First principles investigation of the elasticity of ice VIII and ice X

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Determination of the structure, physical properties, and phase relations of high-pressure ice is important for physical, geophysical and planetary sciences. Hydrogen bonded molecular phases ice VIII and ice VII have known to transform to an atomic crystal phase ice X at ~60-100 GPa by the hydrogen bond symmetrization. However, the phase boundaries between ice VII/VIII and ice X phases have not been sufficiently determined so far, primarily due to the existence of intermediate "dynamically ordered" ice VII and X phases at the phase boundary between ice VII/VIII and X. In the dynamically ordered ice VII and X phases, the proton distribution becomes unimodal at the midpoint of two neighboring oxygen, even though the underlying potential still remains double-well shape. The dynamically ordered ice VII was suggested to have highly compressible character between 40 to 60 GPa due to the quantum effects of protons (Sugimura et al. 2008). On the other hand, the sound velocities of ice VII were measured at room temperature up to 80 GPa by the brillouin scattering experiments (Ahart et al. 2011). Nonetheless, the velocities were smoothly increases with pressure up to 80 GPa and no indication of phase transitions into the dynamically ordered ice VII/X nor ice X. Therefore, the purpose of this presentation is to investigate how the elastic properties of ice are changed by the hydrogen bond symmetrization of ice and discuss the location of the phase boundary between ice VIII/VII and X phases from the viewpoint of elasticity.

The elastic constants of ice VIII and ice X phases under pressure are determined at static 0 K conditions using first principles calculation. The step-like increase of the elastic constants of ice VIII phase occurred at 100-110 GPa by the hydrogen bond symmetrization. Those elastic constants and their slopes with pressure are completely different between ice X and VIII. Therefore, these phases can be distinguished by the elasticity. On the other hand, the experimental elastic constant of C_{11} of ice VII gradually change from ice VIII like asymmetric hydrogen bond character to symmetric hydrogen bond character within wide pressure range. The present study suggests that the transition from ice VII to ice X starts around 30 GPa and completes at 110 GPa.