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Pressure and Temperature Effects on the Antiferrodistortive Phase Transition and Phonon Softening in $SrTiO_3$ SHIH-CHANG WENG, Univ of Illinois - Urbana, RUQING XU, AYMAN SAID, Advanced Photon Source, Argonne National Lab, XINYUE FANG, Univ of Illinois - Urbana, SHIH-LIN CHANG, National Synchrotron Radiation Research Center, TAI-C. CHIANG, Univ of Illinois - Urbana — Strontium titanate undergoes an antiferrodistortive transition accompanied by a cubic-to-tetragonal structural distortion. This transition can be induced at ambient pressure by lowering the temperature down to 105 K or at room-temperature by applying hydrostatic pressure up to 9.6 GPa. The hydrostatic pressure leads to the same type of symmetry breaking and phonon softening at the R point in the Brillouin zone as the temperature does, but give a much larger volume reduction. Herein we report our results of pressure-induced phonon softening determined by inelastic X-ray scattering using a diamond-anvil cell for the required pressure. The phonon softening behavior follows a power law and is accompanied by a central peak. The comparison between pressure and thermal effects is presented. First-principles calculations were preformed as a function of pressure (or unit cell volume), and the results support that the distorted structure becomes stabilized under hydrostatic pressure.

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