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Annual Report 2003, Spring-8
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This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.
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This study is for in-situ investigation of chemical bonding and molecular structure of low z-elements and simple molecular solids at high pressures and temperatures using 3rd-generation synchrotron x-ray diffraction. To understand the contribution of the empty d–electron orbital of Mg in relation to the formation of molecular solids like MgO, which is one of the important Earth lower mantle materials and MgB$_2$, which has recently been the focus of intense superconducting material research, we have performed double-sided laser heating experiments using a diamond anvil cell (DAC). Understanding the structural stability and the formation of the above Mg-compounds requires studying Mg itself as well as the relevant compounds.

BL10XU at the SPring-8 was used to study phase stability and make accurate equation of state (EOS) determinations of Mg coupled with external heating and the double-sided laser heating technique. Monochromatic x-ray at 30 keV (0.4135 Å) was focused to about 40µm at the sample and the diffracted x-ray were recorded using a high-resolution image plate (3000x3000 pixels with a 0.1mm resolution per pixel).

EOS parameters for hcp and bcc Mg were determined by fitting to a Birch-Murnaghan equation. An isothermal compression of Mg at 300 K up to 100 GPa provides EOS parameters (B$_0$, B$_0''$, and V$_0$) comparable for both hcp and bcc phases, which is similar to the cases for hcp and fcc phases measured in cobalt and xenon. Similar EOS parameters for both low and high pressure phases with a very small or no measurable volume discontinuity at the phase transition pressure suggests that the hcp-bcc structural transition of Mg may be driven by a stacking fault due to a shear instability as seen in xenon and cobalt. Compared to the recent estimation determined using a large volume press [1], our B$_0$ is smaller by more than 10% suggesting that the difference may be due to non-hydrostatic conditions. The phase boundary of Mg up to 650 K was determined using external resistive heating in air. The results show a noticeable hysteresis during forward and backward transitions. The initial negative slope of the phase boundary agrees very well with the value predicted by theory[2].

Double-side laser heating at several pressures below 20 GPa (Fig. 1) with simultaneous in-situ x-ray diffraction indicates that hcp is the dominant stable phase and a double hexagonal close packed structure (dhcp) is not seen at high temperatures and high pressures, unlike the observations of recent studies of Mg using a large volume press, claiming dhcp below 20 GPa between 1350 and 1050 K. We suggest that the dhcp may appear as nonequilibrium phase induced by shear stress.

![Fig. 1. Photomicrograph of Mg sample surrounded by MgO under pressure. Note the laser spot in the middle of the Mg sample indicating high temperature near melting. The entire culet size is 0.3 mm in diameter.


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