small sample masses, as NdO+ via conventional solid source mass spectrometry, to determine the Sm-Nd age difference between the core and bulk crystals. Using a peak metamorphic P-T condition of 8 kb, 820 C, the core (67.3 Ma) and bulk (60.9 Ma) ages of the British Columbian garnet sample yield a cooling rate of 8 C/Myr, which is in very good agreement with the cooling rates that we have derived by modeling the retrograde Fe-Mg zoning in the same garnet, and resetting of the bulk Sm-Nd garnet cooling age with respect to the U-Pb zircon age. Propagating the uncertainties of the inferred peak metamorphic condition, the three independent methods yield a cooling rate of 4-8 C/Myr for the British Columbian sample. The Salinian sample, on the other hand, yields indistinguishable core (78.2 $\pm$ 2.7 Ma) and bulk (77.9 $\pm$ 2.9 Ma) ages, as expected from its fast cooling history, which can be constrained by the results of earlier studies. Since the Sm-Nd decay system in garnet has relatively high closure temperature (usually more than 650 C), the technique developed in this paper fills an important gap in thermochronology since the commonly used thermochronometers are applicable only at significantly lower temperatures.

V12I-04 1645h INVITED

The Rates and Timescales of Collisional Orogenesis; Insights From Metamorphic Monazite and the Importance of Garnet

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Much of our understanding of the processes involved in the prograde portion of the orogenic cycle comes from physical and computational models, rather than from geological observation. Although significant progress has been made in the numerical and physical simulation of orogenesis, few constraints exist that permit these models to be rigorously tested. Tools, reliant principally upon metamorphic garnet, that allow the prograde pressure and temperature history to be determined have been applied successfully to a number of orogenic systems. However, it appears the major stumbling block is the necessary time constraints. Traditional methods involve either accessory phase or rock-forming mineral chronometry. Both methods have their drawbacks, for instance, it is difficult to attach an accessory phase age to P-T, and conversely it is notoriously difficult to get precise and accurate ages from rock-forming mineral chronometers (although several new methods have proved successful). To ameliorate this situation, several workers, including ourselves, have been actively seeking methods that allow accessory phase chronometers to be linked to P-T, with particular success being achieved with monazite and xenotime. Fundamentally these methods are of two types: (i) those that are based on detailed textural and chemical studies of the samples in question, or (ii) the empirically or experimentally calibrated accessory phase thermometers. Metamorphic garnet is fundamental to both these methods. Through a combination of these approaches with *in situ* accessory mineral dating (SHRIMP, LA-MC-ICPMS) we have been able to constrain the timing of prograde metamorphism, and determine heating and burial rates for several orogenic regions, including the Asian and Indian Himalaya and the Canadian Cordillera.

V12I-05 1705h INVITED

Garnet Deformation Microstructures: TEM vs. EBSD

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The development of electron backscatter diffraction (EBSD) and orientation contrast (OC) analysis enable us to study the microstructure of minerals and to measure the orientation of all crystallographic axes in thin sections with resolution down to sub micrometer scale. One of the great advantages of this methods is that it is now possible to study cubic crystals, such as garnet, which are isotropic for light. The application of this new technique to the study of garnets revealed an unexpected wide variety of microstructures, which are not all related to the deformation of garnet. The orientation distribution analyses help to distinguish between brittle or plastic deformation, grain or subgrain boundaries and growth defects. Garnet microstructures related to plastic deformation are characterized by the development of rotation axes if a transect across several garnet subgrains is measured with small crystallographic mismatches ($< 3^{o}$) across cell boundaries. Each specific rotation axis is directly related to the activated slip system. If more than one slip system is involved, the identification of individual is not always possible. In order to fully characterize the deformation microstructure additional transmission electron microscopical (TEM) work is needed. Here we present new data on garnet deformation microstructures characterized by EBSD and TEM techniques. In some cases a connection between cell boundary and chemical composition is observed by comparing OC, BSE and element mapping. The same area is studied by analytical TEM and shows subgrain boundaries as well as indications for brittle failure with subsequent refilling of a newly grown garnet. In the case of subgrain boundaries a higher diffusivity is expected along dislocation cores. In order to get a more general view about the net effect of microstructuring of garnet, bulk diffusion calculations were performed for homogeneously distributed defects and a network of subgrain boundaries. Assuming the same enhancement of diffusion by microstructuring as in metal, garnet remains an open system for homogeneously distributed defects below 600 to 650^{o}C at strain rates in the order of 10-12 s^{-1}. A closely spaced network of subgrain boundaries will affect bulk diffusion at even higher temperatures. Our data suggest that deformation microstructures in garnet are more frequent than previously assumed and that microstructures may significantly enhance bulk diffusion coefficients. As a consequence the microstructure of garnet must be considered when applying geo-chronological or thermo-barometrical techniques.

V12I-06 1725h

Crystallographic-Preferred Orientation vs. Shape-Preferred Orientation of Mineral Inclusions in Garnet

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Mineral inclusions in garnet are used to infer assemblages and textures that existed prior to entrapment and equilibration, and may be used to establish P-T conditions and paths. These applications rest on the assumption that inclusion shape and composition represent pre-entrapment features. If inclusions are texturally modified during syn- to post-entrapment processes, inclusion textures that appear to represent structural fabrics passively overgrown by garnet may instead represent textural and chemical interaction of inclusions with host. It is therefore necessary to determine the relationship, if any, of the crystallographic-preferred orientation (CPO) and shape-preferred orientation (SPO) of inclusions in garnet. An example of a case in which inclusion SPO might not correlate with CPO, and therefore may not represent a pre-entrapment fabric, is observed in high-grade metamorphic rocks in which the inclusions develop facets parallel to garnet crystallographic axes; that is, the inclusions are negative crystals. Because the inclusion shapes result from post-entrapment modification, the SPO defined by the facets has no meaning as a fabric indicator. Preliminary electron back-scattered diffraction (EBSD) data collected from faceted quartz and plagioclase inclusions in a sillimanite gneiss (peak T > 725 degrees C) indicate no correlation between the facet-defined SPO and the CPOs of the inclusions. Ongoing work examines the relationship between SPO and CPO for rocks representing a range of metamorphic grades and P-T-t-deformation histories.

V12I-07 1740h

Unravelling Garnet Aggregate Microstructures: Multiple Nucleation and Coalescence Versus Brittle Deformation

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Very particular garnet porphyroblast microstructures relating to a growth process that implies multiple nucleation plus grain-boundary energy minimisation driven rotation of individual garnet grains during coalescence to a single crystal (Spiess et al., 2001) have the capability to constrain the step limiting factors of reaction progress during metamorphism. Indeed, the degree of coalescence, and hence the type of microstructure that evolves by this process, relates to significantly different ratios of interface reaction rates vs. diffusion rates (Dobbs et al., 2003), and reasonably to differences in the metamorphic settings. The main importance of these coalescence microstructures might indeed be in the recognition of such interrelationships. However, similar garnet microstructures can also form by brittle deformation of a single porphyroblast, rather than by coalescence of an aggregate of individual grains. Because the implications from such deformation microstructures are totally different, there is need to unambiguously recognising their distinguishing features. We have analysed the microstructure of a garnet porphyroblast that has been deformed to an ellipsoidal aggregate of garnet grains during brittle deformation within a mylonite zone. We have used EBSD and OC to analyse the garnet substructures as well as the degree of crystallographic misorientation between adjacent grains, and we have used X-ray mapping plus quantitative EDS microchemical analysis to unravel any significant compositional zoning. The data we have obtained clearly show that coalescence microstructures are completely different from brittle deformation microstructures. Specifically, for the brittle deformed garnet porphyroblast we have observed that: 1) X-ray mapping does not reveal zoning patterns that support multiple nucleation and the setting up of growth rate differentials throughout the ellipsoidal porphyroblast domain; 2) OC images do not show substructures of microfaceted sub-domains that relate to impingement; 3) Uncorrelated EBSD data are statistically random, and the crystallographic orientation of adjacent grains do not show any tendency for a reduction in misorientation. In addition, our data also suggests that during brittle deformation fracturing of garnet to an aggregate of grains is controlled by the existing stress field, the distribution of quartz inclusions, and the crystallography of garnet. This latter aspect is also confirmed by the dispersion path of EBSD data plotted within pole figures. References: Spiess R., Peruzzo L., Prior D.J. and Wheeler J., 2001. Development of garnet porphyroblasts by multiple nucleation, coalescence and boundary driven rotations. Journal of Metamorphic Geology, 19, 269-290. Dobbs H. T., Peruzzo L., Seno F., Spiess R. and Prior D. J. 2003. Unravelling the Schneeberg garnet puzzle: a numerical model of multiple nucleation and coalescence. Contributions to Mineralogy and Petrology (published online first).

V12J MCC: 3006 Monday 1600h

Crustal and Mantle Processes in Ophiolites and Ocean Crust Generation II *(joint with GP, OS, T)*

Presiding: **Y Dilek,** Miami University**; W Bach,** Woods Hole Oceanographic Institution

V12J-01 1600h

Unconformities in Slow-Spread Oceanic Crust: Implications for Spreading Processes and Dismembered Ophiolites

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Parallel studies of ophiolites and oceanic lithosphere have provided progressively more sophisticated and complex views of processes at mid-ocean ridge spreading centers. Investigations of major seafloor escarpments in slow-spread lithosphere provide tectonic windows into the geology of oceanic crust that may be interpreted in terms of spreading processes. Traditional models of oceanic crust, largely based on the internal structure of ophiolite complexes, anticipate a laterally persistent, predictable layered assemblage of rock units including the familiar sequence of pillow basalts, sheeted dikes, and gabbroic rocks overlying mantle peridotites. However, direct observations in slow-spread oceanic crust of the Mid-Atlantic Ridge commonly reveal a diverse array of crustal structures generated at a slow-spreading rate and variable magma supply. One of the most common features of crustal sections found in these settings are unconformities in which relatively fresh basaltic lavas and/or sedimentary rocks directly overlie other variably deformed and metamorphosed crustal or upper mantle rock units. Crustal sections in different areas document these types of unconformities over serpentinized peridotites, metagabbros, and lava/dike units. Despite the common exposure of relatively deep crustal and

even upper mantle material, sheeted dike complexes are rare in these settings. Major unconformities represent discontinuities in magmatic accretion during continued tectonic extension, which may be common along slow-spreading ridges. Given their peculiar structural settings, crustal structures exposed in these tectonic windows should not be regarded as typical of even slow-spread oceanic lithosphere, but rather as part of a spectrum of structures that reflect crustal accretion with a highly variable and inconsistent magma supply. Some ophiolite complexes that appear to have been dismembered may owe their structural complexity to processes at spreading centers rather than post-obduction processes and may provide details of spreading unconformities.

V12J-02 1615h

Crustal Accretion and Cooling of the Lower Crust at Fast-Spreading Ridges: Thermal Models Consistent with Petrological and Geophysical Observations from Active Ridges and Ophiolites

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We have developed thermal models of oceanic crustal accretion at fast-spreading ridges that explicitly include petrological variation and allow the distribution of crystallisation and hydrothermal cooling to be varied. These models are used to relate geophysical observations from active ridges to petrological and geological observations from ophiolites. We ran a large number of models with different distributions of crystallisation and found that this distribution is not strongly constrained by a combination of seismic tomography and large-scale petrological observations from the Oman ophiolite. When constraints from seismic reflection and compliance surveys are also included, we find that models where 25–100% of the lower crust is formed by crystallisation in the shallow melt lens and 25–100% of the lower crust crystallises at its final depth can match the observations. Therefore, further observations are required to better constrain the distribution of crystallisation at fast-spreading ridges. Different distributions of crystallisation produce different distributions of heat release, and therefore require different distributions of hydrothermal cooling within the crust. When crystallisation occurs in the lower crust, hydrothermal cooling must extend to near-Moho depths within <5 km of the axis in order for the predicted distribution of melt to be consistent with the geophysical observations. Both petrographic and petrological observations from gabbros of the Oman ophiolite have now been used to determine relative cooling rates within the lower crust, and such observations may provide constraints on the distribution of crystallisation and hydrothermal cooling. In order to investigate these constraints, we calculated temperature-time paths from our models and, using the temperature-dependent partitioning and diffusion of Ca between olivine and clinopyroxene, predicted the concentration profiles of Ca in olivine from lower crustal gabbros. Cooling rates inferred from the Oman observations are consistent with conductive cooling. However, we found that this apparent conductive profile can be produced even when extensive hydrothermal cooling takes place to Moho depths within 1 km of the ridge axis. This profile is generated by conduction from the mantle to the lower crust at distances of < 10 km from the axis. Such heating can reset the concentrations of Ca in olivine, producing profiles that appear to be due to either conductive or bi-modal cooling.

V12J-03 1630h

Structure and Tectonics of the Moho and Surrounding Part of the Oman Ophiolite, West Sohar

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We report on a field study and subsequent analysis of ophiolites, which are on-shore examples of the ancient oceanic lithosphere, in the Bat area of Wadi Zabin and its southern extension areas in the Northern Oman Mountains. The study focuses on the extensive flow and shear structures including mylonite thrust faults, and folds. These mylonite thrust faults and folds are mapped and structurally analyzed. Each rock body, except for the later stage intrusive bodies, is always associated with strong shear zones. Exposures of regionally persistent serpentinized peridotite appears to have formed at the bottom of a dome at Bat, bounded by faults to W and covered with massive and layered gabbro to E. The mylonite and schist of ultramafic composition strikes NW approximately parallel to the inferred paleo-spreading direction suggesting that it may represent a detachment fault plastically deformed, with dextral dragged slip zones. Small-scale isoclinal folds asymmetric folds and thrusts characterize the deformation both in the mylonite and shear zones. Consideration of these structural characteristics, attitude and vergences indicate that the flow and shear structures occurred at several stages, first under high temperature conditions to form ductile deformations, and later semi brittle deformations. This deduction is consistent with an early spreading phase and a later stage of converging tectonics, possibly at the obduction stage.

V12J-04 1645h

Thermal Control on High Temperature Hydrothermal Circulation at Fast Spreading Ridges

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A deep and high-T (up to 1000°C) hydrothermal contamination of the oceanic crust at the ridge axis has been documented in the Oman ophiolite, and is confirmed by recent Sr and O isotopic investigations (Bosch et al. submitted). In the deep and hot gabbros, the main water channels are submillimetric microcracks with a dominantly vertical attitude. We propose that the mechanism allowing seawater ingression in the lower gabros, at temperatures above 700°C, is anisotropy of thermal contraction, opening microcracks that are controlled by fabric. The exceptionally large anisotropy of thermal contraction (109%) of single crystal of calcic plagioclase, when coupled with the strong lattice fabrics in the lower gabbros results in the maximum thermal contraction direction to be parallel to maximum crystals elongation L1. This direction in the oceanic ridge referential is horizontal and is perpendicular to microcracks dominant orientation. This high-T hydrothermal alteration in gabbros reaches the Moho. In the underlying peridotites, preliminary Sr isotopic data on clinopyroxene from wehrlites suggest that seawater was able to ingress at crystallization temperature for clinopyroxene. Interestingly, in these peridotites with horizontal foliation, thermal contraction, calculated as above from fabrics and thermal expansion coefficients in olivine, is vertical, being responsible for subhorizontal cracking, as deduced from serpentine dominant veining. Thus, during off-axis drifting of newly accreted lithosphere, thermal contraction opens vertical cracks, favoring seawater ingression down to the Moho. Below, in peridotites, the horizontal microcrack system would favor closing of hydrothermal circuit at Moho level.

V12J-05 1700h INVITED

Burst of High Temperature Seawater Injection Throughout Accreting Oceanic Crust- A Model Derived From the Oman Ophiolite

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Following the discovery of a high temperature (800°C) and a very high temperature (1000°C) hydrothermal alteration in the crust of the Oman ophiolite, a systematic structural and petrological study has been conducted throughout the entire ophiolite, backed by isotopic geochemistry that is developed in a companion abstract. The results show that the crustal gabbros are extensively altered down to Moho by a large seawater flux, which was channeled through identified recharge and discharge circuits. A physical model explains how microcracks, constituting the recharge system, can propagate through the hot, accreting gabbros at the ridge of origin and how, in spite of their submillimeter width, they provide the large volume of seawater necessary for the observed alteration. Building on these results, we show here that the activity of these microcracks is highly episodic, with bursts of activity lasting only a few days, and that are followed by quiescence periods of a few tens of years. This model of high temperature, oceanic hydrothermal alteration has several implications concerning fast spreading oceanic ridges and related ophiolites.

V12J-06 1715h

Hydrous Partial Melting Within the Deep Oceanic Crust

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Our knowledge on the structure, composition, and mineralogy of the in-situ lower oceanic crust (layer 3) and the mechanism how it is formed is poor. Petrological models for its generation, seismic and thermal models require an effective cooling of the deep oceanic crust. The current model implies a conductive mechanism for the cooling, and hydrothermal circulation is regarded to play a small role in transport of heat and masses in the deep oceanic crust (Wilcock, 2003). Here we demonstrate that hydrothermal circulation within the gabbroic layer starts at much higher temperatures (900° - 1000°C) as up to now believed. Water-rich fluids causes hydrous partial melting in a large scale, which is manifested by characteristic microtextures visible within many investigated rocks of all reference locations for oceanic gabbros (sampled by the Ocean Drilling Program (ODP Legs 147, 153, 176) and from the Oman ophiolite). The observed process has the potential for significant transfer of heat and masses between the upper and lower oceanic crust. The interpretation of the observed microstructures as products of hydrous partial melting is based on experimental work. Water-saturated melting experiments on a variety of natural gabbros between 900 and 1000°C at 200 MPa produced silicic melts similar in composition to oceanic plagiogranites (Koepke et al., 2003 in press). The newly formed minerals form a characteristic paragenesis consisting of plagioclase, orthopyroxene and pargasitic amphibole. In all experiments the An content of the new plagioclases is higher compared to that of the protolith, even at the lowest investigated temperature. It can be observed that olivine and clinopyroxene of the protolith react to orthopyroxene and pargasite. Very similar features can be observed in the natural gabbros. The most striking feature are zones within the plagioclase grains showing a strong enrichment in An component, often with An contents which are 20 to 25 mol% higher than those of the host plagioclase. Primary olivines and clinopyroxenes in contact with such zones very often react to orthopyroxene and pargasitic amphibole as in our experiments. These phases rim olivine and clinopyroxene and grows "interstitially", typical petrographic characteristics of a late-stage magmatic phase. Koepke J., Feig S.T., Snow J. and Freise M., 2003 in press. Contrib. Mineral. Petrol. Wilcock W.S.D., 2003. Geophys. Res. Abstr., 5: 13273.

V12J-07 1730h

Variable Seawater-Peridotite Interactions - First Insights From ODP Leg 209, MAR 15°N

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Serpentinization of peridotites at slow-spreading mid-ocean ridges has important consequences for the rheology of the oceanic lithosphere, geochemical budgets of the oceans, and microbial processes within, at, and above the seafloor. ODP Leg 209 recovered peridotites that show a remarkable variability of hydrothermal alteration reactions and intensities, including talc-tremolite alteration of pyroxenes associated with incipient serpentinization of olivine, complete alteration of peridotites to serpentine and magnetite followed by the destruction of magnetite and replacement of serpentine

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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, H_2, 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-oxyhydroxide 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 $^{87}Sr/^{86}Sr$ 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 10^6 kg^2/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. Migliori, 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 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.