The 493rd Geodynamics Seminar

First principles investigation of the high-pressure behavior of the FeOOH-AlOOH-phase H ($MgSiO_4H_2$) system

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Abstract

It is believed that water is carried into the Earth's deep interior by hydrous minerals such as dense hydrous magnesium silicates (DHMSs) in the descending cold plate. A number of studies have been conducted to determine the high-pressure behaviors of DHMSs. In recent years, we discovered a new DHMS, phase H, stable at lower mantle pressure condition; and the solid solution formed by phase H and d-AlOOH has been proposed as the most important carrier of water to the deepest part of Earth's mantle (Tsuchiya 2013, Nishi et al. 2014, Ohira et al. 2014). However, those hydrous phases are not denser than surrounding (dry) mantle minerals (Tsuchiya and Mookherjee 2015) and their gravitational stability in deeper part of the Earth is questionable. Therefore, the effect of denser elements such as Fe on the stability of DHMS is intrinsically connected to the ability of these phases to transport water into Earth's deep interior. In order to assess the effect of Fe on the phase relation of phase H and d-AlOOH, we determined the high-pressure behavior of the end-member composition of this system, e-FeOOH. We have discovered a new high-pressure phase transition in FeOOH at lower mantle conditions using both theoretical and experimental methods. Here we show the high-pressure structures and physical properties of the FeOOH-AlOOH-phase H system using first principles calculation and discuss possible geophysical implications.

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