

Water behaviour on layered silicate minerals such as brucite

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Introduction

Water in the earth's crust and mantle has significant effect on the rupture strength of rocks, rheological property and magma generation of island arc. Assuming that the water in the earth's crust and mantle exists as liquid state, the water behaviour is decided by the interaction between mineral surfaces and water. However the interaction is hardly known yet [1]. In recent years, adsorbed water on mica surfaces has attracted considerable interest as the possibility of icelike structure formation. An ice-like structure on the hydrated surface of muscovite mica has been reported by scanning polarization force microscopy (SPFM) [2]. Besides the most stable structure of water on muscovite mica surface was investigated by using the ab initio molecular dynamics (ab initio MD) simulation method [3]. They proposed that at monolayer coverage water molecules make a fully connected two-dimensional hydrogen bond network, and the ice-like structure is stable even at 300 K. In this work, we focused attention on the water behaviour on brucite (0 0 0 1), gibbsite (0 0 1), and muscovite (0 0 1) surfaces. Since brucite is typical mineral having hydroxyl on the cleavage surfaces, it is most suitable to study the water behaviour on the surface having hydroxyl. Brucite is one of the important hydrous minerals to investigate the water behaviour in the transition zone of mantle [4].

Methods

Ab initio model potentials for water-mineral surfaces interactions were obtained by fitting the parameters to ab initio electronic structure data, computed using the first-principles method based on density functional theory. Using this ab initio model potentials between water and mineral surfaces, molecular dynamics simulations of a water thin film with a thickness of ca. 1.25 nm embedded between the surfaces were performed at the ambient conditions. Molecular dynamics simulations were performed by MXDORTO [5] and MXDTRICL [6] developed by Kawamura. The orientation, self-diffusion coefficient, reorientation time, and dielectric dispersion of water were calculated to know the water behaviour near mineral surfaces.

Results and Discussion

The results in brucite surfaces are discussed below. Compared with the water located in the middle layer between brucite surfaces, self-diffusion coefficient of nearest surfaces increase by a factor of 1.45 and the reorientation time decrease by a factor of 0.77. This rapid mobility of water on brucite results from the weak interaction between water and brucite, and hydroxyl of brucite surface play a significant role on weakening the water-surface interaction.

The dielectric constant and behaviour of water between brucite as well as gibbsite and muscovite surfaces at wide range temperature and pressure conditions will be shown at this conference.

References

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