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Compression and structure of brucite to 31 GPa from synchrotron X-ray diffraction and infrared spectroscopy studies

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Abstract

Synchrotron X-ray powder diffraction and infrared (IR) spectroscopy studies on natural brucite were conducted up to 31 GPa using diamond-anvil cell (DAC) techniques at beamlines X17C and U2A of National Synchrotron Light Source (NSLS). The lattice parameters and unit-cell volumes were refined in $P\bar{3}m1$ space group throughout the experimental pressure range. The anisotropy of lattice compression decreases with pressure due to a more compressible **c** axis and the compression becomes nearly isotropic in the pressure range of 10–25 GPa. The unit-cell volumes are fitted to the third-order Birch-Murnaghan equation of state, yielding $K_0 = 39.4(1.3)$ GPa, $K_0' = 8.4(0.4)$ for the bulk modulus and its pressure-derivative, respectively. No phase transition or amorphization was resolved from the X-ray diffraction data up to 29 GPa, however, starting from ~4 GPa, a new infrared vibration band (~3638 cm^{-1}) 60 cm^{-1} below the OH stretching A_{2u} band of brucite was found to coexist with the A_{2u} band and its intensity continuously increases with pressure. The new OH stretching band has a more pronounced redshift as a function of pressure (–4.7 cm^{-1}/GPa) than the A_{2u} band (–0.7 cm^{-1}/GPa). Comparison with first-principles calculations suggests that a structural change involving the disordered H sublattice is capable of reconciling the observations from X-ray diffraction and infrared spectroscopy studies.

Keywords: Brucite, equation of state, X-ray diffraction, infrared spectroscopy