Coupled substitution of Fe^{3+} and H^+ for Si in wadsleyite

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Wadsleyite is the most abundant mineral in the upper part of the mantle transition zone (MTZ) and can incorporate up to 3 wt% water in its crystal structure. Incorporation of water (or hydrogen) in wadsleyite influences its elasticity, atomic diffusivity, creep strength, crystallographic preferred orientation, grain-growth kinetics and electrical conductivity. Moreover, water affects phase boundaries relevant to wadsleyite. Consequently, determination of the substitution mechanisms of hydrogen in wadsleyite is fundamentally important to addressing the effects of water on the above properties of the upper MTZ. The major substitution mechanism of hydrogen in Fe-free hydrous wadsleyite is protonation of oxygen having no bonding to Si (non-silicate oxygen, O1). Recently, coupled substitution of Fe³⁺ and H⁺ for Si was proposed as a new protonation mechanism in Fe-bearing hydrous wadsleyite (Bolfan-Casanova et al. 2012; Smyth et al. 2014; Kawazoe et al. 2016). I will review the previous studies and introduce experimental evidence to support the coupled substitution of Fe³⁺ and H⁺ for Si in wadsleyite.

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