

lating flow stress accompanied by progressive subgrain rotation and massive fluid-assisted grain boundary migration, leading to a much lower flow stress than in the dry material. The observed flow behavior and strength can only be explained when composite dislocation and solution-precipitation creep in combination with grain boundary migration recrystallization are taken into account. Most of the resulting recrystallized grain size distributions of wet polycrystalline halite were found to be close to lognormal with a median grain size and standard deviation that decrease with increasing stress and temperature. The data allowed testing of available models for the development of steady state dynamic recrystallized grain size distributions. From the observed flow behavior, we infer that dynamic recrystallization does not lead to major rheological weakening in materials exhibiting relatively fast grain boundary migration. Therefore, it is unlikely that rheological weakening by grain boundary migration is sufficient to lead to strain localization in geological materials that in general exhibit lower migration rates than wet polycrystalline halite.

MR62A-1061 1330h POSTER

Crystallographic Preferred Orientations and Seismic Properties of Gabbroic Rocks

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The crystallographic preferred orientations (CPO) of mineral phases in gabbroic rocks are a key component for our understanding of the physical properties (rheology, seismic velocities and anisotropy, ...) of the lower continental crust and oceanic crust. In the past, the CPO of gabbros were rarely analyzed, because of the difficulty of measuring low-symmetry crystal (plagioclase, clinopyroxene) orientation using the universal stage. The recent use of the EBSD (Electron Back-Scattered Diffraction) technique in geosciences makes the measurement of these minerals much easier, using a scanning electron microscope.

We present a series of EBSD measurements of CPO in gabbroic rocks from the Oman ophiolite, from the lower crust at the South-West Indian ridge (ODP Hole 735B), and from igneous intrusions in the Itabuna belt (Sao Francisco craton, Bahia, Brazil). The measured samples cover a wide range of flow conditions, from magmatic flow to plastic flow at the ductile/brittle transition, with an emphasis on the high-temperature structures.

Plagioclase is the dominant mineral phase and forms the solid framework. Its fabrics generally display a girdle of [100] in the foliation plane, with a maximum parallel to the mineral lineation, a point maximum of [010] normal to the foliation, and a weaker concentration of [001] in magmatically deformed samples. Moving from magmatic flow to dislocation creep, the fabrics tend to retain their strong [010] point maximum and to have weaker [100] and stronger [001] maxima.

The fast direction of elastic wave propagation in plagioclase is [010]. Consequently, the effect of plagioclase in a foliated gabbro (i.e. fast direction normal to foliation) tends to be opposite to the one of olivine and clinopyroxene (i.e. fast direction parallel to lineation), resulting in a weak anisotropy, with a fast-propagation direction strongly dependent on the modal composition of the gabbro. Results are compared to the more classical fabrics and seismic properties of mantle peridotites.

MR62A-1062 1330h POSTER

Application of Impression Creep and Microindentation Hardness Tests in Experimental Rock Deformation

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The perspectives of indentation techniques for the investigation of the rheology of minerals and rocks are explored. Microindentation hardness tests using a Vickers pyramid geometry on various minerals show that this method is suitable to investigate the

strength of minerals in the low-temperature plasticity regime. Experiments on the pyroxene solid solution series jadeite-diopside revealed a good correlation between hardness and shear modulus indicating that jadeite and diopside belong to the same isomechanical group. Hardness tests on olivine provided insight into its strength anisotropy. Orientation analysis of SEM scale slip lines allowed the determination of the activated slip systems, with the crystal orientation determined by EBSD. Impression creep tests using a cylindrical indenter were performed to study the high-temperature deformation behaviour of materials at low strain rates. This method was originally established in engineering materials science, but has not previously been applied to minerals. Creep parameters obtained by impression creep tests compare well to those obtained in conventional uniaxial creep tests. The microstructure around the indents and its evolution along strain and strain rate gradients can be studied. Both methods require a minimum of sample preparation. While microindentation hardness tests can be performed on small grains within natural aggregates, impression creep tests are suitable for both single crystals and polycrystalline aggregates.

MR62A-1063 1330h POSTER

Influence of Interlayer Bonding on the Frictional Behavior of Sheet-Structure Minerals

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We compare the frictional strengths of 16 sheet-structure minerals, measured under oven-dried and water-saturated conditions, to identify the factors that cause them to be relatively weak compared to most other rock-forming minerals. We ran room-temperature frictional sliding experiments on sawcut rock samples containing a 1-mm layer of gouge of a given mineral separate. The samples were vacuum-dried at 120 degrees C overnight and then immediately tested in a triaxial apparatus at 100 MPa normal stress and 0.5 micrometers/sec sliding velocity. The samples were sheared dry to 4 mm displacement, then water was introduced to a pressure of 10 MPa and sliding was resumed at 100 MPa effective normal stress. Preliminary work (Morrow et al., 2000, *Geophys. Res. Lett.*, v. 27, pp. 815-818) indicated a possible correlation between the coefficient of friction of a dry gouge and the strength of its interlayer bonds, and the new results verify this correlation. The dry values of coefficient of friction range upwards from about 0.2 for graphite, levelling off at about 0.8 for margarite, clintonite, gibbsite, kaolinite, and lizardite. SEM examinations support the hypothesis that for those gouges with a dry coefficient of friction less than 0.8, shear occurs by breaking through the interlayer bonds to form new cleavage surfaces. For samples whose dry coefficient of friction is approximately 0.8, consistent with Byerlee's law, the interlayer bonds are sufficiently strong that other frictional processes dominate. This correlation suggests that the energy input associated with a given value of the coefficient of friction may be calibrated against laboratory cleavage measurements (e.g., about 5000 mJ/sq. m surface energy of muscovite cleaved in a vacuum; dry coefficient of friction of 0.6). The addition of water causes strength to decrease for every mineral except graphite. The range of values for water-saturated coefficient of friction is 0.2 for talc and graphite to 0.7 for the brittle micas margarite and clintonite. If these minerals are separated into groups with similar crystal structures, the water-saturated coefficient of friction increases with increasing interlayer bond strength in each group. We propose that the water in the saturated gouges exists as thin, structured films that are bonded to the plate surfaces proportional in part to the mineral's surface energy; the water-saturated coefficient of friction would then reflect the stresses required to shear through the water films. Increasing temperature and pressure would tend to reduce the width of the water films and cause the strength to increase towards the limiting dry value.

MR62A-1064 1330h POSTER

Primary Grain Shapes and Grain Preferred Orientations: Why NO Analysis of Finite Strain is Complete Without Their Incorporation

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The final shapes and orientations of fabric elements (e.g. quartz grains in a sandstone) used to quantify

the intensity of finite strain experienced by a rock is the product of distortions, volume changes, and rotations on a pre-tectonic primary fabric. Unfortunately, most studies reporting quantitative assessments of finite strain assume initially spherical shapes, non-spherical but randomly or uniformly oriented fabric elements, or that the effect of primary fabrics are identifiable even after straining.

In this study we have compiled the results of >150 fabric ellipsoid determinations from a variety of undeformed sedimentary and volcanic rock types including multiple fabric elements (e.g. crystals, pumice) from within the volcanics. While depending greatly upon the rock type and the particular fabric element in question, the primary fabric ellipsoids determined here range from those that only slightly departed from a sphere (e.g. sandstones: 1.3: 1.1: 1; pebbly mudstone: 1.25: 1.15: 1; HBL in volcanics: 1.2: 1.1: 1) to those which are extremely oblate (e.g. pumice: 3.2:2.4:1; shale: 1.5: 1.4:1). These results highlight the need for caution when selecting the type of fabric element used in strain analyses. This arises from the observation that some populations of fabric elements, such as pumice, not only yield relatively high initial mean axial ratios but also exhibit a broad range of initial axial ratios. Additionally, since the final fabric ellipsoid is the multiplicative product of the primary ellipsoid and the superimposed strain ellipsoid, the data generated in this study indicate that even for the fabric elements that yield relatively small primary fabric intensities the effect on the final ellipsoid may be dramatic. For example, the 2D combination of a primary fabric ellipse with a ratio of 1.3:1 with a strain ellipse of 2:1 would result in a final ellipse of 2.6:1, an apparent 30% more extension if the preexisting fabric is not accounted for.

Because the orientations of the primary fabric ellipsoids reported here rarely exhibit consistent relationships to bedding directed removal of the primary fabric contribution is not generally possible. We suggest, however, that the most appropriate means of correcting for the affect of a primary fabric is to multiply the finite fabric ellipsoid by the reciprocal of the mean primary fabric ellipsoid axis by axis for every axis combination. This process, therefore, brackets the range of possible final strain intensities.

MR62B MCC: Hall C Saturday 1330h

Elasticity and Constitution of the Earth's Interior I Posters (joint with S, T, V, DI)

Presiding: S V Sinogeikin, University of Illinois; R M Wentzcovitch, University of Minnesota

MR62B-1065 1330h POSTER

Equation of state of K+Fe at high pressure: K in the Earth's core?

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X-ray diffraction to 60 GPa of potassium heated with iron reveals a 2-3% inflation of the hexagonal close-packed unit-cell volume of Fe, suggesting that K dissolves into the ϵ -Fe phase at pressures above ~25 GPa. The equation of state of this K-Fe phase is well described by the Birch-Murnaghan formalism [Birch, 1978], with a zero-pressure isothermal bulk modulus slightly higher than that of ϵ -Fe: $K_{0T} = 240 (\pm 10)$ GPa, assuming a pressure derivative $K_{0T}' = 4$. Our results are compatible with both theoretical [e.g., Bukowski, 1979] and experimental work [Parker et al., 1996] indicating that K transforms from alkali to transition-metal character under pressure. The implication is that potassium can indeed be incorporated into the core early during Earth history, and thus provide an additional source of heat for the geodynamo and mantle dynamics.

MR62B-1066 1330h POSTER

Stability of bcc-Iron in the Earth Core: The End of Controversy

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We have performed *ab initio*, embedded atom (EAM) and classical molecular dynamics (MD) study of the stability of the body-centered cubic (bcc) phase of iron under conditions of the Earth inner core. The EAM and *ab initio* MD are based on the results of the Full Potential Linear Muffin Tin Orbital (FP-LMTO) and projector-augmented-wave (PAW) implementation of density functional theory. The results of different models consistently point to the stability of the bcc iron phase. The calculated temperature of hexagonal (*hcp*) to bcc phase transition at the volume of $7.2 \text{ \AA}^3/\text{atom}$ is between 4000 and 5000 K, according to different models. This is in good agreement with shockwave experiments, which show the existence of an intermediate phase between *hcp* and liquid phase. The bcc phase melts at the temperature of 6600 K at the pressure of 323.5 GPa, which is by 300 K higher than the melting temperature of the *hcp* phase. While the experiments are yet to confirm our finding, we conclude, that the present state of theory points to the stability of the bcc phase in the Earth inner core. The phase boundary between *hcp* and bcc phases is close to the "low" melting curve of iron, which now can be interpreted as the boundary of a solid-solid transition. The interpretation allows to dismiss the major controversy between the "low" and "high" iron melting temperatures. Under the circumstances, when there is no data on the state of the iron under conditions of the Earth inner core and theory predicts the bcc iron as a stable phase under those TP conditions, the Earth inner core has to be considered consisting of bcc iron. Since bcc iron is less dense than *hcp* iron, the presumable amount of light elements in the core is less than was thought before. The melting temperature of iron in the center of the Earth, when the bcc phase is taken into account, is 6900 K.

MR62B-1067 1330h POSTER

Phase Relations in the System Fe-FeSi at 21GPa

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Silicon is a light element likely incorporated in the molten core. Melting relations and subsolidus mineralogy in the system Fe-FeSi at high pressures are fundamentally important for understanding the physico-chemical state of the core. In this study, we have investigated the phase relations in Fe-FeSi system at 21 GPa in a temperature range from 1350 to 2050°C in a multi-anvil apparatus. We used mechanical mixtures of powder Fe and FeSi as starting materials loaded into an Al₂O₃ capsule. Experimental results showed that CsCl-type FeSi coexisted with Fe₃Si₂ when using Fe(+28wt% Si) starting material at subsolidus temperatures (Dobson et al., 2002, *Ame. Mine.*). The results further demonstrated the solid solution between Fe and Fe₃Si₂ (Fe+25.1wt% Si) at 1350 to 2050°C. We did not find any experimental evidence for the miscibility gap as suggested by Lin et al. (2002, *Science*). The Fe(+0.25.1wt% Si) phase most likely has the fcc structure in the present high-pressure and high-temperature conditions, although the X-ray diffraction patterns of the recovered samples show the bcc structure. Further results will be presented on the basis of in-situ X-ray observations.

MR62B-1068 1330h POSTER

Hydrogen in Iron at High Pressures and Temperatures

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Seismic data indicate both the inner and outer core of the Earth is less dense than pure iron at core pressures and temperatures. The density deficit suggests

that light elements as iron compounds are contained in the inner and outer core. The preferred candidates for the light element are hydrogen, sulfur, oxygen, silicon, and carbon. The possibility that hydrogen was dissolved into the Earth's core was proposed 25 years ago [1] and experimental works show that H has many qualities that make it a good candidate for the light element in the core [i.e. 2, 3]. However, information on iron hydride is limited and the crystal structure and the stability of iron hydride, including the equilibrium solubility of hydrogen, is unknown at higher temperatures and higher pressures. We carried out in situ X-ray diffraction experiments using electrically heated diamond-anvil cells (DACs) in order to determine the phase relation and equation of state on iron hydride. A series of experiments was performed on samples of iron and hydrogen loaded into DACs. X-ray diffraction patterns of iron hydride were collected using monochromatic synchrotron x-ray radiation and the imaging plate at the BL-13A beamline at the Photon Factory, National Laboratory for High Energy Physics (KEK). Pressure was determined by the ruby fluorescence method. As a preliminary result, we found that iron hydride which has a double hexagonal close-packed structure is stable the temperature between 300 K and 654 K at about 15 GPa. A second-order Birch-Murnaghan equation of state fitted to the pressure-volume data yields the isothermal bulk modulus of 129 (± 2) GPa and zero-pressure volume of 56.0 (± 0.3) \AA^3 , assuming the pressure derivative of bulk modulus of 4. The results are in a good agreement with those reported by Badding et al. [1991]. The composition FeH_x with $x=0.88$ (± 0.03) at zero pressure, which seems to be constant up to 25 GPa at room temperature, is obtained using the volume of iron hydride, *hcp* iron [4] and hydrogen [5]. References: [1] Stevenson, *Nature* 268, 130 (1977). [2] Fukai et al., *Jpn. J. Appl. Phys.* 21, L318 (1982). [3] Badding et al., *Science* 253, 421 (1991). [4] Uchida et al. *JGR* 106, B10, 21799 (2001). [5] Fukai, *High-Pressure Research*, Syono and Manghani, eds., AGU, Tokyo/Washington D. C., 373, (1992).

MR62B-1069 1330h POSTER

Elasticity of Antiferromagnetic *hcp* Iron

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The thermodynamic properties of the high pressure polymorph of iron (*hcp*, ϵ) under compression are an essential component of our understanding of Earth's core, with particular importance of compression behavior and elasticity. While at core pressure the equation of state and bulk moduli from experiment and computational mineral physics agree well, there is considerable discrepancy in compressional and shear elasticity below 100 GPa [1,2].

Using accurate first principles theory we previously [2] found an orthorhombic magnetic ground state for *hcp* iron (afmII, stable up to ~ 50 GPa) that considerably improves the agreement of the equation of state between experiment and theory. By computing the full elastic constant tensor of the magnetic superstructure (nine independent elastic constants) we evaluate the influence of magnetic correlations on the elasticity of *hcp* iron. We apply state of the art all electron density functional theory (implemented in the Linearized Augmented Plane Wave method) with a GGA exchange correlation potential, and compute elastic constants from strain energy, relaxing the positions of the atoms in the *hcp* cell.

We find that for afmII both the longitudinal and shear moduli are reduced considerably, resulting in a lower shear modulus over the compression range where afmII is predicted to be stable. This yields overall better agreement in aggregate acoustic properties with experimental studies, although there remains some disagreement in the shear wave velocity. We further find enhanced single crystal anisotropy for the afmII structure over non-magnetic *hcp* iron.

[1] H. K. Mao et al., *Nature* 396, 741 (1998); *ibid.* 399, 280 (1999); *Science* 292, 914 (2001); [2] G. Steinle-Neumann et al., *Phys. Rev. B* 60, 791 (1999)

MR62B-1070 1330h POSTER

Constraints on the Composition of the Outer Core From the Equations of State and Other Properties of Liquid Fe,S,Si-alloys.

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The seminal work of F. Birch (Birch, 1952) opened the perspective of deriving the chemical composition of the Earth from the comparison of the elastic properties of Earth materials as probed by seismic data and those measured experimentally on various compounds. Our present knowledge of the terrestrial outer core is that it consists of 85-95wt% Fe (Poirier, PEPI, 85, p.319, 1994; Laio, *Science*, 287, p.1027, 2000), light element(s) adding up to 100%. Several and independent geochemical models predict that both S and Si are present in the core (Allegre et al., EPSL, 134, p. 515, 1995; Javoy, GRL, 22, p.2219, 1995; Dreibus, GCA, 60, P.1125, 1996), with 7-10wt%Si and 1-3wt%S. Meanwhile, at ambient pressure, the Fe-S-Si system presents a very large domain of immiscibility (Raghavan, 1988) with the coexistence of two liquids (FeS and FeSi). This observation has largely lead to reject the simultaneous presence of S and Si in the Earth's core

We investigated the physical properties of liquid Fe and liquid Fealloys at high pressure, using large volume presses (Paris-Edinburgh cell up to 6 GPa, multi-anvil apparatus up to 27 GPa). From our experimental results, three major issues will be addressed: 1) what are the equations of state of Fe-x%S and Fe-x%Si liquids?, 2) what are the structural changes in the liquid at the atomic scale with increasing pressure and temperature, and their dependency upon the nature and amount of alloying light element, and 3) how the miscibility gap evolves in the Fe-S-Si system at high pressure?

Answering these questions will help us to constrain the composition of the outer core not only by following the ingenious method of F. Birch but also by investigating the formation of the Earth's core, in the 0-5 GPa range.

MR62B-1071 1330h POSTER

Shear Elastic Constants for Metals and Silicates from Stonely Waves in the Diamond Anvil Cell

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Despite progress in the accurate determination of equation-of-state properties for mantle and core constituents under deep Earth conditions, key elastic properties remain poorly understood. While pressure and temperature-dependence of the bulk modulus is reasonably constrained on the basis of high precision volume measurements, full sets of elastic constants and, in particular, the shear modulus are substantially more difficult to measure or estimate. At this point several measurements and theories are not in accord. Two key applications are in understanding the nature of lateral variations in velocity in the deep mantle and in understanding the nature of elastic anisotropy in the inner core. Lateral change in composition is often assumed to underlie the anti-correlation of bulk and shear elastic properties in the lower mantle. The degree of lattice preferred orientation in the inner core is not at all clear on the basis of existing data or theory.

It is experimentally possible to generate interfacial elastic waves between samples and the pressure medium in a diamond anvil cell using the impulsive stimulated light scattering (ISLS) technique. The measured velocities provide strong constraints on the shear modulus. The method has been applied to the measurement of elasticity of iron and tantalum to pressures above 30 GPa. Measurements are also possible in silicates prepared with a thin metal film on the surface. However, interfacial waves do not exist for some combinations of elastic properties and in some cases, the velocities are more sensitive to the properties of the pressure medium than the sample. The general utility of ISLS to excite interfacial waves and examples for metals and silicates are discussed.

MR62B-1072 1330h POSTER

Elastic wave velocities of iron-bearing Ringwoodite ($\text{Mg}_{0.8}\text{Fe}_{0.2}\text{SiO}_2$) to 12GPa at room temperatureYuji Higo¹ (81-89-927-8405; higo@sci.ehime-u.ac.jp)Baosheng Li² (1-631-632-9642; bli@notes.cc.suny.edu)Toru Inoue¹ (81-89-927-9658; inou@sci.ehime-u.ac.jp)Tetsuo Irifune¹ (81-89-927-9645; irifune@dpc.ehime-u.ac.jp)Robert C. Liebermann² (631-632-8214; robert.liebermann@sunysb.edu)¹GRC, Ehime University, 2-5 Bunkyou-cho, Matsuyama 790-8577, Japan²Department of Earth and Space Sciences, SUNY at Stony Brook, Stony Brook, NY, NY 11794

At present, it is widely accepted that olivine is the most important mineral in the Earth's upper mantle. The elastic property changes associated with the phase transformations to its high-pressure polymorphs are very important parameters to constrain the composition of the mantle transition zone. In this study, we measured the elastic wave velocity of iron-bearing Ringwoodite ($\text{Mg}_{0.8}\text{Fe}_{0.2}\text{SiO}_4$). The specimen was hot-pressed at 18GPa and 1273K in a 2000-ton Uniaxial Split Sphere Apparatus (ORANGE-2000: GRC at Ehime university). The recovered polycrystalline specimen was characterized by x-ray diffraction, EPMA, ultrasonic techniques, and the density was determined by Archimedes method, and found to be single-phase and fine-grained. Bench top measurements of the compressional and shear wave velocities yielded $V_p=9.10$ km/s and $V_s=5.52$ km/s. High-pressure ultrasonic measurement was carried out in a 1000-ton Uniaxial Split-Cylinder Apparatus (USCA-1000: SUNY) at pressures up to 12GPa at room temperature using ZnTe as internal pressure marker. The sample was surrounded by lead to minimize the deviatoric stress. Also in this experiment, the travel times of the Al_2O_3 buffer rod were used for pressure calculation. The travel times of the buffer rod under the same cell geometry have been calibrated as a function of sample pressure by the thermal equation of state of NaCl using in-situ X-ray diffraction techniques. The results of our high-pressure experiment, including the elastic moduli and their pressure dependence, effect of iron on the elastic moduli, as well as their implication for the mantle transition zone, will be presented.

URL: <http://ccserv.adm.ehime-u.ac.jp/~grc/e.html>

MR62B-1073 1330h POSTER

Magnesiowüstite ($\text{Mg}_{0.64}\text{Fe}_{0.36}\text{O}$) Thermal Equation of State to 25 GPa and 2073 KW van Westrenen¹ (w.van_westrenen@gl.ciw.edu); J Li¹ (j.li@gl.ciw.edu); Y Fei¹ (fei@gl.ciw.edu); JA Van Orman¹ (j.van_orman@gl.ciw.edu); WG Minarik^{1,2} (minarik@gl.ciw.edu); T Komabayashi³ (tkomabay@geo.titech.ac.jp); K Funakoshi⁴ (funakoshi@spring8.or.jp)¹Geophysical Laboratory, Carnegie Inst of Washington, 5251 Broad Branch Rd NW, Washington, DC 20015, United States²Dept of Geology, University of Maryland, College Park, MD 20742, United States³Dept of Earth and Planetary Sciences, Tokyo Inst of Technology, Tokyo 152-8551, Japan⁴Spring-8, JASRI, Hyogo 679-5198, Japan

Magnesiowüstite solid solution, ($\text{Mg}_y\text{Fe}_{1-y}\text{O}$) is the most voluminous oxide in Earth's lower mantle. An accurate thermal equation of state (EOS) for this phase is required to extend thermodynamic properties measured at lower pressures and temperatures to lower mantle conditions. These properties can then be used to compare predictions from thermodynamic modelling with geophysical observations. We have determined the thermal equation of state of magnesiowüstite ($\text{Mg}_{0.64}\text{Fe}_{0.36}\text{O}$) up to 25 GPa and 2073 K. Magnesiowüstite volumes were determined *in situ* at high pressure and temperature using energy-dispersive synchrotron X-ray diffraction at the SPring-8 synchrotron facility. Our data are consistent with an Anderson-type thermal EOS with $K_{T0} = 157 \pm 2$ GPa, $(\delta K_{T0}/\delta P)_T = 4.0 \pm 0.1$, $(\delta K_{T0}/\delta T)_P = -0.031 \pm 0.002$ GPa K^{-1} , $(\delta K_{T0}/\delta T)_V = -0.095 \pm 0.025$ GPa K^{-1} , and $\alpha_{T0} = 4.05 \pm 0.16 \times 10^{-5} + 1.12 \pm 0.22 \times 10^{-8} \times T$. The calculated Anderson-Grüneisen parameter at 300 K is 4.5 ± 0.1 . Most of these parameters are consistent with previous data on the same material (Fei et al., *PCM* 18: 416-422, 1992; Zhang and Kostak, *PEPI* 129: 301-311, 2002), with the possible exception of the thermal expansion coefficient α_{T0} .

($\text{Mg}_{0.64}\text{Fe}_{0.36}\text{O}$) appears to expand more rapidly with temperature than previously assumed, and also more rapidly than pure MgO under the same conditions. This effect cannot be observed at temperatures below 1273 K, and illustrates the importance of high temperature studies for the accurate determination of equations of state of mantle minerals.

MR62B-1074 1330h POSTER

Effects of Iron and Pressure on the c11 Elastic Constant of (Mg,Fe)O Using a New GHz-Ultrasonic Diamond Cell With In-Situ X-ray Diffraction to 10 GPa

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(Mg,Fe)O may be one of the most elastically anisotropic cubic minerals likely to occur in Earth's interior. At ambient *P-T*, pure MgO exhibits ~10% P-wave and ~13% S-wave anisotropy. The landmark single-crystal ultrasonic experiment of Chen et al. (1998) showed that increasing pressure reduces this anisotropy, leading to either zero anisotropy or a switch in sign of the anisotropy factor ($A=2c_{44}+c_{12}$)/ c_{11} expected at ~20 GPa. They also showed that on increasing temperature (at pressure) the value of *A* recovers to bench-top values at only 1000 K (at 8 GPa). The effects of pressure and iron in amounts relevant to Earth's interior on the anisotropic elastic properties of (Mg,Fe)O are not yet known. With this and other questions at hand, we are undertaking hydrostatic single-crystal elasticity measurements on (Mg,Fe)O using GHz-ultrasonic interferometry. Thus far, we have determined the pressure derivative of *c*₁₁ to a maximum hydrostatic pressure of 9 GPa, resulting in linear derivatives ($dc_{11}/dP = 9.4(1)$, $11.7(4)$, $9.8(4)$, and $9.4(2)$ for MgO, and (Mg,Fe)O with 15, 24, and 56 mol% FeO, respectively. This behavior is consistent with our previous results on the compositional dependence of the bulk modulus, which we observed to increase between MgO and (Mg,Fe)O with 25 mol% FeO, before decreasing towards non-stoichiometric $\text{Fe}_{0.95}\text{O}$. Therefore we speculate that the decrease in dc_{11}/dP for the highest Fe-content sample is due at least in part to defects.

The experiments were carried out in a new GHz-ultrasonic diamond cell modeled after the classic tri-pin Merrill-Bassett design. The cell is capable of pressures >10 GPa and features a 60° opening for in-situ single-crystal X-ray diffraction. The anvil seats contain no glue or epoxy so the entire frame (Vascomax 350) may be heated, as we have done readily up to 200°C for annealing. Perhaps most notably, the ultrasonic measurements were made *without* the use of a bonding agent (such as glue or gold) between the sample and the acoustic anvil. We have successfully implemented a novel ultrasonic pressure medium using aerogel, which has the lowest density of any known solid (~0.1 g/cm³) corresponding to about 95% porosity. By wetting the aerogel with a 16:4:1 Methanol:Ethanol:Water fluid, we achieved a hydrostatic but *supportive* pressure medium. The gel appears cloudy at zero pressure, but becomes more transparent above ~0.5 GPa, facilitating optical alignment of the acoustic buffer rod.

Reference: Chen et al. (1998) *Science*, Vol. 280, 1913-1916.

MR62B-1075 1330h POSTER

High Temperature Sound Velocity Measurements with Brillouin spectroscopy on Laser-Heated Samples

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Knowledge of the elasticity of mantle minerals at high temperatures is essential for constructing reliable mineralogical models of the Earth's mantle and interpreting seismological observations. Most of acoustic elasticity measurements up till now have been limited to relatively low temperatures (usually below proposed mantle temperatures) especially if combined with high pressures.

Here we present the first high-temperature Brillouin elasticity measurements of a number of materials (MgO, quartz, silica glass, Al_2O_3) performed with CO₂ laser heating up to or above melting temperatures. In most cases the Brillouin peaks for both compressional and shear velocities remain clear and well defined up to 2500 K (providing that the sample did not melt). Above 2500 K the collection of high-quality Brillouin spectra becomes somewhat problematic due to high thermal background. The temperatures can be measured radiometrically, using the thermal emission of the sample in visible region, or can be inferred on the basis of Raman scattering information or independent sound velocity measurements performed with a resistance heater.

Our initial experiments show that Brillouin scattering coupled with CO₂ laser heating is a viable means of performing sound velocity measurements at extremely high temperatures, significantly beyond those readily made using resistance heating. The work on combining the Brillouin measurement in a diamond cell with laser heating is now in progress and will be discussed.

MR62B-1076 1330h POSTER

What is wrong with Decker's pressure scale

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Decker's equation of state for NaCl (Decker 1971) is examined with respect to *P-V-T*, ultrasonic and shock wave data of MgO and NaCl. At room temperature up to 10 GPa, it has been found that Decker's pressure scale is systematically about 6-8% lower than that estimated from the ultrasonic data of MgO. Similar corrections may also be applied as a first order approximation at high temperatures up to 800°C. The correction is about 3-4% higher than the equation preferred by Birch (1978, 1986), but agrees well with the one derived with a higher value of *K'*, which as noticed by Birch, does not violate the shock data of NaCl. *K'* of NaCl hence may be underestimated in the early experiments due to the problem in pressure calibration. The analysis of the shock wave data of NaCl also indicates that even the fourth-order Birch-Murnaghan equation of state may not be sufficient to represent the pressure-volume relationship of a soft material like NaCl. The detailed corrections at higher pressures and temperatures are still unclear as they are limited by the uncertainties of the data. The study suggests that most of the uncertainties are systematic and introduced by the deviatoric stress and the systematic errors in temperature measurements. For a consistent pressure scale, those errors should be eliminated in future experiments.

MR62B-1077 1330h POSTER

High Pressure Crystal Chemistry of Hydrous Ringwoodite

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Single crystals of hydrous Fe₉₀ ringwoodite up to 800 μm in diameter have been synthesized in a multi-anvil press at 1400°C and 20 GPa. The crystals are deep blue in color and contain approximately 0.8 percent H₂O by weight as measured by IR spectroscopy.

The unit cell parameter of this material has been refined by single-crystal X-ray diffraction at 15 different pressures up to 3.8 GPa. Pressure was determined by refinement of the unit cell volume of a standard quartz crystal. Preliminary values for the bulk modulus give a *K*₀ = 172 ± 9 GPa and *K* = 5.1 ± 1.6 over the range studied.

The crystal structure of this material has been refined at six pressures up to 3.8 GPa. Refinements were

obtained from an average of 13 unique data with values of $R_f < 5\%$. Preliminary estimates of the polyhedral compressibilities are $1.0 \times 10^{-2} \text{ GPa}^{-1}$ ($K = 100 \text{ GPa}$) for Mg^{VI} and $6.3 \times 10^{-3} \text{ GPa}^{-1}$ ($K = 160 \text{ GPa}$) for Si^{IV} .

Comparison of the present data with previous results shows a systematic decrease in the bulk modulus of ringwoodite with H content. This decrease is larger than the effect of temperature within the allowable ranges of each so that an increase in H_2O content of one percent would have an effect on the bulk modulus equivalent to raising the temperature by 500°C .

MR62B-1078 1330h POSTER

Elastic Constants of Chrome-Diopside: Application of Resonant Ultrasound Spectroscopy to Monoclinic Single Crystals

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Although clinopyroxene represents from 15 to 25% of the upper mantle, its elastic properties have not been studied as extensively as those of other mantle minerals, in part, because of its low crystal symmetry. The right-rectangular parallelepiped resonance (RPR) form of resonant ultrasound spectroscopy (RUS) is applied to monoclinic crystal symmetry to determine the 13 adiabatic elastic constants, C_{ij} , of single-crystal chrome-diopside $\text{Di}_{0.93}\text{Hd}_{0.03}\text{Ur}_{0.02}\text{X}_{0.02}$ (Di, diopside; Hd, hedenbergite; Ur, ureyite; X, other or unknown). These data represent the first successful application of the RPR method to determine the complete elastic tensor of a monoclinic single-crystal, thus demonstrating the feasibility of this method for studying elasticity of low symmetry crystals. The lowest 62 modal frequencies of a gem quality specimen were measured and identified at ambient temperature and pressure. Inverting the modal frequencies results in respective C_{11} , C_{22} , C_{33} , C_{44} , C_{55} , C_{66} , C_{12} , C_{13} , C_{23} , C_{15} , C_{25} , C_{35} , and C_{46} values (GPa) of 228.1(1.0), 181.1(0.6), 245.4(1.3), 73.9(0.3), 68.2(0.2), 78.1(0.2), 78.8(0.5), 70.2(0.7), 61.1(0.7), 7.9(0.5), 5.9(0.5), 39.7(0.4), and 6.4(0.2), where numbers in parentheses indicate experimental uncertainty. The corresponding isotropic bulk, K_S , and shear, G , moduli are 116.5 (0.7) and 72.8(0.2) GPa, respectively. When comparing these results with other pyroxene data, we find systematic correlations between M2 site composition and C_{ij} values for most, but not all, moduli. Unusual compositional dependence near end member diopside is seen for a few moduli, and is propagated to K_S and especially G , which should prompt a re-examination of some C_{ij} values of end member diopside.

MR62B-1079 1330h POSTER

Single Crystal Compression Study of Hydrous Wadsleyite II

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Wadsleyite II is a hydrous silicate spinelloid phase and a possible constituent of the Earth's Transition Zone that may occur between the stability regions of wadsleyite (spinelloid III) and ringwoodite (spinel). Its crystal structure is similar to spinelloid IV, which occurs between the fields of spinelloid III and V in the anhydrous Ni aluminosilicate system. The space group is *Imma* with $a = 5.69$; $b = 29.0$; and $c = 8.24$. Two crystals of this phase of slightly different compositions, Fo90 and Fo88 have been studied by high-pressure single-crystal X-ray diffraction in the diamond anvil cell to pressures of about 5.6 GPa. The two crystals contain 2.1 and 2.8% H_2O by weight. They also contain significant amounts of trivalent cations Fe, Al, and Cr. The two samples have been characterized by electron microprobe, single-crystal X-ray diffraction, high-resolution transmission electron microscopy, and IR and Mossbauer spectroscopy.

Preliminary fits of the unit cell volumes at various pressures to a second-order Birch-Murnaghan equation of state give bulk moduli of $150 \pm 9 \text{ GPa}$ for the Fo90 sample containing 2.1% H_2O and $127 \pm 12 \text{ GPa}$ for the Fo88 sample containing 2.8% H_2O . These preliminary bulk moduli are consistent with a systematic decrease in bulk modulus with H content similar to that

observed in wadsleyite. The presence of wadsleyite II in the Transition Zone would tend to obscure the transition of wadsleyite to ringwoodite near a depth of 525 km.

MR62B-1080 1330h POSTER

Superheating of Crystalline Solids: Theory, Experiment, Simulation and Applications to Static and Dynamic High-pressure Melting

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Systematics of superheating ($\Theta = \Delta T/T_m$, where ΔT is the amount of superheating and T_m melting temperature) of crystalline solids as a function of heating rate (Q) are established by defining a dimensionless energy barrier for nucleation, $\beta = 16\pi\gamma_{sl}^3/(3kT_m\Delta H_m^2)$ where γ_{sl} is the solid-liquid interfacial energy, ΔH_m is the heat of fusion and k Boltzmann constant. Under conditions that lead to homogeneous nucleation (e.g., ultrafast internal heating), superheating is more pronounced.

Sound speed and shock temperature measurements on various materials (Fe, V, Mo, Ta, W, CsBr, KBr, SiO_2 , and Mg_2SiO_4) under planar impact ($Q \sim 10^{12} \text{ K/s}$) leads to superheating of $\Theta = 0.2 - 0.6$. Comparable superheating was achieved during intense laser irradiation ($Q \sim 10^{12} - 10^{15} \text{ K/s}$) on Al, Pb and GaAs. These observations are captured by the $\Theta - \beta - Q$ systematics. Homogeneous nucleation is inherent in molecular dynamics simulations of perfect bulk crystals with typical heating rates $Q (\sim 10^{12} - 10^{13} \text{ K/s})$ similar to those in shock wave loading and intense laser irradiation. Single-phase and two-phase simulations of melting of *fcc* metals (Al, Ni, Cu, Rh, Pd, Ag, Ir, Pt, and Au), a *bcc* metal (Ta), oxides (MgO and SiO_2) with various types of force field (FF) such as embedded atom method potential, first-principle potential and Morse-stretch charge equilibrium FF etc., have demonstrated superheating consistent with the superheating systematics.

Despite of the large range of melting temperatures observed, the extrapolation of melting curves from diamond-anvil-cell experiments on V, Mo, Ta and W remain discrepant with shock wave results even when superheating and experiment uncertainties are taken into account. In the case of Fe, the discrepancy is less pronounced. This may result from a not yet explored solid-solid phase transition.

URL: <http://www.gps.caltech.edu/~sluo>

MR62B-1081 1330h POSTER

Equation of State and Phase Diagram of Silica: Geophysical Applications

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New results in static synthesis, shock wave loading and molecular dynamics modeling of high-pressure polymorphs of silica have advanced our understanding of silica as a prototype system of interest for geophysics and materials science (Luo et al., *GRL*, 2002; Luo et al., *Physics-USpekhi*, 2002). The shock wave equation of state (EOS) and static high-pressure results of fused quartz, quartz, coesite and stishovite, and phase diagram of silica up to megabar regime, are presented based on previous and current studies. These results bear important geophysical applications. Thermodynamic calculation of the reaction of $\text{MgSiO}_3(\text{perovskite}) \rightarrow \text{MgO}(\text{periclase}) + \text{SiO}_2(\text{stishovite})$ demonstrated that MgSiO_3 perovskite is thermodynamically stable relative to the oxide assemblage at lower mantle conditions. The EOS and phase diagram of silica system also allow a rigorous calculation of the thermodynamic states and kinetics on Hugoniot and release of shocked silica, which

are of great importance for the interpretation of natural and laboratory impacts. The thermodynamic states of shocked quartz upon loading and release (including mixed phase regime) are determined based on Debye's model when applicable, and measured release pressure-particle-velocity paths (Podurets et al., *Izv.*, 1976). The calculated shock and post-shock temperatures are in agreement with experiments (Lyzenya et al., *JGR*, 1983; Boslough, *JGR*, 1988), and appear to validate the method of measuring post-shock temperature. Interesting physical phenomena such as superheating, amorphization and polymorphism are shown to be present upon both loading and unloading.

URL: <http://www.gps.caltech.edu/~sluo>

MR62B-1082 1330h POSTER

Crystal chemistry and mineral physics of silicate perovskite in the Earth's lower mantle

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The lower mantle constitutes more than half of the Earth's interior by volume, and is believed to consist predominantly of (Mg,Fe)SiO₃ perovskite, with up to ~20% (Mg,Fe)O magnesio-wadsite. The oxidation state, site occupancy, and spin state of iron in perovskite has significant control over the physical and chemical properties of the lower mantle, including sub- and super-solidus phase relations, transport properties, elasticity, trace-element partitioning, and geomagnetism. In order to determine the effect of pressure, temperature and composition on the oxidation state, site occupancy, and spin state of iron in perovskite, we have synthesized a number of silicate perovskite with different iron and aluminum contents. The synthesized samples were examined using an electron probe microanalyzer, a microbeam X-ray diffractometer, a Mossbauer spectrometer, and an X-ray emission spectrometer. Our data will be applied to understand the physical and chemical properties and processes in the lower mantle, as well as the electronic properties in highly correlated 3d compounds.

MR62B-1083 1330h POSTER

Tetragonal Structure of CaSiO₃ perovskite at 20–46 GPa

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CaSiO₃ perovskite is one of the major phases in the transition zone and lower mantle. Although its stability has been confirmed to 134 GPa, its crystal structure is less certain and several recent first-principles calculations predict a non-cubic structure of CaSiO₃ perovskite at mantle pressures. The low resolution of energy-dispersive X-ray diffraction that was previously used did not allow the detection of any deviation from cubic symmetry that involved a peak splittings (< 0.7 %).

We conducted high-resolution X-ray diffraction measurements using synchrotron radiation sources (CHESS and SSRL). Image plates were used to collect diffraction from monochromatic X-rays (17 keV, 25 keV). Pure wollastonite powder was mixed with platinum which serves as both a pressure standard and laser absorber. Argon was loaded as both pressure medium and thermal insulator. Ruby chips were also loaded to provide a secondary pressure calibration. In order to synthesize CaSiO₃ perovskite and anneal differential stresses, samples were heated to more than 1500 K using a continuous Nd:YAG laser before each X-ray diffraction measurement.

We observed peak splittings for the 200 and 211 diffraction lines, attributable to a tetragonal distortion of CaSiO₃ perovskite at 24–46 GPa. The *c* axis of the tetragonal phase is shorter than the *a* axes by 0.3–0.7 %, and the bulk modulus is 255(5) GPa for $K' = 4$. The observed diffraction patterns are consistent with the tetragonal distortion being induced by either a rigid octahedral rotation around the tetragonal *a* axes or an anisotropic distortion of SiO₆ octahedra, rather than a

rigid octahedral rotation around the tetragonal c axis as proposed by some first-principles calculations. This discovery may have important implications for the elastic moduli and anisotropy, and element partitioning in CaSiO_3 perovskite at lower-mantle pressures.

MR62B-1084 1330h POSTER

High Pressure Structural Properties of FeAlO_3

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Recent diamond anvil cell experiments carried out at the GSECARS sector of the Advanced Photon Source indicate that FeAlO_3 transforms between 5 and 7 GPa to a tetragonal garnet structure ($a = 11.529 \text{ \AA}$, $c = 11.046 \text{ \AA}$). At 20–25 GPa, the garnet phase becomes unstable with respect to an orthorhombic perovskite phase (space group $Pbnm$, $a = 4.584 \text{ \AA}$, $b = 4.883 \text{ \AA}$, $c = 6.669 \text{ \AA}$). Atomistic simulations of these structures made using an empirical potential model show that at low pressure the fully-ordered garnet phase is metastable with respect to the ambient pressure phase, and a disordered phase can become stable as a result of its higher entropy. Theoretical results also show that the perovskite phase becomes stable at 25 GPa, in agreement with experiment. Similarities in compression behavior between MgSiO_3 suggest that the MgSiO_3 - FeAlO_3 join provides a suitable model system for the study of Fe^{3+} in aluminous perovskite at lower mantle conditions.

MR62B-1085 1330h POSTER

Kinetics of the Pyroxene-Garnet Transformation: Preliminary Results

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Previous experimental studies have shown that in a "pyrolyte" mantle, Ca-poor pyroxene is completely dissolved into garnet at about 10 GPa, and Ca-rich pyroxene at about 16 GPa. Current mineralogical view of the Earth's upper mantle and the transition zone is mainly based on these results with the assumption that the pyroxene-garnet transformation proceeds with relative ease under the mantle conditions. In order to assess the validity of this critical assumption, knowledge about kinetics of the transformation is required. Here we report the preliminary results from an experimental study designed to investigate kinetics of the pyroxene to garnet transformation.

A 2000-ton uniaxial-split-sphere high-pressure apparatus was used to achieve mantle conditions of 6 to 14.5 GPa and 1200–1400 °C. Powdered KLB-1, whose bulk composition is close to "pyrolyte", was used as starting material. The powder sample was annealed at 6 GPa and 1300 °C for at least 4 hours before the target pressure and temperature were applied. Run duration ranged from 4 to 21 hours. Run products were analyzed using a micro-fractometer and an electron microprobe. It was found that substantial amount of Ca-poor pyroxene was still present in all samples, including the sample in which olivine has completely transformed to wadsleyite. Concentrations of oxide indicators for phase transition in garnet, such as SiO_2 , CaO , and Al_2O_3 , were fairly unchanged from the pre-annealed material, suggesting that the transformation is extremely slow in occurring. We also observed exolutions of Ca-rich pyroxene or garnet in Ca-poor pyroxene, but they were too small to be analyzed. These results indicate that the pyroxene-garnet phase transformation can take complicated paths, and metastable pyroxene may exist in the Earth's lower upper mantle and the transition zone.

MR62B-1086 1330h POSTER

First principles prediction of the akimotoite-to-perovskite transition in MgSiO_3

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The akimotoite-to-perovskite phase transition in MgSiO_3 is expected to contribute to the structure of the "660" km discontinuity in colder regions of the mantle. The transformation has a negative Clapeyron slope, behavior that has important implications for mantle dynamics. We have used first principles calculations to illuminate the origin of the negative slope and to test the ability of theoretical methods to predict the temperature dependence of phase transformation boundaries. We used density functional perturbation theory to investigate the structure, vibrational modes, and thermodynamic properties of akimotoite and perovskite.

We find that the negative Clapeyron slope can be attributed to the larger density of states of low frequency vibrations in the perovskite phase. Such vibrations consist of 1) Mg displacements: increased magnesium coordination and larger Mg-O bond lengths in perovskite lower vibrational frequencies of modes involving these displacements; 2) octahedral rotations: a lower degree of polyhedral connectivity in perovskite introduces low frequency nearly rigid unit modes. The larger density of state of low frequency modes in perovskite accounts also for the increase in other thermodynamic properties across the phase transition. This detailed calculation of a solid-solid phase boundary provides new insights into our ability to predict high pressure-temperature transformations by first principles.

MR62B-1087 1330h POSTER

Stability of Magnesite under the Lower Mantle Conditions

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MgCO_3 magnesite is an important mineral of some sedimentary rocks, and is probably the only stable carbonate in the deep mantle [1]. It was suggested that magnesite disproportionates to form an assemblage of $\text{MgO} + \text{C}$ (diamond) + O_2 at pressures above 40–50 GPa [2]. We have examined this hypothesis and investigated stability of magnesite under the lower mantle conditions using a laser-heated diamond anvil cell with a synchrotron radiation [3]. The sample was a mixture of natural magnesite and a small amount of the platinum black powders. The latter powder was used as a heat absorber in laser heating as well as a pressure marker at high temperature. An Al_2O_3 powder was used as a thermal insulator between the sample and the diamond anvil. The sample was enclosed in a hole of a Re gasket. All experiments were carried out under the condition of 15–110 GPa and 1800–3000 K at the Spring-8 high pressure beamline BL10XU. The x-ray beam was monochromatized to the wavelength of 0.3571–0.4130 angstrom and was collimated to 20 micrometer in diameter. In spite of the proposed stability limit of magnesite, we did not see any evidence for the dissociation at the investigated pressures and temperatures. On the other hand, although magnesite with a trigonal structure was stable at pressures up to 110 GPa, it transformed to an unknown phase with an orthorhombic structure at 110 GPa and 2200 K. The present results show that magnesite is stable down to depths of 2500 km and remains the major host phase of

carbon throughout the most part of the lower mantle. The newly found phase could be stable at deeper parts, and may play an important role in the slab-mantle-core interactions. [1] T. Katsura et al., Proc. Japan Acad. B67, 57 (1991) [2] L. Liu, Contrib. Mineral. Petrol. 134, 170 (1999)

[3] T. Watanuki et al., Rev. Sci. Instrum. 72, 1289 (2001)

MR71A MCC: 122 Sunday 0830h

Applications of Neutron Scattering in Earth Sciences I (joint with V, DI)

Presiding: N L Ross, Virginia

Polytechnic Institute and State

University; J Parise, State University

of New York, Stony Brook

MR71A-01 0835h INVITED

Insights into Analogue Perovskite Solid Solutions from High-Resolution Neutron Powder Diffraction

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Neutron powder diffraction provides a powerful tool for the study of phase transitions as a function of pressure, temperature, or chemical composition. The structural information obtainable from powders using diffractometers such as HRPD (ISIS, UK) or D2B (ILL, France) rivals, and in some respects exceeds what may be possible using conventional crystallographic techniques reliant on single crystals.

We have used both instruments to explore the subtle phase transitions observed in the $(\text{Ca}_x\text{Sr}_{1-x})\text{TiO}_3$ and $(\text{Sr}_x\text{Ba}_{1-x})\text{SnO}_3$ solid solutions. We have also used low resolution high flux instruments to explore the thermal dependence of the superlattice behavior below the cubic to tetragonal phase transition in $(\text{Ca}_x\text{Sr}_{1-x})\text{TiO}_3$. In each case a sequence of phase transitions from Pm-3m through I4/mcm to Pbnm is seen as a function of composition, and is driven by the change in average radius of the B-cation. This sequence of transitions is the same as expected for a magnesium silicate perovskite structure on increasing temperature. It is now recognised that lower mantle perovskite is likely aluminous, with solid solution towards either a stoichiometric or oxygen-defect end-member. The analogue systems we have characterised have been doped with trivalent cations on the B site to explore the effect of such substitution on the sequence of phase transitions. High-temperature neutron diffraction shows that oxygen defects stabilize the higher symmetry structures, lowering T_C for the transition to cubic.

New developments in high-T high-P neutron diffraction techniques will allow the extension of these ambient pressure studies to the investigation of the influence of pressure as a variable, and hence the extension of such analogue studies to the whole range of variables experienced in the lower mantle. These will be briefly outlined.

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Neutron Diffraction Study of Silicate Perovskites

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The oxygen deficiency and cation-site distribution of silicate perovskite control its physical and chemical properties, including density, bulk modulus, defect mobility, ionic transport, flow behavior, oxidation states, hydration, and minor-element solubility. These properties of perovskite, in turn control the geophysical and