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A kinetical study of proton dynamics of brucite and portlandite

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Brucite is $Mg(OH)_2$ compound and the crystal structure of brucite is recognized as a prototype of hydrous layered minerals with complicated structures. Various physical and chemical properties of some minerals with the brucite structure such as brucite itself and portlandite, $Ca(OH)_2$have been investigated. It is especially interesting to understand proton dynamics in hydrous minerals, because the proton diffusion should be closely related to mechanism and kinetics of plastic deformation, hydration, dehydration and so on. Nevertheless, proton diffusion studies on brucite structured minerals have been surprisingly scarce. Recently Noguchi and Shinoda (2010) conducted H-D exchange diffusion experiments on portlandite and Guo et al.(2013) performed proton diffusion experiments on brucite at high pressure. However, it is difficult to understand mechanism of proton diffusion of brucite structured minerals systematically, because their experimental conditions such as pressure and temperature are different. In this study, we performed deuterated experiments for brucite, hydrated experiments for deuterated brucite and deuterated experiments for portlandite at several temperatures and at an atomospheric pressure.

All sample powders were prepared by hydrothermal synthesis and checked the qualities by X-ray diffraction, infrared absorption spectroscopy and SEM. The H-D exchange experiments at several temperatures were performed with a vertical tube furnace in which bubbling dried N_2 gas through D_2O (or H_2O) was introduced. A crucible filled with the sample powder was hung in the middle of the tube furnace. A small amount of the sample powder was picked out at appropriate time intervals and IR measurements for it were performed to know time variation of the molar ratio of D to H.

The diffusion rate depends on temperature and is faster at higher temperature. The diffusion rate also depends on the molar ratio of D to H. Rate control process of proton diffusion in brucite structured minerals will be discussed from diffusion coefficients, activation energies and frequency factors determined.

Keywords: Proton dynamics, H-D exchange, brucite, portlandite, kinetics