Computational study of the quantum fluctuation on the δ-AlOOH crystal structure

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δ-AlOOH is a high pressure phase of the diaspore and boehmite, the aluminous hydrous minerals. The phase can stably exist around the pressure-temperature condition of subducting slab, and take a role of transporting water into the core-mantle boundary, suggested by Sano et al. The crystal structure of δ-AlOOH has P21nm symmetry in the ordinary pressure condition and Pnnm symmetry in higher pressure condition than 10 GPa. These structures are identified by the location of the hydrogen of the O-H-O hydrogen bond either a side or center between oxygen atoms, respectively. The critical pressure of phase transition becomes higher by the deuteration effect as also reported by the above researchers. Because the deuteration generally decreases the effect of nuclear quantum fluctuation of hydrogen, the quantum fluctuation contributes the phase transition condition. In present study, we explored the geometry of δ-AlOOH using the path integral molecular dynamics and conventional molecular dynamics methods, where former method includes both the quantum and thermal fluctuations of the crystal structure and latter one includes only the thermal fluctuations. In our results, the quantum effect reduced the volume of P21nm phase and enlarged the volume of Pnnm phase. The reduction of the quantum pressure of the proton in a double well potential such as the P21nm structure have been discussed for ice VII by Sugimura et al, while Pnmm phase has single well potential for the hydrogen atom. These trends of the quantum pressure agree the P-V curve of δ-AlOOH and δ-AlOOD in experimental measurements.

Keywords: aluminous hydrous mineral, δ-AlOOH, isotope effect, quantum fluctuation

