Shigeharu Kittaka et al., J Phys Chem Biophys 2017, 7:4(Suppl)
DOI: 10.4172/2161-0398-C1-025

Neutron scattering study of super cooled water confined in mesoporous silicas, MCM-41 and SBA-16: Role of component pores and their size

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The nature of super-cooled water in confinement is an important subject that involves many aspects of natural sciences. Strong hydrogen bonds lead to the formation of structured collective entities in liquid water, finally resulting in crystallization of ice. Since the development of synthetic methods of well-defined porous silicas of various sizes, cylindrical, spherical, etc., experimental and theoretical analysis of pore water has significantly developed. The present interest is to find how the collective entities of water grow in fine pores of different shapes and what dynamic motions are there. Neutron spin echo (NSE) measurements were conducted on heavy water confined in cylindrically porous MCM-41 and spherically porous SBA-16 in the temperature range 210–290 K. Deuterium has a nuclear spin of 1 and thus has a highly coherent scattering cross-section that is convenient for the study of the dynamics of collective entities of heavy water. In the spherical pores of SBA-16, the translational motion of heavy water was strongly inhibited, even at 290 K. Rotational motion, however, was observed clearly in the temperature range 230–290 K and was analysed by the Vogel–Fulcher–Tammann relation. The relaxation time of the rotational motion of heavy water increased with a decrease in temperature. For heavy water in the cylindrically porous MCM-41, the relaxation time increased with reducing the temperature, as in SBA-16, but much more sharply. The larger value for the former is ascribed to the linear growth of hydrogen bonds in the cylindrical pores. In contrast, in the spherical space of SBA-16, spherical growth of heavy water clusters could permit a faster dynamic rotational motion. NSE measurements of light water in SBA-16 showed the translational diffusion of discrete water molecules there, indicative of the occurrence of breaking and recombination of hydrogen bonds in the collective entities.

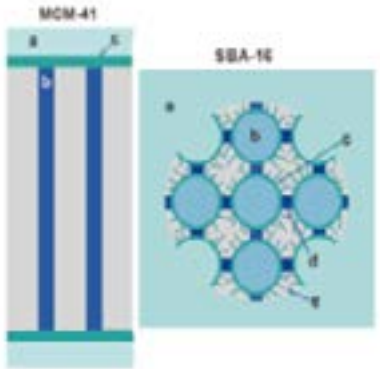

Fig. 1 Water contacting with MCM-41 and SBA-16.

Biography

Shigeharu Kittaka has his expertise in surface chemistry of metal oxide-water systems: electrification of metal oxides in water, fine spherical particle formation and surface structure, layer structure of $V_2O_5 \cdot nH_2O$ by intercalation of water and organic molecules and electrical properties, phase changes of molecular liquids: water, ammonia, alcohol etc.

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