

OCTA

Integrated simulation system for soft materials

APPLICATION REPORT

Nagoya University, Doi Project
Research and Development of the Platform
for Designing High Functional Materials

Computer Aided Materials Design Joint Research
Japan Chemical Innovation Institute (JCII)

FEB. 22 2002

Acknowledgment

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Contents

No.	Title
EAR1-001-03	Prediction of rheological properties of linear polymers.
EAR1-002-01	Analysis of the interfaces of the phase separated structures in ultra thin polymer films.
EAR1-003-01	Prediction of electro-rheological effect of binary polymer blends.
EAR1-004-02	Analysis of polymer melts confined between nanoscale gap.
EAR1-005-01	Molecular dynamics study of poly (ethylene oxide) (PEO) containing LiI salt.
EAR1-006-01	Molecular dynamics simulation of alkane crystallization processes. - Effect of short-chain branching -
EAR2-007-03	Micro- and macro-phase separations of AB block copolymer / A and B homopolymers blends.
EAR2-011-02	Prediction of elastic properties of thermoplastic elastomer.
EAR2-012-02	Simulation study of phase separated structures of blends of long and short block copolymers.
EAR2-013-02	Prediction of the domain structure in ternary polymer blend.
EAR2-014-02	Inspection of the domain structure for actual polymer blends.
EAR2-015-01	Parameterization of the Gay-Bern potential for nCB and molecular dynamics simulation of 5CB.
EAR2-016-02	Derivation of coarse-grained potential for polyethylene.
EAR2-017-02	Interaction between polymer grafted walls.
EAR2-018-01	The simulation of the shrinking process of NIPA gels. - The stress-diffusion coupling model for dynamics of gels -
EAR3-019-01	An analysis of loop/bridge ratio of triblock copolymer.
EAR3-020-02	Study of the relation between χ parameter and Lennard-Jones parameter.
EAR3-021-02	Study of interface strength of polymer blend.
EAR3-022-01	The influence of short chain branching on polymer crystallization process. - Molecular dynamics simulation -
EAR3-023-01	Estimation of optical transmittance of polymer materials using spherulites growth model.
EAR3-024-01	Mechanical properties of topological gel. - Molecular dynamics simulation -
EAR3-025-02	Analysis of the structure of polymer blend system.
EAR3-026-01	Calculation of elastic modulus of polymer blend.
EAR3-027-01	Prediction of strain energy on photo-resist patterns.
EAR3-028-01	Prediction of the uniaxial elongational viscosity of polydisperse polystyrene(PS) melt.
EAR3-029-01	Shear viscosity of star polymers.
EAR4-030-02	Prediction of interfacial tension of an A/B polymer blend.
EAR4-031-02	Study of interface strength of polymer blend with polydispersity.

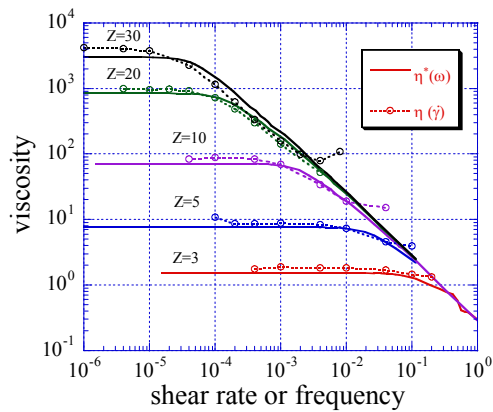
Title	Prediction of rheological properties of linear polymers.
Researchers	Hiroyasu Tasaki, Jyun-ichi Takimoto and Masao Doi
Purpose of this study	Development and research of a new simulation method for the prediction of the rheological properties of linear polymers with arbitrary molecular weight distributions.
System (Material)	Linear monodisperse or polydisperse polymer system (PS, PE, ... etc.)
Program (including analysis)	PASTA
Method & Some important input parameters	<p>(Method) Stochastic simulation based on the slip-link model, takes account of contour length fluctuation, reptation and constraint renewal (constraint release or constraint creation).</p> <p>(Inputs) Molecular Weight : $Z = M / M_e$ (M : Molecular weight Me : Entanglement molecular weight) Numbers of polymer : n Some set of Z and n is available.</p>
Advance & Problem	<p>(Advance) - Applications to the linear polymers have shown good agreement with experiments(shear flow, uniaxial elongational flow, stress relaxation in step strain shear experiment, ...etc.)</p> <p>(Problem) - Prediction of the rheological properties of polymers with extremely broad molecular weight distributions and long chain branching structures.</p>
References	<p>[Manuscript]</p> <p>[Presentation at conferences (Meetings)] 47th Rheology tohronkai, p.263 (1999)</p>
KeyWords (in English)	Rheology, tube model, entanglement, contour length fluctuation, constraint release, viscosity, viscoelasticity, Cox-Merz rule, Doi-Edwards, linear, monodisperse, binary blend, shear modulus, shear flow, elongational flow

Results (Remarks)

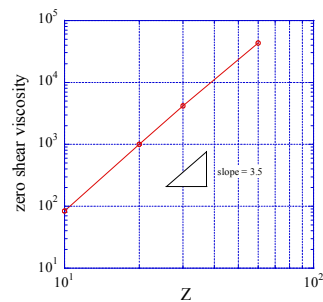
Output : Stress

Shear viscosity, uniaxial elongational viscosity,
relaxation modulus and linear viscoelastic functions($G'(\omega)$, $G''(\omega)$,
 $\eta^*(\omega)$) ... etc.

[Example of analysis]

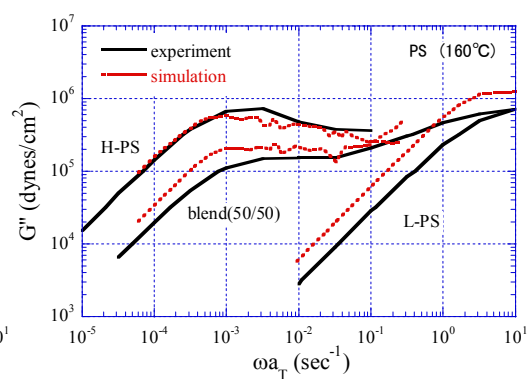
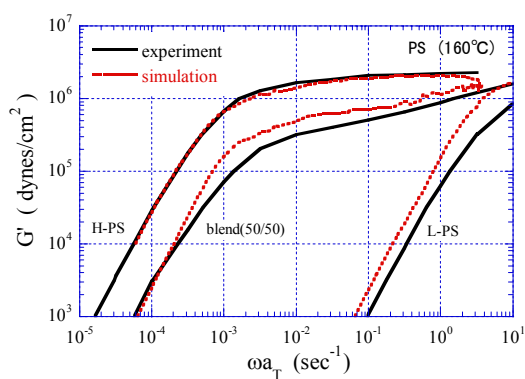


Cox-Merz rule



Molecular weight dependency of
zero shear viscosity (3.5th power of Z)

	Experiment	Simulation
H-PS	Mw 581,000	Z32
L-PS	Mw 58,700	Z 3 (=Mw/Me)



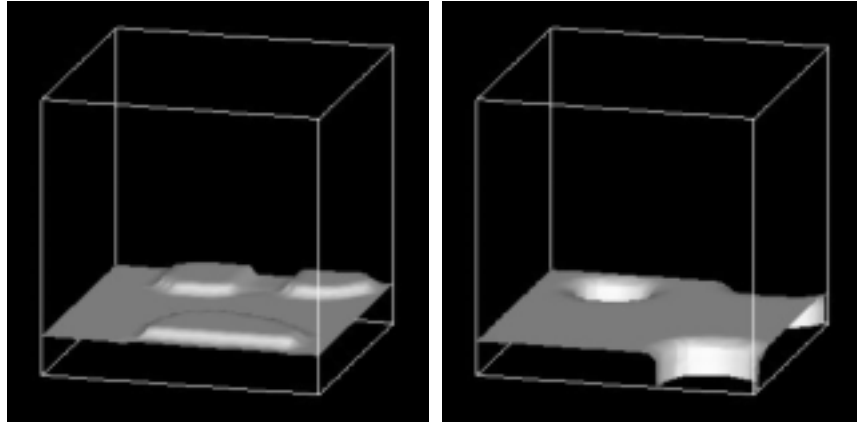
Comparison of simulation to experiment
in storage moduli(G') and loss moduli

Title	Analysis of the interfaces of the phase separated structures in ultra thin polymer films
Researchers	Hiroshi Morita, Toshihiro Kawakatsu, and Masao Doi
Purpose of this study	Development and research of the method to analyze the phase separated structures of ultra thin polymer films which would be constructed by spin cast.
System (Material)	Homopolymer blend system (target : PS/PVME)
Program (including analysis)	MesoSimulator990827 version
Method & Some important input parameters	<p>(Method) Dynamic mean field density functional method (Scheutjens-Fleer model + Cahn-Hilliard eq.)</p> <p>(Inputs) Polymer Polymer A (corresponds to PS), polymer B (corresponds to PVME), Void(for air layer). volume fraction, length, and species for each polymer must be set. Parameters of interactions Potential from wall (like χ parameter) Segment-segment interaction parameter(χ)</p>
Advance & Problem	<p>(Advance) - We can simulate the surface roughening structure at free surface of thin films consistently with experiments. (Experimental: Macromolecules, 28, 934, (1995)) - We can simulate the cylindrical phase separated structure in thin films under the surface roughening conditions. (Experimental: Macromolecules, 29, 3232, (1996)) - Construction of the phase diagrams of surface roughening conditions using the equilibrium of interfacial tension was succeeded. - The obtained film thickness by our simulation was from 10 nm to 20 nm.(using $(R_g)^2 = Nb^2$)</p> <p>(Problem) - Quantitative correspondence between the simulation and experiments. (including χ parameters)</p>
References	<p>[Manuscript]</p> <p>[Presentation at conferences (Meetings)] International Polymer Conference99(at Yokohama 1999.10)</p>
KeyWords (in English)	Thin film, surface roughening, interfacial tension, phase diagram, cylindrical structure, mean field, dynamic density functional method, neumann triangle

Results (Remarks)

Output : Density field and it's time dependent.

Analysis : Phase separation dynamics.



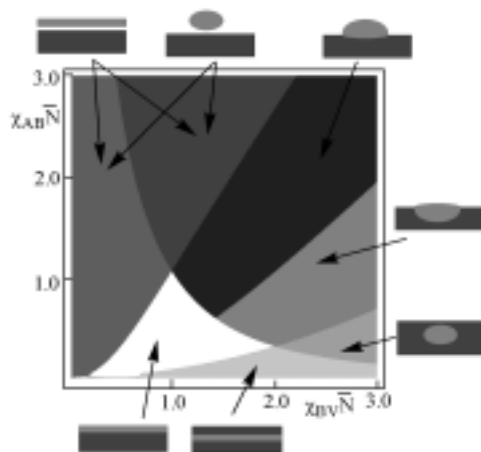
Figures: Interfacial structures of thin polymer blend films

Left Figure: Computational results of the surface roughening structure at free surface (at the case of roughening) .

Right Figure: Computational results of the cylindrical phase separated structure. (interfacial structure of polymer A)

[Example of analysis]

Phase diagram for the surface roughening at free surface.

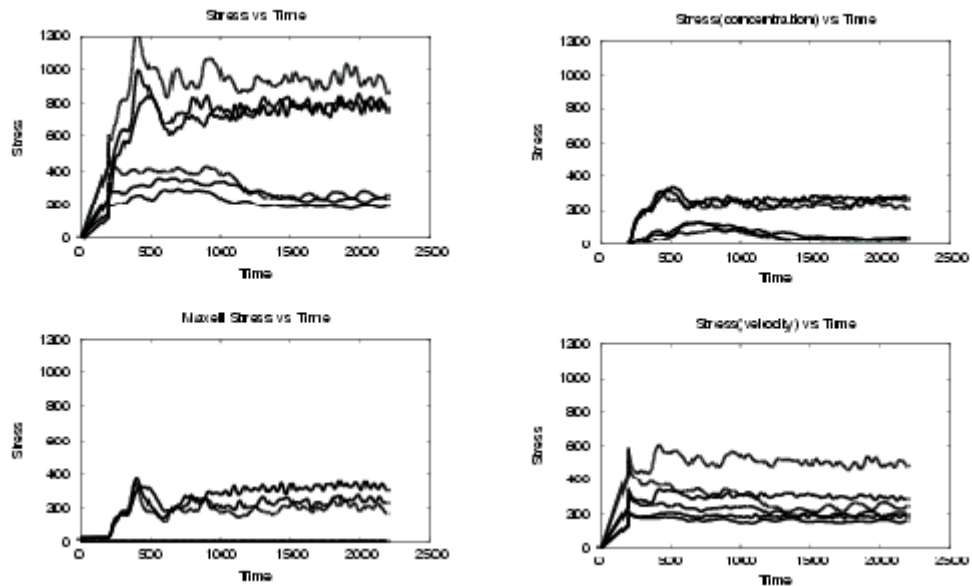


Title	Prediction of electro-rheological effect of binary polymer blends.
Researchers	Takashi Taniguchi
Purpose of this study	Prediction of morphologies of the domain structure and rheological properties of binary polymer blends under shear flows and external electric fields.
System (Material)	Homopolymer blend system (target : DMS/UPPG)
Program (including analysis)	MUFFIN ver 1.0 Visualization, graph of stress-time functions.
Method & Some important input parameters	(Method) Simulator for Dielectric binary fluid 1. Navier stokes equation 2. Maxwell equation 3. Cahn-Hillard equation including hydrodynamic effect (Inputs) Shear Rate, dielectric constant and viscosity for each component, χ parameter, segment lengths, strength of the imposed electric field
Advance & Problem	(Advance) (Problem)
References	[Manuscript] [Presentation at conferences (Meetings)] The 3 rd Tohwa University International Conference on Statistical Physics (Tohwa StatPhys '99 Nov, 8-12) The 47 th Rheological Society of Japan Meeting (1999.10) Meeting of ER-study group(at Yamagata Univ. 1999.10)
KeyWords (in English)	Rheology, Electro-rheological effect, dielectric constant, polymer blend, Electric field, shear flow, oscillatory flow, Cahn-Hillard equation, Maxwell stress, Maxwell equation.

Results (Remarks)

Output:

Time development of shear stress for various electric field strength.



Figures: Total stress versus time (top left) ,
Stress coming from surface tension of domain boundaries (top right),
Maxwell stress (bottom left) and Newtonian stress (bottom right).

Title	Analysis of polymer melts confined between nanoscale gap
Researchers	Takeshi Aoyagi, Tatsuya Shoji, Fumio Sawa, Hiroo Fukunaga, Jun-ichi Takimoto and Masao Doi
Purpose of this study	To clarify the mechanism of the specific behaviors of polymer melts confined between nanoscale gap, which is observed experimentally.
System (Material)	Poly-isoprene thin film confined between mica plate. (3nm-100nm gap)
Program (including analysis)	COGNAC v1.0, 2.0 Trajectory analysis utility (self diffusion, normal modes etc.)
Method & Some important input parameters	(Method) Coarse-grained molecular dynamics with bead-spring polymer chain model. (Inputs) Bead-spring model: degree of polymerization, number of molecule interaction potential: bead-bead, bead-wall simulation conditions: temperature, density, time step etc.
Advance & Problem	(Advance) The thickness of the surface layer, estimated from the analysis of the static polymer structure, is about 1.0–1.5 times the radius of gyration R_g in the bulk, and is independent of the distance between the walls and the wall–polymer interaction. The relaxation time of the polymers, obtained from the autocorrelation of normal modes, increases with increasing the strength of the wall–polymer interaction and with decreasing the distance between the walls. These wall effects are observed at a distance much larger than R_g . This result is in agreement with the recent dielectric measurements of <i>cis</i> -polyisoprene confined between mica surfaces. (Problem) The result of normal force is not consistent with the previous literature, where repulsive force has been reported for polymer adsorbing walls. A possible reason for this discrepancy is that we used a structureless wall potential, which allows the adsorbed polymers to slide freely along the surface, while real polymers are pinned on the surface.
References	[Manuscript] J.Chem.Phys. 115 (1) 552 (2001) [Presentation at conferences (Meetings)] Polymer preprint Japan, 48 (13), 3562 (1999) 47 th Rheology tohronkai, p265 (1999)
KeyWords (in English)	confined system, isoprene, mica, nanoscale gap, nanorheology, coarse grained molecular dynamics, bead-spring model

Results (Remarks)

<Simulation results>

The component of radius of gyration perpendicular to the wall (Fig.3(a) in ref.) and the relaxation time τ_R (Fig.6 in ref.) as a function of the distance between wall Z .

τ_R slows down around the distance $Z=30\sim 40$ ($1/Z=0.025\sim 0.033$). $\langle Rg^2 \rangle^{1/2}$ of this polymer chain model is about 3.2.

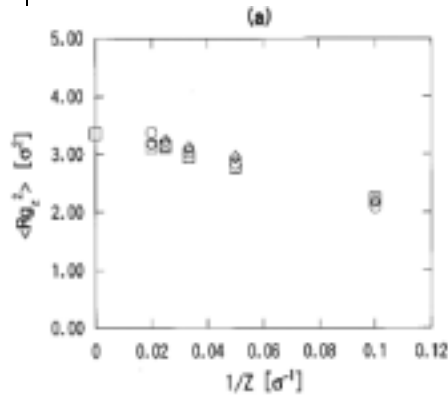


FIG. 3. Component of $\langle R_g^2 \rangle$ as a function of the distance between the walls, Z . (a) Component perpendicular to the wall and (b) component parallel to the wall, plotted vs $1/Z$. The results of the bulk simulation are shown at $1/Z=0$, $\epsilon''=5.0\epsilon$ (circles), $\epsilon''=1.0\epsilon$ (squares), and $\epsilon''=1.0\epsilon$ with a cutoff at 1.0ϵ (diamonds).

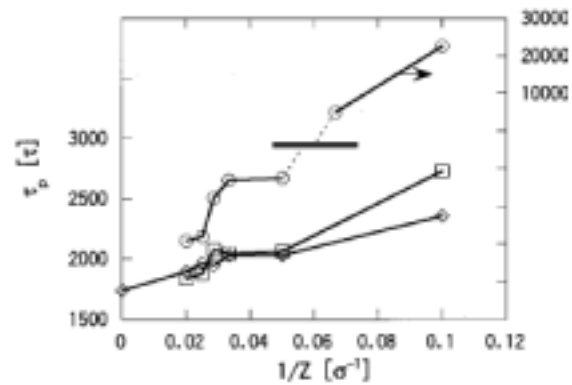


FIG. 6. Relaxation time $\tau_{p=1}$ as a function of Z . The results of the bulk simulation are shown at $1/Z=0$, $\epsilon''=5.0\epsilon$ (circles), $\epsilon''=1.0\epsilon$ (squares), and $\epsilon''=1.0\epsilon$ with the cutoff at 1.0ϵ (diamonds).

<Example of experimental results>

Y.Cho, H.Watanabe and S.Granick, J.Chem.Phys., **110**, 9688 (1999)

Dielectric relaxation of polyisoprene confined between mica plate.

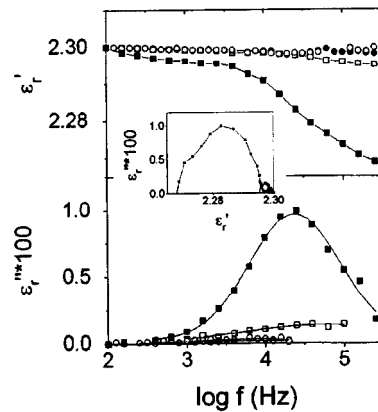


FIG. 7. Comparison of measurements made in parallel-plate geometry concerning spin-coated films of *cis*-polyisoprene ($M_n=6000 \text{ g mol}^{-1}$, $M_w/M_n=1.04$) confined between atomically smooth muscovite mica. The normalized responses in phase with the electric field [$\epsilon'_r(f)$, the top panel] and 90° out of phase [$\epsilon''_r(f)$, the bottom panel], are plotted against Hertizian frequency, f , after normalization using Eqs. (8) and (9). The data concern films of macroscopic thickness (closed squares), 572 Å thickness (open squares), 285 Å thickness (closed circles), and 64 Å thickness (open circles). Thickness was determined by multiple beam interferometry. The inset shows $\epsilon''_r(f)$ plotted against $\epsilon'_r(f)$, i.e., a Cole-Cole plot.

Title	Molecular dynamics study of poly (ethylene oxide) (PEO) containing LiI salt
Researchers	F. Sawa, T. Aoyagi, T. Tatsuya, H. Fukunaga, J. Takimoto and Masao Doi
Purpose of this study	To get an insight into the transport mechanism of Li ion in PEO. Application: Li ion battery
System (Material)	PEO and LiI salt.
Program (including analysis)	COGNAC v1.3
Method & Some important input parameters	<p>(Method) Molecular dynamics simulation modeled by united atom model with empirical potentials. To calculate coulomb interaction, charges are sited at non-bonding interaction sites as point charges.</p> <p>(Inputs) Degree of polymerization and number of molecule. Bonding interaction (bond, angle and torsion potentials were used) and non-bonding interaction (OPLS). Temperature was set at 363K.</p>
Advance & Problem	<p>(Advance) -It was observed that Li⁺ in PEO melts has two characteristic modes of motion. -It was also observed that Li⁺ and I⁻ form ion cluster with increasing salt concentration consistently with experiments.</p> <p>(Problem) -Tremendous additional calculation is required for quantitative evaluation of diffusion coefficient deriving ionic conductivity.</p>
References	<p>[Manuscript] Progress of Theoretical Physics Supplement No. 138 (2000) (Accepted)</p> <p>[Presentation at conferences (Meetings)] The 5th International Conference on Computational Physics (ICCP5 (1999)) CMD18-European Physical Society (2000) Polymer Preprints Japan (2000)</p>
KeyWords (in English)	MD, PEO, Li, LiI, conductivity, OPLS, ewald, united atom model

Results (Remarks)

Output:

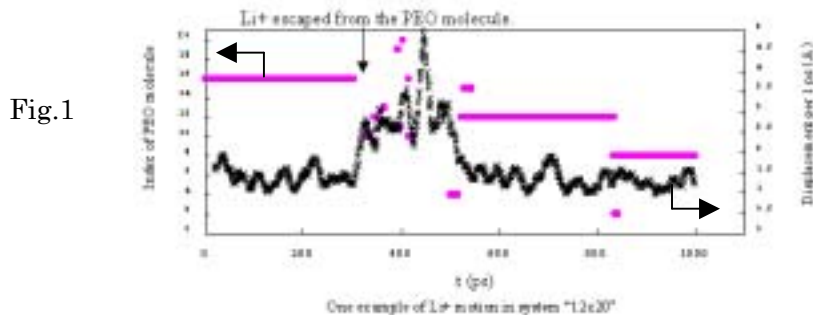


Fig.1)

One example of Li^+ motion in the system. (Degree of polymerization : 12)

The circles indicate the index number of PEO molecule with which this Li^+ forms a complex, and the cross symbols indicate the displacement of the Li^+ per 1 ps.

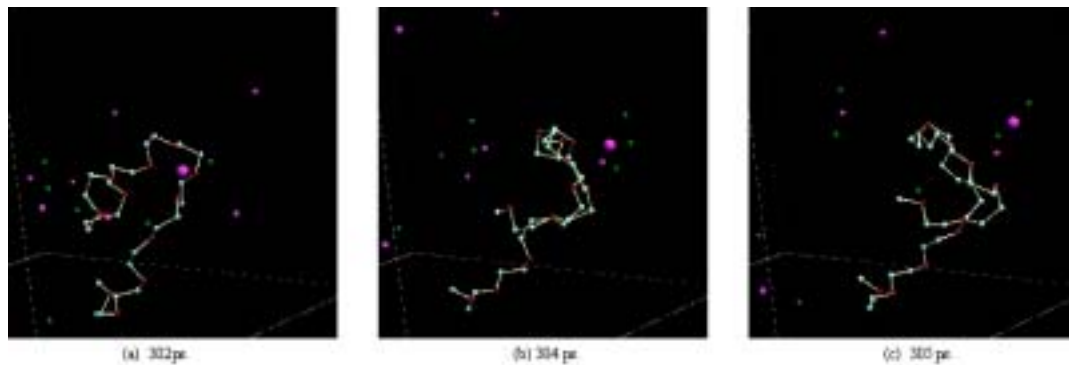


Fig.2

Fig.2)

The snapshots in each time step. The Li^+ (referred at Fig.1) is drawn as large balls for visual.

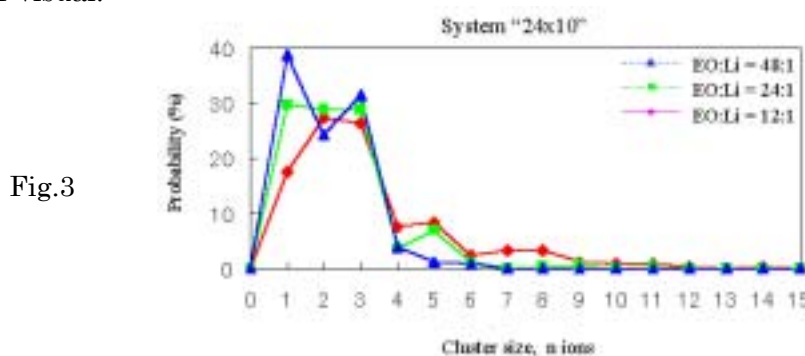


Fig.3)

Size distribution of the ionic cluster for various salt concentrations. The larger ion cluster (consists of Li^+ and I^-) was formed with increasing salt concentration (Degree of polymerization : 24).

Title	Molecular dynamics simulation of alkane crystallization processes: - Effect of short-chain branching-
Researchers	T. Shoji, T. Aoyagi, H. Fukunaga, F. Sawa, J. Takimoto and M. Doi
Purpose of this study	The purpose of this study is to make clear the effects of short-chain branching in primary nucleation and growth processes of polymer by using molecular dynamics(MD) simulation method.
System (Material)	linear alkane: n-decane short-branched alkane 1: 2methyl-nonane short-branched alkane 2: 5methyl-nonane
Program (including analysis)	Program: COGNAC v1.3 Analysis: trajectory analyzer (order parameter, conformation analysis)
Method & Some important input parameters	(Method) Molecular dynamics simulation modeled by united atom model with empirical potentials. (Inputs) polymer architecture(degree of polymerization) united atom models potentials(bond ,bending, torsion, non-bond) calculation conditions(temperature, pressure, density, time steps)
Advance & Problem	(Advance) Ordered crystal structure was not observed for the branched chains by quenching to the temperature where the linear chain formed crystal. The suppression of the crystallization due to the branching was enhanced when the branching was located close to the middle of the backbone. (Problem) Observation of crystallization process for linear / branched chain's blend system could give useful information on the effect of the branching structure.
References	[Manuscript] Submitted/Accepted(/) Polymer Preprints Japan, Vol.48, No.14, 3955 (1999) 219 th ACS National Meeting(2000) International Symposium on Platform for Designing High Functional Materials(2000)
KeyWords (in English)	molecular dynamics(MD) simulation , the united atom model , short-chain branching , crystallization , the nucleation and growth n-decane, 2methyl-nonane, 5methyl-nonane

Results (Remarks)

Output:

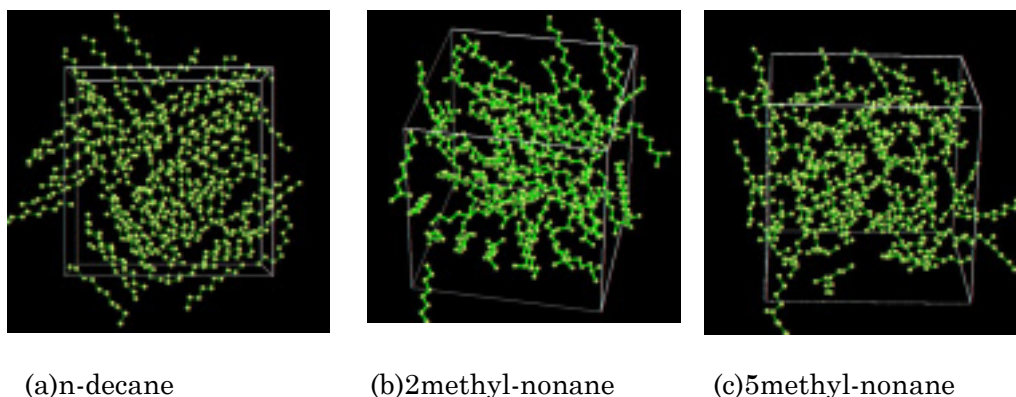


Fig.1 The snapshots of the different chains systems at 11 nano seconds after quenching to 180K from 420K. The n-decane chains (a) show ordered structure and create several of crystal domains. On the other hand, 2methyl-nonane chains (b) made the partial ordered conformations, but most of chains are still random. 5methyl-nonane chains (c) have no ordering structures.

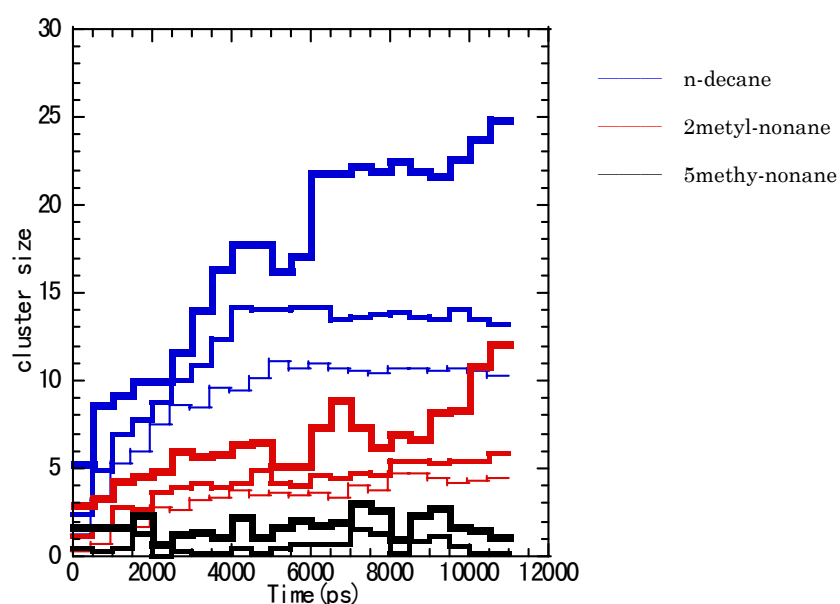


Fig.2 The crystal domain cluster sizes averaged each 500ps vs time. Thick lines represent maximum crystal domain cluster sizes, the middle thick lines the second largest, and the thin lines the third largest. The clusters of n-decane were created at once and grow stably with time until saturating. The clusters of 2methyl-nonane were created but the growth rates were slower. In the case of 5methyl-nonane, The cluster was hardly created. It is obvious that the positions of short-chain branching have influence and strongly hinder nucleation and growth in primary crystallization processes. The effect is prominent when the branching was located around the middle of the backbone.

Title	Micro- and macro-phase separations of AB block copolymer / A and B homopolymers blends
Researchers	Hiroya Kodama, Shigeyuki Komura and Keizo Tamura
Purpose of this study	The aim of this study is to see the effect of molecular weight of individual components on internal structures formed by phase-separated interfaces, where block copolymers accumulate. Origin of polymeric microemulsion structures observed by Bates et al. is also of interest.
System (Material)	diPE-PEP/PE/PEP blends. F. Bates, et al., Phys. Rev. Lett. 79 (1997) 849.
Program (including analysis)	a tentative SCF program(equivalent to SUSHI)
Method & Some important input parameters	(Method) Numerical calculations based on a self-consistent mean-field method. Characteristic length of structures and free energy profiles are analyzed. (Input parameters) chain length of block copolymer and homopolymers χ parameter composition
Advance & Problem	(Advance) Equilibrium micro- and macro-phase separated structures of blends of AB block copolymer and A and B homopolymers are studied using a self-consistent field theory by means of numerical calculations. It has been shown that block copolymer brush formed at AB interfaces becomes dry as homopolymers become longer relative to the block copolymers. In the case that the homopolymers are longer than block copolymers, three-phase coexistence among lamellar, A-rich and B-rich homogeneous phases is observed. Analysis of the free energy profiles in extremely swollen lamellar phase reveals marginal stability of such periodic structures against fluctuations of interfacial separations. (Problem) Stability of polymeric microemulsion can not be discussed, because the fluctuation effect of interfacial configurations is neglected in ordinary SCF treatment.
References	[Manuscript] Accepted (2000/10/25) H. Kodama, S. Komura and T. Tamura, <i>Europhys. Lett.</i> 53 (2001) 46 [Presentation] 1999/11/8-12 Tohwa StatPhys'99, Japan
KeyWords (in English)	mean-field theory, ternary blend, block copolymers, phase separation, microemulsions, lamellar phase

Results (Remarks)

[Inputs]

A homopolymers: chain length N_A , monomer volume fraction Φ_A

B homopolymers: chain length N_B , monomer volume fraction Φ_B

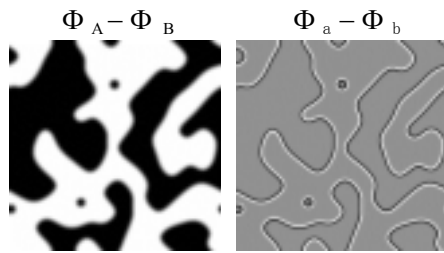
Symmetric AB diblock copolymers: chain length N_{AB} ,
monomer volume fractions: A block; Φ_a , B block; Φ_b

χ -parameter between A and B
volume fraction

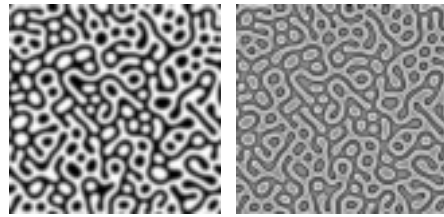
A, B homopolymer; 1:1, A block; θ

[Results]

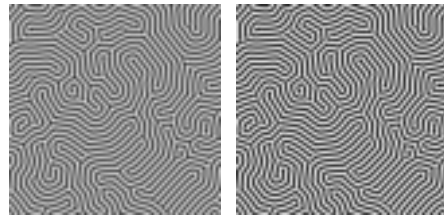
monomer volume fraction profiles



$\theta = 0.1$

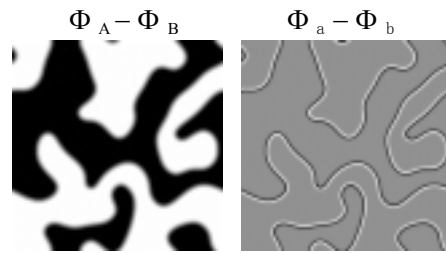


$\theta = 0.4$

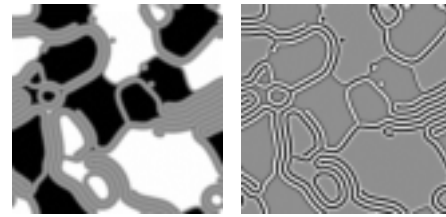


$\theta = 0.9$

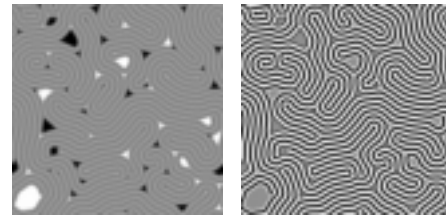
$N_A=N_B=4, N_{AB}=8, \chi=2$



$\theta = 0.1$



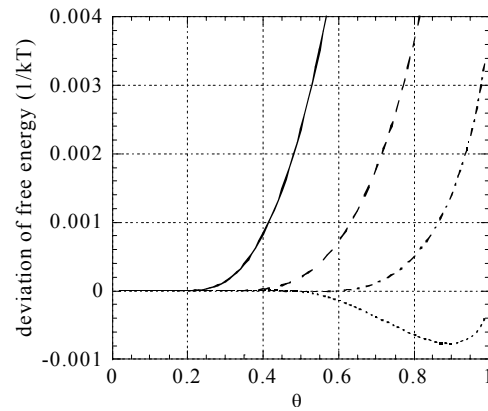
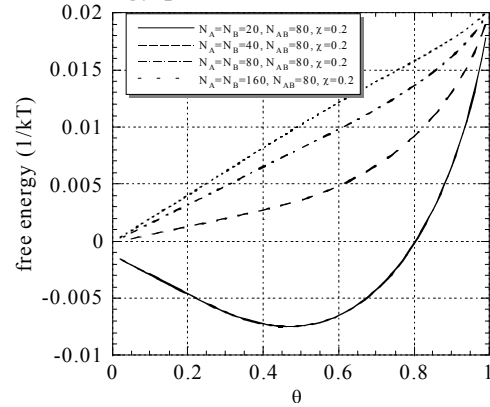
$\theta = 0.4$



$\theta = 0.9$

$N_A=N_B=16, N_{AB}=8, \chi=2$

free energy profiles



Title	Prediction of elastic properties of thermoplastic elastomer
Researchers	Takeshi Aoyagi, Jun-ichi Takimoto, Masao Doi
Purpose of this study	Prediction of elastic behaviors of thermoplastic elastomer with micro domain structure. Development of an efficient algorithm for generating initial structure of phase separated polymer melts.
System (Material)	Thermoplastic elastomer Block copolymer consisting hard and soft segments. (i.e. Styrene-Butadiene-Styrene, Polyurethane)
Program (including analysis)	COGNAC v3 SUSHI 3
Method & Some important Input parameters	(Method) 1. Generate initial configuration based on the distribution of volume fraction obtained by SUSI calculation with density biased potential. 2. Elongation unit cell during MD simulation (Inputs) 1. Polymer architecture (i.e. A3B24A3 triblock) 2. χ parameter 3. Interaction parameter for bead-spring model
Advance & Problem	(Advance) - Initial chain configurations, which have micro phase separated structure, are generated efficiently. - The elastic properties of thermoplastic elastomer are reproduced using coarse-grained molecular dynamics simulation. (Future work) - Application to realistic materials. - Study a systematic way to determine parameters (χ parameter, interaction parameter for MD etc.) and chain architecture to reproduce mechanical properties of real materials quantitatively.
References	[Presentation at conferences (Meetings)] MRS 2000 spring meeting (San Francisco) Abstracts p260 Polymer preprint Japan 49 (3), 443 (2000)
KeyWords (in English)	thermoplastic elastomer, coarse grained molecular dynamics, dynamics density functional , microdomain

Results (Remarks)

Model: A3B24A3 triblock copolymer

$$\chi_{AB} = 1.8$$

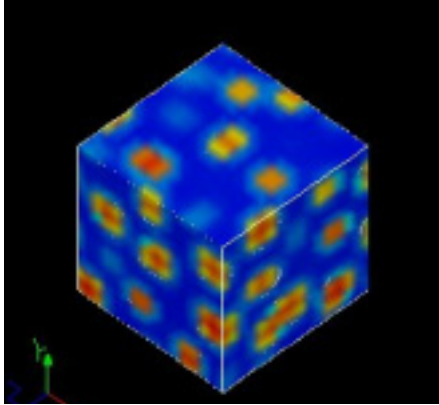


Figure 1 Density distribution by dynamics density functional calculation

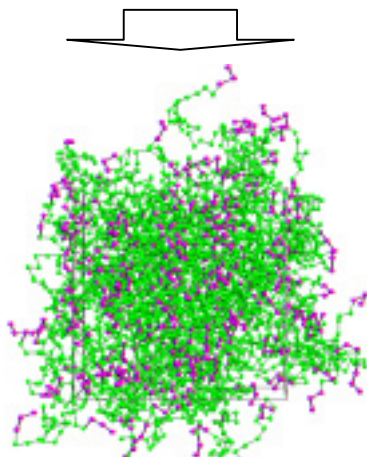


Figure 2 Initial chain configuration

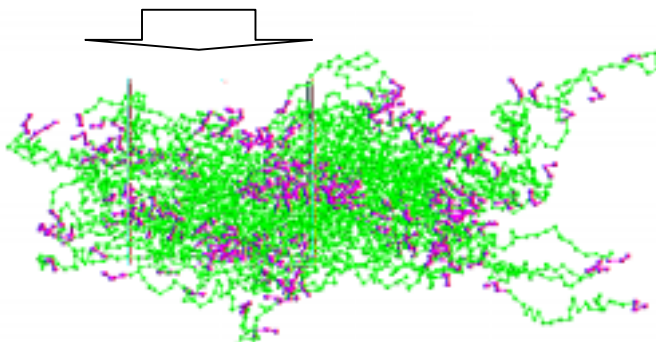


Figure 3 Elongated chain structure

Initial polymer chain configuration (Figure 2) is generated from density distribution, which is obtained from dynamics density functional calculation (Figure 1). Coarse grained molecular dynamics simulation with simple elongation is performed using micro phase separated initial structure. Figure 3 shows elongated chain structure and Figure 4 shows stress-strain curve. Comparing multiphase (Domain) and random initial structure, we found clear effect of pseudo network structure of micro domain structure for rubber elasticity.

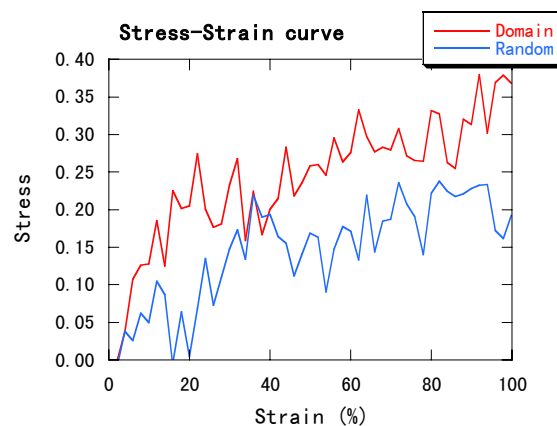


Figure 4 Stress-strain curve by coarse-grained molecular dynamics simulation

Title	Simulation study of phase separated structures of blends of long and short block copolymers
Researchers	Hiroshi Morita, Toshihiro Kawakatsu, Masao Doi, Daisuke Yamaguchi, Mikihiro Takenaka, and Takeji Hashimoto
Purpose of this study	Reproduction of the phase separated structures obtained by experiments. Analysis of the competition of the process between micro and macro phase separation.
System (Material)	Long A-B/ short A-B blend. (A-B corresponds to PS-PI in experiments.)
Program (including analysis)	MesoSimulator990827version
Method & Some important input parameters	<p>(Method) Dynamic mean field density functional method (Scheutjens - Fleer model + Cahn - Hilliard eq.)</p> <p>(Inputs) Polymer Polymer A (corresponds to PS), Polymer B (corresponds to PVME), Void(for air layer), volume fraction, length, and species for each polymer must be set. Parameters of interactions potential from wall (like χ parameter) segment-segment interaction parameter(χ)</p>
Advance & Problem	<p>(Advance) We succeeded to reproduce several phase-separated structures observed in experiments. Furthermore, we can calculate the macro phase separated structures. Scattering function analysis was also performed.</p> <p>(Problem) We have strict restriction on the unit cell dimension to 2^n to obtain scattering functions. This restriction causes difficulty to identify some of phase separated structures.</p>
References	<p>[Manuscript] Submitted/Accepted(/)</p> <p>[Presentation at conferences (Meetings)] International symposium of Doi Project.</p>
KeyWords (in English)	Blends of nearly-symmetric long and short block copolymers, macro phase separation, micro phase separation, dynamical process, scattering function, dynamic density functional method

Results (Remarks)

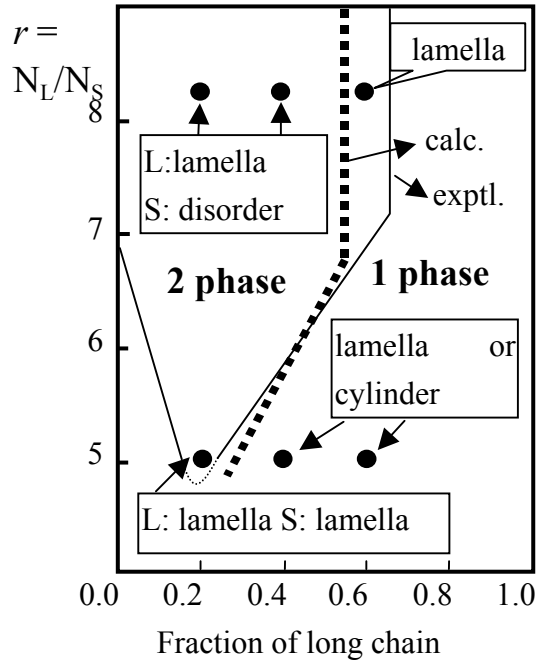


Fig. 1 A phase diagram obtained by experiments and 2D simulations. Dotted and solid lines indicate the boundary between one phase and two phase regions from experiments and calculations, respectively.

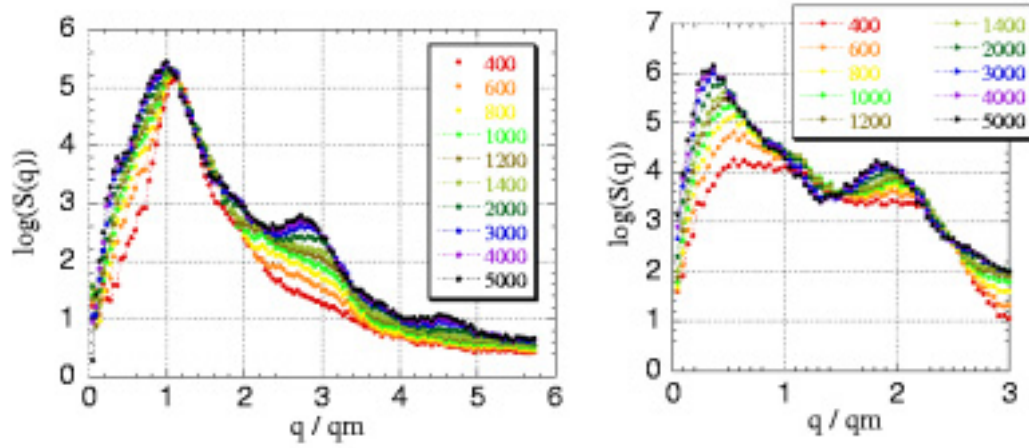
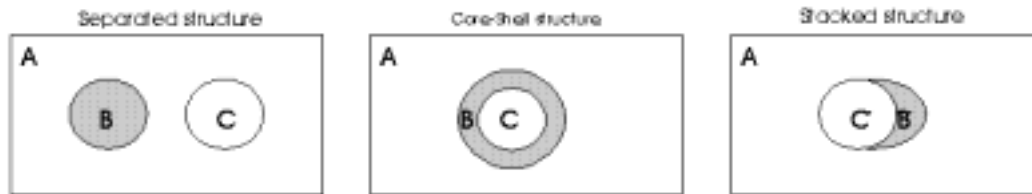


Fig. 2 Circular averaged scattering functions at the time=400, 600, 800, 1000, 1200, 1400, 2000, 3000, 4000, and 5000. (a) and (b) show the scattering functions of $\phi_A - \phi_B$ and $\phi_{Long} - \phi_{Short}$, respectively. The wave number q is scaled by the peak position q at time = 5000.

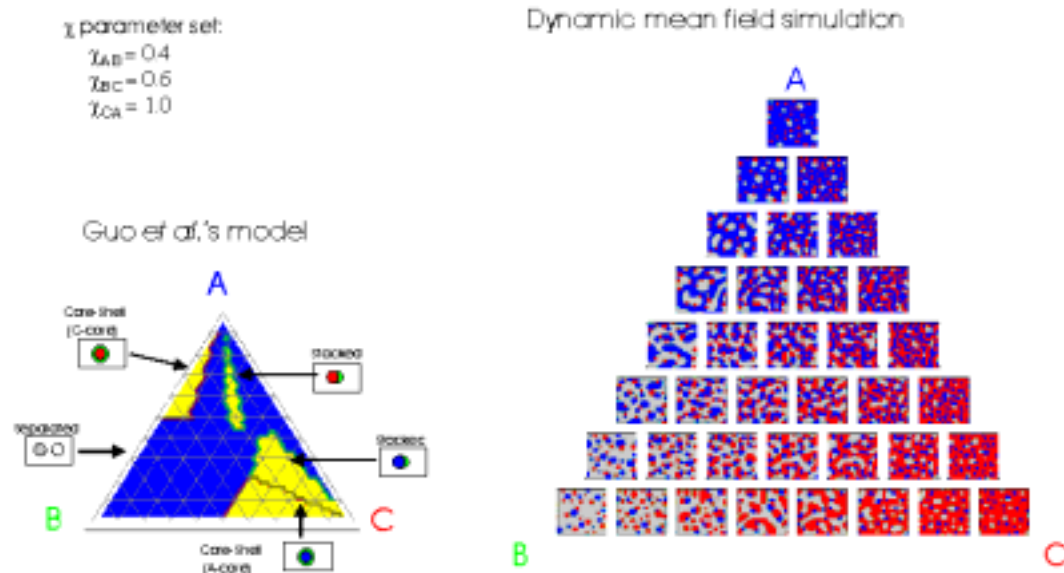
Title	Prediction of the domain structure in ternary polymer blend
Researchers	Shinzi Urashita, Toshibiro Kawakatsu, and Masao Doi
Purpose of this study	To clarify the relationship among the domain structure, the interaction parameters, and the volume fraction of the ternary polymer blends, the Scheutjens-Fleer-Fry mean field calculation for a model system was performed.
System (Material)	The model system of ternary polymer blend
Program (including analysis)	Mesosimulator Release 981127, Release990304 Mesosimulator-Viewer (analysis tool)
Method & Some important input parameters	(Method) the Scheutjens-Fleer-Fry mean field theory, the model of Guo <i>et al.</i> (Input) the interaction parameter, chain length, the blend ratio
Advance & Problem	We reproduce the domain structure change as the change of the interaction parameter and the blend ratio for same set of polymer blends. This results were consistent with the estimation based on Guo <i>et al.</i> model (<i>Polymer</i> , 38 , 785 (1997)).
Reference	[Manuscript] Accepted <i>Prog. Theor. Phys. Suppl.</i> 412, No. 138 (2000) [Presentation] The 5th International Conference on Computational Physics (ICCP5) P2-30 (1999)
KeyWord (in English)	Ternary polymer blend, domain morphology, core-shell structure, dispersed structure, stacked structure, interfacial tension, Guo <i>et al.</i> model

Results (Remarks)

For analysis, the domain structure was classified into three classes: separated, core-shell and stacked structures.



Based on this classification, we obtained the phase diagram of ternary homopolymer blend by using the interfacial energy estimation (Guo model) and the dynamic mean field simulation. The following figures are one of the example for a set of interaction parameters.

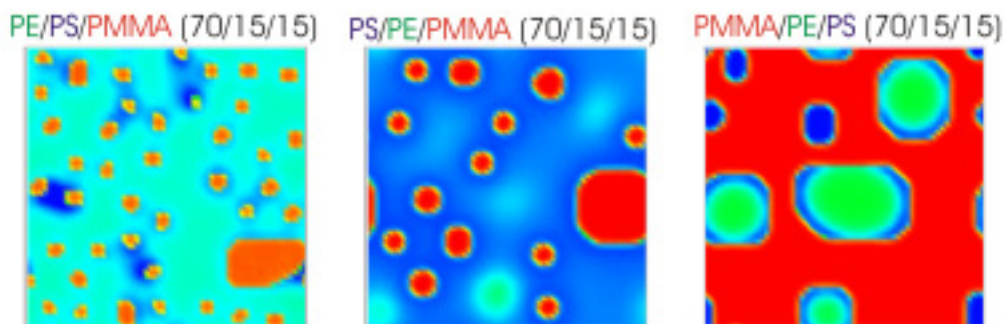


By the Guo *et al.* model, we can reproduce the domain structure near the region of the triangle corner in phase diagram. We should perform the dynamic mean field simulation to predict the domain structure in the other region.

Title	Inspection of the domain structure for actual polymer blends
Researchers	Shinzi Urashita
Purpose of this study	To verify the Scheutjens-Fleer-Fry mean field calculation as the application to the actual polymer system, reproducing the domain structure by using the estimated interaction parameters for actual polymer blends was performed.
System (Material)	Ternary polymer blend Polyethylene / Polystyrene / Poly (methyl methacrylate) blend, Polyethylene / Polypropylene / Polystyrene blend
Program (including analysis)	Mesosimulator Release 981127, Release 990304 Mesosimulator-Viewer (analysis tool)
Method & Some important input parameters	(Method) the Scheutjens-Fleer-Fry mean field theory Hofyzer & van Krevlen's method, Hoy's method (Input) Interaction parameter, chain length, Kuhn length, blend ratio, density
Advance & Problem	Advance: For the estimated system, calculated results were consistent with the experiments. Problem: Verification of the parameters including the interaction parameter is indispensable for quantitative calculation.
Reference	
KeyWord (in English)	Ternary polymer blend, domain morphology, chi-parameter, Hofyzer & van Krevlen's method, Hoy's method, group contribution method

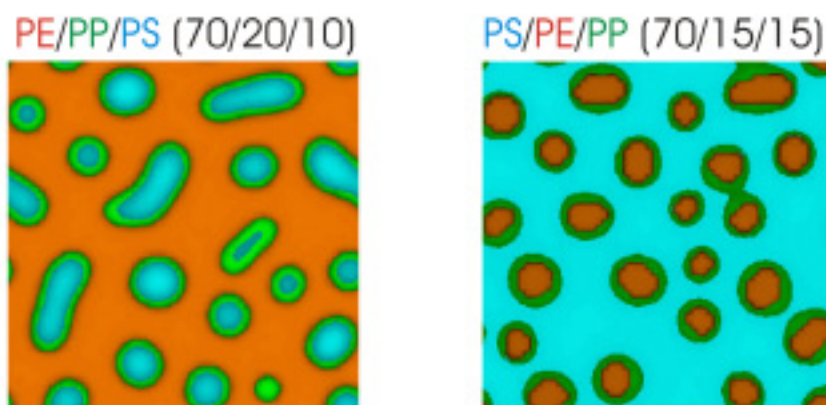
Results (Remarks)

I estimated the domain structure of the polymer blends by the Scheutjens-Fleer-Fry dynamic mean field simulation with the interaction parameters estimated by van Krevelen's method. The following figures are the results of the polyethylene / polystyrene / poly (methyl methacrylate) for various blend ratio.



In the case that polyethylene or poly (methyl methacrylate) is major part, the minor components make the core-shell structure. In the other case where polystyrene is major part, the minor components make separated droplet.

I also estimated the domain structure of the blends of polyethylene / polypropylene / polystyrene for various blend ratio.



In the case that polyethylene or polystyrene is major part, the minor components make the core-shell structure like the previous figure.

The results are consistent with the experimental results.

(H. F. Guo, S. Packirisamy, N. V. Gvozdic and D. J. Meier *Polymer* **38**, 785 (1997))

Title	Parameterization of the Gay-Bern potential for nCB and molecular dynamics simulation of 5CB
Researchers	Hiroo Fukunaga, Jun-ichi Takimoto, Masao Doi
Purpose of this study	In most of mesogens, the tail plays an important role in determining their phase behavior. The purpose of this study is to examine the dependence of the phase behavior on the parameters of the coarse-grained potential, and to analyze the effect of the tail.
System (Material)	5CB(4-n-pentyl-4'-cyanobiphenyl)
Program (including analysis)	COGNAC v1.2 hand-made analysis tool(order parameter, RDF)
Method & Some important input parameters	(Method) Molecular dynamics simulation using the model, where an 5CB molecule is divided into a rigid part and a flexible part. (Input) Number of molecules, NPT ensemble, Gay-Berne potential, Lennard-Jones potential, temperature, pressure
Advance & Problem	Advance: We have carried out MD simulations of 5CB to examine the parameter dependency of the structure, the density of the ordered state and the transition temperature. We found that if the length of the rigid core is kept constant, the isotropic phase becomes favored with increasing the aspect ratio of the core. This can be explained as the effect of the thickness of the tail part. Problem: We would require to include the terminal dipole.
Reference	[Manuscript] : Accepted Prog. Theoret. Phys. Suppl., 138, 396 (2000). Mol. Cryst. Liquid Cryst., in press. [Presentation at conferences (Meetings)] The 5th International Conference on Computational Physics (ICCP5) (1999) Japan Liquid Crystal Society conference(1999,2000) The 18 th International Liquid Crystal Conference (ILCC2000) (2000)
KeyWord (in English)	molecular dynamics (MD) simulation , Gay-Berne (GB) potential, Lennard-Jones (LJ) potential, OPLS potential, liquid crystal, nematic, nCB(4-n-alkyl-4'-cyanobiphenyl)

Results (Remarks)

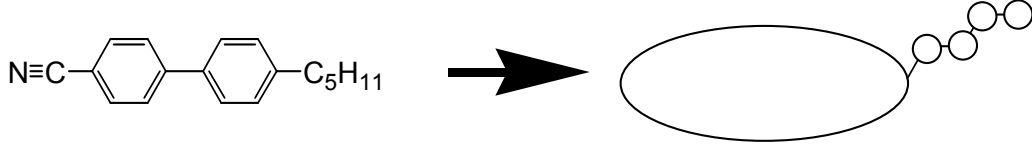


Fig.1 GB-LJ hybrid model for 5CB molecule.

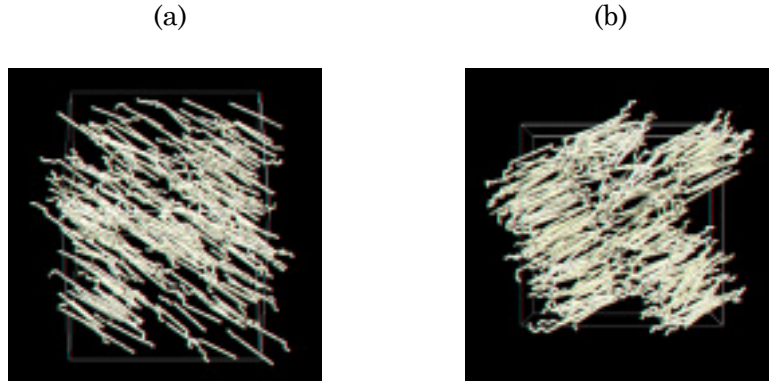


Fig.2 Snap shot of the liquid crystal phase obtained using the GB potential represented by (a) length-breadth ratio of 3.4 and (b) 4.0 for 5CB molecule.

Appendix

Gay-Berne potential

$$\begin{aligned}
 U(\hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j, \mathbf{r}_{ij}) &= 4\varepsilon(\hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j, \mathbf{r}_{ij}) \left[\left(\frac{\sigma_0}{r_{ij} - \sigma(\hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j, \mathbf{r}_{ij}) + \sigma_0} \right)^{12} - \left(\frac{\sigma_0}{r_{ij} - \sigma(\hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j, \mathbf{r}_{ij}) + \sigma_0} \right)^6 \right] \\
 \sigma(\hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j, \mathbf{r}_{ij}) &= \sigma_0 \left[1 - \frac{\chi}{2} \left\{ \frac{((\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_i) + (\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_j))^2}{1 + \chi(\hat{\mathbf{u}}_i \cdot \hat{\mathbf{u}}_j)} + \frac{((\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_i) - (\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_j))^2}{1 - \chi(\hat{\mathbf{u}}_i \cdot \hat{\mathbf{u}}_j)} \right\} \right]^{-1/2} \\
 \varepsilon(\hat{\mathbf{u}}_i, \hat{\mathbf{u}}_j, \mathbf{r}_{ij}) &= \varepsilon_0 \left[1 - \chi^2 (\hat{\mathbf{u}}_i \cdot \hat{\mathbf{u}}_j)^2 \right]^{-\nu/2} \left[1 - \frac{\chi'}{2} \left\{ \frac{((\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_i) + (\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_j))^2}{1 + \chi'(\hat{\mathbf{u}}_i \cdot \hat{\mathbf{u}}_j)} + \frac{((\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_i) - (\hat{\mathbf{r}}_{ij} \cdot \hat{\mathbf{u}}_j))^2}{1 - \chi'(\hat{\mathbf{u}}_i \cdot \hat{\mathbf{u}}_j)} \right\} \right]^\mu \\
 \chi &= \left[\frac{(\sigma_e / \sigma_s)^2 - 1}{(\sigma_e / \sigma_s)^2 + 1} \right] & \chi' &= \left[\frac{(\varepsilon_s / \varepsilon_e)^{1/\mu} - 1}{(\varepsilon_s / \varepsilon_e)^{1/\mu} + 1} \right]
 \end{aligned}$$

Title	Derivation of coarse-grained potential for polyethylene
Researchers	Hiroo Fukunaga, Toshihiro, Kawakatsu, Jun-ichi Takimoto, Masao Doi
Purpose of this study	In this study, we propose a new method to derive a set of coarse-grained potentials for polyethylene.
System (Material)	Polyethylene
Program (including analysis)	COGNAC v1.2 spline smoothing
Method & Some important input parameters	(Method) While the effective bonded potentials are determined by simply taking the logarithm of the corresponding distribution functions calculated from the microscopic simulations, the effective non-bonded potentials are evaluated using the canonical ensemble average for the fixed non-bonded distance. (Input) Number of atoms, NVT or NPT ensemble, temperature, pressure
Advance & Problem	Advance: The coarse-grained model combined with the aforementioned effective potentials can reproduce the radii of gyration, the distribution functions of the coarse-grained variables and the densities. Problem: We would require to take the correlation effects between bonded variables and between bonded and non-bonded variables.
Reference	[Manuscript] : Accepted Comput. Phys. Commun., in press [Presentation at conferences (Meetings)] Japan Molecular simulation conference 2000 Conference on Computational Physics 2000
KeyWord (in English)	molecular dynamics (MD) simulation , Gay-Berne (GB) potential, Lennard-Jones (LJ) potential, OPLS potential, liquid crystal, nematic, nCB(4-n-alkyl-4'-cyanobiphenyl)

Results (Remarks)

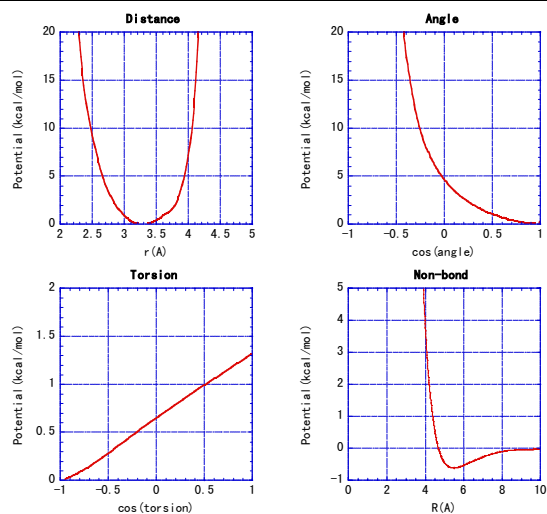


Fig.1 Coarse-grained potentials based on the distribution functions obtained by atomistic MD simulation.

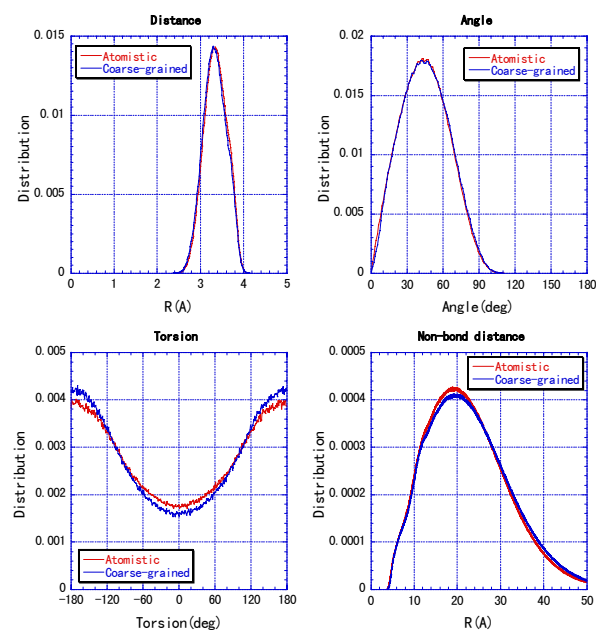


Fig.2 Comparison of distribution functions obtained by atomistic and coarse-grained MD simulations.

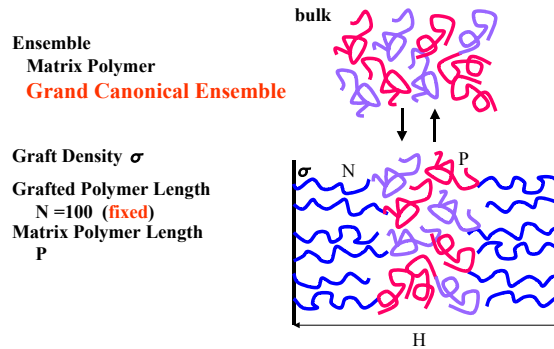
Title	Interaction between polymer grafted walls
Researchers	Takashi Honda, Hiroya Kodama, Toshihiro Kawakatsu
Purpose of this study	Calculate the interaction between colloidal particles and predict the dispersity of the particles.
System (Material)	Polymer solutions with polymer grafted particles.
Program (including analysis)	InterfaceSimulator-branch-SurfaceVer. 1.0 / SUSHI Ver. 3.0
Method & Some important input parameters	<p>(Method) Static SCF(Self-consistent field) method</p> <p>(Inputs) Grafting density, Chain length of grafted chain, Composition of the polymer solution</p>
Advance & Problem	<p>(Advance) We can estimate the interaction whether it is attractive or repulsive between polymer grafted particles in the polymer solution.</p> <p>(Problem) We assume that the radius of the particle is large enough than the polymer length and the surface grafted by polymers is assumed as the plane surface. It is need to consider different model to calculate the system with small particles.</p>
References	<p>[Manuscript] Submitted/Accepted(/)</p> <p>[Presentation at conferences (Meetings)] ACS National Meeting(at San Francisco 2000 Mar.), Computers in Chemistry #148</p>
KeyWords (in English)	SCE, graft, free energy, excess free energy, brush

Results (Remarks)

Simulation model: One dimensional model

The two walls grafted by polymers were dipped into the polymer solutions. The length of the grafting chain and the chain in the solution were N and P .

We set the $N=100$ and vary the P . The interaction between the segments are set to zero (good solvent solution)

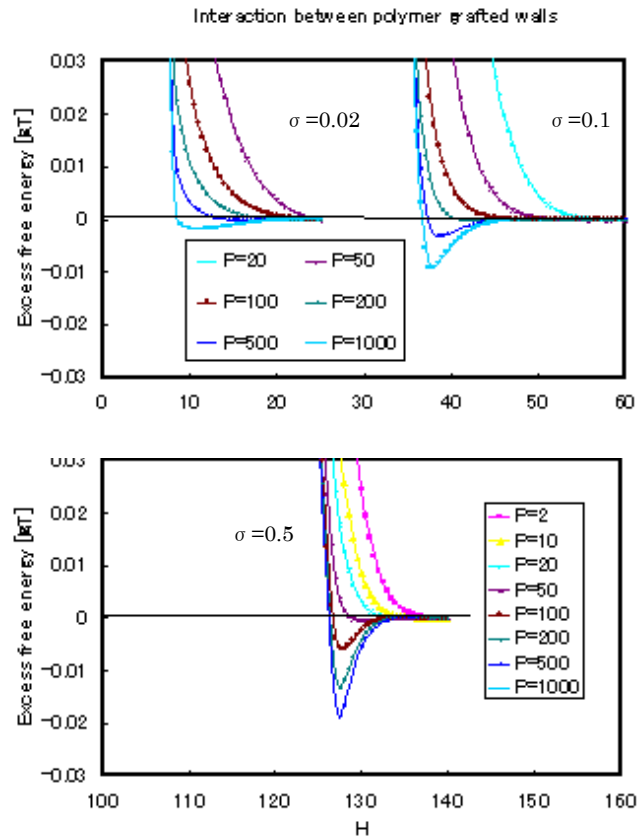


Output: Excess free energy (It can be considered as the interaction energy.)

The concentration of the polymer solution set to 50 %. The result is follows.

The condition of attractive interaction can be seen with large P .

The large grafting density enhances the effect.



Title	The simulation of the shrinking process of NIPA gels - the stress-diffusion coupling model for dynamics of gels -
Researchers	Tatsuya Yamaue, Takashi Taniguchi, and Masao Doi
Purpose of this study	<p>Many kinds of external stimuli, such as, temperature, pH, photons, ions, electric current (field), e.t.c. , can control the volume of the gel. In the case of volume phase transition, an enormous change in volume can be induced by an infinitesimal change of one of the these stimuli and this is of great importance in its application, as an actuator, sensor, switching device, DDS and so on.</p> <p>The dynamics of the volume-phase transition process of gels has been described by the collective diffusion model of gel networks, which well reproduces the liner phenomena. But, it was found experimentally that the shrinking process is strongly decelerated and stopped transiently in a "plateau period" due to the formation of surface skin. In the end of the "plateau period", various patterns appear and the gels restart to shrink. The collective diffusion model of gel networks can't reproduce these non-liner phenomena, such as surface skin which functions in DDS. Here we have constructed the Stress-Diffusion Coupling Model of gels, in which the general deformation of polymer networks, the continuity of solvent and the coupling between solvent diffusion and network stress are considered, and formulated the simulation scheme for large deformation of gels. Using this model we have simulated the shrinking process of slab NIPA(N-isopropyl-acrylamide) thermo-responsive gels undergoing spinodal decomposition by finite element method with delaunay triangulation in comparison with the collective diffusion model of gel networks.</p>
System (Material)	<p>NIPA(N-isopropyl-acrylamide) Gels [experiments] E.S.Matsuo and T.Tanaka, J.Chem.Phys. 89, 1695 (1988) A.Suzuki, S.Yoshikawa and G.Bai, J.Chem.Phys. 111, 360 (1999)</p>
Program	MUFFIN – GELS - , ver1.0
Method & Some important input parameters	<p>(Method) Model1: Stress-diffusion coupling model Model2: Corrective diffusion model of polymer networks (Inputs) Standard NIPA(N-isopropyl-acrylamide) gels with water solvent. polymer volume Fraction in reference state = 0.5 crosslinking number density in reference state = 0.05 - 0.20 Ginzburg-Landau free energy for mixing free energy</p>
Advance & Problem	<p>(Advance) The stress-diffusion coupling model, which can describe the actual solvent diffusion of gels, can reproduce the non-liner phenomena in the volume phase transition process, which related to the constraint phenomena of the solvent diffusion.</p> <p>(Problem) Furthermore, we will start the research of 3D simulation , electric field effects for ionic gels and another simulation scheme of the stress-diffusion coupling model, in which we consider the direct simulation of two fluids model among analysis of the velocity of solvent flow.</p>

References KeyWords (in English)	<p>[Manuscript] Submitted/Accepted(/)</p> <p>T.Y,et.al.,Progress of Theoretical Physics Supplement138(2000),416.</p> <p>T.Y,et.al.,AIP Conference Proceedings 519 (2000), 423.</p> <p>T.Y,et.al.,Transactions Material Research Society of Japan, in Press.</p> <p>[Presentation at conferences (Meetings)]</p> <p>Jul 1999,NATO-ASI, Soft & Fragile matter, Summer Seminar.</p> <p>Oct 1999, 48th. Kobunshi-Toronkai.</p> <p>Oct 1999, ICCP5.</p> <p>Nov 1999, The 3rd. Tohwa University International Conference.</p> <p>Dec 1999, 11th. Material Research Society, Japan.</p> <p>Jan 2000, 11th. Kobunshi-Gels Kenkyu-Toronkai</p> <p>NIPA(N-isopropyl-acrylamide) thermo-responsive gels, stress-diffusion coupling model, corrective diffusion of polymer networks, shrinking process, plateau period, surface skin layer, pattern formations, finite element method(FEM), lagrange picture</p>
Results (Remarks)	<div data-bbox="357 853 1235 1144"> </div> <div data-bbox="603 1151 991 1182"> <p>Left : Model2, Right : Model1</p> </div> <div data-bbox="288 1189 1305 1368"> </div> <div data-bbox="389 1375 1204 1406"> <p>Model2, Left : Soft Cases (spinodal region), Right : Hard Cases</p> </div> <div data-bbox="331 1413 1262 1688"> </div> <div data-bbox="389 1695 1204 1727"> <p>Model1, Left : Soft Cases (spinodal region), Right : Hard Cases</p> </div> <p>By the stress-diffusion coupling model, in the spinodal region, we have reproduced the "plateau period" in the shrinking process of thermo-responsive gels. During the "plateau period", the instability grows and the "bubble-like" inner patterns due to the phase separation appear. After finishing the formation of inner patterns of gels, the gels restart to shrink. Those results nicely reproduce the phenomena which were experimentally observed. In the liner shrinking process, in which gels shrink uniformly, the results of the collective diffusion model of gel networks and the stress-diffusion coupled model equal.</p>

Title	An analysis of loop/bridge ratio of triblock copolymer
Researchers	Takeshi Aoyagi, Jun-ichi Takimoto, Masao Doi
Purpose of this study	An analysis of loop/bridge ratio of triblock copolymer in various microdomain structures. Study a relation between loop/bridge structure and macroscopic properties.
System (Material)	Triblock copolymer (i.e. Styrene-Isoprene-Styrene, Styrene-Butadiene-Styrene)
Program (including analysis)	COGNAC v3 SUSHI 3
Method & Some important Input parameters	<p>(Method)</p> <ol style="list-style-type: none"> 1. Generate initial configuration based on the distribution of volume fraction of each segments obtained by SUSHI calculation with density biased Monte Carlo method. 2. The function of the mask conditions of SUSHI is used to constrain the one end segment of 0.1% chain in a domain. Then, loop/bridge ratio is calculated from the distribution of the other end segment. 3. A Python script is used to analyze loop/bridge ratio of chain configuration of COGNAC. <p>(Inputs)</p> <ol style="list-style-type: none"> 1. Polymer architecture (i.e. A3B24A3 triblock) 2. χ parameter
Advance & Problem	<p>(Advance)</p> <ol style="list-style-type: none"> 1. We developed an efficient method to generate an initial chain configuration for MD from the distribution of volume fraction of segment. 2. Loop/bridge ratio in lamella morphology agrees with theoretical and experimental results. 3. Loop/bridge ratio is predicted in cylinder and bcc morphology. <p>(Future work)</p> <p>A study of the relation between loop/bridge structure and properties (e.g. rubber elasticity) to predict an optimized chain structure.</p>
References	[Presentation at conferences (Meetings)] Polymer preprint Japan 49 (9), 2569 (2000)
KeyWords (in English)	coarse grained molecular dynamics, mean field calculation, block copolymer, loop conformation, bridge conformation, microdomain

Results (Remarks)

Figure 1 shows the distribution of volume fraction of the end segment, which is constrained by the mask conditions of SUSHI in a cylinder morphology. The distribution of one end which is constrained in the center domain (Fig.1(a)) and the other end (Fig.1.(b)) are shown. Loop/bridge ratio is calculated from the volume fraction in the center domain (loop) and the other domains (bridge) in Fig.1(b). Figure 2 shows a snapshot structure of triblock copolymer in the cylinder domain.

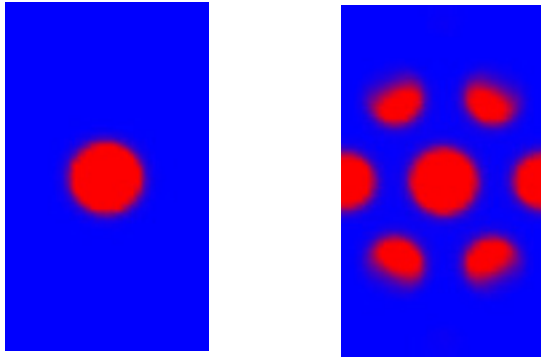


Figure 1. Volume fraction of the end segments of ABA triblock copolymer in a cylinder morphology. (a) fixed end, (b) free end

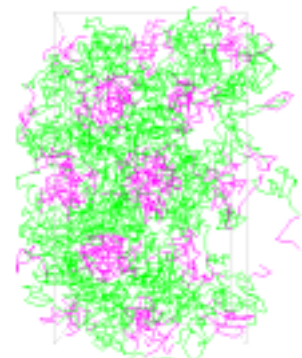


Figure 2. Snapshot structure of ABA triblock copolymer in a cylinder morphology

Table 1-3 show bridge ration of triblock copolymer in lamella, cylinder and bcc morphology.

Table1 Bridge ratio in lamella morphology

Polymer	χ	Lattice size/# of lamella	lamella length	ϕ_{bridge} (SCF)	ϕ_{bridge} (MD)
A10B20A10	2.0	32/4	8.0	0.45	0.49
A20B40A20	1.0	39/3	13.0	0.45	0.44
A40B80A40	1.0	40/2	20.0	0.41	0.41

Table2 Bridge ratio in cylinder morphology

Polymer	χ	Volume fraction ϕ_A	lattice size	ϕ_{bridge} (SCF)	ϕ_{bridge} (MD)
A5B40A5	1.5	0.20	8.0	0.63	0.65
A6B28A6	1.25	0.30	9.0	0.63	0.65

Table3 Bridge ratio in BCC morphology

Polymer	χ	Volume fraction ϕ_A	lattice size	ϕ_{bridge} (SCF)	ϕ_{bridge} (MD)
A3B54A3	3.0	0.10	11.0	0.76	0.77
A5B40A5	1.0	0.20	10.0	0.78	0.81
A6B28A6	0.75	0.30	8.5	0.80	0.83

Title	Study of the relation between χ parameter and Lennard-Jones parameter
Researchers	Takeshi Aoyagi, Jun-ichi Takimoto, Masao Doi
Purpose of this study	Study of the relation between χ parameter and Lennard-Jones parameter for quantitative zooming.
System (Material)	Immisible polymer blend / block copolymer system
Program (including analysis)	COGNAC v3 SUSHI v3
Method & Some important input parameters	<p>(Method)</p> <ol style="list-style-type: none"> 1. Generate initial configuration based on the distribution of volume fraction obtained by SUSI calculation with density biased Monte Carlo method. 2. Staggered reflective boundary conditions are applied. 3. Study the quantitative relation between χ parameter and Lennard-Jones parameter from the surface thickness <p>(Inputs)</p> <ol style="list-style-type: none"> 1. Polymer architecture, i.e. A100/B100 2. χ parameter and Lennard-Jones parameter
Advance & Problem	<p>(Advance)</p> <p>A quantitative relation between χ parameter and Lennard-Jones parameter is obtained.</p> <p>(Future plan)</p> <p>A quantitative assessment applying to realistic polymer system.</p>
References	<p>[Presentation]</p> <p>14-th bunshi simulation toronkai p141 (2001)</p> <p>ICAPP2001 Yonezawa(2001/10)</p> <p>[Manuscript]</p> <p>Proceeding of ICAPP2001 Yonezawa</p>
KeyWords (in English)	coarse grained molecular dynamics, polymer blend, interface, SCF calculation, χ parameter, Lennard-Jones parameter

Results (Remarks)

Figure 1 shows the calculated surface thickness as a function of χ parameter and Lennard-Jones parameter. Lennard-Jones parameter is to a symmetric value, i.e. $\epsilon_{AA} = \epsilon_{BB}$ and $\epsilon_{AB} = \epsilon_{AA} + \delta\epsilon$. In the case of Fig.1, cutoff distance is set to $2^{1/6}\sigma$. Thus, miscibility and the thickness of interface decrease as $\delta\epsilon$ increases. The diameters of LJ potential are set to $\sigma_{AA} = \sigma_{BB} = \sigma_{AB} = 1\sigma$. Chain length, N is set to 20 and 100. The surface thickness and energetic parameters are plotted with scaled by N . Figure 2 shows the relation between χ and $\delta\epsilon$ in the case of cutoff distance are $2^{1/6}\sigma$ (Fig.2(a)) and 2.5σ (Fig.2(b))

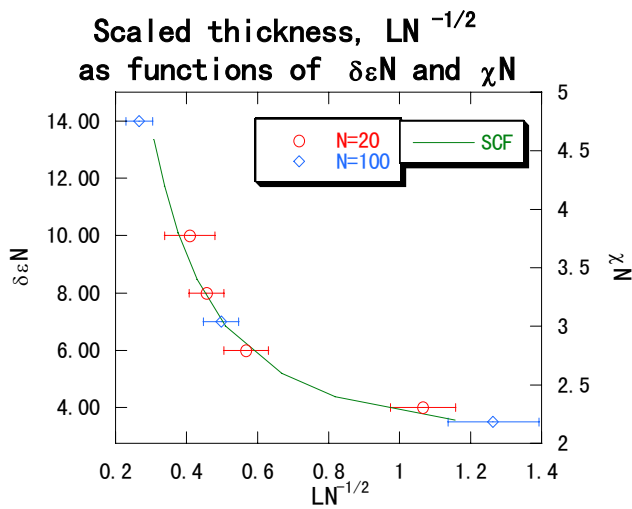


Figure 1

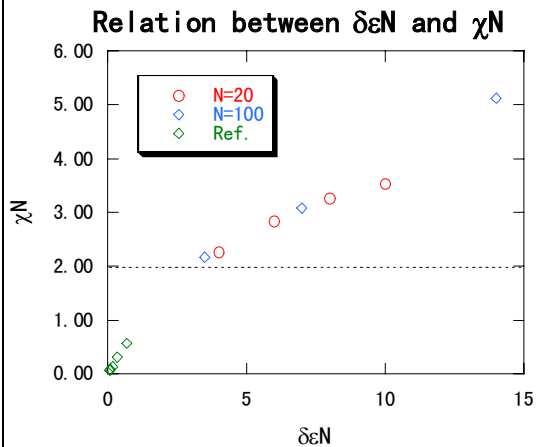


Figure2 (a)

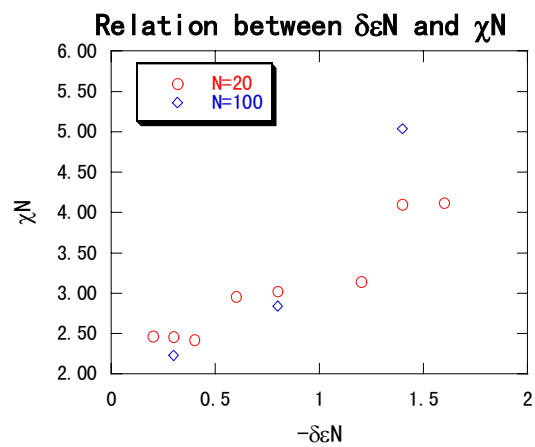


Figure2 (b)

Ref. G.S.Grest,M-D.Lacasse and K.Kremer, J.Chem.Phys. 105, 10583 (1996)

No. EAR3-021-02

First registration:2001/8/13 New: 2001/11/16

Title	Study of interface strength of polymer blend
Researchers	Takeshi Aoyagi, Jun-ichi Takimoto, Masao Doi
Purpose of this study	To study the effect of miscibility, chain length and elongation rate to surface strength of polymer blend.
System (Material)	Immisible polymer blend system
Program (including analysis)	COGNAC v3 SUSHI v3
Method & Some important input parameters	<p>(Method)</p> <ol style="list-style-type: none"> 1. Generate initial configuration based on the distribution of volume fraction obtained by SUSI calculation with density biased Monte Carlo method. 2. Staggered reflective boundary conditions are applied. 3. Elongation unit cell during MD simulation <p>(Inputs)</p> <ol style="list-style-type: none"> 1. Polymer architecture, i.e. A100/B100 2. χ parameter 3. Interaction parameter for bead-spring model
Advance & Problem	<p>(Advance)</p> <ol style="list-style-type: none"> 1. Efficient method and boundary condition are developed to model initial structure of interface of polymer blend. 2. The effects of miscibility, chain length and elongation rate to the stress behavior at elongation of interface are clarified. <p>(Problem)</p> <ol style="list-style-type: none"> 1. quantitative assessment applying to realistic polymer system. 2. Application to semi crystalline polymer.
References	<p>[Presentation]</p> <ul style="list-style-type: none"> - 50-th koubunshi toronkai (2001/9) - ICAPP2001 Yonezawa(2001/10) <p>[Manuscript]</p> <ul style="list-style-type: none"> - Proceeding of ICAPP2001 Yonezawa
KeyWords (in English)	coarse grained molecular dynamics, polymer blend, interface, SCF calculation, surface fracture, bulk failure

Results (Remarks)

Figure 1 shows snapshots of the interface of polymer blend during elongation. The chain length N is 100 in this case. When the attractive interaction between two segments of blended polymers are strong and the thickness of interface is thick enough, ($\sim R_g$), bulk failure is observed during elongation (Fig.1(a)). Furthermore, a fibril like structure is observed during elongation. On the other hand, in the case of weak attractive interaction, the thickness interface becomes thin and the fracture of interface is observed (Fig.1(b))

Figure 2 shows stress-strain behavior during elongation. The results of two different strain rate are shown in the figure. In the case of fast strain rate (Fig.2(a)), maximum stress is higher than slow strain rate (Fig.2(b)) and the strain at maximum stress are larger. Also, the long tail of strain is observed at the faster strain rate. In both cases, stress-strain behavior shows almost the same as homogenous bulk ($\delta\epsilon N=0.0$) except $-\delta\epsilon N=10.0$ case, which has very weak attractive interaction between the polymers and thin interface (shown in Fig.1(b)). These results correspond to the difference between bulk failure and fracture of interface depending on the interaction between segments and thickness of surface.

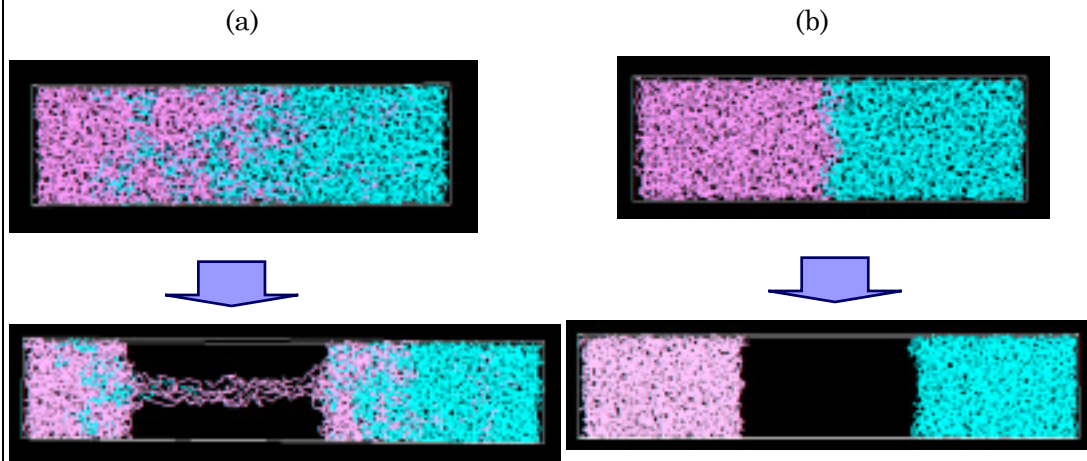


Fig.1 Snapshot structure of polymer blend at interface during elongation, (a) thick interface ($-\delta\epsilon N=0.3$), (b) thin interface ($-\delta\epsilon N=10.0$).

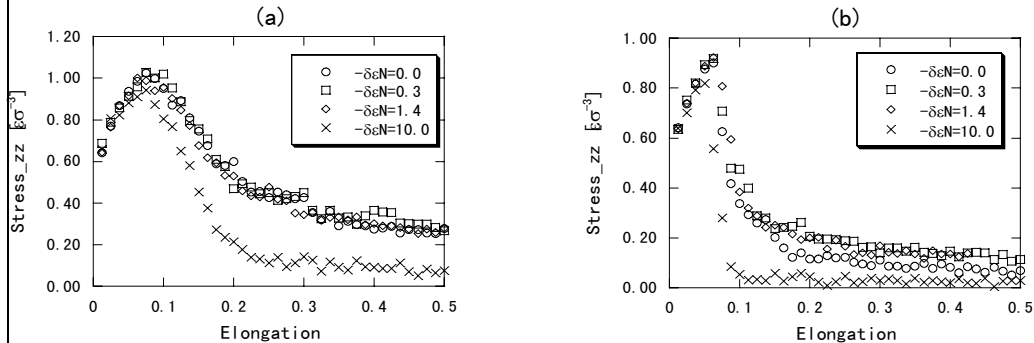


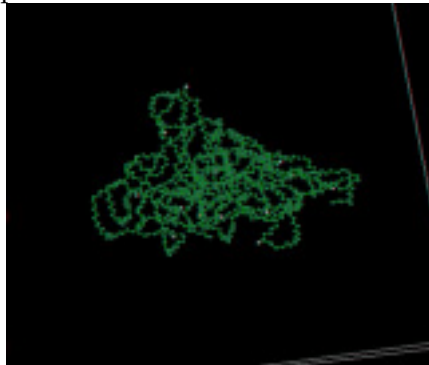
Fig.2 Stress-strain curve of polymer blend at interface.

Initial strain rate, $d\epsilon/dt$: (a) $2.08 \times 10^{-3} [\tau^{-1}]$ (b) $2.08 \times 10^{-4} [\tau^{-1}]$

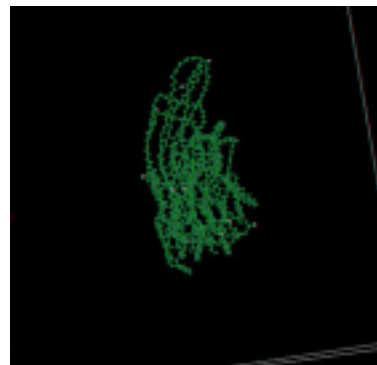
Title	The influence of short chain branching on polymer crystallization process -molecular dynamics simulation-		
Researchers	Tatusya Shoji, Jun-ichi Takimoto, and Masao Doi		
Purpose of this study	To investigate the influence of arrangement of and number of short chain branching on main chain on polyethylene crystallization process by using molecular dynamics simulation.		
System (Material)	sample name	architecture	branching arrangement
	lin	linear (no branching)	
	b10re	10 methyl branching	regular
	b15re	15 methyl branching	regular
	b15ra	15 methyl branching	random
Program (including analysis)	COGNAC version 3 analysis: trajectory analyzer (order parameter、conformation)		
Method & Some important input parameters	(Method) Coarse-grained molecular dynamics using united atom models potentials (Inputs) -polymer architecture(degree of polymerization) -united atom models potentials(bond ,bending, torsion, non-bond) -calculation conditions(temperature, density, time steps, etc...)		
Advance & Problem	(Advance) We investigated the influence of arrangement of and number of short chain branching on main chain on the nucleation and growth process of crystallization of isolated one chain polyethylene by using molecular dynamics simulation. All of branched beads were swept out from inner lamella and finally located at the folding points of crystalline lamella interface. The arrangement and number of branching changed the averaged thickness of the lamella stem. We consider that it is possible to control the thickness of lamella by the primary structure of polymer.		
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)] Polymer Preprints Japan (49 (8), 2032 (2000))		
KeyWords (in English)	molecular dynamics(MD) simulation , the united atom model , methyl branching , crystallization , the nucleation and growth interval of insertion,		

Results (Remarks)

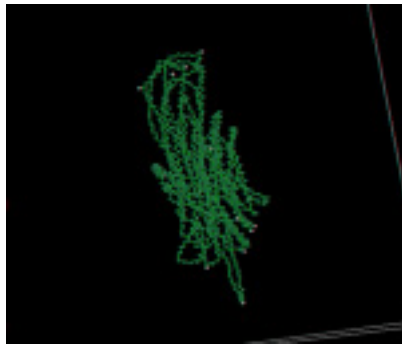
Output:



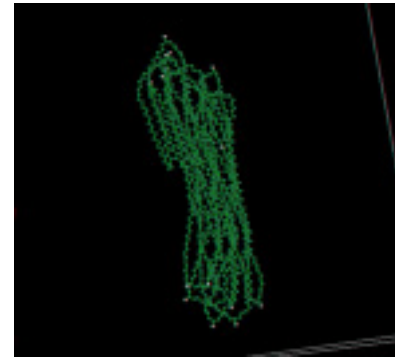
(a) $t=0$



(b) $t=50\text{ps}$



(c) $t=100\text{ps}$



(d) $t=1\text{ns}$

Fig.1 Snapshots of b15re until 1ns after quenching.

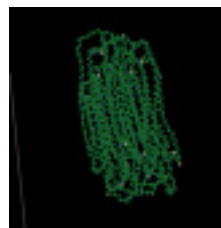
Fig.1 shows snapshots of b15re until 1ns after quenching. The crystallization process of the branched polymer consists two steps. In the first step, the branched parts are quickly pushed out from the random coordinates to surface of a coil, and give rise to fold as starting point of chain-folding, and form the local ordered stems. In the second step, the linear chain parts form gradually ordered structures and finally becomes crystalline lamella structures with chain-folded interfaces.



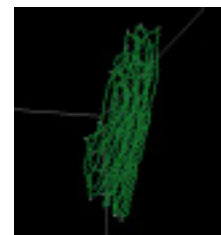
(a) lin



(b) b10re



(c) b15ra



(d) b15re

Fig.2 Snapshots of four sample after crystallization.

Fig.2 shows the final structures of the four samples after crystallization. The thickness of each sample was (a) 52, (b) 49, (c) 47, or (d) 71 Angstrom. Therefore we consider that it is possible to control the thickness of lamella by the primary structure of polymer.

Title	Estimation of optical transmittance of polymer materials using spherulites growth model
Researchers	Naoki Kobayashi, and Takashi Taniguchi
Purpose of this study	We estimate light transmittance of polyethylene using computer simulations based on spherulites growth.
System (Material)	Polyethylene
Program (including analysis)	Optical transmittance simulator ("TURBAN in MUFFIN")
Method & Some important input parameters	<p>(Method)</p> <p>TURBAN consists of two parts: (i) Computer simulation of spherulite growth on Avrami conditions, and (ii) Computer simulation of the optical transmittance based on Maxwell equation using the obtained spherulite structures.</p> <p>(Inputs)</p> <ul style="list-style-type: none"> -Nucleation density or nucleation rate. -Spherulite growth rate. -Spatial scale. -Crystallinity. -Refractive indices of each crystal axis direction and amorphous parts.
Advance & Problem	<p>(Advance)</p> <p>We can estimate a light transmittance of polymeric materials with spherulite system by computer simulation.</p> <p>(Problem)</p> <p>Input and output interface of the simulator TURBAN is not in UDF file format.</p>
References	<p>[Manuscript] Submitted/Accepted(/)</p> <p>[Presentation at conferences (Meetings)]</p> <p>50th SPSJ Annual meeting (at Osaka 2001,May)</p> <p>50th SPSJ Conference (at Tokyo 2001,Sept.)</p>
KeyWords (in English)	polyethylene, transmittance, spherulite, films, simulation, turbidity

Results (Remarks)

We carry out computer simulations of spherulites growth on Avrami conditions. Fig.1 shows the images of simulation of 3D spherulite growth with inhomogeneous nucleation. Using the obtained spherulites structures, we estimate a turbidity of the polyethylene materials. Fig.2 shows the turbidity spectra against light wavelength for various spherulite average diameters. The result of the simulation is in good agreement with an experimental result of polyethylene haze(Fig.3).

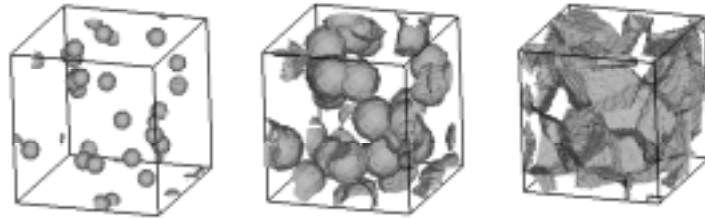


Fig.1 Simulation images of spherulites growth.

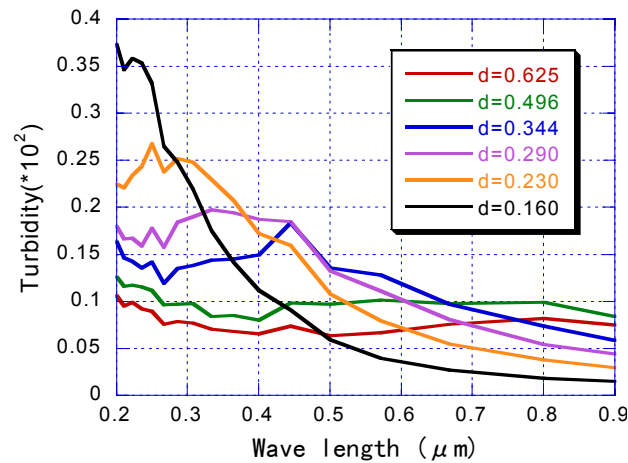


Fig.2 Turbidity spectra from the simulation with various spherulite average diameters.

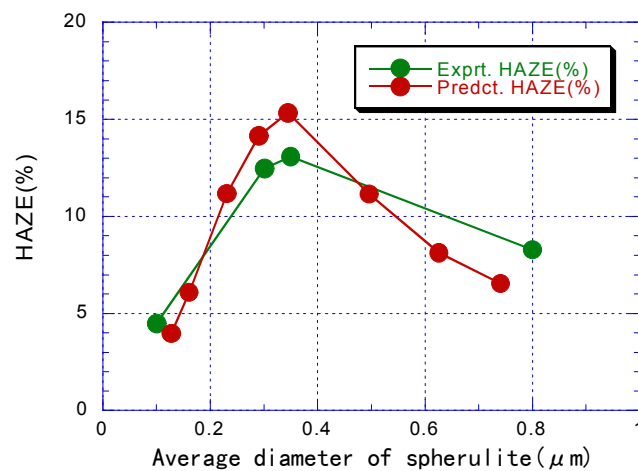


Fig.3 Predicted HAZE and experimental[1] HAZE.

[1] Lei Wang, M. R. Kamal and A. D. Rey, *Polym. Eng. Sci.*, **41**, 358 (2001).

Title	Mechanical properties of topological gel. - Molecular dynamics simulation -
Researchers	Fumio Sawa, Takeshi Aoyagi and Masao Doi
Purpose of this study	Topological gel is a new type of a gel which has cross-links that can slide along the backbone of the polymer chain composing the gel network. We have carried out molecular dynamics simulations of topological gel to study the effect of sliding cross-links on the mechanical properties.
System (Material)	This system consists of linear polymers end-capped by large molecules and connected by cyclic molecules.
Program	COGNAC ver.3.08
Method & Some important input parameters	<p>(Method) COGNAC ver.3.08 was used for current simulation, however, initial coordinates and topology of system was made by a Python script. And also, some of analysis was done by hand made script(Python).</p> <p>(Inputs) System: Number of linear polymers and cyclic molecules. Potentials: Bonding (bond and angle) and Nonbonding(Lennard-Jones and Lennard-Jones-Gay-Berne) potential was used. Simulation: Temperature, density and other parameters.</p>
Advance & Problem	<p>(Advance) By COGNAC simulation, it was clarified that topological gel has characteristic mechanical properties. Moreover, by comparison with chemical gel, topological gel is thought to have higher entropical elasticity than chemical gel.</p> <p>(Problem) The examined rate of elongation is much higher than that of experimental condition. The ratio of the elongation rate and velocity of the cyclic molecules sliding on each linear polymer is thought to be the main factor of elasticity. However, comparison between simulation results and experiments can be possible with taking account of its ratio.</p>
References	<p>[Manuscript] Submitted/Accepted(/)</p> <p>[Presentation at conferences (Meetings)]</p> <p>39'th Kobunshi-Zairyou-Jiyuu-Toronkai (2001)</p> <p>50'th Symposium on Macromolecules (2001)</p>
KeyWords (in English)	molecular dynamics, topological gel, mechanical properties

Results (Remarks)

<Results>

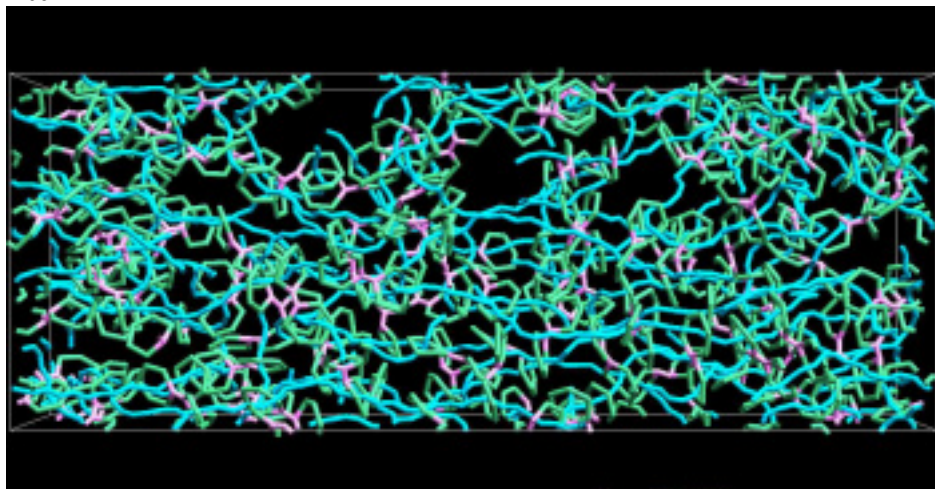


Fig.1

Fig.1)

A snapshot of the system. Linear polymers are colored blue, and cyclic molecules are green. Red objects are cross-links.

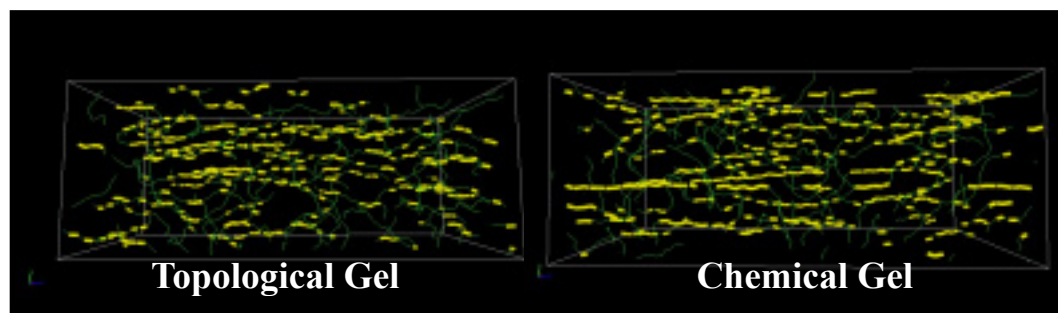


Fig.2

Fig.2)

Snapshots of gels(left: topological gel, right: chemical gel) at the conditions at elongation of 1.75. The elongational direction is horizontal. Chemical gel has some specific polymers aligning to elongation.

Fig.3)

Stress(σ) versus elongation(λ).

(cd7:topological gel,
cd7c: chemical gel)

Topological gel seems to have higher capacity of elongation more than chemical gel.

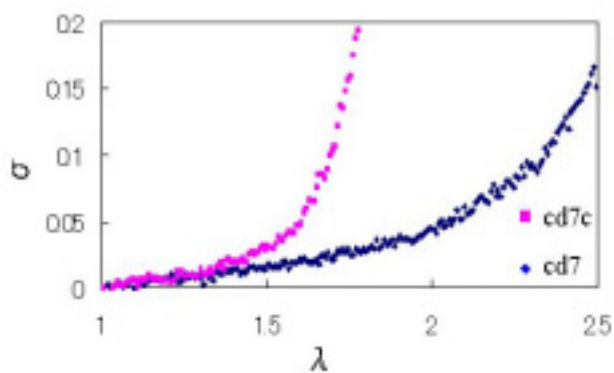
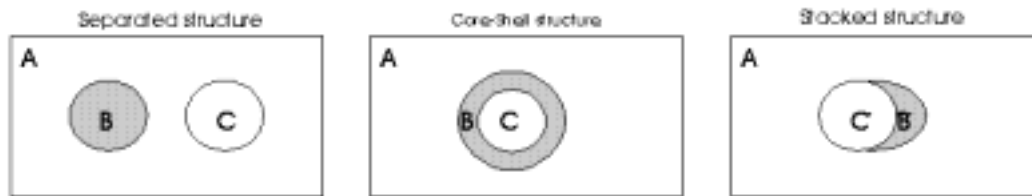


Fig.3

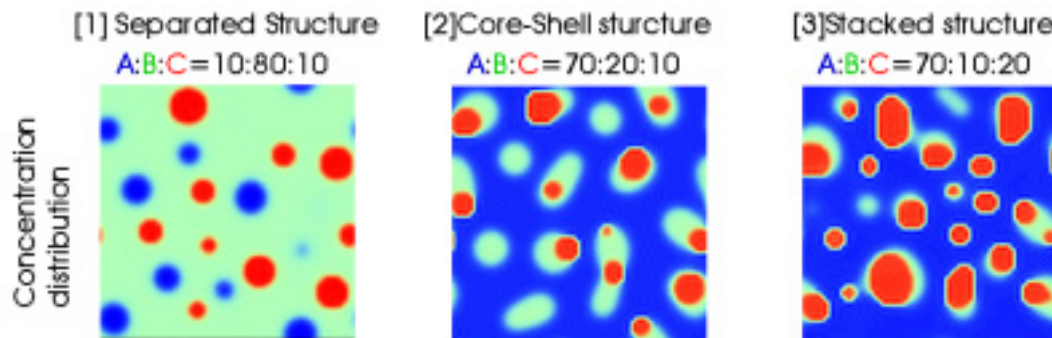
Title	Analysis of the structure of polymer blend system
Researchers	Shinji Urashita
Purpose of this study	To predict and estimate physical properties of polymer alloy, it is expected that we recognize the domain structure identification. Therefore, the methods for objective classification of each type of domain structures are useful.
System (Material)	Ternary polymer blend system
Program (including analysis)	MesoSimulator Release990304, dynamic mean fields simulation program Geoman: calculation tool for the Euler characteristic Conturn: generation tool for the colored contour
Method & Some important input parameters	(Method) the Scheutjens-Fleer-Fry mean field theory, labeling algorithm, bi-cubic spline interpolation (Inputs) Interaction parameter, chain length, blend ratio, concentration field
Advance & Problem	(Advance) - By using Euler characteristic plot, the domain identification for ternary polymer blend is successful. - Typical example for the domain identification is shown for the separated, core-shell, and stacked structures.
References	[Presentation at conferences (Meetings)] "The prediction of the domain morphology of polymer blend by using dynamic mean field simulation", S.Urashita and T.Kawakatsu, 14 th Molecular Simulation Symposium of Japan, 2P06 (2001)
KeyWords (in English)	Minkowski functionals, Euler characteristic, Domain morphology, Ternary polymer blend

Results (Remarks)

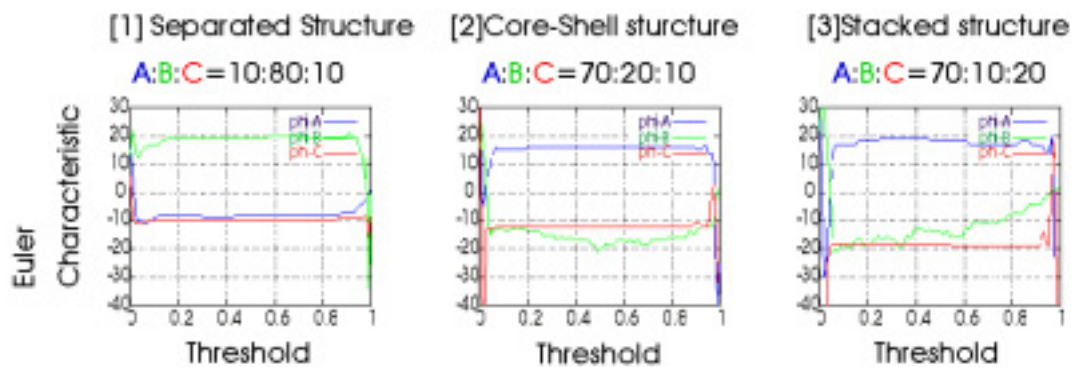
Typical domain structures for ternary polymer blend are following:



The simulation based on the Scheutjens-Fleer-Fry dynamic mean field theory generates the corresponding structures and the colored contours for each structure are given.



It is difficult to distinguish the structure [2] and [3] by eyes, thus method the Euler characteristic, it is one of Minkowski functionals and is defined as $\chi(\rho) = N_{\rho}^{(7)} - N_{\rho}^{(t)}$, is adopted for the guidepost of the domain identification. By using the colored contours, the plots for the Euler characteristic and threshold concentration are shown in the below.



It is clearly distinguished for each domain structures by the plots.

No. EAR3-026-02

First registration: 2001/11/ 1 New: 2001/11/22

Title	Calculation of elastic modulus of polymer blend
Researchers	Masahiro Noda, Makoto Sasaki, Takashi Taniguchi, and Masao Doi
Purpose of this study	Calculation of elastic modulus of polymer blend with phase separated structure
System (Material)	Polymer blend system (PP/SEBS)
Program (including analysis)	MUFFIN ver.2 (MSPD)
Method & Some important input parameters	(Method) Calculation and analysis of strain and strain energy by linear elastic theory (Inputs) elastic modulus of each blend component(bulk modulus and shear modulus), density field
Advance & Problem	(Advance) - We can calculate the elastic modulus of the system with phase separated structure. These values are in good agreement with the value predicted theoretically. - We can use SUSHI or MUFFIN_MSPD data as an input of the density field required for this calculation.
References	[Manuscript] Application report "AMUSE"
KeyWords (in English)	polymer blend, PP, SEBS, linear elasticity, phase separation, bulk modulus, shear modulus, Young's modulus, strain energy

Results (Remarks)

Output: strain, strain energy etc.
Analysis: total elastic modulus

[Example of analysis]

Input parameter

-Elastic modulus
<PP>
 $G=1.0(\text{MPa})$, $K=833.333(\text{MPa})$
<SEBS>
 $G=0.50(\text{MPa})$, $K=2000(\text{MPa})$

Method

-Simulation of independent displacements, at least two or more kinds
-Total strain energy f and distortion is plotted based on the following equation (Fig.1-b).

$$\Sigma f = G_{ave} \Sigma \left(e_{ij} - \frac{1}{d} \delta_{ij} e_{ii} \right)^2 + K_{ave} \Sigma \frac{(e_{ii})^2}{2}$$

-The cross point is averaged elastic modulus to be calculated.

Results

As a result of this technique applied to sphere (dispersed), bicontinuous structure, the modulus was described by the following simple models. (Fig. 2).

$$E = \phi_1 E_1 + \phi_2 E_2 \quad \dots \text{parallel model}$$

$$E^{1/5} = \phi_1 E_1^{1/5} + \phi_2 E_2^{1/5} \quad \dots \text{Davies model}$$

$$\frac{1}{E} = \frac{\phi_1}{E_1} + \frac{\phi_2}{E_2} \quad \dots \text{series model}$$

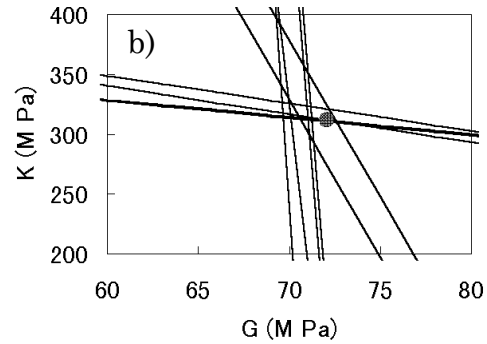
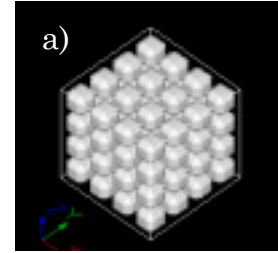


Fig.1a) Example of dispersed structure (white: SEBS).

b) Example of analysis of the simulation using the structure shown in Fig.1-a).

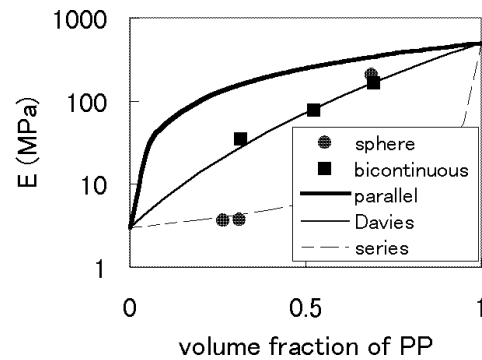


Fig.2

Comparison with the simulation and the theoretical equations. Symbols are for the simulation and lines are for the theory.

No. EAR3-027-01

First registration: 2001/11/ 1 New: 2001/11/ 1

Title	Prediction of strain energy on photo-resist patterns
Researchers	Masahiro Noda, Makoto Sasaki, and Masao Doi
Purpose of this study	Prediction of strain energy on cantilever supposing photo-resist pattern
System (Material)	Photo-resist (Polymer thin film)
Program (including analysis)	MUFFIN ver.2 (MSPD)
Method & Some important input parameters	(Method) Calculation and analysis of strain and strain energy by linear elastic theory (Inputs) Elastic modulus of polymer thin film(bulk modulus and shear modulus), stress
Advance & Problem	(Advance) - We succeeded to calculate the strain energy distribution on photo-resist pattern. - Critical aspect ratio which is hard to be determined by experiment can be predicted by the analysis. (Problem) - estimation of elastic modulus of polymer thin film and stress
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)]
KeyWords (in English)	photo-resist, bulk modulus, shear modulus, Young's modulus, strain energy

Results (Remarks)

Output: strain, strain energy etc.

Analysis: aspect ratio of resist pattern

[Example of analysis]

Input parameter

-Elastic modulus

$G=1.72(\text{GPa})$

$K=16.7(\text{GPa})$

($E=5.00(\text{GPa})$)

-Stress

-500(KPa) perpendicular to x_{max} plane
(z_{min} plane is fixed.)

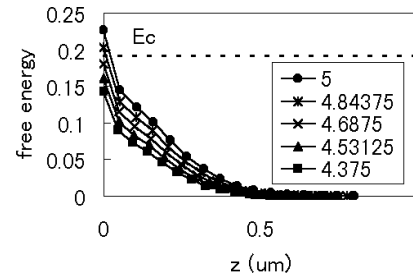
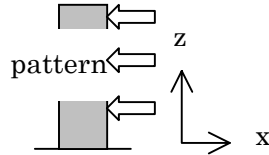


Fig.1 Height dependence of the strain energy, changing the aspect ratio (pattern width: $0.16\mu\text{m}$, z : $0.7\text{--}0.8\mu\text{m}$).

Method

-The maximum strain energy is computed, with changing pattern form (Fig. 1).

-The critical aspect ratio for the collapse (A_c) can be determined from the relation between the aspect ratio and the energy with the critical strain energy(E_c) (Fig. 2).

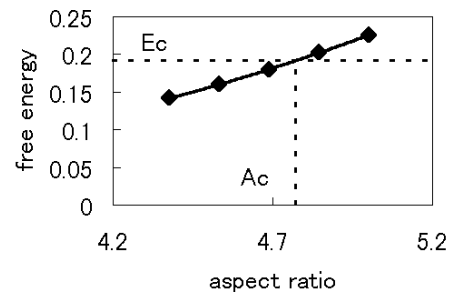


Fig.2 Relation between the aspect ratio and the maximum strain energy (pattern width: $0.16\mu\text{m}$).

Results

-The critical collapse aspect ratio was obtained for the photo-resist pattern $0.1\mu\text{m}$ or less (Fig. 3).

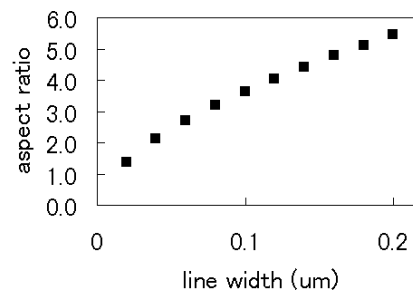


Fig.3 Relation between line width and a critical aspect ratio.

Title	Prediction of the uniaxial elongational viscosity of polydisperse Polystyrene(PS) melt.
Researchers	Hiroyasu Tasaki, Jyun-ichi Takimoto and Masao Doi
Purpose of this study	Prediction of the uniaxial elongational viscosities of polymers.
System (Material)	-PS($M_w = 2.85 \times 10^5$, $M_w/M_n = 2.0$) -PS + 1.5wt.% high molecular weight PS(HMW-PS, $M_w = 3.2 \times 10^6$)
Program (including analysis)	PASTA (Smoothing and 2D-plotting programs)
Method & Some important input parameters	(Method) Stochastic simulation based on the Slip-link model, which takes account of the reptation, contour length fluctuation and constraint renewal (constraint release or constraint creation). (Inputs) Molecular Weight : $Z = M / M_e$ (M : Molecular weight, M_e : Entanglement molecular weight) Numbers of polymer : n *Some set of Z and n is available. MaxStretchRatio : Extended chain length / Equilibrium chain length (or 0 for Gauss chain)
Advance & Problem	(Advance) - The strain hardening of elongational viscosities, which has strong effect on the processability of polymer, is very sensitive to the existence of very high molecular weight components. Our simulation method can predict the effects of molecular weight distribution and high molecular weight component on the strain hardening quantitatively. (Problem) - Prediction of the rheological properties of polymers with extremely broad molecular weight distributions and branching structures, such as pom-pom and comb.
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)] - 47 th Rheology tohronkai, p.263 (1999) - J. Takimoto, H. Tasaki and M. Doi, Proceeding of XIIIth International Congress on Rheology, Cambridge, UK, 2 , 97 (2000) - H. Tasaki, J. Takimoto, M. Doi, Proceeding of Materials Science for the 21st Century, Osaka, Japan, B , 15 (2001)
KeyWords (in English)	Rheology, slip-link model, entanglement, constraint release, constraint renewal, contour length fluctuation, polystyrene, elongational viscoelasticity, strain hardening, PASTA

Results (Remarks)

(1) We prepared 10^4 chains in a computer to mimic the GPC data.

Input :	Z	n	MaxStretchRatio
	3.1	354	4.4
	3.5	394	4.4
		
	107.4	2	4.4

(2) First, we calculated the dynamic moduli, and determined two model parameters (the time scale and the stress scale) by fitting the simulation results to the experiment.

(3) Then we calculated the elongational viscosities at the same strain rates as experiments. Uniaxial elongational stress (σ_E) is calculated by following equation.

$$\sigma_E = N_1 + \frac{1}{2} N_2$$

N1: First normal stress difference

N2: Second normal stress difference

[Example of analysis]

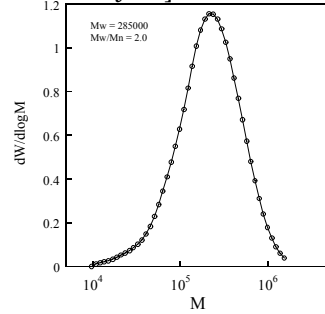


Fig.1 GPC profile

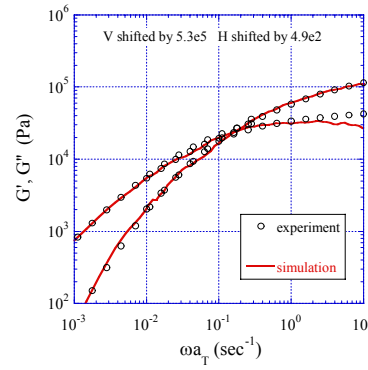


Fig.2 Storage modulus(G') and Loss modulus(G'')

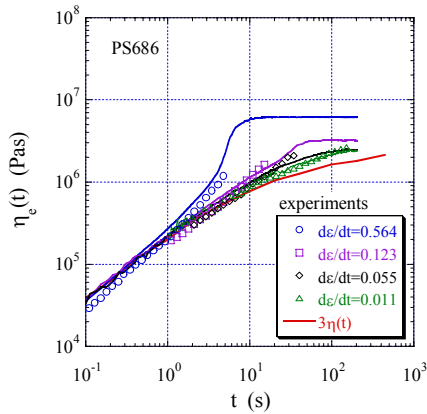


Fig.3 Elongational viscosity of polydisperse system. Symbols and lines represent the experiments and simulations, respectively

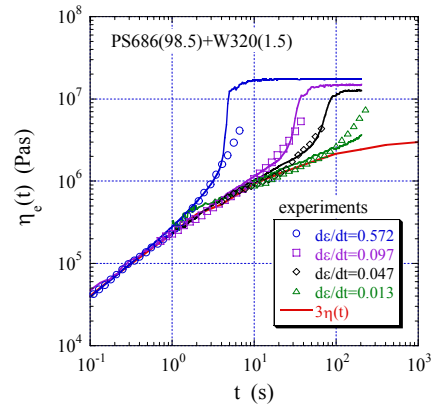


Fig.4 Elongational viscosity of polydisperse system containing 1.5wt.% HMW-PS

Title	Shear viscosity of star polymers.
Researchers	Jyun-ichi Takimoto, Hiroyasu Tasaki and Masao Doi
Purpose of this study	Prediction of the shear viscosities of star polymers.
System (Material)	Star polymers and blend of linear and star polymers
Program (including analysis)	PASTA (Smoothing and 2D-plotting programs)
Method & Some important input parameters	<p>(Method) Stochastic simulation based on the slip-link model. It is assumed that the junction point of the arms does not move except moving due to the macroscopic flow of the sample.</p> <p>(Inputs) -Number of entanglements of the arm : $Z_a = M_a / M_e$ (M_a : Molecular weight of arms, M_e : Entanglement molecular weight) -Number of arms : n_a *Some set of Z_a and n_a is available. -MaxStretchRatio : Extended chain length / Equilibrium chain length</p>
Advance & Problem	<p>(Advance) The shear viscosities of liner and star polymers at high shear rate are similarly independent of the molecular weight. In case of linear polymers, Convective Constraint Release(CCR) is a dominant relaxation mechanism under fast flow. Since the end of an arm is free, it is assumed that the relaxation of star polymers at high shear rate is also governed by CCR of the arms. The rate of CCR is depend on the shear rate, the shear stress of liner and star polymers show good agreement at high shear rate independent of the molecular weight.</p> <p>(Problem) Prediction of the rheological properties of polymers with other type branching structures, such as pom-pom and comb.</p>
References	<p>[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)] H. Tasaki, J. Takimoto, M. Doi, Proceeding of Materials Science for the 21st Century, Osaka, Japan, B, 15 (2001)</p>
KeyWords (in English)	<p>Rheology, slip-link model, entanglement, constraint release, constraint renewal, contour length fluctuation, linear polymer, arm, star polymer, viscoelasticity, shear viscosity, zero shear viscosity, PASTA</p>

Results (Remarks)

[Example of analysis]

In the case of star polymers, it is assumed that the junction point of the arms does not move except moving due to the macroscopic flow of the sample. Under this assumption, each arm of a star polymer can be dealt with independently. Of course, an entanglement between each arm is taken into consideration. Therefore, each arm can carry out a simulation like a linear polymer except for the point of not performing reptation. However, the Rouse relaxation time of an arm whose molecular weight is Z_a (Accurately, $Z_a = M_a / M_e$) is given as $\tau_R = 4\tau_e Z_a^2$, that is, it is necessary to use the Rouse relaxation time of the linear chain of a molecular weight Z_a .

In addition, this simulation technique gives the result for which it does not depend on the number of the arm about rheological properties of star polymers.

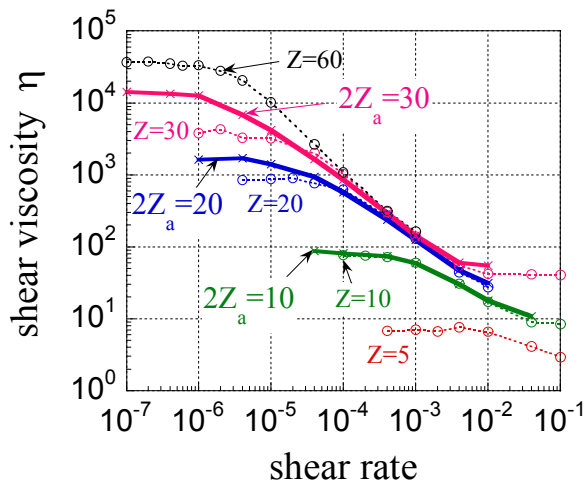


Fig.1 Shear viscosity of the linear and star polymers.

Thick solid lines and thin broken lines with symbols represent the star polymers and linear polymers, respectively.

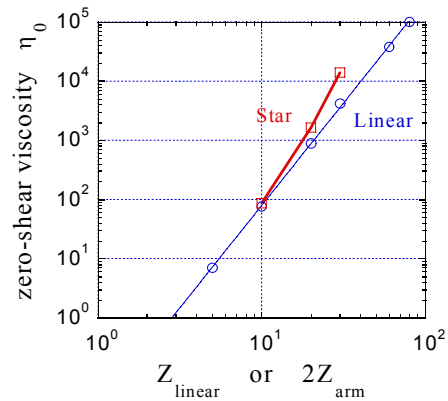


Fig.2 Molecular weight (Z or Z_a) dependency of the zero shear viscosity.

No. EAR4-030-02

First registration: 2002/ 2/16 New: 2002/ 2/21

Title	Prediction of interfacial tension of an A/B polymer blend
Researchers	Katsuyuki Yokomizo, Hiroya Kodama, Takashi Honda, Toshihiro Kawakatsu and Masao Doi
Purpose of this study	Analysis of polydispersity effects on the interfacial tension of an A/B homo polymer blend
System (Material)	Polymer blends with polydispersity
Program (including analysis)	SUSHI, FluidSimulator
Method & Some important input parameters	<p>(Method) 1-dimensional canonical SCF (statics)</p> <p>(Inputs) Flory-Huggins segment interaction parameter Volume fraction and segment numbers of each polymer</p>
Advance & Problem	<p>(Advance) - FluidSimulator equilibrates the system and calculates the volume fraction profiles of all components and the interfacial excess free energy (interfacial tension). - Components can be polymers (homo-polymers, block- or graft-copolymers, etc) or solvents.</p> <p>(Problem) - Molecular design of compatibilizer</p>
References	<p>[Manuscript] Submitted/Accepted(/)</p> <p>[Presentation at conferences (Meetings)]</p>
KeyWords (in English)	interfacial excess free energy, polymer architecture, polydispersity, equilibrium interfaces,

Results (Remarks)

Output: interfacial excess free energy, etc.

Analysis: polydispersity effects on the interfacial tension

[Example of analysis]

- The effects of polydispersity on the polymer interfaces are investigated for A/B binary homopolymer mixtures where both polymers have molecular weight distributions. The equilibrium structure of the polymer blend is obtained by the 1-dimensional static SCF calculation under the Neumann boundary condition. Let us denote the segment density of the i type chains as ϕ_i^α where α specifies each of the coexisting equilibrium phase. Using ϕ_i^α and the equilibrium free energy F , one can calculate the free energy of the bulk phase f^{bulk} and the equilibrium chemical potential of each component μ_i .

- Then, the excess free energy F^{excess} is calculated as follows. The volume fraction, segment numbers and system size are expressed as ϕ_i^0 , N_i and L .

$$f^{\text{bulk}} = \sum_i \frac{\phi_i^\alpha}{N_i} \ln \frac{\phi_i^\alpha}{N_i} + \frac{1}{2} \sum_{ij} \chi_{ij} \phi_i^\alpha \phi_j^\alpha$$

$$\mu_i = 1 + \ln \frac{\phi_i^\alpha}{N_i} + N_i \sum_j \left(\chi_{ij} \phi_j^\alpha - \frac{\phi_j^\alpha}{N_j} \right) - \frac{1}{2} N_i \sum_{ij} \chi_{ij} \phi_i^\alpha \phi_j^\alpha$$

$$F^{\text{excess}} = LF - Lf^{\text{bulk}} - L \sum_i \frac{\mu_i (\phi_i^0 - \phi_i^\alpha)}{N_i}$$

Results

- We investigated molecular weight dependence of the excess free energy by changing the chain length and the volume fraction
- Each system shows almost the same behavior, which resembles to that of the molecular weight dependence of a mono disperse polymer blend system.
- It asymptotically approaches the theoretical value of the interfacial tension obtained by Helfand and Tagami⁽¹⁾ in the limit of infinite molecular weight.

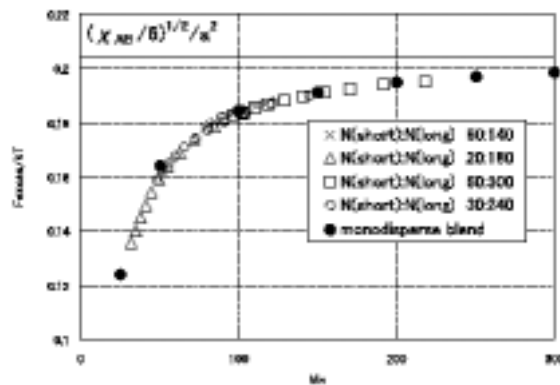


Fig.1 Molecular weight dependence of the excess free energy. (χ_{AB} : 0.25)

(1) Helfand, E. and Tagami, Y. : J.Chem.Phys., 62, 1327 (1975)

Title	Study of interface strength of polymer blend with polydispersity
Researchers	Katsuyuki Yokomizo, Takeshi Aoyagi, Takashi Honda, Hiroya Kodama, Toshihiro Kawakatsu, Masao Doi
Purpose of this study	Analysis of the effect of miscibility, polydispersity in chain length on the interfacial strength of polymer blend.
System (Material)	Immiscible polymer blend with polydispersity.
Program (including analysis)	COGNAC v3 SUSHI v3
Method & Some important input parameters	<p>(Method)</p> <ol style="list-style-type: none"> 1. Generate initial configuration based on the distribution of volume fraction obtained by SUSHI calculation with density biased Monte Carlo method. 2. Staggered reflective boundary conditions are applied. 3. Elongation unit cell during MD simulation <p>(Inputs)</p> <ol style="list-style-type: none"> 1. Polymer architecture, i.e. A55/A550/B55/B550 2. χ parameter 3. Interaction parameter for bead-spring model
Advance & Problem	<p>(Advance)</p> <ol style="list-style-type: none"> 1. Efficient method and boundary condition are developed to model initial structure of interface of polymer blend. 2. The effects of miscibility, polydispersity in chain length on the stress and strain behavior of interfaces are clarified. <p>(Problem)</p> <ol style="list-style-type: none"> 1. A quantitative assessment applying to realistic polymer system. 2. Application to semi-crystalline polymer.
References	<p>[Presentation]</p> <p>50-th koubunshi toronkai (2001/9)</p> <p>ICAPP2001 Yonezawa(2001/10)</p> <p>[Manuscript]</p> <p>Proceeding of ICAPP2001 Yonezawa</p>
KeyWords (in English)	coarse grained molecular dynamics, polymer blend, interface, SCF calculation, interfacial fracture, bulk failure, depletion

Results (Remarks)

- Three model systems were considered. The model-1 and model-2 are monodisperse systems with the same number-averaged molecular weight M_n but have different values of the interaction parameter. The model-3 is a polydisperse system with the same values of M_n and χ_{AB} .
- The stress-strain curves and the snapshot pictures of the interfacial region after the elongation are shown in Fig.1.
- A yielding point is clearly observed in each case. We found that the yield stress and the yield strain of the monodisperse system increase with increasing interfacial thickness. On the other hand, for the system with large interfacial thickness, both the yield stress and the yield strain become smaller than those for the monodisperse system with the same interfacial thickness.
- From the observation of the structure after the elongation, we found that the yield phenomenon of the polydisperse system is dominated by the failure of the interface where the long chains are depleted. Please see Fig.2.
- For the monodisperse system, the yield phenomenon is dominated by a void formation in the bulk phase.

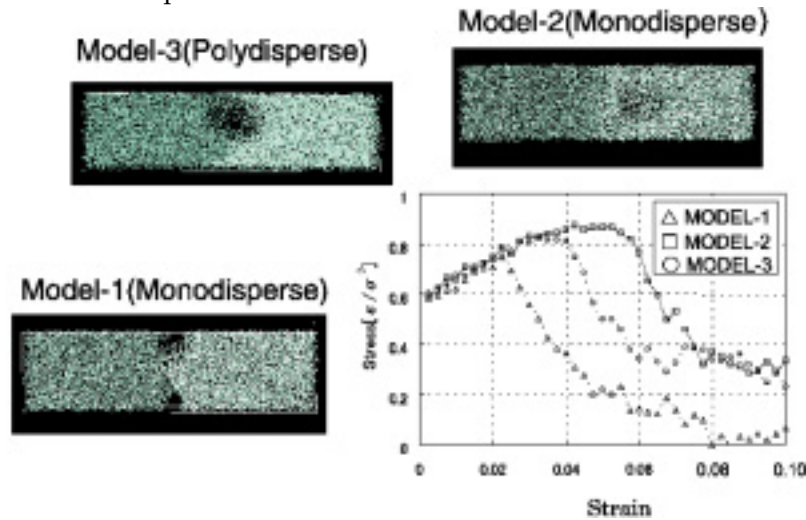


Fig.1 Stress - strain curves and snapshots of the interfacial structure after elongation.

Model-1 : $N_s=N_t=100$, $\chi_{AB}=0.25$. Model-2 : $N_s=N_t=100$, $\chi_{AB}=0.10$. Model-3 : $N_s=55$, $N_t=550$, $\chi_{AB}=0.10$

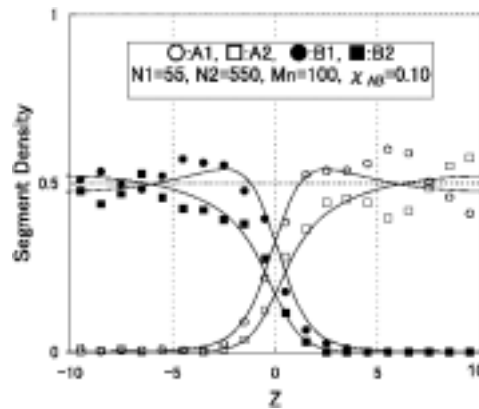


Fig.2 Density profiles of the segments belonging to each type of chains obtained from COGNAC (symbols) and from SUSHI (curves).