Ice-like Behavior of Ultra-Confined Water

TIMOTHY PRISK, ALEXANDER KOLESNIKOV, EUGENE MAMONTOV, LAWRENCE ANOVITZ, Oak Ridge National Laboratory — Water confined within microporous minerals presents an extreme example of fluid confinement, where the water molecule is trapped within cages or pore channels which are not much larger than the water molecule itself. Hemimorphite $\text{Zn}_4\text{Si}_2\text{O}_7(\text{OH})_2\cdot\text{H}_2\text{O}$ is a microporous silicate mineral containing confined molecular water which interacts with the crystal structure by means of hydrogen bonding. The water molecule forms a set of coplanar hydrogen bonds with the hydroxyl groups, forming a system of two-dimensional ice within the pore channel. In this presentation, we report quasi-elastic and inelastic neutron scattering studies of water and hydroxyl proton dynamics within hemimorphite. The scattering data reveal strong anisotropy in the vibrational behavior of the water molecule, with the scissors and stretching normal mode motions occurring only on a single crystallographic plane. The effective density of states of the protons extracted from the scattering data reproduces the water contribution to the mineral’s heat capacity.

$^1$This research conducted at the Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

Timothy Prisk
Oak Ridge National Lab

Date submitted: 12 Nov 2014

Electronic form version 1.4