



TITLE:

# <Division of Multidisciplinary Chemistry>Polymer Materials Science

AUTHOR(S):

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CITATION:

<Division of Multidisciplinary Chemistry>Polymer Materials Science. ICR  
annual report 2020, 27: 36-37

ISSUE DATE:

2020

URL:

<http://hdl.handle.net/2433/262847>

RIGHT:

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# Division of Multidisciplinary Chemistry – Polymer Materials Science –

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



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## 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    Polymer Properties  
Self Assembly    Softmatter  
Hierarchical Structure

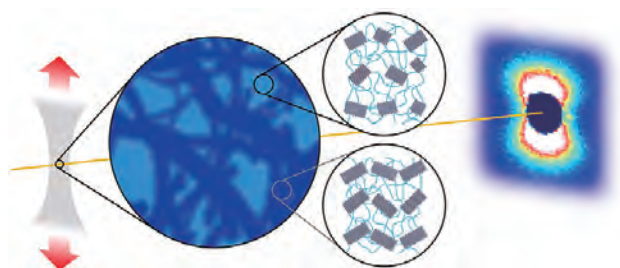


## Selected Publications

Kishimoto, M.; Mita, K.; Ogawa, H.; Takenaka, M., Effect of Submicron Structures on the Mechanical Behavior of Polyethylene, *Macromolecules*, **53**, 9097-9107 (2020).  
Ogawa, H.; Ono, S.; Nishikawa, Y.; Fujiwara, A.; Kabe, T.; Takenaka, M., Improving Grazing-incidence Small-angle X-ray Scattering-computed Tomography Images by Total Variation Minimization, *J. Appl. Cryst.*, **53**, 140-147 (2020).  
Okamoto, M.; Mita, K.; Uekusa, T.; Takenaka, M.; Shibayama, M., Development of Elastic Recovering 4-methyl-1-pentene/propylene Copolymer, *Polymer*, **191**, [122269-1]-[122269-10] (2020).  
Nishitsuji, S.; Watanabe, Y.; Takebe, T.; Fujii, N.; Okano, M.; Takenaka, M., X-ray Scattering Study on the Changes in the Morphology of Low-modulus Polypropylene Under Cyclic Uniaxial Elongation, *Polym. J.*, **5**, 279-287 (2020).

## Effect of Submicron Structures on the Mechanical Behavior of Polyethylene

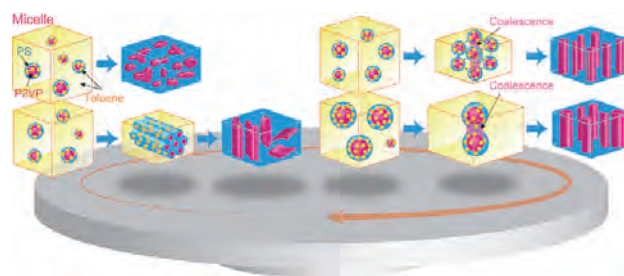
We investigated changes in the hierarchical structures of polyethylene (PE) during tensile testing by means of time-resolved ultra small-angle scattering (USAXS), small-angle, and wide-angle X-ray scattering. We discovered the enhancement of density fluctuation on the submicron scale by USAXS, which led to the generation of voids and necking. The spatial inhomogeneity of the stress fields associated with density or crystallinity fluctuation on the submicron scale induced the inhomogeneous flow during stretching. In other words, the change in the higher order structure than in the lamellar structure dominated the mechanical properties of PE. The enhancement of the fluctuation in linear low-density polyethylene (LLDPE) was smaller than that in high-density polyethylene (HDPE). Mechanical melting in the LLDPE suppressed the inhomogeneous flow and delayed the generation of voids and necking. As a result, the LLDPE exhibited two yield points on a S-S curve, while the HDPE exhibited one yield point. We believe that these results support the universality of the viscoelastic effect, which has been proposed to explain the fracture mechanisms of other systems such as semi-dilute polymer solutions and glassy materials.



**Figure 1.** Schematic illustrations of the changes in the hierarchical structures in the PE during stretching.

## Molecular Weight Effect on the Transition Process of Symmetric PS-*b*-P2VP during Spin-Coating

We studied the transition behavior in symmetric poly(styrene-*b*-2-vinyl pyridine) (PS-*b*-P2VP) with different molecular weights during spin-coating from a toluene solution by using grazing-incidence small-angle X-ray scattering (GISAXS). For the lowest molecular weight condition used here (the number-average molecular weight,  $M_n$ , was 16,500), the disordered micelles transitioned into disordered structures during evaporation. When  $M_n = 50,000$ , the micelles transitioned into hexagonally packed cylindrical structures parallel to the substrate and then into lamellar structures. The effect of selective solvent evaporation on the transition process became significant when  $M_n$  was larger than 84,000. For  $M_n = 84,000$  and 199,000, the micelles first transitioned into spheres on the body-centered cubic lattice (BCC), where the BCC (110) plane was aligned perpendicular to the substrate. Then, the spheres coalesced into loosely packed cylindrical structures. The convection effect of the solvent caused this coalescence, and vitrification prohibited continued transitioning into the lamellar structures from the cylindrical structures. PS-*b*-P2VP with  $M_n = 428,000$  self-assembled into loosely packed cylindrical structures perpendicular to the substrate; thin films were formed after the transition from micelles into BCC structures. However, the BCC (110) plane did become aligned perpendicular to the substrate because the high viscosity prevented alignment due to convection during the solvent evaporation.



**Figure 2.** Schematic representation of the structural formation of PS-*b*-P2VP with molecular weights in the spin-coating process.