Properties of Ultra-Confined Water: Effects on Phase Stability

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Water in sub-nanometer channels in silicate minerals presents an extreme case of confinement similar to those along grain boundaries. The specific properties, however, vary tremendously with the specific mineral. For example, a "quantum tunneling state" occurs in water molecules confined in 5 Å channels in beryl, characterized by extended proton and electron delocalization. The average kinetic energy of the water protons is ~30% less than in bulk liquid or solid water. Such behavior is not observed in nearly isostructural cordierite. In hemimorphite, water molecules form a planar hydrogen bond network with hydroxyl groups on the crystal framework. The incoherent dynamic structure factor reveals two thermally activated relaxation processes, a faster on a subpicosecond time scale and a slower on a 10-100 ps time scale, between 70-130 K. The slow process is an in-plane reorientation analogous to rotational diffusion. The fast process is a localized motion of the water molecule with no apparent analogs within known bulk or confined water phases. Thus, once water in the subsurface becomes confined to nanoscale grain boundaries it is unlikely that its properties match those of the bulk material. Thus, mineral stability and solubility may depend directly on the structural environment of water in a given geoenvironment.

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