functionals we conclude that the uncertainty in our results cannot explain the large discrepancy between theory and experiment and that a new experimental determination of the MgO melting line may be in order. The melting slope that we calculate, if extrapolated to higher pressures, has strong implications for the composition of the earth's lower mantle.

A. Zerr and R. Boehler, Nature 371, 506 (1994).

V21B MCC: 3001-3003 Tuesday 0800h

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

Presiding: **D Forsyth,** Brown University**; K E Donnelly,** Lamont-Doherty Earth Observatory

V21B-01 0800h

Hot Cracks in the Pacific Plate

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Lineations in the gravity field are widespread on the Pacific plate but are not yet explained by plate tectonics. We propose that they represent warps caused by accumulation of thermoelastic stress in the cooling lithosphere. Stress is relieved along parallel cracks where young volcanic ridges sometimes develop. Both the crack spacing and gravity amplitude are predicted by the elastic plate theory and variational principle. The absence of the gravity lineations in the young lithosphere provides an upper bound on the fracture energy of the lithosphere. Our model suggests that both the gravity lineations and the volcanic ridges are a natural consequence of lithospheric cooling.

V21B-02 0815h

Fractures, not Plumes, Have Controlled Major Seamount Volcanism in the Pacific over 170 Million Years

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The distribution of guyots and atolls and large volcanic islands on the Pacific plate can be used to outline the likely connection between stresses acting on the plate and the gradual development of large, linear volcanic chains over the past 170 Ma. We construe three general periods with different stress regimes in the history of the Pacific plate. 1) During the Jurassic and Early Cretaceous, the Pacific plate was surrounded by ridge segments and there were no major stress alignments within it. Within-plate volcanism thus assumed the scattered arrangement for the condition of no tectonic stress (1), and the large Magellan and Wake seamount clusters formed. Near the eastern boundaries of the plate, complex and shifting patterns of ridge reorganization dictated formation of very long, splayed, near-axis ridges such as Horizon Guyot and Necker Ridge. 2) At about 90 Ma, the growing middle-aged Pacific plate achieved its first persistent stress regime with the formation of subduction boundaries along its western or northwestern margin. The plate was no longer static but began to move over the asthenosphere and into the mantle. Subduction boundaries and the overall direction of subduction are uncertain, but this imparted a general yet not fully stable component of tension across the plate, producing the NNW Gilbert-Marshall, Line and Emperor Seamount ridges, generally orthogonal to the overall direction of least principal stress. The Line Island seamount chain, being near ridge axes, sustained a variable stress regime. It thus has no age progression of rocks dated between 70-90 Ma (2), great width, and a dual orientations of ridges. 3) By 47 Ma, nearly half of the boundaries of the Pacific plate now were trenches spanning from the Aleutians to New Zealand. In addition, northward migration of the Indian plate and Australia caught a major portion of the westerly moving Pacific plate between the northeast corner of the Tonga Trench and the Aleutians. The plate could not shift laterally in response to whatever was occurring along its eastern spreading boundaries. A very consistent and strong stress regime therefore developed across the Pacific plate with a NNE direction of least principal stress. The change in stress orientation may have taken up to 10 million years, during an interval marked by little or no volcanic productivity at the western end of the Hawaiian chain. Since that time, the predominant alignment of both linear island chains and Puka Puka-type ridges, from the Kodiak-Bowie chain in the Gulf of Alaska to the Louisville Ridge south of the Antarctic convergence, has been orthogonal to this direction. Development of large-volume persistent chains and shorter small-volume chains indicates patterns of differential stress in the plate, variable fertility and geochemistry of the asthenosphere and/or shallow convective overturn of the asthenosphere rather than the action of mantle plumes of different sizes and depths of origin. Tapping of enriched mantle by widespread volcano clusters during the Mesozoic suggests the presence of a shallow asthenospheric source layer rather than multiple narrow conduits. (1) Hieronymus, C.F., and Bercovici, D. 2000. Earth Planet. Sci. Lett. 181, 539-554. (2) Davis, A.S., Gray, L.B., Clague, D.A., and Hein, J.R., 2002 Geochem. Geophys. Geosyst. 3: 10.1029/2001GC0000190, 1-28.

V21B-03 0835h INVITED

Viscous Fingering of Miscible Fluids in Laboratory Experiments and the Oceanic Mantle Asthenosphere

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Oceanic intraplate volcanism at a range of spatial scales is not simply explained by the fixed hotspot paradigm. The Pukapuka ridge, spanning 2000 km of the Pacific plate, forms from a geochemically enriched OIB source but propagates toward the EPR at rates greatly exceeding plate motion. A rapid localized flow of mantle material eastward to the EPR from the Pacific Superswell region is suggested. A similar mechanism could also explain the regularly spaced gravity lineations aligned with plate motion observed over large areas of the Pacific seafloor. At a smaller scale, seamounts between oceanic spreading ridges and nearby volcanic hotspots often form in uniformly spaced parallel ridges or chains, perhaps associated with material transport toward the spreading axis. The Sojourn, Hotu-Matua, and Rano Rahi seamount fields as well as the Musician seamounts are other examples of these parallel volcanic chains. Viscous fingering that develops as low viscosity mantle displaces higher viscosity mantle in the asthenosphere may be one explanation for these regular patterns in material transport. To better understand the dynamics facilitating such viscous fingering instability, we perform laboratory fluid experiments with two miscible fluids consisting of high viscosity sugar solutions. Fluid is injected into the gap between two horizontal plates initially filled with the higher viscosity fluid. The radial pattern of fluid flow that develops is observed for varying viscosity ratios, plate spacing, injection rate, and injection hole diameter. Fingering behavior is observed for viscosity ratios greater than about 10. Both injection rate and plate spacing influence the fingering wavelength and morphology. The fingering wavelength to spacing ratio of $\sim$13 is nearly constant and a factor of 3 higher than previously reported results. A complex interaction between the fluids near the bounding surfaces may change the effective fluid layer thickness. Our preliminary results suggest that if viscous fingering is responsible for the dominant 200 km wavelength gravity lineations observed for the south Pacific seafloor, the thickness of the layer guiding mantle flow should be less than 20 km. Could this be a thin, melt rich region at the top of the asthenosphere? Ongoing work is considering the potentially important effect of a moving plate at one boundary of the fluid layer.

V

V21B-04 0850h

Secondary Hotspots in the South Pacific as a Result of Mantle Plumelets and Lithospheric Extension?

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By far the largest number of secondary hotspots (cf. Courtillet et al., 2003) can be found in the "South Pacific Thermal and Isotopic Anomaly" (SOPITA) or "Superswell" region. Its Cretaceous counterpart is preserved in a large range of seamounts and guyots found in the "West Pacific Seamount Province" (WPSP). The seamounts in these regions display very distinct and long-lived isotopic signatures (Staudigel et al., 1991; Koppers et al., 2003) that can be used to combine source region chemistry and seamount geochronology to map out mantle melting anomalies over geological time. These mappings may resolve many important questions regarding the stationary character, continuity and longevity of the melting anomalies in the South Pacific mantle and its secondary hotspots. Of all secondary hotspots that are currently active in the SOPITA we could identify only two hotspots that appear to be long-lived and that have Cretaceous counterparts in the WPSP. Plate reconstructions show that the "HIMU-type" Southern Wake seamounts may have originated from the Mangaia-Rurutu "hotline" in the Cook-Austral Islands, whereas the "EMI-type" Magellan seamounts may have originated from the Rarotonga hotspot. All other hotspots in the SOPITA and WPSP are short-lived (or intermittently active) as evidenced by the presence of numerous seamount trail "segments" representing no more than 10-40 Myr of volcanism. Our observations violate one or more assumptions of the classical Wilson-Morgan hotspot hypothesis: (1) none of the South Pacific hotspots are continuously active, (2) most are short-lived, (3) some show evidence of hotspot motion, and (4) most of them have poor linear age progressions, if any at all. On top of this we have evidence for volcanism along "hotlines" and the "superposition" of hotspots. The simple and elegant "hotspot" model, therefore, seems insufficient to explain the age distribution and source region characteristics of intra-plate volcanoes in the South Pacific. This has lead to new models that retain the concept of mantle plumes, but these lack both simplicity and predictive power. New models that call on "extension" are indeed simple and they may explain most characteristics of Earth's intra-plate volcanism, but they also have limited predictive power, making it more difficult to test for their validity. We argue that we require a combination of processes: one that forces regional magmatism from a large-scale source of buoyancy from below (like the rise of plumelets shooting off the top of a superplume) and one process that acts from above, as intra-plate extension opens up pathways that allow the lithosphere to be penetrated by magma.

V21B-05 0905h

Geochemical constraints on melting proccess in the GLIMPSE region

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The GLIMPSE region, where there are cross grain gravity lineaments, has abundant volcanism that permits tests of melting conditions and mantle sources associated with these important off-axis features. The Sojourn and Brown Ridges are extensive linear features, subparralel to one another and perpendicular to the East Pacific Rise (EPR), which lies to the east. The Brown Ridge lies further to the east of Sojourn, ending ∼60 km or less from the EPR. South of the two ridges, Hotu and Matua are central complexes punctuated by dozens of smaller cones. Fresh lava flows with no topographic expression also cover portions of the sea floor in the general area. The recent flows on flat lying terrain include a flow northwest of the Sojourn Ridge, arguing for recent volcanism in the west as well as in the east. Samples from two cruises show that compositions range from highly depleted to strongly enriched. Sojourn Ridge samples show a general increase in enrichment with increasing distance from the EPR. On the Brown Ridge sporadic spikes of enrichment with no systematic geographic distribution occur and are associated with limited isotopic variations that are similar to those observed on the EPR, suggesting very recent enrichment and depletion events near the spreading axis. In contrast Hotu and Matua samples largely consist of incompatible element enriched lavas with isotopic compositions similar to Easter Island. Evidence for recent volcanism is found throughout the region. In the west, SiO_2 contents are significantly lower, reflecting higher pressures of formation and therefore little lithospheric thinning in the west. On the Brown Ridge in the east, recent volcanism also is apparent, but low SiO_2 contents are not observed reflecting younger and thinner lithosphere.

V21B-06 0920h

Origin of Cross-Grain Gravity Lineations and Intraplate Volcanic Ridges: Constraints and Ideas From the GLIMPSE Experiment

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Three hypotheses have been advanced in the literature for the origin of cross-grain gravity lineations and associated volcanic ridges in the Pacific: small-scale convective rolls aligned by asthenospheric shear in the direction of absolute plate motion; lithospheric boudinage or cracking by remotely applied stresses; and mini-plumes or hotspots. Inspired by the compositional anomalies and age progression along the Pukapuka ridge, we have suggested a fourth possibility; that the volcanic ridge and seamount chains are associated with rapid transport of volatile-rich, low viscosity mantle in the asthenosphere back toward the East Pacific Rise. The GLIMPSE experiment was designed to provide constraints on these conceptual models by measuring crustal thickness variations, seismic velocity anomalies in the underlying mantle, density anomalies as revealed through bathymetry and gravity, variations in mantle composition and the depth and degree of melting as indicated by major and trace elements and isotopic composition of the melt products, thickness of the brittle lithosphere shown by depth extent of microearthquakes, and age progression of volcanism. The study area west of the East Pacific Rise and just south of the Garrett fracture zone includes the Hotu-Matua volcanic complex, which has recent volcanic activity distributed over a region about 60 km across and 200 km long, and the Sojourn/Brown ridges, which are the largest and most continuous of these intraplate volcanic ridges. A year-long deployment of ocean-bottom seismometers, extensive underway geophysical surveying and dredging and geochemical analysis of basalts indicates that there are distinct differences between the processes of formation of the Hotu/Matua and Sojourn/Brown chains. Our current interpretation is that, rather than the gravity lineations beginning to form in seafloor 4-5 Ma old, they die out as the East Pacific Rise spreading center is approached.

V21B-07 0940h

Lithospheric and Melt Anomaly Control of Foundation Chain Volcanism

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The Foundation Chain is a small chain of seamounts and volcanic ridges extending northwestward from the Pacific-Antarctic spreading ridge. $^{40}Ar/^{39}Ar$ age data show linear migration of volcanism along-chain at a rate of 91±2mm/yr for the past 22 Myr (O'Connor et al., 1998). The case history of the Foundation Chain is notable because it is a rare example of a hotspot melting anomaly that has been traversed by a fossil microplate and is now being encroached by the active Pacific-Antarctic spreading ridge. Prior to the Selkirk Microplate encountering the melt anomaly the Foundation Chain formed as broad elongate zones of scattered, synchronous volcanism cross-cutting the overall NW-SE trend of the chain (O'Connor et al., 2002). But once the significantly older microplate began capping the melt anomaly about 14 Myr ago, the chain narrowed abruptly into a single line of discrete seamounts, only broadening again about 5 Myr ago when sufficiently young lithosphere again started drifting over the melting anomaly. Measured ages show a dominant trend of coeval, yet structurally disconnected, segments of Foundation Chain VERs developing in a series of en echelon, elongate 'zones' of coeval volcanism cross-cutting the overall NW-SE seamount trend (O'Connor et al., 2001). These elongate zones developed at intervals of approximately 1 Myr while maintaining a basically steady-state orientation and size as the Pacific-Antarctic spreading ridge migrated closer to the melt anomaly. Although VER development was controlled in part by local factors (e.g. location of nearest spreading ridge segment, lithospheric thickness and stress), long-lived attributes of the Foundation melt anomaly (e.g. size, orientation, periodicity) must have played a pivotal role. Foundation volcanism can be suppressed across elongate melt 'zones' if the capping tectonic plate is too thick for melts to penetrate to the surface (O'Connor et al., 2001, 2002). The lack of a seamount chain connecting the Foundation and the Austral volcanoes can be similarly explained, thus extending the age of the Foundation melting anomaly back to at least 34 Myr ago (McNutt et al., 1997). While lithospheric architecture controls if and where Foundation volcanism occurs (e.g., chain broadening and narrowing), it cannot explain the origin of the underlying long-lived melting anomaly. The timing and distribution of Foundation Chain volcanism requires a long-lived process that creates broad melting anomalies of fundamentally constant size and orientation under a moving Pacific lithosphere with an apparent periodicity of about once per Myr (O'Connor et al., 2001, 2002). Thus, the Foundation Chain is a product of lithospheric architecture and a first-order mantle process controlling the existence and behavior of an underlying long-lived melt anomaly.

V21C MCC: Level 1 Tuesday 0830h

Volcanic Emissions to the Troposphere: Posters II *(joint with A, B)*

Presiding: **F M Schwandner,** Institute of Mineralogy and Petrography**; D L Lopez,** Ohio University

V21C-0522 0830h POSTER

Acid Loading of Soils by Magmatic CO_2 at Mammoth Mountain, California

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Areas of tree kill appeared in the early 1990's after a shallow intrusion of magma under the south flank of Mammoth Mountain, California. Subsequent field measurements have revealed high concentrations of soil CO_2 in these areas, the locations of which are controlled by faults and fractures that serve as conduits for magmatic CO_2 streaming to the surface from depth. Detailed surveys at the largest of these tree-kill areas, Horseshoe Lake, about 14 ha in size, have consistently shown soil CO_2 concentrations that range up to 90% or greater in the shallow soil layers. Continuous soil CO_2 monitoring stations established in 1995 at Horseshoe Lake reveal a pattern of both short-term and seasonal variations in magmatic CO_2. Because the pressure of CO_2 is externally fixed by CO_2 streaming to the surface, carbonic acid activity is constrained by open-system buffering of magmatic CO_2. Eight years of intensive soil CO_2 monitoring have documented a consistent pattern whereby pH values as low as 4 can be achieved in the soil solution during spring melting of the winter snow pack. Coupled with the seasonal drop in pH, aluminum, which can also be toxic to forest ecosystems, is released from soils in those areas with the highest CO_2 concentrations. After more than a decade of exposure to elevated levels of CO_2 and repeated cycles of acid loading, along with nearly complete tree and vegetation mortality and the release of Al^{3+}, the soils at Horseshoe Lake and the other areas of tree kill may not recover their ability to sustain any significant level of forest production for several years, even if the CO_2 degassing should stop immediately. The level of in-situ acid loading by magmatic CO_2 in the tree kill areas around Mammoth Mountain rivals that of the better known process of rain-out of acid gases from volcanic plumes in the troposphere.

V21C-0523 0830h POSTER

Two Decades of Degassing at Kilauea Volcano, Hawaii: Perspectives on Island Impacts

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The ongoing eruption of Kilauea provides an opportunity to examine how volcanic emissions impact the natural and human environment of the island of