American Mineralogist, Volume 101, pages 2514–2524, 2016

Formation of hydrous stishovite from coesite in high-pressure hydrothermal environments

Kristina Spektor[1,†], Johanna Nylen[1], Renny Mathew[1], Mattias Edén[1], Emil Stoyanov[2], Alexandra Navrotsky[2], Kurt Leinenweber[3], and Ulrich Häussermann[1,*]

[1]Department of Materials and Environmental Chemistry, Stockholm University, SE-10691 Stockholm, Sweden
[2]NEAT ORU, University of California at Davis, One Shields Avenue, Davis, California 95616, U.S.A.
[3]Department of Chemistry and Biochemistry, Arizona State University, Tempe, Arizona 85287-1604, U.S.A.

Abstract

In low-temperature, high-pressure hydrothermal environments coesite transforms into hydrous forms of stishovite. We studied hydrous stishovite produced from hydrothermal treatment of silica glass as initial SiO_2 source at temperatures of 350–550 °C and pressures around 10 GPa. The *P-T* quenched samples were analyzed by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), thermal analysis, and IR and magic-angle spinning (MAS) NMR spectroscopy. The presence of significant amounts of H_2O (ranging from 0.5 to 3 wt%) is shown from thermogravimetric measurements. PXRD reveals that at temperatures below 400 °C, hydrous stishovite is obtained as two distinct phases that may relate to the solid ice-VII environment present at prevailing *P-T* conditions. Initially formed hydrous stishovite is metastable and dehydrates over time in the low-temperature, high-pressure hydrothermal environment. The primary mechanism of H incorporation in stishovite is a direct substitution of $4H^+$ for Si^{4+} yielding unique octahedral hydrogarnet defects. In IR spectra this defect manifests itself by two broad but distinct bands at 2650 and 2900 cm^{-1}, indicating strong hydrogen bonding. These bands are shifted in the deuteride to 2029 and 2163 cm^{-1}, respectively. Protons of the octahedral hydrogarnet defect produce ^1H MAS NMR signals in the 9–12 ppm region. The presence of multiple resonances suggests that the octahedral defect is associated with various proton arrangements. At elevated temperatures, the NMR signals narrow considerably because of proton dynamics.

Keywords: Coesite-stishovite transition, hydrous minerals, octahedral defects, high-pressure hydrothermal environments