Effects of surface functional groups of carbon on water adsorption process and phase transition of confined water in nanopore

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The anomalous behavior of water in carbon nanopores has been attracted from the scientific viewpoint and the importance for current and future various applications. We used measurements of adsorption rate, X-ray scattering and differential scanning calorimetry to investigate water behavior in carbon nanopores. We focused on the effects of surface functional groups on the water adsorption process and the phase transition of confined water. The functional groups act as the initial site of water adsorption and determine hydrophilicity of carbon walls. We consider the functional groups as the important factor of elucidating water/carbon system.

The density fluctuation obtained from X-ray scattering measurements revealed that the coalescence of water clusters occurs at lower relative pressure in carbon with more functional groups. Furthermore, the density fluctuation has a negative correlation with the adsorption rate constant. The increase in the density fluctuation corresponds to the inhomogeneous water adsorption or the formation of water clusters. These results suggest that water clusters in pore inhibit the diffusion of water vapor and decrease the adsorption rate.

Using differential scanning calorimetry, we found that the adsorbed water can be divided into two groups in different environments. One is water inside the pores, the other is water adsorbed after the completion of pore filling. The melting temperature of water inside pores is lower than that of bulk water and is slightly dependent on the amount of functional groups. The melting temperature of water inside pores tends to be the higher with increasing the functional groups, but the difference is very small. Additionally, it was observed by X-ray diffraction that the formation of ice Ih and amorphous ice inside pores occurs continuously with lowering temperature.

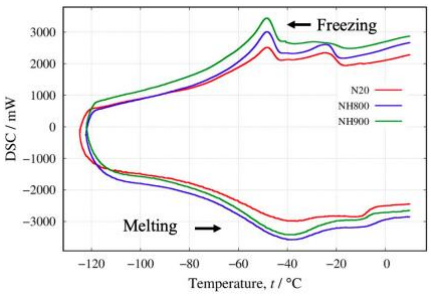

Fig. DSC profiles of activated carbon N20, NH800, NH900 (average pore width w = 1.0 nm). The amount of functional groups is N20 > NH800 > NH900.