

## High-pressure phase transition and equation of state of hydrous aluminous silica

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Stishovite is the polymorph of SiO<sub>2</sub> with tetragonal rutile structure that is stable in subducted basaltic lithologies at depths of the mantle transition zone and the lower mantle. It is known that stishovite undergoes a second-order ferroelastic transition to an orthorhombic CaCl<sub>2</sub>-type phase above 50 GPa at room temperature, where extensive elastic shear softening is expected [1]. Previous studies showed that Al incorporation can considerably decrease the transition pressure [2], while it is still debated whether H has similar effects [3]. Here we report the equations of state, structural evolution and phase transformation of stishovite and CaCl<sub>2</sub>-structured samples having approx. 5 (Al5) and 11 mol% AlOOH (Al11). The Al11 sample shows orthorhombic symmetry from ambient conditions up to 50 GPa, which is the maximum pressure investigated. Al5, on the other hand, is tetragonal at ambient conditions and becomes orthorhombic upon compression at about 15 GPa. However, based on preliminary structural refinements and Raman spectroscopy measurements on Al5 at high pressure, the soft optic mode and octahedral tilting, which are related to elastic softening, remain the same as in the tetragonal phase until 20 GPa. Based on the observed different behaviors of spontaneous strains, octahedral tilting and soft optic mode in the CaCl<sub>2</sub>-type structure of Al5, we argue that H incorporation and H-bond symmetrization may modify the character of the phase transition, and thus affect the elastic properties of stishovite and CaCl<sub>2</sub>-type in the lower mantle.

[1] Carpenter, Hemley & Mao (2000), *Journal of Geophysical Research*, 105, 807–816.

[2] Lakshtanov, Sinogeikin, Litasov, Prakapenka, Hellwig, Wang, et al. (2007), *Proceedings of the National Academy of Sciences of the United States of America*, 104(34), 13588–13590.

[3] Umamoto, Kawamura, Hirose & Wentzcovitch (2016), *Physics of the Earth and Planetary Interiors*, 255, 18–26.