

Springfield, MO, USA, August 28, 2003) were able to obtain SO<sub>2</sub> and NO<sub>2</sub> readings of 9.8 and 0.72 Mg/d, respectively. The NO<sub>2</sub> measurement was based on the spectra wavelength range of 411 to 415 nm. Laboratory and field testing is planned to further evaluate the precision, accuracy and applications of this type of instrument for remote sensing of volcanic plumes and to evaluate its performance relative to the correlation spectrometer (COSPEC), the accepted standard for volcanic SO<sub>2</sub> measurements.

## V11C-0514 0830h POSTER

### Probing Volcanic Eruption Clouds With the Airs Spectrometer on Aqua: A New Tool for Quantifying Sulfur Dioxide and Ash Emissions

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Since its launch on EOS/Aqua in May 2002, the Atmospheric Infrared Sounder (AIRS) has successfully detected SO<sub>2</sub> and ash clouds emitted during a number of volcanic eruptions. Detection of SO<sub>2</sub> is achieved using the strong infrared absorption band of the gas centered around 7.3  $\mu$ m. For upper tropospheric volcanic clouds, preliminary AIRS SO<sub>2</sub> retrievals performed using a version of the AIRS radiative transfer algorithm that includes variable SO<sub>2</sub> indicate good agreement with SO<sub>2</sub> amounts detected by the ultraviolet Total Ozone Mapping Spectrometer (TOMS) where coincident data are available. However, the higher spatial, spectral and temporal resolution of AIRS provides much improved coverage of volcanic emissions at lower altitudes, such as the October 2002 eruption of Mt.Etna (Italy). AIRS retrievals of SO<sub>2</sub> and ash optical depths and effective particle radii in volcanic clouds from several eruptions will be presented, including Etna, Ruang (Indonesia, September 2002), Reventador (Ecuador, November 2002), Anatahan (Mariana Islands, May 2003) and Soufriere Hills (Montserrat, July 2003). These examples demonstrate the potential of AIRS data to improve measurements of volcanic SO<sub>2</sub> and ash loading following eruptions, and to refine our understanding of volcanic cloud composition, structure and evolution.

## V11C-0515 0830h POSTER

### Coupling a Lagrangian Dispersion Model and Remote Sensing Data for Quantification of Volcanic Ash Transport and Deposition

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Use of remote sensing techniques, particularly the band 4 (10.3-11.3  $\mu$ m) minus band 5 (11.5-12.5  $\mu$ m) "split-window", is the predominant method for monitoring the long-term movement of airborne volcanic emissions such as ash, water vapor, and other gases. The split-window technique works well for moderately concentrated clouds, and there are methods based on radiative transfer that may provide quantitative information about total mass and particle size (Wen and Rose, 1994). However atmospheric dispersion, sedimentation and wet deposition eventually lead to the loss of discernible signals in the split window. Fortunately, numerical dispersion models do not have a low-concentration limit and are capable of longer term tracking. Model simulations also provide relative concentration changes with time. Only after post-event analysis is it possible to obtain quantitative concentration information as a function of space and time. A new technique combining remote sensing data with model simulations which may help provide near real-time information of cloud concentrations has been developed. This technique uses information gathered from several relatively recent eruptions for which total eruption volume and fallout distributions have been determined. Using the fallout distribution measurements and model simulations, the deposition rates at a function of location and time can be calculated. Combining this information with net eruption volume, ash cloud concentrations can be quantified from the model simulations and further correlated with the remote sensing data. The low-concentration limit of the split-window technique can then be obtained. Using this information, cloud concentrations can be obtained from model simulations

for cases when concentration levels are too low or remote sensing data is simply not available. Although the required data for this technique is somewhat scarce, initial results are encouraging and will be discussed. The results from this technique will be compared with those based on radiative transfer models. Also, some of the new numerical modeling techniques implemented to provide more precise information about deposition rates will be presented.

## V11C-0516 0830h POSTER

### Correlation of SO<sub>2</sub> Gas Emissions, Seismicity and Thermal Signals at Santiaguito, Guatemala

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With vertical explosions occurring approximately every 40-50 minutes, the Santiaguito dome at Santa Maria Volcano is an ideal system for examining short-term data patterns. A 3-week long field experiment was performed in January 2003 at the Santiaguito Volcano Observatory in order to record high temporal resolution measurements of volcanic activity. We collected digital seismic data from a single vertical component seismometer located approximately 4 km southeast of the active Caliente vent. A portable infrared thermal monitoring unit was deployed daily to record the temperature of the plume as it left the vent at an acquisition rate of 300 measurements per minute. A miniature ultraviolet spectrometer (MUSE) was also deployed daily to measure the SO<sub>2</sub> gas emissions just above the vent. This instrument is based on the differential optical absorption spectroscopy (DOAS) technique and allowed for continuous readings at a rate of 36 measurements per minute from approximately 6.5 km south of the Caliente vent. At abstract time, the seismic data is not analyzed, but there is a strong correlation between the SO<sub>2</sub> emission and thermal data showing that the expelled gas heats the dome extensively as it is emitted, with a possibility of different signatures indicating certain types of activity such as pyroclastic flows. It is expected that, with the addition of seismic data and the application of analysis of periodicity using Fourier Transforms, the data will elucidate conduit processes, providing additional vital constraints to sub-surface models.

## V11C-0517 0830h POSTER

### Photometric Observations of Aerosol Plumes From Volcanoes in Guatemala, El Salvador, and Nicaragua

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Visible to near infrared sun-photometers were used to measure spectral optical depths in order to infer particle size distributions of volcanic aerosols in plumes from volcanoes in the Central American arc. Data were taken from the following volcanoes on the listed dates in 2002: Pacaya, Guatemala on January 14, 16, 20 and 21; Santa Ana, El Salvador on January 24 and 26; San Miguel, El Salvador on January 28; and San Cristobal, Nicaragua on February 3. These volcanoes were chosen for study because of: good calibration of the sun-photometer (Pacaya), the presence (and effects) of a crater lake (Santa Ana) and a paucity of previous measurements (San Miguel and San Cristobal). The optical properties of these tropospheric volcanic aerosols will be retrieved after the removal of the background optical depth. Through the application of the Angstrom

equation and a King-type inversion, the Angstrom coefficients, the particle size distribution, and the effective radius (Reff) will be determined (Watson and Oppenheimer, 2000; 2001). Through these methods we hope to increase the understanding of emission and conversion processes of tropospheric volcanic aerosols. We hope the interpretation of these data will help elucidate environmental and climatic effects of these aerosols on local to global scales, and provide insight into modulation of aerosol emissions through the presence of a crater lake.

## V11C-0518 0830h POSTER

### SO<sub>2</sub> loss rates at Lascar volcano, Chile: preliminary results and interpretations from 2002 measurements

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The measurement of volcanic SO<sub>2</sub> emission rates is commonly performed on cross sections of the plume some distance downwind from the active vent, some time after its interaction with other volcanogenic gases (primarily water), particles and droplets of volcanogenic and/or meteoric origin, and atmospheric gases. The emission rates being measured therefore do not necessarily represent the real fluxes emitted by the volcano; instead they are underestimated due to the conversion of SO<sub>2</sub> to SO<sub>4</sub><sup>-2</sup> (Oppenheimer et al., 1998). Near source plume chemistry is not well understood, but can have significant effects on climatologically active species, which is why it is important to quantify volcanic SO<sub>2</sub> conversion rates as a function of meteorological environment and plume age. A mini-UV spectrometer and a Microtops II sun photometer were used to measure SO<sub>2</sub> emission rates and aerosol particle size distributions at Lascar volcano, Central Andes, during the months of October and November 2002. Direct gas measurements from fumaroles in the crater were made on November 1. These represent the first gas samples ever collected directly in the crater. Lascar volcano represents one of the end-members of the environmental spectrum, being a high volcano (summit altitude at >5600 meters above sea level) in a dry atmosphere (average RH<15%). Its location allows for simultaneous near-vent and downwind measurements at similar altitudes. Here we present our preliminary results from November 2, 2002, taken at a variety of azimuthal angles (effective distances from the plume) from the vent downwind to about 20 km, during a two-hour period (0900-1100 local time). This represents a time downwind of up to ~42 minutes, based on a plume speed of ~8 m/sec. Initial interpretations and correlations with the direct measurements are also presented. The data obtained from a Kestrel 4000 weather station will help clarify the effects of Lascar's high, dry, and extremely transmissive atmosphere upon SO<sub>2</sub> conversion rates.

## V11D MCC: Level 1 Monday 0830h

### State of the Art in Theory of Materials: Methods and Applications I Posters (*joint with P, MR, DI*)

**Presiding:** B Winkler, Institut für Mineralogie, Abt. Kristallographie, Johann Wolfgang Goethe-Universität; B Kiefer, New Mexico State University

## V11D-0519 0830h POSTER

### Influence of water on the compressional mechanism of $\beta$ and $\gamma$ spinels

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It is widely accepted that the atmosphere and the oceans of the Earth are formed by degassing of the Earth's mantle. Most of the water may have been lost or it may still be stored in the Earth's mantle. If considerable amounts of water are present in the Earth's mantle, such water plays a key role in the geodynamics of the Earth's interior, because it affects the melting temperature and the transport properties of minerals as well as their elastic properties. Recent high pressure experiments suggested that main components of the transition zone of the Earth's mantle, the wadsleyite and the ringwoodite, can store significant amount of water [1, 2]. More recently, the lower mantle minerals, consisting of Mg-perovskite, magnesio-wustite and Ca-perovskite, can potentially store considerable amounts of water [3]. However, the effects of water solution on their physical properties and the substitution mechanisms of water in these materials have not yet been fully understood. Then the first principles calculations within the density functional theory are performed here to investigate change in compressional mechanism of hydrous wadsleyite ( $\beta$ -Mg<sub>2</sub>SiO<sub>4</sub>) and ringwoodite ( $\gamma$ -Mg<sub>2</sub>SiO<sub>4</sub>), and substitution mechanisms of water in these minerals. Here two types of substitution mechanisms have been examined for wadsleyite changing the positions of substituted water molecule. Observed cell parameters and bulk moduli of the anhydrous and hydrous wadsleyites are well reproduced by the present calculations. Bulk moduli of these two calculated hydrous wadsleyite become significantly lower than that of water-free one, which strongly supports the high pressure experiment. For ringwoodite, we also examined two types of substitution models corresponding to the experimental stoichiometries, in which Mg<sup>2+</sup> and Si<sup>4+</sup> ions are replaced by two and four H<sup>+</sup> in the first and second models, respectively. Resultant reduction of the bulk moduli due to water incorporations reproduces the experimental ones as well as the case for wadsleyite. The influence of water incorporations on the transition pressure from  $\beta$  to  $\gamma$  spinels are also examined here using the free energies here calculated. Present calculations show that this transition pressure become larger by a few GPa when these minerals contain water. [1] Inoue et al., Geophys. Res. Lett. 22, 117-120 (1995). [2] Yusa et al., Geophys. Res. Lett. 27, 413-416 (2000). [3] Murakami et al., Science 295, 1885-1887 (2002).

## V11D-0520 0830h POSTER

### First-principles Study Of Hydrous Minerals, $\delta$ -AlOOH And Phase D (= G) Under High Pressure

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The existence of water in the earth is paid attention because it is thought that the presence of water affects the physical properties of earth constituent minerals. We report the physical property and crystal structure of  $\delta$ -AlOOH and phase D under high pressure.  $\delta$ -AlOOH is a new high pressure phase of boemite and diaspore and phase D is a highest pressure phase of dense hydrous magnesium silicate (DHMS). These phases are important as a possible water reservoir in the subducting slab and as a potentially water supplier into the Earth's lower mantle. While many experiments have been carried out for the quest of stable hydrous and nominal anhydrous minerals in earth's interior, its particular states of hydrogen or hydrogen bond in these minerals under high pressure have not been well clarified. In order to investigate pressure effects on structure of these hydrous minerals and its nature of hydrogen bond, we conducted first-principles theoretical calculation in which implemented Troullier-Martins pseudopotential and plane wave basis sets. Throughout the calculation in this study, we used GGA-PBE for exchange correlation functional. We found that the hydrogen bonds of both phases have symmetric character under high pressure about 30 GPa. We report structures, bulk moduli and O-H stretching frequencies of

$\delta$ -AlOOH and phase D relevant to asymmetric and symmetric hydrogen bond. The bulk modulus of symmetric hydrogen bond phase of  $\delta$ -AlOOH is more than 20% harder than that of asymmetric one. The subtle change of hydrogen position with pressure causes remarkable alteration of hydrogen bond strength and thus significantly changes bulk properties and compression behavior.

## V11D-0521 0830h POSTER

### Liquid Water from Linear-Scaling First-Principles Molecular Dynamics

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The atomic-scale simulation of hydrothermal fluids in interaction with rock surfaces requires a good description of both the fluid and the chemistry at the interface. Even if empirical force-field models or hybrid schemes can offer satisfactory results in some cases, many systems of interest demand a complete first-principles description, extremely demanding from a computational point of view. A promising method for that purpose is that of linear-scaling density-functional molecular dynamics, which will be able to face the needed sizes and complexities more efficiently than traditional methods. We explore here the performance of our linear-scaling method, based on atomic orbitals of finite support, in the description of pure water in ambient conditions. Structural (pair correlation functions) and dynamical (self-diffusion, velocity autocorrelation) characteristics are obtained and compared with experiments and previous ab initio and empirical results, showing that the linear-scaling description is very satisfactory. A study of the dynamics of hydrogen bonds will be presented as well, as a characterisation of the network-liquid character of water, very relevant to its behaviour when interacting with surfaces or solutes, hydrophobic or hydrophilic. The first-principles description offers a quite different picture from what obtained from empirical models: hydrogen bonds live longer than expected.

## V11D-0522 0830h POSTER

### Layer shift phase transition in kaolins by computer

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In contrast to our previous understanding of dehydration and decomposition of hydrous layered silicates under pressure recent experiments on a simple clay polytype, Al<sub>2</sub>Si<sub>2</sub>O<sub>5</sub>(OH)<sub>4</sub> dickite, show a single crystal - single crystal phase transition. This phase transition is characterized by a shift of the layers with respect to one another, and could provide evidence for a general type of phase transition in the layered structure of hydrated silicate frameworks. Not many clay minerals form crystals large enough to permit single-crystal X-ray diffraction studies, therefore, we use ab-initio solid state physics methods to investigate the possibility of the layer-shift phase transition under compression. We have performed computations using ultra-soft pseudopotentials in a planewave method (VASP) to study the energetics and structure of dickite and the other two kaolin polytypes, kaolinite and nacrite, as well as their observed or predicted high pressure forms, over a considerable compression range. The static computations were performed without symmetry constraints, at constant volume, with relaxation of the shape of the unit-cell and positions of the atoms. We analyze in detail the energetics of the kaolin polytypes and their structural response to compression. With these calculations we predict the layer shift phase transition to be of general character in the kaolin polytypes, and indicate that this may indeed be a phase transition that is of general character in layered hydrous minerals. If such a transition occurs in other hydrated minerals of the ocean floor during subduction, the release of water into the overlying mantle wedge may be delayed to greater depths.

## V11D-0523 0830h POSTER

### The Role of Shear in the Onset of Iron's *bcc* to *hcp* Stress-Induced Phase Transition

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Iron presents a martensitic phase transition from *bcc* to *hcp* at an approximate pressure of 13 GPa. The exact onset pressure has been determined to have values ranging from 9 to 16 GPa by several different experimental results. We propose a multiscale model for Iron, with all necessary quantities computed exclusively from first-principles. In this model, we account for all shear components of the deformation, finding that they play a crucial role in its onset, even for very small amounts of shear. Briefly, the model consists of constructing the energy landscape in all six-components of strain. Then, for a given deformation of a representative sample, we minimize its energy by possibly accommodating martensitic laminates inside it, in the spirit of a spinodal decomposition. We will describe the model in detail and show how the onset pressure varies when shear is present, as well as the mixed states encountered upon transformation.

## V11D-0524 0830h POSTER

### Finite-temperature Properties of bcc Fe

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We have used a tight-binding model fit to first-principles linearized augmented plane wave computations to compute finite temperature magnetic properties of bcc Fe. The tight-binding model was used to compute total energies and magnetic fields as functions of magnetic moment for ferromagnetic and antiferromagnetic spin arrangements. The derived energies were used to fit parameters for an effective Hamiltonian whose energy could be evaluated very rapidly. We used an energy expression (slightly modified) from Rosengard and Johansson (PRB 55, 14975, 1997). This effective Hamiltonian contains onsite terms which are functions of moment, and Heisenberg-like interactions, which are functions of the moments on a pair of atoms. We have performed a preliminary parametrization for first-neighbors and including only  $m_i \cdot m_j$  interaction terms. Monte Carlo simulations (800,000 steps per run) using the Metropolis algorithm were performed using this effective Hamiltonian for supercells of 128 atoms. As the temperature increased the total magnetic moment of the system decreased to zero, yielding the Curie temperature, T<sub>c</sub>. Preliminary results for -27, and -1 GPa are 1000 and 800K, respectively. This model will be used to find the magnetic contributions to the equation of state.

## V11D-0525 0830h POSTER

### Understanding Fe-K Alloying at High Pressure Using Density Functional Theory

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Recent experiments in the diamond anvil cell and multianvil apparatus indicate that potassium (K) can be alloyed with iron (Fe) at high pressure which has important implications for the thermal state and history of Earth's interior. Due to the volatility of K, however, the extent of alloying remains unclear in the experiments. Here we investigate by means of first principles calculations the nature and consequences of alloying K into the high pressure polymorph of Fe, hexagonal close packed (hcp), and try to use the results to analyze the experimental data. We perform density functional based computations on hcp Fe supercells of various sizes (32, 48, and 96 atoms) in which K is substituted, using the projector augmented wave method as implemented in VASP. In agreement with experiments we find that substitutional incorporation of K into Fe causes the hcp structure to expand. The atomic size of K in the hcp Fe matrix collapses rapidly as a function of pressure, and is essentially indistinguishable to that of iron at core pressures. We find in agreement with experiments and theory on pure K that at high pressure the bonding character becomes more transition metal like, with electronic d-states of K at the Fermi energy. As magnetism has been found to have a significant effect on computed physical properties of iron up to pressures of 50 GPa we have performed select computations to investigate magnetism. We find magnetism to persist in the bulk of the structure despite the incorporation of the non-magnetic K atom.

#### V11D-0526 0830h POSTER

##### Quasi-harmonic Predictions Of Structural Parameters At High P,T

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Reliable computations of materials properties at high pressures and temperatures (P,T) is possible as long as one has the essential knowledge of crystal structures and structural parameters at the same conditions. Variable cell shape molecular dynamics enabled ten years ago these computations in complex structures. However, its routine application is still not a reality because of the highly demanding nature of these computations. Besides, this technique should not predictive below the Debye T. Here we introduce a complementary, often alternative, and extremely simple procedure that allows one to determine complex crystal structures from first principles high P,T free energy computations within the quasi-harmonic approximation. We have applied it to predict the structure of MgSiO<sub>3</sub>-perovskite up to 4000 K and 150 GPa and have successfully tested it against available crystallographic data.

#### V11D-0527 0830h POSTER

##### Modelling the Cores of Dislocations Minerals

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Dislocations influence many properties of minerals, including plastic deformation, growth and dissolution, diffusion and the formation of polytypes. Some of these properties can be understood using concepts based on a description of the mineral as an elastic continuum. However, for those properties where a description of the core is important, such an approach fails and an atomic scale view must be sought. So far atomic scale modelling of the core of dislocations has been restricted to simple cubic materials and metals. We describe a recently developed a protocol for the simulation of the

core of dislocations in complex ionic and semi-ionic materials at atomic resolution. The methodology, as implemented in the program GULP [1], involves embedding an atomistic model of the dislocation core, and its immediate surroundings, in a representation of the rest of the crystal based on anisotropic linear elasticity. The simulated system is periodic in 1-dimension and follows from the developments made by, for example, Hoagland *et al.* [2], but it is not limited to simple cubic materials. The above methodology is illustrated by reference to applications involving varied mineral systems including upper mantle silicates, simple oxides and topologically more complex materials. These studies throw light on varied aspects of mineralogy, from studies of crystal growth processes associated with the emergence of screw dislocations at the surface of minerals, to the plasticity of minerals in the Earth's mantle. Studies of plasticity and dislocations in mantle minerals have been an active area of experimental science for many years, but this is, we believe, the first systematic attempt to model the core of dislocations in a range of complex ionic systems. [1] Gale, J. D. and A. L. Rohl (2003) *The General Utility Lattice Program (GULP)*. Molecular Simulations **29** pp. 291-341. [2] Hoagland, R. G., J. P. Hirth, P. C. Gehlen (1976) *Atomic simulation of the dislocation core structure and Peierls stress in alkali halide*. Philosophical Magazine **34** 413-439.

#### V11D-0528 0830h POSTER

##### Molecular Dynamics Simulations of Diffusion in a Silica Melt

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Computer modelling of silicate melts enables the study of pressure-temperature conditions not easily obtainable by traditional experimentation (e.g. 1). Diffusion in melts under various conditions is critical to our understanding of a variety of processes such as melt crystallisation, magma mixing and the behaviour of trace elements during magma ascent that underpins the field of igneous petrogenesis. It can also provide information on melt structure via diffusion mechanisms and their activation energies. In the present paper, the magnitude and mechanism of diffusion of silicon and oxygen in molten silica has been investigated by molecular dynamics using a modified BKS potential (2). A range of melt temperatures and pressures were studied with a view to understanding the relationship between temperature, pressure, diffusion and melt structure. At each P-T point studied, the system was equilibrated for between 1 million and 40 million 1fs steps depending on the conditions, with data collection over the same time range. The potential was adjusted to overcome problems with instability in the particle velocities at high temperature. The simulations were run at the Oxford University Supercomputing centre, UK. Systems of 144, 288, 576 and 1152 particles were investigated. In addition, two different sets of periodic boundary conditions were used - cubic and truncated octahedral. The latter was found to provide a better ratio of simulated time to compute time. The present data extend the range of data available and indicate a pronounced non-linearity in the temperature dependence of diffusion, as shown by plots of log10D with 1/T. The second derivative is greatest around 3500K. At least two different diffusion mechanisms may operate at lower and higher temperatures with differing activation energies. Comparison with previous molecular dynamics data shows broad agreement with most studies. Although the data presented do include some low temperature runs, comparison with experimental data is still difficult because of the differences in temperatures and pressures that are attainable by experimentation and computation. However, the extrapolated data agree reasonably well. (1) Fraser DG, Cagin T, Demiralp E, Goddard WA (1998) New transferable interatomic potentials for simulating melting of Mg silicates near the base of the mantle. A.G.U. abstract (2) Van Beest BWH, Kramer GJ, Van Santen RA (1990) Force fields for silicas and aluminophosphates based on ab-initio calculations. Phys Rev Lett **64**: 1995

#### V11D-0529 0830h POSTER

##### Atomistic Simulations of PbTiO<sub>3</sub>, PMN, and PMN-PT: using shell model potentials fitted to first principles results

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The origin of the high piezoelectric response observed in complex perovskites such as PbZn<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub>-PbTiO<sub>3</sub> (PZN-PT) or PbMg<sub>1/3</sub>Nb<sub>2/3</sub>O<sub>3</sub>-PbTiO<sub>3</sub> (PMN-PT) is not well understood. These systems are of both industrial and basic material science interest. In the past decade much progress has been made in understanding the behavior of ordered ferroelectrics using first-principles methods. The direct application of first-principles methods to examine finite-temperature properties of these larger, disordered systems is still not computationally feasible. One appealing approach is to fit interatomic potentials to select first-principles data of ordered structures, and then use Molecular Dynamics to simulate more relevant systems. We have developed a shell model potential to describe PbTiO<sub>3</sub> and PMN by fitting to first-principles results. At zero pressure, the model reproduces the temperature behavior of PbTiO<sub>3</sub>, but with a smaller transition temperature than experimentally observed. We then fit a shell model potential for the complex PMN based on the transferability of the interatomic potentials. We have examined several proposed ordered and disordered structures for PMN. We find that even for ordered PMN, quenching the structure gives a non-polar state, but with local polarization (off-center ions) indicative of relaxor behavior. For certain structures, we have observed the loss of short-range polarization order at high temperatures, indicative of the experimentally observed Burns temperature. We will also discuss the affect of electric fields on the behavior of PMN. Due to the transferability of the potential we can directly simulate PMN-PT and we will report on preliminary results for this material.

#### V11D-0530 0830h POSTER

##### First principles studies of the system Fe<sub>2</sub>O<sub>3</sub> - FeTiO<sub>3</sub>; phase stability and magnetism

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Spin polarized electronic structure (VASP) calculations of total energies and magnetic moments for ordered supercells in the system Fe<sub>2</sub>O<sub>3</sub> - FeTiO<sub>3</sub> suggest that some layered superstructures are more stable than an isocompositional mechanical mixture of hematite (Fe<sub>2</sub>O<sub>3</sub>) plus ilmenite (FeTiO<sub>3</sub>). This result contradicts established ideas about hematite-ilmenite phase relations (e.g. Burton and Davidson, Adv. Phys. Geochem. V7, pp 86, 1988). It suggests that there may be stable phases which contribute to the "lamellar magnetism" named by Robinson et al. (Nature 418, 517-2002). It is not clear if these results are artifacts of the approximations made in spin polarized local spin density functional calculations. In addition, the electronic structure of a 30 atom layered supercell [FTFFFT... F is an Fe-layer (T is a Ti-layer) perpendicular to the hexagonal c-axis] has been studied. Preliminary results indicate charge ordering similar to that predicted by Robinson et al. (2002).

#### V11D-0531 0830h POSTER

##### Monte Carlo Simulations of Feldspar Dissolution Kinetics

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We present a kinetic model based on Monte Carlo simulation to better understand the fundamental behavior of mineral dissolution. This model is applied to the dissolution of crystallographically defined Ca-Na feldspar surfaces. Adsorption energies of H<sub>2</sub>O and H<sub>3</sub>O<sup>+</sup> molecules to Al-O-Si and Si-O-Si bonds and activation energies to break these bonds were calculated using ab initio and DFT techniques (Xiao and Lutttge, 2002). These data were obtained by taking into account both solvation effects and the immersion of molecular clusters in a dielectric continuum, i.e., water. The role of cations in the dissolution of the feldspar structure is assumed trivial and most attention is focused on the behavior of Si/Al tetrahedra. The role of the crystal



structure, order/disorder phenomena, bonding characteristics of Si and Al atoms, and possible surface defects like screw dislocations and point defects are discussed. Our model allows detailed investigation of the endmembers of the plagioclase series, albite and anorthite. We analyzed the movement of steps, congruency of dissolution, inhibition, anisotropy effects, and surface composition as a function of both saturation state of the solution and crystallographic orientation of the crystal surface. Additionally, we compared the dissolution rates of albite and anorthite in the context of their ratio of Si-O-Si to Al-O-Si bonds. These results will be extended to the whole feldspar series so as to predict the fundamental behavior of feldspar dissolution and evaluate the general role of Si-O-Si and Al-O-Si bond behavior.

## V11E MCC: Level 1 Monday 0830h

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

**Presiding:** W G Minarik, University of Maryland

## V11E-0532 0830h POSTER

### Using Breccia-Hosted Spinel of Abyssal Peridotites to Obtain a Representative Local Mantle Composition

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Surprisingly little is known about the extent, scale, and causes of local (outcrop/dredge) heterogeneity in the oceanic mantle. Our primary sources of information are abyssal peridotites, which are fragments of the residual MORB mantle tectonically exposed on the ocean floor at mid-ocean ridges. On a ridge scale it is impossible to objectively pick representative samples for detailed petrological and geochemical analyses, due to analytical limitations and financial restrictions, as well as operator-biased sample selection. This is particularly important for the ultraslow spreading Gakkel Ridge (Arctic Ocean), where thousands of individual peridotite specimens from nearly forty sampling locations are available. Preliminary conventional (i.e. major and trace element mineral analyses in-situ) petrological investigations at Gakkel Ridge have revealed variable dredge-scale heterogeneities, which are related to regional changes in the extent and relative proportion of melting/melt-migration. In order to better assess the extent and distribution of dredge-scale chemical variations, we have separated spinel grains out of carbonate-cemented peridotite breccias that were collected along with normal serpentinized peridotites (and which are common on the ocean floor). The rationale for this is that the spinel clasts may provide a more representative composition of the local outcrop, or slope from which the serpentinite fragments were sedimented by mass wasting. In a pilot study, we selected 29 breccia samples from 7 dredge hauls. For each of these dredge hauls major and trace element mineral data of more than 8 normal residual abyssal peridotite (RAP) samples are available. The major element spinel compositions of the RAP hand specimens (n=95) were then compared with those obtained on breccia-hosted (BH) spinels (n=1300) from the same dredge haul. The agreement between BH spinels and those from the RAP is very good. As expected, BH-spinels cover a larger range than RAP-spinels, although each individual breccia only covers a part of the entire spectrum within a single dredge. This may mean that the spinels are derived quite locally and not mixed much. The Cr#-Ti systematics of the spinels can be used to infer degrees of melting, extent of reaction with percolating melts, and spatial distribution and abundance of dunites channels. Besides spinels from residual peridotites, the breccias host spinels from peridotites affected by high-level melt percolation, such as plagioclase-bearing peridotites or ones affected by crosscutting dykelets. In most cases, it is possible to distinguish the non-residual from the residual ones (e.g. dredge D34: 40% residual, 50% dunitic, 10% vein-influenced; n=162). Despite some limitations (higher spinel mode in dunite, possible preferential weathering of dunite), this may prove a useful

tool to estimate the local proportions of residual mantle, melt transport channels, and the volume of mantle affected by late-stage crosscutting dykelets.

## V11E-0533 0830h POSTER

### Petrological insights of the first recovered chromitites from Site 1271, ODP Leg 209, MAR 15°N

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ODP Leg 209 recovered several podiform chromitites at Site 1271, Mid-Atlantic Ridge close to the 15° 20'N fracture zone. These chromitites are the first sampled from the Mid-Atlantic Ridge. Furthermore, Site 1271 is only the second chromitite locality that has been found along any Mid-Ocean Ridges. The first chromitite found, which from near the East Pacific Rise at Hess Deep at ODP Site 895 (Arai and Matsukage, 1996), is a single, elongate, discontinuous train of chromite grains <1 cm wide. In contrast, the Site 1271 chromitites are rounded rather than elongate, have sharp contacts with surrounding peridotite, and are clearly massive. It has been proposed that the formation of chromitite occurs during subduction-related arc magmatism only, because the formation requires hydrous magmas (Matveev and Ballhaus, 2002). Therefore high Cr#s have been cited as evidence that most ophiolites with high Cr# in mantle spinels do not form at normal Mid-Ocean ridges. Based on our results, confirming the Hess Deep observation, it is clear that chromitites are not restricted to arc magmatism. However, there is abundant high-temperature amphibole in core from Site 1271, some of which could be igneous. Based on the of unusually high-Cr# (>0.6) in spinels from harzburgite and dunite dredged from the Mid-Atlantic Ridge in the 14° to 16°N region (Bonatti et al., 1992; Dick and Kelemen, 1992; Sobolev et al., 1992) and the general observation that spinels in chromitites have higher Cr# than spinels in residual mantle peridotites (e.g., Dick and Bullen, 1984), we anticipate that the Cr#s Site 1271 chromitites are the highest yet found in spinel from Mid-Ocean ridge setting. High Cr#s can provide insight into the processes of chromitite formation and may give rise to new interpretation of ophiolite provenance.

## V11E-0534 0830h POSTER

### Mont Albert to Buck Mountain: Provenance of Appalachian Ophiolite Chromites Using Osmium Isotopes

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Osmium <sup>187</sup>Os/<sup>188</sup>Os isotopic ratios have been determined for chrome-rich spinels from a suite of Appalachian ophiolites thought to represent Iapetus margin mantle formed and emplaced during the Ordovician. Because Re is incompatible during mantle melting while Os is compatible, non-radiogenic initial <sup>187</sup>Os/<sup>188</sup>Os can constrain the average source and the timing of melt extraction, especially as Os is concentrated in chromite. Radiogenic ratios indicate contamination from aged sources with high Re/Os, such as mafic or continental crust. In rocks where spinel is the only remaining primary mineral, these properties can constrain the tectonic environment of formation as well as active-margin Os transport. There is little correction for <sup>187</sup>Os in-growth since the Ordovician due to very low sample Re. Each ultramafic unit (from Mont Albert on the Gaspé Peninsula of Québec down to the Blue Ridge of North Carolina) forms a unique cluster of <sup>187</sup>Os/<sup>188</sup>Os ratios, spanning 1 to 3%, but the whole range is about 10%. This corresponds to a range of initial  $\gamma$ Os of -1 to +9, where  $\gamma$ Os is the percent deviation from a chondritic source at the age of formation (roughly 500 Ma). Within ophiolites where detailed mapping and other geochemical information are available, there is a correlation between mantle-like Os and tholeiitic basalts; radiogenic Os and boninites (Thetford Mines). Continental arc-related mantle chromites (Baltimore Mafic Complex;  $\gamma$ Os +4 to +7) are the most radiogenic. The least radiogenic are chromites from the Staten Island serpentinite and Mont Albert ( $\gamma$ Os -1 and 0, respectively), either indicating formation from a previously depleted source or that they predate the other Taconic ophiolites. The restricted range of each

ophiolite, compared to the whole of the data set, allow provenance links to be made between isolated bodies. For example, the Buck Creek, NC ultramafic complex, which has undergone granulite facies metamorphism, (Tenthorey et al., 1996) has a similar <sup>187</sup>Os/<sup>188</sup>Os to other Ordovician NC Blue Ridge dunites ( $\gamma$ Os = +6.5 to +8.5), but distinctly different from a NC Piedmont chromitite ( $\gamma$ Os = +2, Falls Lake mélange, Stoddard et al., 1989) that is inferred to be Neoproterozoic in age.

## V11E-0535 0830h POSTER

### Asymmetric Zoning in Peridotitic Spinel - Disequilibrium Melt/Rock Reaction in the Oceanic Mantle

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Models of melt migration and melt/rock reactions in the mantle are based on the assumption of an instantaneous local equilibrium (Kelemen et al., 1992). These local equilibrium models have been thought to provide the most realistic outline for future investigations so far. Plagioclase hercynites from Gakkel Ridge are characterised by strong compositional variations in all phases with an overall range of spinel Cr# from 10-55 of the sample suite often in a single thin section. The spinels show distinct asymmetric zonation that is not in accordance with orientation, shape of the grains or other textural indicators. The zoning is best developed where the spinel grains are rimmed by plagioclase. Plagioclase trace element composition show that they originate by an intruding depleted melt. Symmetrical zoning with consistent orientation of Al-rich and Al-poor regions with respect to lineation and grain shape like in mylonitic peridotites from the Miyamori ophiolitic complex (Ozawa, 1988) was not observed. The Gakkel Ridge samples show only weak deformation; therefore a different explanation is required. Residual spinel peridotites from the same dredge are generally unzoned and have homogeneous compositions. The absence of crosscutting veins and the extreme chemical disequilibrium suggest melt injection conditions very close to the hercynite solidus. The asymmetric zoning shows that diffuse reactive melt migration can take place at low melt/rock ratios in local disequilibrium conditions. If this is a general process then the assumption of local equilibrium cannot be made, at least in a major part of the melting system. Kelemen, P. et al. (1992) Nature, 358, p. 635-641; Ozawa, K. (1988) Nature, 338, p. 141-144.

## V11E-0536 0830h POSTER

### Melt Percolation and Melt Rock Interaction in the Ophiolitic Peridotites of the Alpine Apennine System (Italy): a Main Step in the Rift Evolution of the Jurassic Ligurian Tethys

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Ophiolites exposed along the Alpine - Apennine chain represent the oceanic lithosphere of the Jurassic Ligurian Tethys basin which separated the Europe and Adria plates. Pre-oceanic rifting of the Europe-Adria lithosphere caused: i) the tectonic exhumation of the sub-continental lithospheric mantle, and ii) the adiabatic upwelling and decompression partial melting of the asthenosphere. Mantle peridotites of the Alpine-Apennine ophiolites (Lanzo (Western Alps) Erro-Tobbio (Liguria), Ligurides (Northern Apennines), Monte Maggiore (Corsica)) are variably depleted spinel hercynites. They show a complete equilibrium recrystallisation under spinel-facies conditions at T = 900-1100°C, attained during their accretion to the