Anharmonicity of OH vibration in brucite under high pressure

Keiji Shinoda[1]

[1] Geosciences, Osaka City Univ.

The crystal structure of brucite (Mg(OH)2) is the CdI2 structure with MgO6 octahedral layers (brucite layer) stacked along the c-axis and the OH dipole oriented parallel to the c-axis on a three-fold axis. The hydrogen bond between a hydroxyl on a brucite layer (donors OH) and an oxygen on the next layer (acceptors O') is very weak as evidenced by the (001) perfect cleavage. Brucite is widely studied as a prototype of hydrous magnesium silicates. Kruger et at. (1989) observed a pressure induced IR absorption peak at 3650cm-1 and assigned it to a hot band from the first excited state to the overtone. Although some possibilities of structural changes of OH in brucite had been proposed, a clear view of any phase transition was not clear. Shinoda & Aikawa (1998) also observed a pressure induced absorption peak at 3650cm-1 with DAC and polarized IR spectroscopy, and assigned it to a new OH dipole formed by proton transfer between donor OH and nearest neighbor acceptor O' under pressure. Shinoda et al. (2002) observed pressure induced OH dipole under high temperature and high pressure with HTDAC under synchrotron IR microscope at BL43IR of SPring-8, and suggested a possibility of a high pressure phase transition of brucite. In this study, NIR-IR absorption spectra of brucite were measured under high pressure with DAC, and fundamental and overtone absorption peak of OH dipole were assigned. From overtone spectra of OH in brucite, anharmonicity of OH vibration of brucite under high pressure is discussed.