Dynamics of Water and Methanol Molecules in Binary Liquid Mixture Confined in Mesopores of MCM-41.

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We had investigated dynamics of water and methanol molecules in pure liquid confined in mesopores of MCM-41 by using quasi-elastic neutron scattering (QENS), and found that both of rotational and translational motions of these molecules in MCM-41 become slower compared with those in bulk liquid around room temperature. In the present study, dynamics of water and methanol molecules in binary liquid mixture confined in MCM-41 was investigated. MCM-41 is one of the most suitable sample to study confined liquids, since it has highly controlled cylindrical nano-space with very narrow pore size distribution.

MCM-41 sample, whose pore diameters were 3.74 nm, were prepared by the method of Beck et al. To observe dynamics of water and methanol molecules separately, we prepared two kinds of partially deuterated binary liquid mixture of water and methanol (molar ratio 1:1), i.e., H2O-CD3OH and D2O-CH3OD. The former gives QENS spectra mainly due to water molecules and the latter those mainly due to methanol ones, especially methyl group in it. For the QENS measurements, we prepared five MCM-41 samples whose pores were filled with different adsorbate: H2O-CD3OH and D2O-CH3OD, H2O, CD3OH, CH3OD. The QENS measurements of these five pore-filled MCM-41 samples, corresponding five bulk-liquid samples, a dried MCM-41 sample and an empty cell were carried out by using time-of-flight type spectrometer AGNES installed at the JRR-3M reactor of Japan Atomic Energy Research Institute. The wavelength of neutron beam was 0.422 nm, the momentum transfer (Q) range 6.4-25.0 nm-1, and the temperature range 200-300 K.

QENS spectra of H2O-CD3OH and D2O-CH3OD confined in MCM-41 as well as corresponding bulk-liquid samples at Q = 18.0 nm-1 and T = 300 K are shown in Figure 1. Here, the displayed spectra are the difference between raw spectra and spectra of the dried sample, and thus contain the contributions only from the confined liquid. All the spectra are normalized ones, in which peak maxima have been coincided with each other to emphasize the change in quasi-elastic wings of the spectra. By comparing line widths of the spectra, it is found that motions of methanol molecules is faster than those of water molecules for both bulk and confined liquid. It is also found that molecular motions in confined liquid are slower than those in bulk liquid for both water and methanol molecules. Detailed analysis is now in progress.

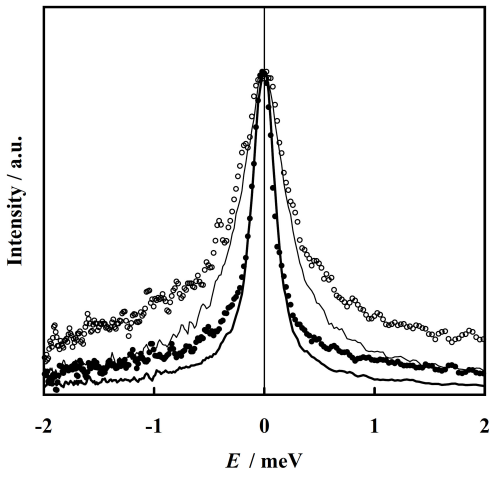

Fig. 1. QENS spectra of confined samples of H2O-CD3OH (bold line) and D2O-CH3OD (open circles) and bulk samples of H2O-CD3OH (fine line) and D2O-CH3OD (closed circles) at Q = 18.0 nm-1 and T = 300 K.