Soft X-Ray Absorption Spectroscopy for Observing Chemical Processes in Solution

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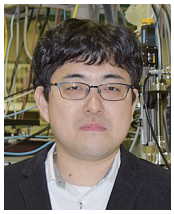

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Soft X-ray absorption spectroscopy (XAS) observes local structures of liquids with different light elements. We have developed liquid cells and devices with precise absorbance control and observed several chemical processes in solution by using *operando* XAS.[1,2] In this year, we have investigated the process of hydrophobic cluster formation in aqueous ethanol solutions by using XAS.[3]

1. Hydrophobic Cluster Formation in Aqueous Ethanol Solutions

Hydrophobic cluster structures in aqueous ethanol solutions at different concentrations have been investigated by XAS.[3] In the O K-edge XAS, we have found that hydrogen bond structures among water molecules are enhanced in the middle concentration region by the hydrophobic interaction of the ethyl groups in ethanol. On the other hand, in the C K-edge XAS, the lower energy features arise from a transition from the terminal methyl C 1s electron to an unoccupied orbital of 3s Rydberg character and show characteristic four concentration regions. From the comparison of C K-edge XAS with the inner-shell calculations, we have revealed the intermolecular interactions of ethanol with water at different concentration regions and found that ethanol clusters are easily formed in the middle concentration region due to the hydrophobic interaction of the ethyl group in ethanol, resulting in the enhancement of the hydrogen bond structures among water molecules.

References

1) M. Nagasaka and N. Kosugi, *Chem. Lett.* **50**, 956–964 (2021).
2) M. Nagasaka, H. Yuzawa and N. Kosugi, *Anal. Sci.* **36**, 95–105 (2020).
3) M. Nagasaka, M. Bouvier, H. Yuzawa and N. Kosugi, *J. Phys. Chem. B* **126**, 4948–4955 (2022).

Twisted Structure Analysis of Soft Matters by Resonant Soft X-Ray Scattering

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Soft matters exhibit their intriguing properties due to mesoscopic physical structures by self-organizations. To understand properties of soft matters, we need to investigate their structure in the mesoscopic scale. We developed a new resonant soft x-ray scattering method which has various kind of selectivities such as elements, groups and molecular alignments.[1]

1. Twisted Structure of Helical-Nanofilament

Twisted structure can be often observed in soft matter. However, since electron density modulations resulting from the twisted structures are weak, conventional small angle x-ray scattering method is difficult to observe it. The resonant soft x-ray scattering measurements can probe twisted structures and obtain pitch of twisted structure. This is because a resonant process strongly depends on an angle between molecule and polarization vector of incident soft x-ray. In this year, we performed resonant soft x-ray scattering experiments at UVSOR BL3U for a helical-nanofilament of liquid-crystal matter.

We successfully obtained diffraction images at the wavelength of 4.34 nm (285 eV), which correspond to C 1s-to-π* core excitations. From the analysis of images, we found a resonant enhancement of diffractions corresponding to a twist pitch of 80 nm. We also found that twist pitch depends on the sample compositions and its temperatures.

Reference

1) B. A. Collins and E. Gann, *J. Polym. Sci.* **60**, 1199 (2022).