

Spectroscopic and scattering studies on syndiotactic polystyrene cocrystals

F. Kaneko¹, A. Radulescu², H. Iwase³, S. Takata⁴, H. Nakagawa⁵, M. Nishiura⁶, and Z. Hou⁶

¹Graduate School of Osaka Univ., Osaka, Japan; ²JCNS at MLZ, Garching, Germany; ³CROSS, Ibaraki, Japan; ⁴J-Parc Center, Ibaraki, Japan; ⁵JAEA, Ibaraki, Japan; ⁶Organometallic Chem. Lab., RIKEN, Saitama, Japan.

ABSTRACT: Syndiotactic polystyrene (sPS) has a unique property to form cocrystals with a variety of chemical compounds. The cocrystals can be generated not only as crystalline solid states but also as gel states from solutions. Under certain conditions, the sPS cocrystal exhibits some characteristic structural changes, such as the substitution of the guest molecule and the transformation to a crystal polymorph of sPS, ejecting the guest molecules from the cavities.

To obtain different kinds of structural information from such polymer cocrystal systems, we have developed a measurement system combining neutron scattering and FTIR spectroscopy, as shown in Fig 1.¹

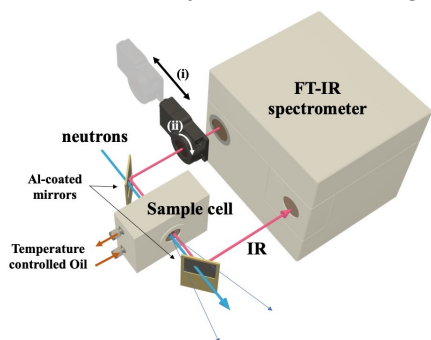


Figure 1: The optical system of the simultaneous SANS/WANS/Polarized-FTIR measuring system installed at TAIKAN diffractometer in J-Parc.

We have applied this system to explore the properties of sPS cocrystals. Figs 2 and 3 show our experimental results on the adsorption of water molecules onto the sPS co-crystal with deuterated sPS as host and hydrogenated PEG (MW: ca. 600) as guest.

The sample was exposed to either H₂O or D₂O vapor at different concentrations (based on saturated vapor pressure at 60°C).

As shown in Fig. 2, the IR bands due to H₂O and D₂O components, which clearly appear at lower frequencies than those of their vapors, change in intensities sensitively depending on their respective humidities, suggesting their adsorption to the PEG component.

Figure 3 shows how the SANS profile changes with the humidity. Although the change in D₂O concentration does not alter the SANS profile much, the switch from D₂O to H₂O causes a noticeable change in the lamellar reflection, suggesting that water is chiefly absorbed in the crystalline region containing the PEG component.

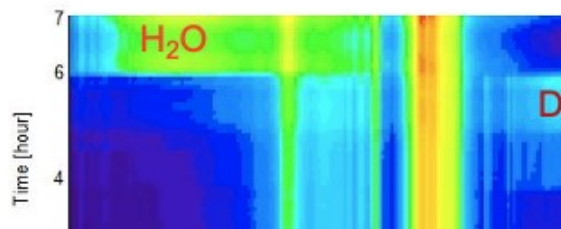


Figure 2: IR spectral changes in response to humidity changes for D₂O and H₂O.

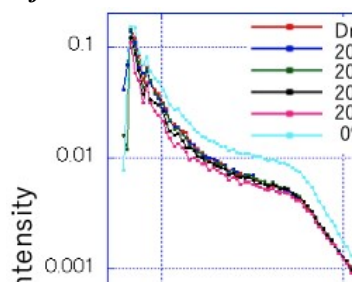


Figure 3: SANS profile variation of sPS/PEG co-crystals dependent on D₂O and H₂O concentrations

KEY WORDS: Syndiotactic Polystyrene, Neutron scattering, FTIR spectroscopy, Simultaneous measurement systems, SANS, WANS

References

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2. F. Kaneko, T. Kawaguchi, A. Radulescu, et al. *Rev. Sci. Instr.* 90, 093906, 2019.