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Title	An analysis of loop/bridge ratio of triblock copolymer
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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. Stylene-Isoprene-Stylene, Stylene-Butadiene-Stylene)
Program (including analysis)	COGNAC v3 SUSHI 3
Method & Some important Input parameters	(Method) 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. (Inputs) 1. Polymer architecture (i.e. A3B24A3 triblock) 2. χ parameter
Advance & Problem	(Advance) 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. (Future work) A study of the relation between loop/bridge structure and properties (e.g. rubber elasticity) to predict an optimized chain structure.
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.

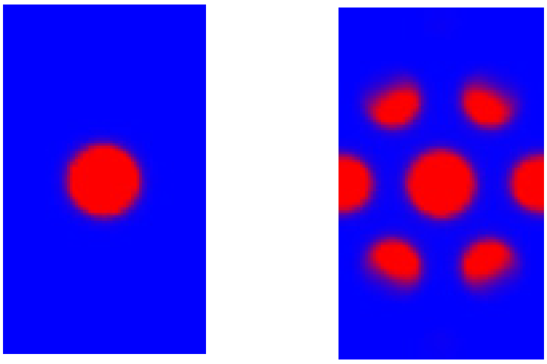

Figure 1. Volume fraction of the end segments of ABA triblock copolymer in a cylinder morphology. (a) fixed end, (b)free end

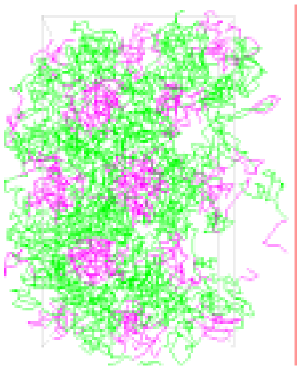

Figure 2. Snapshot structure of ABA triblock copolymer in a cylinder morphology

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