P14 |

Phase transition behaviour of water confined in titania mesopores

T. Muthulakshmi, D. Dutta, Priya Maheshwari and P. K. Pujari*

Radiochemistry Division, Bhabha Atomic Research centre, Mumbai, INDIA

*email: pujari@barc.gov.in

Phase transition of water under nano-confinement is an active area of research due to its relevance in fundamental physics as well as in biological and technological applications. In the present work, the phase transition behaviour of water confined in titania mesopores with different levels of hydration has been investigated using temperature dependent positron annihilation Doppler broadening and lifetime spectroscopy. The mesoporous titania was synthesized by one-pot sol-gel method using Pluronic F127 as template. The synthesized titania has a pure anatase phase with pore size of 4.8 nm and the BET surface area of 109 m^2/g. The titania matrix doesn't favour positronium (Ps) formation. The observed *ortho*-positronium (*o*-Ps) *pick-off* lifetime in hydrated titania represents Ps formation and annihilation in confined water. The change in slope with temperature in the Doppler broadened *S*-parameter and *o*-Ps pick-off lifetime (τ_p) profile is indicative of the phase transition of confined water. It is manifested from the profiles that the phase transition behavior varies with the levels of hydration in titania mesopores. As the hydration level decreases, the H-bonding network among water molecules gets disrupted and the interaction with the pore surface is modified which result in the variation in phase transition behavior. In the fully hydrated titania, water is present both at the surface and the core of the pore, whereas in the partially hydrated pore, the bulk-like core water becomes less. Hence, the effect of surface interaction becomes more prominent as the hydration level decreases. With the decrease in temperature both the τ_p and *S*-parameter values show decreasing trend that saturate at very low temperature limit. In the fully hydrated titania a sharp change in the slope of τ_p is observed just below the bulk freezing point of water (273K) indicative of freezing of bulk like water present in the matrix. A further change in the slope was observed below 250K indicating the ice-nucleation of confined supercooled water. The value of τ_p and the *S*-parameter remain constant below 200K suggesting the completion of the growth of ice nuclei inside the pore. In the partially hydrated titania, on the other hand, the low temperature transition is observed to be extended till 180K. Below 180K, both the τ_p and the *S*-parameter values remain almost constant. The role of hydrogen bonding network on the low temperature phase transition of confined water will be discussed in more details.