First-principles investigations on the elastic and vibrational properties of hydrous wadsleyite under pressure

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Existence of hydrogen in the deep earth interior is paid attention because it is known to significantly affect the physical properties such as viscosity, melting temperature, and elastic properties of the earth constituent minerals. Wadsleyite is thought to be a primary constituent in the upper part of the Earth's transition zone and this phase can be a significant water reservoir in the Earth. We have investigated and clarified the high pressure structural and elastic properties of hydrous wadsleyite using first principles calculation [1]. We demonstrated that our structural models show good agreements with high pressure experimental studies and the seismic velocities of hydrous wadsleyite decrease almost linearly with increasing the degree of hydration. For the next step, we have also calculated vibrational properties of hydrous wadsleyite under pressure based on our structural models. Comparing our data with existing Raman and IR measurements, we discuss the possible hydrogen positions and the effect of water on structural properties of hydrous wadsleyite under pressure.

[1] Tsuchiya & Tsuchiya (2009) *J. Geophys. Res.* **114**, B02206.

Ab initio assessment of high-*P,T* thermodynamics in multi-component mineral systems: Application to postperovskite phase equilibria in the MgSiO$_3$–Al$_2$O$_3$ system

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First principles density functional simulations have been applied with great success to investigate high-pressure crystallographic and thermodynamic properties of various classes of materials from elemental and molecular solids, oxides and other compounds to complex silicate minerals. It is definitely worthy to extend this powerful technique to high-*P,T* thermodynamics of multi-phase and multi-component systems, which are, in particular, of significant geophysical interest. Since such studies are so far limited mainly in the research field of relatively simple alloy systems, we try to develop the computation techniques for solid solution thermodynamics of Earth and planetary materials with much more complex structural and compositional degree of freedom, with including statistical effects and phonon effects.

As the first example, we have assessed high-*P,T* post-perovskite phase equilibria in the MgSiO$_3$–Al$_2$O$_3$ pseudobinary system [1], which is thought to be closely related to the deep mantle D" seismic discontinuity. Although earlier studies based on the static cationic substitution properties reported a significant divariant loop suggesting no sharp transition expected to occur in this system, present calculations demonstrate that Al$_2$O$_3$ produces a narrow perovskite-post-perovskite coexisting *P,T* area ($\Delta P \sim 1$ GPa) for the pyrolitic Al concentration, which is sufficiently responsible to the seismic discontinuity. We also found that the perovskite structure spontaneously changes to the Rh$_2$O$_3$(II) structure with increasing the Al concentration involving very small displacements of the Mg-site cations. Results suggest that the technique appears to work well even for complex mineral solid solution systems.

[1] Tsuchiya & Tsuchiya (2009) *Proc. Natl. Acad. Sci. USA* **105**, 19160.