Contribution ID: **21** Type: **Oral**

Research on syndiotactic polystyrene complexes with simultaneous measurements of small-angle and wide-angle neutron scattering with FTIR spectrocopy

Syndiotactic polystyrene (sPS) has a unique property to form molecular complexes with a variety of chemical compounds, from low mass molecules to polymeric compounds. The guest molecules are stored in the cavities surrounded by the phenyl side groups of sPS. The sPS complex can be generated not only as crystalline solid states but also as gel states from solutions and glass samples. Under certain conditions, the sPS complex exhibits some characteristic structural changes, such as the substitution of the guest molecules and the transformation to a crystal polymorph of sPS ejecting the guest molecules from the cavities. Small angle neutron scattering (SANS) is a versatile and convenient method to investigate the higher order structure of molecular assembly systems. It is a quite suitable tool to follow and analyze the structural changes and formation process of sPS complexes; by exploiting the significant difference in scattering length between fully deuterated and protonated compounds we can deduce the information how the guest molecules are distributed in the sPS complex system. In order to assist the analysis of SANS data, we developed a simultaneous SANS/FTIR measuring system by employing the KWS-2 diffractometer at MLZ Germany(1,2), which is able to add the molecular level information such as conformation and concentration. Furthermore, we recently introduced this methodology to a neutron scattering instrument covering a wider scattering angle range (BL-15 Taikan at JPARC, Japan), which makes it possible to access the hierarchical structures in polymer complexes, from the higher order structures to the interior structure within the crystal lattice. We have applied the simultaneous measurement method to the studies on the temperature dependent structure changes of sPS cocrystals and the sPS gelation process from binary-solute solutions.

1. F. Kaneko, N. Seto, et al., *Chem. Lett.* 44 (2015), 497-499.
2. F. Kaneko, N. Seto, et al., *J. Appl. Cryst.* 49 (2016), 1420–1427.

Preferred topic

Characterization - large instruments

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