

Hydration Process of Zinc Ion Restricted in Cylindrical Carbon Nanospace

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The hydration structures of metal ion restricted in carbon nanospace are quite different from those in bulk solution. Recently, we reported the dehydration structure around a zinc ion confined in cylindrical micropore of single-wall carbon nanotube (SWCNT)¹⁾. In this work, we studied the variation of hydration structure during adsorption process of water vapor on zinc-ion deposited SWCNT by XAFS technique.

We used two kinds of SWCNTs (HP-SWCNT and LP-SWCNT) whose pore widths are 1.4 and 0.9 nm, respectively. Each SWCNT was dispersed in aqueous solution of zinc acetate to impregnate zinc ion into the micropore. SWCNTs adsorbed by zinc ion (denoted by HP-SWCNT-Zn and LP-SWCNT-Zn) were evacuated at 423 K followed by adsorption of water vapor. Both XAFS and time-dependent XAFS (QXAFS) spectra were collected on Zn *K*-edge (9661 eV) at KEK-PF.

Figure 1 shows the QXAFS spectra at Zn *K*-edge for HP-SWCNT-Zn during the adsorption process of water vapor. The white-line intensity, which is the absorbance near the absorption edge of Zn *K*-edge, having higher symmetrical structure is generally stronger than that of lower one. Therefore, the present results reflect that the structural variation around a zinc ion confined in the micropore of HP-SWCNT can proceed with two steps, although the structure in the micropore of LP-SWCNT changes from evacuated to hydration states monotonously. Figure 2 shows the variation of white-line intensity at each equilibrium pressure and water vapor adsorption isotherm at 303 K on HP-SWCNT-Zn. The white-line intensity is decreased at $P/P_0 = 0.4 \sim 0.5$ and water vapor is rapidly adsorbed into micropore of HP-SWCNT at same region. This indicates the hydration structure around a zinc ion is varied by the total amounts of adsorbed water.

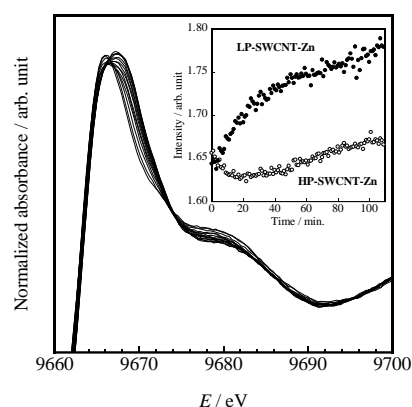


Figure 1. QXAFS spectra at Zn *K*-edge for HP-SWCNT-Zn during the adsorption process of water vapor for 110 min. The inset plots the white-line intensity of HP-SWCNT-Zn and LP-SWCNT-Zn during the adsorption process of water vapor.

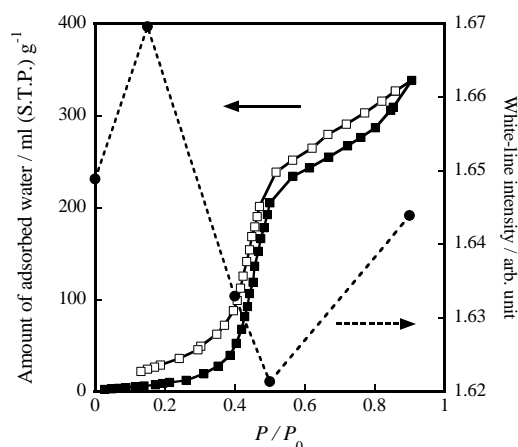


Figure 2. Water vapor adsorption-desorption isotherm (solid line) at 303 K on HP-SWCNT-Zn and white-line intensity (dotted line) at each equilibrium pressure.

1) M. Nishi et al., *Nanoscale*, **5**, 2080, (2013).