

Temperature Dependence of water dynamics in nano-porous material FSM

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In absorption water in the pore of mesoporous silica such as FSM-16 (Folded Sheets Mesoporous Materials), briefly, it can be considered that two kinds of water from which mobility is different exist. One is the absorbed water beside the pore wall (mono-layer water) and another is other absorbed water in the pore. Especially, the mobility of mono-layer water is strictly restricted by the hydrogen bonding to the surface hydroxyl group. The dynamics of mono-layer water would be different from that of other water.

In order to obtain the activation energy of the absorption water in FSM16 pore, we have investigated the dynamics of mono-layer water and full-layer water by using AGNES in the temperature range 150K-318K. On the basis of the result of adsorption isotherm of FSM, the absorption amount of water in the sample was adjusted by steam pressure. The observed spectra of mono-layer sample were analyzed with the model function, given by the convolution of a Gaussian and a Lorentzian function (L1). For the full-layer sample, the spectra were expressed by the convolution function using double Lorentzian function (L1, L2). Here, L1 and L2 are contributions from mono-layer and the other water, respectively. To extract HWHM of L2, two of fitting parameters were fixed. HWHM values of L1 were fixed to values obtained from mono-layer measurements. The ratio of the intensity for L1 and L2 was also fixed in that of the amount of absorption water. As the resolution function, the spectrum of same sample at 150K was used. Fig.1 shows the temperature dependence of HWHM of L2 as a function of the squared scattering vector. This result is well represented by random diffusion model shown as solid lines. Fig.2 shows Arrhenius plot of the

diffusion coefficient of the mono-layer and full-layer sample. Consequently, the values of activation energy of the mono-layer and full-layer sample were 2.5 and 4.7 kcal/mol, respectively. It is interesting to note that the tendency of the temperature dependence of the diffusion coefficient of full-layer water is in good agreement with that of bulk-water [1].

Reference

- [1] T.Takamuku et. al. J.Phys. Chem. B 1997 101 5730-5739

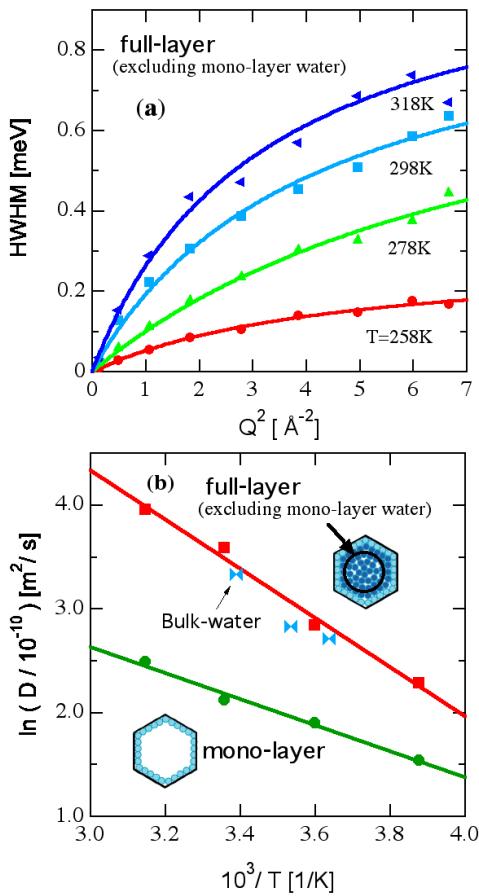


Fig. 1. (a) Temperature dependence of HWHM of L2. Solid lines represents the random jump diffusion fit. (b) Arrhenius plot of the diffusion coefficient of mono-layer water and the other water in FSM16.