

Title	Study of the relation between χ parameter and Lennard-Jones parameter
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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	(Method) 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 (Inputs) 1. Polymer architecture, i.e. A100/B100 2. χ parameter and Lennard-Jones parameter
Advance & Problem	(Advance) A quantitative relation between χ parameter and Lennard-Jones parameter is obtained. (Future plan) A quantitative assessment applying to realistic polymer system.
References	[Presentation] 14-th bunshi simulation toronkai p141 (2001) ICAPP2001 Yonezawa(2001/10) [Manuscript] Proceeding of ICAPP2001 Yonezawa
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))

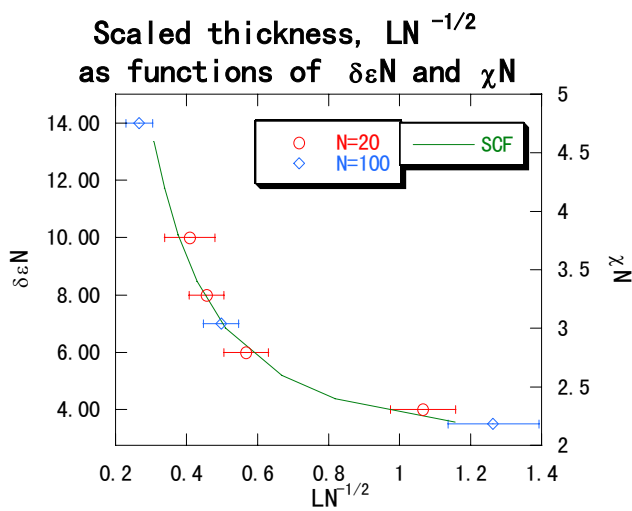


Figure 1

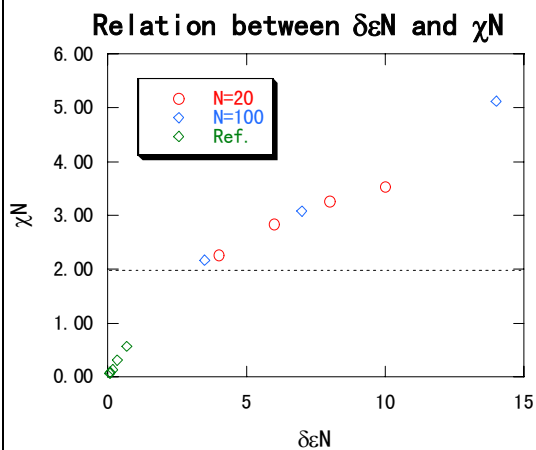


Figure2 (a)

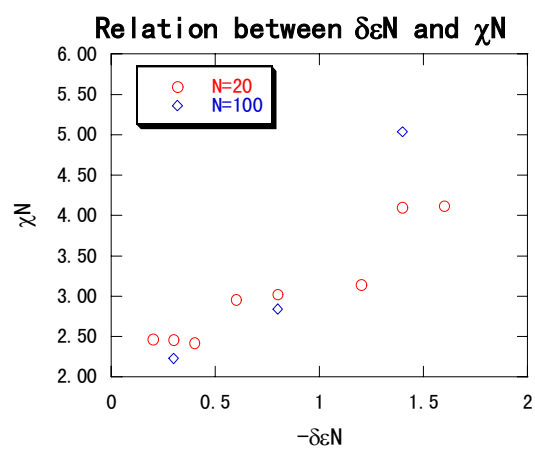


Figure2 (b)

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