Anomalous elastic properties of stishovite from high pressure ultrasonic measurements and *ab initio* calculations

Ting Chen[1], Yongtao Zou[2,3], Xuebing Wang[1], Xintong Qi[1], Robert C. Liebermann[2], and Baosheng Li[2]

[1]Department of Geosciences, Stony Brook University, [2]Mineral Physics Institute, Stony Brook University, [3]now at State Key Laboratory of Superhard Materials, College of Physics, Jilin University, Changchun, China.

Stishovite is a high pressure polymorph of silica which has long been of great interest in geoscience and material science. At ~10 GPa in the Earth's conditions, the relatively low pressure polymorph, coesite, with four coordinated Si, transforms to six-coordinated stishovite. As a result, Stishovite has much higher density (4.287 g/cm^3) and acoustic velocities than coesite (2.909 g/cm^3), which can bring detectable seismic discontinuities considering the abundance of SiO_2 in the Earth's mid-ocean ridge basalt (MORB). At higher pressure ~47 GPa, the rutile structure of stishovite (*P4_2/mnm*) transforms to $CaCl_2$ structure (*Pnnm*) accompanied by the softening of the elastic constant (C_{11}-C_{12}) from both theoretical and experimental studies. This phase transformation has been proposed to explain seismic discontinuities at ~1600 km in the Earth mantle. Understanding the elastic properties as well as structural behaviors of stishovite at high pressure is crucial to further evaluate its seismic signatures in the Earth's mantle.

In this study, we measured the sound wave velocities of polycrystalline stishovite up to ~14 GPa using an ultrasonic interferometry method in conjunction with in-situ X-radiation at the beamline 13-ID-D, GSECARS, Argonne National Lab. These measurements not only expanded the pressure range of previous ultrasonic measurements employing polycrystalline sample by nearly four folds, but also equipped with direct length measurements to ensure higher precision in the derived velocities. We discover that, while the compressional (P) wave velocities increase continuously with pressure, the shear wave velocities, however, remain almost constant in the current pressure range, which is significantly different from most mantle minerals. This suggests that the softening behavior in stishovite initiates far below the transition pressure of ~47 GPa to $CaCl_2$ structure. Complementary to our experimental results, theoretical calculations on stishovite were also performed using density functional theory (DFT) approximation up to 30 GPa. The current experimental P and S velocities are found to be in good agreement with those calculated from DFT. Structural origins for the anomalous elastic behavior were further investigated by a thorough examination of the DFT optimized structures under high pressure.