Spectroscopic and scattering studies on syndiotactic polystyrene cocrystals

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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

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

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

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

Key words: Syndiotactic Polystyrene, Neutron scattering, FTIR spectroscopy, Simultaneous measurement systems, SANS, WANS

References