

Effect of Al³⁺ and H⁺ on the elastic properties of stishovite

**DMITRY L. LAKSHANOV,^{1,*} KONSTANTIN D. LITASOV,² STANISLAV V. SINOGEIKIN,^{1,†}
HOLGER HELLWIG,¹ JIE LI,¹ EIJI OHTANI,² AND JAY D. BASS¹**

¹Department of Geology, University of Illinois at Urbana-Champaign, 1301 W Green Street, Urbana, Illinois 61801, U.S.A.
²Institute of Mineralogy, Petrology and Economic Geology, Tohoku University, Aza Aoba Aramaki, Sendai 980–8578, Japan

ABSTRACT

X-ray diffraction, Brillouin, and Raman scattering measurements were performed on Al³⁺ and H⁺-bearing stishovite at ambient conditions. Samples with different Al³⁺ and H⁺ contents were used to examine the effects of these minor constituents on the density, acoustic velocities, single-crystal and aggregate elastic moduli. The X-ray diffraction and compositional data suggest that the incorporation mechanism of Al³⁺ into stishovite involves the formation of oxygen vacancies, in addition to the incorporation H⁺ in the structure. Our data show an overall linear decrease of the acoustic velocities, single crystal (c_{ij}) and aggregate (K_0 , G_0) elastic moduli as a function of Al³⁺ concentrations. For the sample of stishovite containing 6.07(5) wt% Al₂O₃ and 0.24(2) wt% H₂O we obtained: zero-pressure adiabatic bulk modulus, $K_{s0} = 290(3)$ GPa, and the shear modulus, $G_{s0} = 207(2)$ GPa, with a calculated density of $\rho = 4.16(1)$ g/cm³ based on X-ray diffraction. Stishovite containing 4.37(12) wt% Al₂O₃ and 0.29(3) wt% H₂O possesses higher aggregate moduli: $K_{s0} = 296(3)$ GPa and $G_{s0} = 213(2)$ GPa, with a calculated density of $\rho = 4.21(1)$ g/cm³ based on X-ray diffraction. We conclude that the formation of oxygen vacancies has a stronger effect on the density and thus elastic properties of stishovite than does the incorporation of hydrogen.

Keywords: Stishovite, elasticity, aluminum, hydrogen, mantle, Brillouin spectroscopy, oxygen vacancies