American Mineralogist, Volume 108, pages 1558–1568, 2023

High-pressure phase transition and equation of state of hydrous Al-bearing silica

Giacomo Criniti[1,*], Takayuki Ishii[2,†], Alexander Kurnosov[1], Konstantin Glazyrin[3], and Tiziana Boffa Ballaran[1]

[1]Bayerisches Geoinstitut, Universität Bayreuth, 95440 Bayreuth, Germany
[2]Center for High Pressure Science and Technology Advanced Research, 100094 Beijing, China
[3]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22603 Hamburg, Germany

Abstract

Stishovite, a rutile-structured polymorph of SiO_2, is a main component of subducted basaltic lithologies in the lower mantle. At mid lower-mantle depths, a second-order ferroelastic transition to orthorhombic $CaCl_2$-type (post-stishovite) structure occurs, causing extensive elastic shear softening. Previous studies showed that Al incorporation can decrease the transition pressure, while it is still debated whether H has a similar effect. Here we report the equations of state, structural evolution, and phase transformation of $Si_{0.948}Al_{0.052}O_{1.983}H_{0.018}$ (Al5) stishovite and $Si_{0.886}Al_{0.114}O_{1.980}H_{0.074}$ (Al11) post-stishovite samples using diamond-anvil cells in combination with synchrotron X-ray diffraction and Raman spectroscopy. The Al5 sample transformed to the orthorhombic polymorph upon compression to 16 GPa, displaying a drop of ~12% in its bulk modulus across the transformation. The Al11 sample did not undergo any phase transition in the pressure range investigated. Single-crystal structural refinements and Raman spectroscopy measurements on the Al5 sample show that the soft optic mode B_{1g} is decoupled from the tetragonal-to-orthorhombic structural transformation and shows a plateau in the stability field of post-stishovite, between 20 and 30 GPa. This observation indicates that the transformation is not pseudo-proper ferroelastic as in SiO_2 stishovite and that existing Landau expansions are likely not applicable to H-rich Al-bearing silica samples. Using the equation of state parameters of orthorhombic Al5 and Al11 and literature data on SiO_2 post-stishovite we then discuss the possibility of non-ideal mixing along the SiO_2-AlOOH join.

Keywords: Stishovite, X-ray diffraction, phase transition, equation of state, nominally anhydrous minerals