Intermolecular Structure of Binary Mixture in Confined Spaces: by XRD, ND and RMC

Taku Iiyama[1,2], Masatsugu Yoshimoto[1], Ryusuke Futamura[2], Toshiya Otomo[3]

[1] Faculty of Science, Shinshu University, Matsumoto, Japan
[2]Center for Energy and Environmental Science, Shinshu University, Nagano, Japan
[3]High Energy Accelerator Research Organization, Tsukuba, Japan

Email:tiiyama@shinshu-u.ac.jp

The multi-component adsorption which is the coexistence state of two or more kinds of molecules in the small space is used in many of the applications using porous materials. It is expected that the unusual molecular mixing state in confined spaces. Although the molecular mixing state in the small space is very important for the many of applications, it is not sufficiently clarified, especially, from the experimental microscopic viewpoint by the experimental difficulties.

We have been applying the X-ray diffraction (XRD), neutron diffraction(ND) and small angle X-ray scattering (SAXS) to elucidate the structure of adsorbed molecules in confined carbon spaces [1,2]. Furthermore, the reverse Monte Carlo (RMC) method was applied to obtain the intermolecular structure of confined molecules [3–7]. The broad peaks of XRD can transform to radial distribution function (RDF) of adsorbed phases which is direct structural information of nano-mixture. The combination analysis of XRD and ND gave the separated information of each component of mixture, especially hydrogen atoms. Although RDF is one-dimentional information basically, RMC can provide the 3-dimentional molecular arrangement which reproduces the experimental scattering data. RMC use the geometrical parameters of adsorbents and adsorbate molecules of the multi-component adsorption and solution systems.

We will talk the structure and behaviour of confined ionic liquid, water and organic molecules mixture in carbon micropore[8]. We deduced the intermolecular structure of confined “nano-mixture” by using XRD, ND and RMC analysis.

Reference(s)

[1] R. Futamura, T. Iiyama, A. Hamasaki, S. Ozeki, *Phys. Chem. Chem. Phys.* **2012**, 14, 981.
[2] M. Yoshimoto, R. Futamura, A. Hoshikawa, T. Ishigaki, T. Uchida, T. Iiyama, *Chem. Lett.* **2017**, 46, 923.
[5] T. Iiyama, K. Hagi, T. Urushibara, S. Ozeki, *Coll. Surf. A* **2009**, 347, 133.
[6] A. Tanaka, T. Iiyama, et al, *J. Am. Chem. Soc.* **2010**, 132, 2112.
[7] M. Fukano, et al, *J. Phys. Chem. C* **2013**, 117, 5752.
[8] R. Futamura, S. Ozeki, T. Iiyama, *Carbon* **2015**, 85, 815.