Quasi-elastic neutron scattering study on diffusion dynamics of water molecules in tert-butyl alcohol-water mixture

M. Misawa and M. Nakada
Institute of Science and Technology, Niigata University, Niigata 950-2181, Japan

In a previous paper [1], we reported that the characteristic behavior of the excess partial molar volume Ve of 1-propanol-water mixture was interpreted satisfactorily in terms of the hydrophobic hydration of the fractal surface of alcohol clusters. The fraction of the hydrated water molecules on the fractal surface was determined by means of quasi-elastic neutron scattering. Tert-butyl alcohol (TBA)-water mixture is characterized also by the polydisperse mass fractals [2]. Furthermore, the solution shows the same characteristic behavior of Ve as that of the 1-propanol-water mixture. The purpose of this study is to measure the dynamics of water molecules of the TBA-water mixture and examine whether or not the same interpretation of Ve as applied to the 1-propanol-water mixture is valid for the TBA-water mixture.

Diffusion dynamics of water molecules in the TBA-water mixture has been measured at 25, 47 and 70 °C by using AGNES (C3-1-1) spectrometer, JRR3M at JAEA. In order to observe the dynamics of water molecules, the TBA molecules substituted partially by deuteron (CD3)3COH and the light water molecules H2O were used. The mixtures of TBA content x of 0.0, 0.01, 0.02, 0.04, 0.06, 0.08, 0.10, 0.14 and 0.17 in mole fraction were examined. The dynamical structure factors S(Q,E) in the region of quasi-elastic scattering have been obtained in the range of Qe from 0.376 to 2.504 Aˆ-1.

Detailed analysis on the visualized mesoscale structure of the current solution suggested that the water molecules in the solution were classified into two types at least: one was the bulk-like state and another was the surface-state restricted to the fractal surface of alcohol clusters. Therefore, the S(Q,E)'s from x=0.01 to 0.10 have been analyzed by a linear combination of the S(Q,E)'s for these two states. The fraction α of water molecules located at the fractal surface and the average number Nws of water molecules in the surface-state per TBA molecule (Fig. 1) have been obtained as a function of x. By extrapolating Nws to x=0, we get the value of 19˜21 for Nws. This means that about 19˜21 water molecules are located on the surface of an isolated TBA molecule in water. It is confirmed that the anomalous excess partial molar volume of the TBA-water mixture is explained reasonably well in terms of α in the same way as that for 1-propanol-water mixture [3].

References

[1] M. Misawa, Y. Inamura, D. Hosaka and O. Yamamuro, J. Chem. Phys., 125 (2006) 074502.
[2] M. Misawa, T. Sato, A. Onozuka, K. Maruyama, K. Mori, S. Suzuki and T. Otomo, to be published in J. Appl. Cryst.
[3] M. Nakada, O. Yamamuro, K. Maruyama and M. Misawa, submitted to J. Phys. Soc. Jpn.

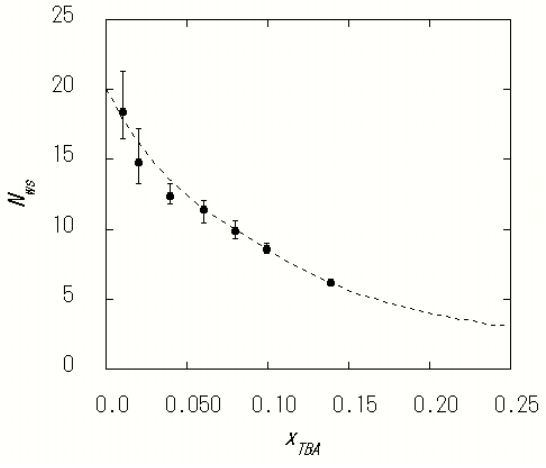

Fig. 1. Composition dependence of Nws for TBA-water mixture at 25 °C.