Division of Multidisciplinary Chemistry
– Polymer Materials Science –

https://www.scl.kyoto-u.ac.jp/~polymat/index.html

Prof
TAKENAKA, Mikihito
(D Eng)

Assoc Prof
OGAWA, Hiroki
(D Eng)

Assist Prof
NAKANISHI, Yohei
(D Eng)

Assist Techn Staff

ISODA, Kumiko

Students

SEKO, Tamio (D2)
HAMAMOTO, Hiroki (D2)
ARAKAWA, Masato (D1)
TAMURA, Yukiko (D1)

KARITANI, Shu (M2)
BANDO, Shunsuke (M2)
MORIMOTO, Ryuji (M2)
NOMURA, Yuki (M2)

SHIRAISHI, Harunori (M1)
HOSOMI, Yu (M1)
SHIMABUKURO, Wataru (M1)
KUBO, Haruki (UG)

TOBITA, Naoto (UG)
YOSHINO, Syunki (UG)

Scope of Research

The structure and molecular motion of polymer substances are studied, mainly using scattering methods such as X-ray, neutron, and light with intent to solve fundamentally important problems in polymer science. The main projects are studied on 1) the morphologies and the dynamics of self-assembling processes in block copolymers, 2) the hierarchical structures in crystalline polymer and rubber-filler systems, 3) the viscoelastic effects in glassy materials, 4) formation processes and ordering structures in polymer thin films.

KEYWORDS

Polymer Physics
Self Assembly
Hierarchical Structure
Polymer Properties
Softmatter

Recent Selected Publications

Nakanishi, Y.; Ishige, R.; Ogawa, H.; Huang, Y.; Sakakibara, K.; Ohno, K.; Kanaya, T.; Takenaka, M.; Tsujii, Y., Unified Explanation for Self-Assembly of Polymer-Brush-Modified Nanoparticles in Ionic Liquids, *Polym. J.*, **55**, 1199-1209 (2023).

Shibata, M.; Nakanishi, Y.; Abe, J.; Arima-Osonoi, H.; Iwase, H.; Shibayama, M.; Motokawa, R.; Kumada, T.; Takata, S.; Yamamoto, K.; Takenaka, M.; Miyazaki, T., Structural Changes of Polystyrene Particles in Subcritical and Supercritical Water Revealed by in situ Small-Angle Neutron Scattering, *Polym. J.*, **55**, 1165-1170 (2023).

Watanabe, Y.; Ogawa, H.; Konishi, T.; Nishitsuji, S.; Ono, S.; Shimizu, N.; Takenaka, M., Distribution of Oriented Lamellar Structures in Injection-Molded High-Density Polyethylene Visualized via the Small Angle X-ray Scattering-Computed Tomography Method, *Macromolecules*, **56(15),** 5964-5973 (2023).

Watanabe, Y.; Nishitsuji, S.; Takenaka, M., Anomalous Small-Angle X-ray Scattering Analyses on Hierarchical Structures of Rubber–Filler Systems, *J. Appl. Crystallogr.*, **56 (2),** 461-467 (2023).

Kishimoto, M.; Takenaka, M.; Iwabuki, H., Spatial Distribution of the Amorphous Region Constrained by Polymer Crystallites, *Macromolecules*, **56 (1),** 207-214 (2023).

Anomalous Small-Angle X-Ray Scattering Analyses on Hierarchical Structures of Rubber–Filler Systems

The hierarchical structures of carbon black (CB) in Poly(styrene-ran-butadiene) (SBR) rubber/CB systems vulcanized with sulfur and ZnO were clarified by using anomalous small-angle X-ray scattering (ASAXS) near the Zn absorption edge. The SBR/CB systems vulcanized with sulfur and ZnO are commonly used and quantitative analyses of the hierarchical structures in the SBR/CB systems are needed. However, the hierarchical structures in the SBR/CB systems have not been well investigated since the strong scattering contrast of Zn hinders the quantitative analyses of the hierarchical structures of CB by using X-ray scattering. In this study, we eliminated the effects of Zn on the scattering intensity and obtained the structure factors of CB in SBR/CB systems by using the ASAXS method. By extrapolating the structure factors of CB to a zero-volume fraction of CB, we were able to estimate the particle structure factor of the CB aggregate and found that the CB aggregates consist of the closely-packed CB primary particles. We also found the existence of the large particles of ZnO and the particles of ZnS in the order of 10 nm in the structure factors of Zn.

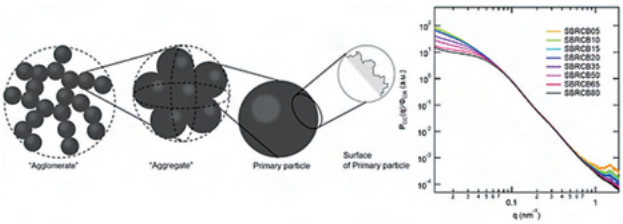

Figure 1. Schematic for hierarchical structures of filler in rubber. Partial scattering function $P_{CC}(q)/\phi_{CB}$ of CB for all samples.

Distribution of Oriented Lamellar Structures in Injection-Molded High-Density Polyethylene Visualized via SAXS-CT Method

We successfully reconstructed the spatial distribution of the orientation of the lamellar structures in injection-molded high-density polyethylene (HDPE) using the small-angle X-ray scattering-computed tomography (SAXS-CT) technique, a combination of the SAXS and CT methods. The skin, subskin, and core layers were identified in the obtained images of the distribution. The orientation and thickness in each layer were found to vary with the injection speed, v. At the slowest v of 5 mm/s, a skin layer is formed along the surface of the sample with the lamellar structure oriented in the injection direction. At the center of the sample, the orientation of the lamellar structure is isotropic, i.e., the core layer. Between the skin and core layers, there is the subskin layer where the lamellar structures are oriented perpendicular and parallel to the injection direction. The thickness of the core layer decreases for $5 \leq v \leq 20$ mm/s because the higher elongation of the polymer chains due to the shear deformation is dominant. For $20 \leq v \leq 40$ mm/s, the strength of the fountain flow and the shear deformation affect the thickness of the layers. The core layer corresponds to the outlet portion of the fountain flow. The increase in the fountain flow amount inhibits the higher orientation of polymer chains, resulting in an almost constant thickness of the core layer with v. In the subskin layer, the increase in the higher elongation of polymer chains with v induces an increase in the thickness for $5 \leq v \leq 20$ mm/s. Although the velocity gradient is even more significant, the suppression of the polymer chain orientation by the fountain flow can result in a nearly constant subskin layer thickness for $20 \leq v \leq 40$ mm/s. The flux of polymers originating from the fountain flow oriented perpendicular to the injection direction is dominant. Unlike the exponential changes in the core and subskin layers, the thickness of the skin layer decreases in proportion to the increase in v potentially because the fountain flow effect increases for $5 \leq v \leq 40$ mm/s, suppressing the shear deformation near the mold.

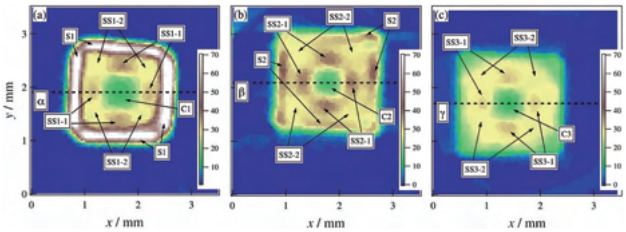

Figure 2. SAXS-CT images in the *X-Y* plane reconstructed from the SAXS profiles at each φ_1 and *Y*. Each injection speed condition is v = 5 mm/s for (a), 20 mm/s for (b), and 40 mm/s for (c). The injection direction is toward the front of the paper.