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First principles investigations of serpentine under pressure

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Serpentine is hydrous phyllosilicate known to be formed in the mantle wedge by a reaction between mantle peridotite and upwelling water released by the decomposition of hydrous minerals in the subducting slab [e.g. Schmidt and Poli,1998]. Partially serpentinized peridotite may be a significant reservoir of water in the mantle wedge and the dehydration of serpentine is considered to have an important contribution to the generation of arc magmatism. This was also extensively investigated in connection with intermediate and deep earthquakes [e.g. Irifune et al. , 1996].

In order to investigate the transporting processes of water into the Earth's interior, the thermodynamic stabilities and the elastic properties of antigorite should be clarified. Antigorite is the high-temperature polymorph of serpentine and thus the relevant phase in the subduction zone. This phase has been reported to show polysomatism depending on the pressure and temperature conditions. Previous TEM study reported that m value (m = number of SiO4 tetrahedra in a wavelength along the ***a*** axis) increases/decreases with pressure/temperature [e.g. Wunder et al. 2001]. However, there is no sufficient structural and thermodynamic corroboration regarding the stable polysome of antigorite along the pressure and temperature conditions of the subducting oceanic plate.

In the present study, we investigated the structure and stability of antigorite with several different m values (m=14~19) using first principles calculation method. We found that antigorite with smaller m values stabilized under pressure. This may contribute the partial dehydration of water during subduction of oceanic plate.