

**MINERALOGY OF PERIDOTITE AND BASALT AT THE EARTH'S LOWER-MANTLE PRESSURES**

S. Ono

Japan Marine Science & Technology Center Institute for Frontier Research On Earth Evolution 2-15 Natsushima-Cho YOKOSUKA-SHI KANAGAWA 237-0061 JAPAN

High-pressure phase equilibria studies provide important constraints on the mineralogy and composition of the earth's interior. However, most of these high-pressure experimental studies have concentrated upon the magnesium-rich simple system. It is generally acknowledged that the phase change of the basaltic crust and surrounding mantle plays significant role in mantle dynamics. In the present study, the cell parameters of minerals in the basaltic (morb) and peridotitic (klb-1) compositions have been determined by a laser-heated diamond anvil cell technique and in situ X-ray method at the synchrotron beam line bl10xu, Spring-8, Japan. The morb and peridotite composition crystallized into assemblages of Mg-perovskite + Ca-perovskite + stishovite + aluminous phase and of Mg-perovskite + Ca-perovskite + magnesiowustite phase, respectively. The results of phase relation are generally consistent with previous studies by multi-anvil press and diamond-anvil cell experiments. The estimated densities of morb were denser than those of the seismic observations (e.g. Prem). Therefore, the oceanic crust may subduct into the base of the lower mantle. This result does not consist with the previous studies (Kesson et al, 1998; Ono et al., 2001). In previous studies, the thermoelastic parameters of minerals of simple compositions were used to estimate the mineral volumes. In this study, however, the mineral volumes were directly determined by in situ X-ray methods. Therefore, the compositional effect of the thermoelastic parameters should be considered to investigate the densities of high-pressure minerals in the multicomponent systems.

**Keywords: IN SITU X-RAY BASALT PERIDOTITE**

**TRANSFORMATIONS IN FLUID WATER AT HIGH PRESSURE AND TEMPERATURE**

J. H. Eggert<sup>1</sup> G. Weck<sup>2</sup> P. Loubeyre<sup>2</sup> D. G. Hicks<sup>1</sup> P. M. Celliers<sup>1</sup> G. W. Collins<sup>1</sup> K. M. Lee<sup>3</sup> L. R. Benedetti<sup>2</sup>

<sup>1</sup>Lawrence Livermore National Laboratory, USA <sup>2</sup>Commissariat à l'Energie Atomique, France <sup>3</sup>University of California, Berkeley, USA

The phase diagram of fluid water has three primary domains: 1) a biological molecular liquid with low coordination number and strong hydrogen bonding, 2) a normal molecular liquid with coordination number near 12 and reduced hydrogen bonding, and 3) a conducting astrophysical fluid associated with dissociation and ionization effects.

This talk will present recent experimental data regarding transitions between these three domains. We have investigated the transition between domains 1) and 2) by performing highly accurate measurements of the structure factor and the density of liquid water and heavy water by X-ray diffraction in a resistively-heated diamond-anvil cell. We observe large changes in the structure factor and a dramatic increase in the coordination number saturating at about 12 above 2 GPa. The transition is not first order but it does occur over a fairly small density range.

We have investigated the transition to domain 3) by performing laser-induced shock experiments on ambient and pre-compressed water samples. We observe that along the primary Hugoniot water first becomes opaque and then reflecting as it enters into domain 3) above about 130 GPa. These optical changes appear to be very temperature dependent as shown by several shots on pre-compressed samples where the final temperature is reduced relative to primary Hugoniot temperatures.

**Keywords: WATER, STRUCTURE FACTOR, DIAMOND ANVIL CELL**

**NOVEL EXTENDED PHASE OF MOLECULAR SOLID CO<sub>2</sub>**

C. Yoo

Lawrence Livermore National Laboratory L-45, PO Box 808 7000 East Ave., LIVERMORE CALIFORNIA 94551 USA

Carbon dioxide at high pressure and temperature occurs in many polymorphs of greatly different crystal structure, chemical bonding and intermolecular interaction. Those phases include two previously well-understood molecular phases of CO<sub>2</sub>-I and III and three recently discovered phases of extended CO<sub>2</sub>-V, strongly associated CO<sub>2</sub>-II, and bent CO<sub>2</sub>-IV.

The crystal structure of CO<sub>2</sub>-V has previously been characterized to be similar to that of SiO<sub>2</sub>-tridymite, with four-fold coordinated carbon atoms. Recently, we have also characterized the crystal structures of CO<sub>2</sub>-II and IV, also being similar to SiO<sub>2</sub>-stishovite and its distorted structure, with pseudo-six fold coordinated carbon atoms. Based on their elongated intramolecular C=O bond distances, well over 1.30 Å, and collapsed intermolecular distances, below 2.38 Å, we conclude that both CO<sub>2</sub>-II and IV are in an intermediate state between molecular and non-molecular solids. Clearly, the crystal structure, chemical bonding, and chemistry of carbon dioxide phases strongly resemble those of SiO<sub>2</sub> polymorphs and thus are of critical importance for understanding the mineralogy and crystal chemistry occurring in the Earth's crust and mantle.

\*Work performed under the auspices of the U.S. DoE by the Llnl, University of California, under contract number w-7405-eng-48. This work has been done in collaborations with V. Iota, J. Park, H. Cynn, K. Visbeck, H. Kohlmann, M. Nicol, and T. Lebihan.

**Keywords: CO<sub>2</sub>, EXTENDED PHASE, MOLECULAR PHASE**

**AB-INITIO SIMULATIONS OF LOW-Z FLUIDS UNDER PRESSURE**

G. Galli E. Schwegler B. Militzer R. Hood F. Gygi

Lawrence Livermore National Laboratory P.O.Box 808 LIVERMORE CA 94551 USA

Results of first-principles simulations of liquid water, oxygen and hydrogen under pressure will be presented and compared with recent experimental data. In particular we will discuss molecular dissociation under pressure and at high temperature, and the way both structural and electronic properties are modified when the fluid undergoes an insulator-to-metal transition. In addition we will present direct first-principles simulations of shock propagation in hydrogen. Our findings will illustrate how ab-initio results can be used to complement experimental data and thus build a detailed and thorough understanding of complex fluids under pressure.

**Keywords: AB-INITIO SIMULATIONS HIGH-PRESSURE WATER HIGH-PRESSURE HYDROGEN**