MITT.ÖSTERR.MINER.GES. 149 (2004)

EQUATION OF STATE AND TRANSITION PRESSURE FOR BRUCITE DEHYDRATION: THEORETICAL APPROACH

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Brucite, $Mg(OH)_2$ is a simple crystalline hydroxide, and is an end-member for hydrous minerals that hosts H_2O in the crust and mantle of the Earth. Owing to its structural simplicity, it serves as useful prototype for layered hydrous minerals.

In order to explore the high pressure behaviour of brucite, *ab initio* total energy calculations based on local density approximation (LDA) and generalized gradient approximation (GGA) of density functional theory have been performed. Using neutron diffraction it has been observed that at high pressures, hydrogen atoms are disordered over the three 6i Wyckoff sites with one-third occupancies where as at ambient pressures they are oriented parallel to *c*-axis (2d Wyckoff site). In order to explore such order-disorder behaviour, we constructed a 3x3x1 super-cell with hydrogen occupying only one of the three 6i sites, and arranged the H atoms such that displacement of each hydrogen atoms from 2d to 6i position forms an enclosed ring. *Ab initio* structural relaxations confirm the mechanical stability, and energetic favorability, as compared with the 2d structure, of this arrangement. We determine the theoretical equation of state for brucite with K_o of 53 GPa and its pressure derivative, K_o' of 6.2, using LDA, and a K_o value of 34 GPa and K_o' of 5.8 with GGA (both corrected for zero pressure and thermal pressures at T = 300 K). We also simulate the transition pressure for the dehydration of brucite at T = 0 K, comparing the enthalpies of $Mg(OH)_2$ and sum of enthalpies of MgO and H_2O (ice-VIII). We are exploring possibilities of formation of symmetric hydrogen bonding at higher pressures. We are also exploring the elastic constants (c_{ij}) for brucite and their pressure dependence.