Mesoscopic investigation to binary mixture of water and cyclohexane by SANS and ND

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Intermolecular structure of adsorbed molecules in hydrophobic confined space (e.g. activated carbons, CNTs, etc) is different from bulk state which is caused by confine effetct and enhanced potential from pore walls especially whose pore width less than 2 nm. Single component case, it is reported that the intermolecular structure of water in hydrophobic slit-shaped pore formed Ice-Ic like structure even at ambient temperature by X-ray diffraction (: XRD), neutron diffraction (: ND) and reverse Monte Carlo modeling [1, 2]. Small angle X-ray scattering measurement and Debye-Bueche (: DB) analysis were revealed that pore filling process of adsorbed water is formation and growing up of water cluster [3]. Contrast variation small angle neutron scattering (CV-SANS) is powerful tool to investigate mesoscopic structure of multicomponent system which is more than three components. In CV-SANS, the scattering length density (: SLD) of solvent is mathced to one of the solvates SLD, and the self scattering term of another component was measured. We applied CV-SANS technique to the multi-adsorption system. In this study, we used water and cyclohexane as adsorbates, and activated carbon fiber, AC (A'd all co. Ltd., w_{ave} = 0.82 nm) as adsorbent. CV-SANS measurement was carried out using BL-20 at MLF in J-PARC. SLD of solvent (water or cyclohexane) changes to the AC SLD(= 6.0×10^{10} cm^{-2}) or void SLD(= 0×10^{10} cm^{-2}). SANS data range is $0.09 < q < 40$ nm^{-1} where $q(= 4\pi\sin\theta / \lambda)$ is scattering vectors, θ is the scattering angle and λ is incident neutron wave length. Correlation length, ξ and zero scattering, I_0 are led to DB [3] and Guinier analysis [4]. We have also led to solid (l_{solid}) and void (l_{void}) average length from correlation length [3].

CV-SANS profiles change with solvent SLD. When cyclohexane SLD is match to AC SLD, l_{solid} is larger than bare AC. Other case, when water SLD is match to AC SLD, l_{solid} is also larger than bare AC, but smaller than cyclohexane matching case. These two results suggested that mesoscopic structure of water and cyclohexane binary mixing in AC pore is not completely separate (e.g. bulk state) but not mixing (e.g. water-ethanol system), and cyclohexane exists vicinity of AC surface, water exists center of pore (far from AC surface). CV-SANS results are supported the differential radial distribution function determined by X-ray and neutron diffraction.

References [1] T. Iiyama et al., *Chemical Physics Letters*, **1997** 274 152-158, [2] MarieClaire BellissentFunel et al., *The Journal of Chemical Physics*, **1996**, 104, 10023-10029, [3] T. Iiyama et al., Colloids and Surfaces A: Physicochem. Eng. Aspects, **2004**, 241, 207-213, [4] Z. Milwwva et al., *carbon.* **2012**, 50, 5062-5075