Division of Multidisciplinary Chemistry
- Molecular Rheology -

http://rheology.minority.jp/en/

Prof
WATANABE, Hiroshi
(D Sc)

Assoc Prof
MASUBUCHI, Yuichi
(D Eng)

Assist Prof
MATSUMIYA, Yumi
(D Eng)

Techn
OKADA, Shinichi

Students

TAKAHASHI, Hideaki (D2)	SATO, Hiroki (M2)	MISHIMA, Eri (M1)
CHEN, Quan (D1)	NAOI, Azusa (M2)	KAWAKITA, Hiroshi (M1)
FURUICHI, Kenji (D1)	HORIO, Kazushi (M2)	KINOSHITA, Taro (M1)
IWASHIGE, Tomohito (M2)	SUZUKI, Takeshi (M1)	MORIYA, Motoaki (M1)
IWAMOTO, Tatsuya (M2)	TANAKA, Satoshi (M1)	UNO, Akiko (UG)

Visitor

Dr PONNUSAMY, Karaichelvi National Institute of Technology, India, 23 April–22 May 2007

Scope of Research

The molecular origin of various rheological properties of material is studied. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluid while heterogeneous polymeric systems exhibit plasticity in addition to these features. For a basic understanding of the features, the molecular motion and structures of various scales are studied for polymeric systems in deformed state. Measurements are performed of rheological properties with various rheometers, of isochronal molecular orientation with flow birefringence, and of auto-correlation of the orientation with dynamic dielectric spectroscopy.

Research Activities (Year 2007)

Publications

Watanabe H, Matsumiya Y, Sawada T, Iwamoto T: Rheological and Dielectric Behavior of Dipole-Inverted (SIS)p-type Multiblock Copolymers: Estimates of Bridge/Loop Fractions for Respective I Blocks and Effect of Loops on High Extensibility of Bridges, *Macromolecules*, **40(19)**, 6885-6897 (2007).

Watanabe H, Matsumiya Y, Takada J, Sasaki H, Matsushima Y, Kuriyama A, Inoue T, Ahn K H, Yu W, Krishnamoorti R: Viscoelastic and Dielectric Behavior of a Polyisoprene/Poly(4-tert-butyl styrene) Miscible Blend, *Macromolecules*, **40(15)**, 5389-5399 (2007).

Matsumiya Y, Matsumoto M, Watanabe H, Kanaya T, Takahashi Y: Nonlinear Rheology and Structural Changes of (BS)n Multiblock Copolymers under Shear Flow, *Macromolecules*, **40**, 3724-3732 (2007).

Matsumiya Y, Inoue T, Watanabe H, Kihara S, Ohshima M: Dielectric Behavior of cis-polyisoprene in Carbon Dioxide under High Pressure, *J. Soc. Rheol. Japan*, **35**, 155-161 (2007).

Arai N, Yasuoka K, Masubuchi Y: Spontaneous Self-assembly Process for Threadlike Micelles, *J. Chem. Phys.*, **126 (24)**, 244905-244907 (2007).

Furuichi K, Nonomura C, Masubuchi Y, Ianniruberto G, Greco F, Marrucci G: Primitive Chain Network Simulations of Damping Functions for Shear, Uniaxial, Biaxial and Planar Deformations, *J. Soc. Rheol. Japan*, **35(2)**, 73-77 (2007).

Presentations

Masubuchi Y, "Molecular Rheology in DNA Solutions", Workshop in Ravello, Ravello, Italy, 15 April 2007 (invited).

Masubuchi Y, Ianniruberto G (Univ. Naples), Greco F (CNR-Italy) and Marrucci G (Univ. Naples), "Primitive Chain Network Simulations for Bidisperse Linear Polymers", AES-ATEMA, Montreal, Canada, 9 August 2007 (invited).

Watanabe H, Constraint Release in Star/Star Blends and

Molecular Rheology by Simulation and DNA

Molecular motion is main resource of polymer rheology since conformational entropy is dominant in free energy. Although for several simple cases such as monodisperse linear polymers description of the molecular motion has been established by the Rouse, Zimm and tube models, the polymer dynamics is still an open problem due to huge degree of freedom in material design of polymers with branching, molecular weight, molecular weight distribution, blends, copolymerization, etc., and hence challenges have been being in progress.

An interesting method to investigate the polymer dynamics is fluorescent microscopy with DNA. Although DNA is a rigid polyelectrolyte indicating distinguished characteristics from synthetic polymers, under certain conditions the observed DNA motion is consistent with the dynamics of synthetic polymers. In addition to the conventional analysis on the fluorescent images we have been developing a method to map the molecular configuration by means of a Monte Calro method where the observed fluorescence is converted to an effective potential field as shown in Figure 1.

If the polymer dynamics can be captured in a certain model, simulations would be achieved to predict the polymer dynamics and rheology. We have been developing a multi-body simulation for entangled polymers utilizing our primitive chain network model where the polymer dynamics is calculated in real 3D space similarly to ordinal molecular dynamics simulations and differently from tube theories. Figure 2 shows a typical snapshot and a result of the prediction.

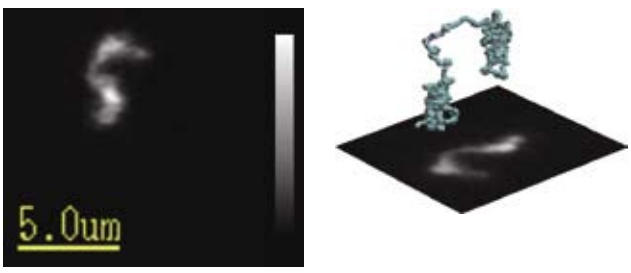

Figure 1. (a) A fluorescent image of a DNA molecule and (b) the constructed polymer configuration.

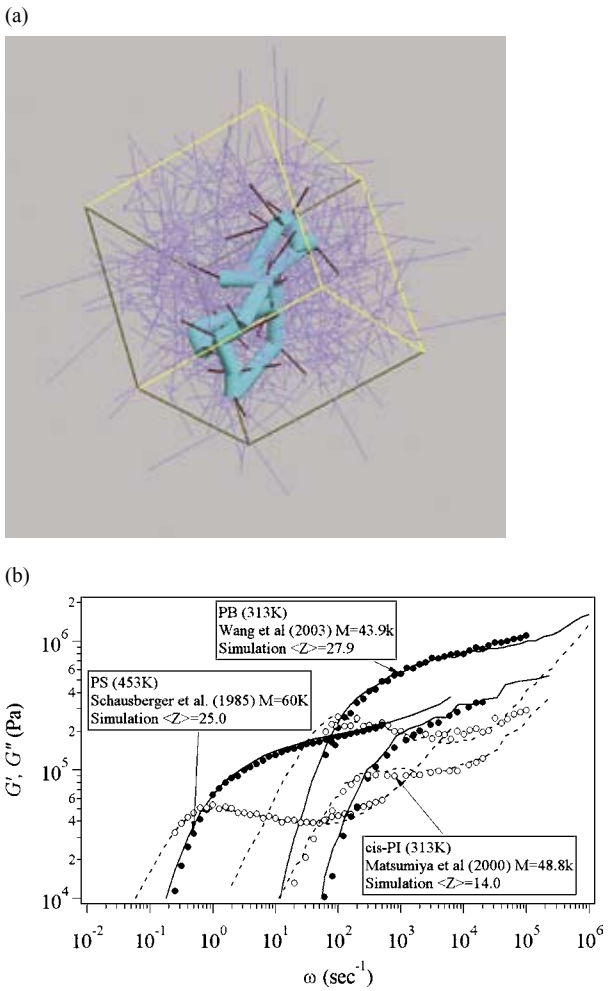

Figure 2. (a) A typical snapshot of the simulation and (b) the prediction of linear viscoelasticity for various polymer melts.

Dynamic Tube Dilation in Monodisperse Star Systems, Rheology of Complex Fluid: Courses and Workshop 2007, 8 July 2007 (invited).

Watanabe H, Rheology and Dynamics of Entangled Polymer Chains: Self-Consistent Coarse-Graining of Length and Time Scales, The 10th pacific Polymer Conference, 4 December 2007 (invited).

Grants

Watanabe H, Creation of Non-equilibrium Soft Matter Physics: Structure and Dynamics of Mesoscopic Systems, Grant-in-Aid for Scientific Research on Priority Areas, 1 October 2006–31 March 2011.

Masubuchi Y, Combined Digital and Analog Molecular Simulation of Polymer Dynamics, Precursory Research for Embryonic Science and Technology, Japan Science and Technology Agency, 1 October 2004–31 March 2008.

Masubuchi Y, Multi-scale Simulations for Soft Matters, Core Research for Evolutional Science and Technology, Japan Science and Technology Agency, 1 October 2006–31 March 2012.

Matsumiya Y, Dynamics of Ionic Liquids in Polymer Networks, Grant-in-Aid for Young Scientists (B), 1 April 2007–31 March 2009.