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The effect of water on the elasticity of minerals

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Hydrous minerals play an important role in the transport of water from the Earth's surface deep into the Earth's mantle. At the same time, water incorporated into the minerals, mainly as OH hydroxyl group, influences their physical properties giving rise to possible seismic anomalies. In the present study, two different minerals, namely stishovite, SiO2, with 5mol% of AlOOH substitution, and Al-phase D, (Al,Fe3+)2SiO6H2, have been studied at high pressure by means of single-crystal X-ray diffraction in a diamond anvil cell using synchrotron radiation at the Extreme Conditions Beamline P02.2 of PETRA III (DESY, Hamburg, Germany).

Stishovite, a rutile-structured polymorph of SiO2, is a main component of subducted basaltic lithologies in the lower mantle. At mid lower-mantle depths, a second-order ferroelastic transition to orthorhombic CaCl2-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 substitution has a similar effect. Here we show that the AlOOH substitution not only reduce the transition pressure of the tetragonal to orthorhombic transition, but also has a major influence on the mechanism of the transition, likely because of the occurrence of symmetric hydrogen bonds at high-pressure. By modelling the individual effect of Al and H on the pressure-temperature conditions at which elastic softening of silica phases is expected, we suggest that this softening may be related to some seismic anomalies observed in the topmost part of Earth's lower mantle, in the proximity of subducted oceanic plates.

Al-phase D, the (Al,Fe3+)2SiO6H2 member of the dense hydrous magnesium silicate (DHMS) phase D, may survive along hot subduction geotherms or even at ambient mantle temperatures in the Earth's transition zone and lower mantle, playing therefore a major role as water reservoir and carrier in the Earth's interior. The evolution of the unit-cell volume of Fe-bearing Al-phase D between room pressure and 38 GPa, determined by means of synchrotron X-ray diffraction in a diamond anvil cell, is well described by a 3rd-order Birch-Murnaghan equation of state. Above 38 GPa, a change in the compression behavior is observed, likely related to the high-to-low spin crossover of octahedrally coordinated Fe3+. Contrary to what observed for A,H-bearing stishovite, the strength of H-bonds and likely their symmetrisation do not greatly affect the elastic properties of phase D solid solutions, independently of their compositions, however change in volumes may be associated with spin crossover transitions for Fe-rich compositions.

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