No. EAR2-011-02 First registration:2000/ 5/16 New: 2001/8/13

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. Stylene-Butadiene-Stylene, 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

$\chi_{AB} = 1.8$

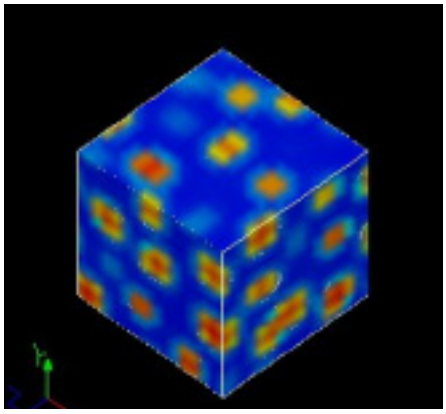

Figure 1 Density distribution by dynamics density functional calculation

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.

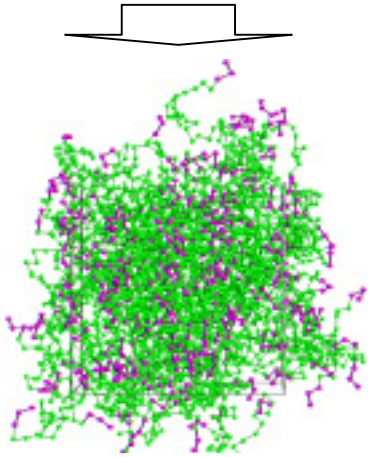

Figure 2 Initial chain configuration

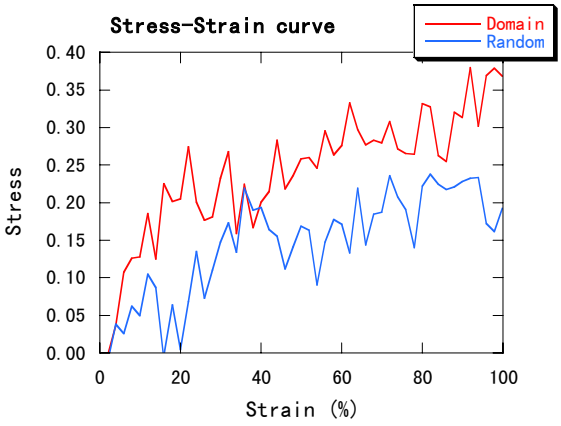

Figure 4 Stress-strain curve by coarse-grained molecular dynamics simulation

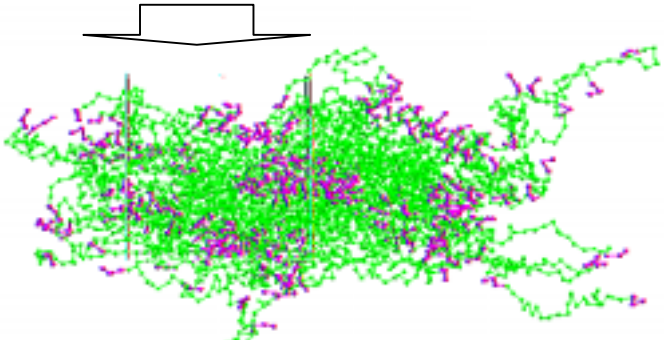

Figure 3 Elongated chain structure