

by talc, variable degrees of serpentine-brucite alteration, and replacement of brucite by iowaite. These rocks provide a unique opportunity to calibrate our observations against recent results from experimental/theoretical geochemical studies and further our understanding of serpentinization and its role in tectonic accretion and microbial colonization of oceanic lithosphere at slow and ultraslow spreading ridges. We propose that at temperatures above 250°C, pyroxenes react to form serpentine, talc, and tremolite, releasing Ca, Si, H₂, and acidity to the reacting fluids that may cause rodingitization in adjacent gabbro bodies. Overall however, rodingites are rare, which may reflect the depleted nature of the mantle protoliths. In the absence of pyroxenes (in dunites) - or at temperatures below 250°C, where pyroxenes react very slowly - the fluids do not become enriched in Ca and Si and serpentine, magnetite, and brucite will form. Many serpentinites lack brucite, tremolite, and talc, because changes in fluid pH and silica activity of the interacting fluids, following the exhaustion of either olivine or pyroxene, caused reaction of these phases to serpentine. Extensive talc alteration of serpentinites and gabbros is usually observed at the intrusive contacts, but large-scale silica metasomatism (or Mg-loss) must be invoked to explain the overall abundance of talc at Site 1268. Significant pyrite/marcasite/hematite veining at Site 1268 indicates fairly oxidizing conditions consistent with the presence of sulfate in the interacting fluids. The first discovery of iowaite in mid-ocean ridge serpentinites (at Site 1272) and the abundant carbonate/Fe-oxhydroxide alteration, locally extending down to 90 meters below seafloor, indicate that water-rock reactions continue at low temperatures and under strongly oxidizing conditions. Pore fluids from nontronite-bearing serpentine muds in fault gouges may provide information about the nature of these late-stage circulating fluids and potential microbial activity.

V12J-08 1745h

An Estimate of Fluid-Flux in Fast-Spreading East Pacific Rise Crust Exposed at Hess Deep

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Hydrothermal circulation at mid-ocean ridges (MORs) has a profound influence on the heat and chemical budgets of the oceanic lithosphere. A geochemical approach for examining the hydrothermal fluid flux at MORs is based on the exchange of Sr-isotopes during fluid-rock interaction recorded by hydrothermally altered rocks. We present a new Sr isotopic dataset for sheeted dykes recovered from tectonic scarps at Hess Deep that in order to evaluate the controls on Sr mobility and Sr-isotopic exchange and calculate the time-integrated fluid flux of this section of fast-spreading East Pacific Rise crust. Similar to hydrothermal alteration patterns evident from mineral assemblages and O-isotope data, Sr-isotope data are spatially complex and do not systematically change with depth. All samples have ⁸⁷Sr/⁸⁶Sr ratios that are shifted towards higher values (0.70251 to 0.70391) than fresh mid-ocean ridge basalt (MORB) (0.70245), due to interaction with seawater-derived, hydrothermal fluids. Strontium concentrations vary from 72 to 121ppm; some dykes are Sr-depleted, others are Sr-enriched, whereas others have Sr contents typical of fresh MORB. Sr mobility is mineralogically controlled such that Sr is liberated where plagioclase is replaced by chlorite plus quartz and is enriched where a small amount (<2%) of epidote is present. Interestingly, the degree of albitization was found to have little control on Sr mobility even though the albite structure favours Sr partitioning. Sr-isotopic exchange was far less influenced by secondary mineral assemblages, except for epidote-bearing samples. In order to gain an estimate of the time-integrated fluid flux we have applied a linear-kinetic fluid-rock exchange model applied by Teagle et al. [2003] for sheeted dykes recovered at ODP Hole 504B. The fluid flux of 1.1 x 10⁶ kg²/m for Hess Deep is lower than that calculated for Hole 504B dykes and far lower than fluid flux estimates based on thermal constraints. We explore the significance of these low fluid fluxes and suggest that the Sr-isotopic budget of hydrothermally altered sheeted dykes is not set during vigorous flow associated with black smokers. Instead, we predict that Sr isotopes are exchanged during less vigorous flow, at or near a ridge axis.

V21A MCC: 3008 Tuesday 0800h

State of the Art in Theory of Materials: Methods and Applications II (joint with P, NG, MR, DI)

Presiding: G Steinle-Neumann, Bayerisches Geoinstitut, University Bayreuth; R M Wentzcovitch, Minnesota Supercomputer Institute

V21A-01 0800h INVITED

Predictive Capabilities for Strongly Correlated Systems: Spectral Density Functional Theory and its Applications

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Density functional theory (DFT) known to work well for weakly correlated materials fails to attack real strongly correlated phenomena, and recent progress in understanding those using many-body model-hamiltonian-based dynamical mean-field theory (DMFT) has triggered developments of new approaches for computational material science in searching for alternatives to DFT. In this talk, one of such new techniques, a spectral density functional theory [1,2], which considers total free energy as a functional of a local electronic Green function, will be discussed. Local dynamical mean-field theory, LDA+U, LDA+DMFT are seen as various approximations within this functional approach, which can be used for practical calculations. Illustrations of the method to compute total energies, local excitational spectra, lattice dynamics and other properties of various systems will be given. [1] S. Savrasov, G. Kotliar, and E. Abrahams, Nature 410, 793 (2001). [2] X. Dai, S. Y. Savrasov, G. Kotliar, A. Miglioni, H. Ledbetter, E. Abrahams, Science 300, 953 (2003).

URL: <http://physics.njit.edu/~savrasov>

V21A-02 0815h

Towards First Principles Spin Dynamics Calculations of the Magnetic Structure of Materials

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At the microscopic level, the same electrons that give rise to metallic cohesion are also responsible for moment formation and the other intrinsic (exchange interactions, anisotropy energies...) and extrinsic (coercivity, remanance) properties of magnetic materials. Despite this complexity it is possible, in many systems, to isolate fast and slow degrees of freedom that are respectively responsible for moment formation and moment dynamics. In first principles spin dynamics (FP-SD) fast moment formation is described by electronic structure methods, whilst the slow moment reorientation is described by a Landau-Lifshitz like equation. In this presentation I will outline the theory of FP-SD based on a the constrained local moment model for calculating the magnetic moments, energy and forcing fields required at each time step in the evolution of the orientational states given by the Landau-Lifshitz equation. In addition I will outline the application of FP-SD to study to the study of complex non-collinear magnetic structures of inhomogeneous systems based of FP methods capable of treating large numbers of atoms. Studies of the magnetic structure of disordered gamma-phase FeMn alloys, Co/FeMn interfaces, and quantum corrals will be used to illustrate the theory. Work sponsored by BES-DMSE US-DOE, under Contract DE-AC05-00OR227725. Computational work performed at CCS-ORNL and NERSC.

V21A-03 0830h

The effect of shear deformations on the transition onset pressure of the bcc to hcp pressure induced martensitic phase transformation in iron.

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At a pressure of approximately 13 GPa iron undergoes a martensitic phase transition from ground state ferro-magnetic bcc to a non-magnetic hcp structure. The exact transformation varies between experiments and is postulated to have a strong dependence on shear stresses during the loading process. To study this shear dependence we have developed a multi-scale model of iron, in which we employ a quantum mechanics based free energy, a kinematically compatible spinodal decomposition of phases, and a dependence on the bcc→hcp transition path(s). Using this model we see that the predicted transformation pressure for pure hydrostatic compression is much higher than expected, however with the inclusion of small initial shear deformations we see the predicted transformation pressure drop considerably and into the experimentally determined pressure range.

V21A-04 0845h INVITED

Quantum Monte Carlo Method for Materials — Random Walks in Slater Determinant Space

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In order to reliably predict materials properties, it is critical to have accurate and robust calculations at the most fundamental level. Often the desired effects of the materials originate from electron interaction and correlation effects, and small errors in treating such effects will result in crucial and qualitative differences in the properties. Density functional approaches, despite its tremendous success in allowing detailed microscopic calculations of a variety of materials, is not always reliable. We have developed a new quantum Monte Carlo (QMC) method [1] for treating electron correlations. Similar to existing QMC methods, it allows calculations of ground-state equilibrium properties in CPU times that scale as a power law with system size. In addition it allows direct incorporation of state-of-the-art techniques (non-local pseudopotentials; high quality basis sets) from the very best mean-field calculations into a true many-body framework. The method projects out the many-body ground state by random walks in the space of Slater determinants. An approximate approach is formulated to control the phase problem with a trial wave function. The method allows the use of any one-particle basis. Using a plane-wave basis and non-local pseudopotentials, we apply the method to Be, Si, P atoms and dimers, and to bulk Si with 2, 16, 54 atom (216 electrons) supercells. Single Slater determinant wave functions from density functional theory calculations were used as the trial wave function with no additional optimization. The calculated dissociation energy of the dimer molecules and the cohesive energy of bulk Si are in excellent agreement with experiment and are comparable to or better than the best existing theoretical results.

[1] Shiwei Zhang and Henry Krakauer, Phys. Rev. Lett., 90, 136401 (2003).

V21A-05 0900h

Quantum Monte Carlo Simulation of High Pressure Materials

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Equation of state information of materials at high pressures is crucial for our understanding of the structure and the evolution of planets. In regimes of extreme density and temperature which are inaccessible to experiments, first principles simulations are an established tool to study materials. In this talk, we present results from quantum Monte Carlo simulations of dense hydrogen and compare with recent shock wave experiments. We discuss implications for the properties of Jovian planets including cooling rates and the distribution of helium and heavier elements. Furthermore, we give an outlook on how these simulation methods can be applied to more complex materials.

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 PbTiO₃, WDA predicts a strain and volume bigger than experiment. We also presented WDA for rare-earth trihydrides, YH₃ and LaH₃. The LDA predicts YH₃ and LaH₃ 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 GGA 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's 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 intermediate 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 Geochim. 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 Musicians 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 ~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.

V21B-04 0850h

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

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