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Elasticity of serpentine: first principles investigation

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Serpentine is formed by a reaction between peridotite and water which is released from hydrous mineral in subducting slab under pressure. Partially serpentinized peridotite may be a significant reservoir for water in the subducted cold slab and is considered to play an important role in subduction zone processes such as generation of arc magmatism.
Serpentine is one of the phyllosilicate minerals where the MgO6 and SiO4 layers are bonded by the weak hydrogen interactions. Therefore, it has been generally believed that serpentine is responsible for the low seismic velocities regions such as some regions at the Pacific and the Philippine Sea slabs (e.g. Nakajima et al. 2009). It has also been reported that strong trench parallel shear wave polarization anisotropy observed at forearc regions is suggested to be caused by the lattice preferred orientation of serpentine (Katayama et al. 2009). However, detailed elastic properties of serpentine have not been sufficiently determined yet.
Antigorite is the most stable polymorph of serpentine during high pressure metamorphism of wet ultramafic rocks. First principles calculation of antigorite is challenging because of its complex crystal structure. Aided by ample computation resources, we calculated the crystal structure and elasticity of antigorite which contains 273 atoms in primitive cell (Capitani and Mellini 2006) up to 10 GPa at 2 GPa interval.
Comparing the velocities of antigorite determined from the present ab initio calculations with the observed seismic velocities of subduction zones, we estimated the degree of serpentinization and possible water contents in subducting slabs. We also analyzed the present results combined with the high-pressure deformation experiments with the lattice preferred orientation of serpentine, in order to explain the strong trench parallel polarization anisotropy observed above subduction zones.

Nakajima et al. (2009) JGR, 114, B08309.
Katayama et al. (2009) Nature, 461, 1114-1118.
Capitani and Mellini (2006) Am Mineral, 91, 394-399