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Compression mechanism of brucite: An investigation by structural refinement under pressure

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ABSTRACT

Synchrotron X-ray powder diffraction study of brucite, $Mg(OH)_2$, was carried out in a diamond anvil cell with an imaging plate detector from 0.6 to 18.0 GPa at room temperature using the angular-dispersive technique on beamline BL-18C at the Photon Factory, KEK, Japan. Using Rietveld analysis, unit-cell parameters as well as atomic positions of the O atoms in brucite have been successfully refined, taking into account the effects of preferred orientation. Variation of the *c*/*a* ratio with pressure indicates that the compression mechanism changes around 10 GPa, above which the compression behavior is isotropic. Based on the changes of the refined atomic positions of the O atoms with pressure, we conclude that the shortening of the interlayer distance controls compression below 10 GPa, whereas above this pressure compression of the oxygen sublattice is the dominant mechanism. Results of the structural refinements also suggest that the MgO_6 octahedral regularity initially approaches a regular configuration with pressure, which then remains unchanged above 10 GPa.