MS18.05.05 THE γ-α Fe_2O_3 TRANSITION. J. S. Olsen, L. Gerward, J. Z. Jiang, S. Morup, T. Peun, Niels Bohr Institute, Ørsted Laboratory, Universitetsparken 5, DK2100 Copenhagen, Denmark, Physics Department, Technical University of Denmark, DK-2800 Lyngby, Denmark, GeoForschungszentrum, Potsdam, D-14473 Potsdam, Germany

The particle size of a solid material affects many of its physical properties. For example, the crystal structure of small particles may not be the same as that of large particles, and phase transition pressures and temperatures may be different. By use of synchrotron radiation and energy dispersive x-ray diffraction, the equation of state of γ-Fe_2O_3 has been measured for pressures up to 50 GPa at ambient temperature in a diamond anvil cell, and at the constant pressure 7 GPa for temperatures up to 1000°C in a multi-anvil cell MAX80. Experiments were performed with γ Fe_2O_3 powder of large particle size (1 μm), and small particle size (7 nm). A comparison of the particle size effect on transition pressures and temperatures of the γ-α phase transformation is presented. From the equation of state we calculate the bulk modulus B_o and its pressure derivative B_o' and compare with available theoretical and experimental data.

MS18.05.06 X-RAY STUDIES OF PRESSURE EFFECTS IN BIOLOGICAL SYSTEMS. Sol M. Gruner, Department of Physics, Princeton University, Princeton, NJ 08544

We have used x-ray diffraction to probe pressure effects on membranes, proteins and polymers. There is little understanding of the structural basis of the many biological effects of pressure in the 0-2 kbar range. Pressure of this magnitude is known to reverse anaesthesia, alter biomembrane properties, unfold or denature protein assemblies and change the activity of enzymes. Since the molecules involved are highly incompressible, the mechanisms involved cannot be a gross reduction in molecular volume. Rather, structural effects are mediated by subtle purturbations in the carefully balanced competition of interactions which give macromolecular assemblies their 3-dimensional conformation and degree of association, such as changes in surface hydration, modifications of fluctuation magnitudes, and anisotropies in compressibility leading to exposure of specific chemical groups. As examples, x-ray results will be presented on the way in which pressure changes the structure of membrane lipid and protein assemblies. Mechanisms whereby these changes may couple to protein activity will be discussed. The discussion will conclude with open questions which may be addressed by pressure-diffraction studies.

MS18.05.07 COMPUTER MODELLING OF PRESSURE-INDUCED PHASE TRANSFORMATIONS IN SOLIDS. John S. Tse and Dennis D. Klug, Steacie Institute for Molecular Sciences National Research Council of Canada Ottawa, Ontario, Canada K1A 0R6, Marco Bernasconi, Max-Planck Institut fur Festkorperforschung Postfach 80 06 65, D-70506 Stuutgart, Germany

The methods of Classical Molecular Dynamics (CMD) and First Principles total energy calculations have been demonstrated to be very valuable in the characterization of pressure-induced transformations in solids. However, each method when applied separately has specific limitations. CMD can be applied to systems with a large number of atoms but it suffers from the inherent difficulties associated with the uncertain accuracy of the potential functions when applied to conditions outside the regime of parameterization. In constrast, First Principles Molecular Dynamics (FPMD) can give highly accurate description of a system under any circumstances, the method is limited to relatively small systems with current computational facilities. The combination of the merits of both methods can lead to a very powerful procedure in the identification of structures at high pressures. In this procedure, possible high pressure crystalline forms are explored via large scale CMD calculations. The space group and internal coordinates of candidate structures are then extracted. FPMD is then used to optimize the unit cell and internal parameters. The diffraction patterns of the optimized structures can then be compared with experiments. This procedure will be illustrated through several examples on the high pressure structures of silica. The FPMD method has also been extended to include the Parrinello-Rahman variable cell scheme recently. The pressure effects on a structure can now be studied directly. New results on selected silica systems using this technique will be presented.

MS18.05.08 SYSTEMATIC CRYSTAL CHEMISTRY OF HIGH-PRESSURE SILICATES: AN INTERACTIVE GRAPHICS DEMONSTRATION R. M. Hazen and R. T. Downs, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road NW, Washington D.C. 20015, phone (202) 696-2410 x2470, e-mail: hazen@gl.ciw.edu

Approximately two dozen structure types with six-coordinated silicon have been synthesized at the high pressures and temperatures characteristic of the earth's deep interior. A new interactive graphics program, XtalDraw, facilitates comparison of these structures and ellucidates their crystal chemical behavior. These investigations reveal recurrent patterns of polyhedral linkages that can be used to classify known phases and to predict new ones. Known phases can be classified according to the arangement of six-coordinated silicon, which occurs as isolated octahedra (in Phase B and majorite garnet), as corner-sharing chains (in titanite-type $CaSi_2O_5$), as corner-sharing layers (in Ca_2SiO_4), as corner-sharing frameworks (in silicate perovskites), or as edge-sharing chains (in stishovite and hollandite). Silicate octahedra also combine with silicate tetrahedra to form a new class of dense alkali or alkaline earth framework silicates.

MS18.05.09 RHEOLOGY MEASUREMENTS AT HIGH PRESSURE AND TEMPERATURE J. Ando, D. J. Weidner, Y. Wang, G. Chen, CHiPR and Dept. of Earth and Space Sciences, U. S. B., Stony Brook, NY 11794; 516-632-8241; email: dweidner@sunysb. edu

Measurement of rheological properties of Earth materials in a multi-anvil devices is accomplished with the aid of a synchrotron generated x-ray probe. Deviatoric stresses are generated by compressing a polycrystalline powder as a result of the interaction between individual grains. The stress is quantified by measurement of the broadening of the diffraction peaks. Generally, the magnitude of the deviatoric stress will exceed the nominal pressure unless the sample fails or flows. The change of the peak width with time defines the strain rate of the sample. Taken together, these data provide constraints on the rheological properties for these conditions.

In situ x-ray diffraction measurements of $MgAl_2O_4$ spinel at 10 GPa confining pressure and temperatures up to 1100C provide an example of such data. Strain rates of the order of 10^{-7} s^{-1} were measured at 600C with deviatoric stresses of the order of a few GPa. The total plastic strain in the sample amounted to a few per cent. The stress-strain rate-temperature conditions quantitatively agree with those for spinel given by Frost and Ashby (*Deformation-Mechanism Maps The Plasticity and Creep of Metals and Ceramics*) and correspond to the plasticity-power law creep boundary for this material.

The current limits of this approach are defined by the resolution of x-ray energy. Future improvements will come using monochromatic sources with high resolution detection systems. This will enable lower stress determinations and hence higher temperatures.