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Title	Study of interface strength of polymer blend
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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	(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. Elongation unit cell during MD simulation (Inputs) 1. Polymer architecture, i.e. A100/B100 2. χ parameter 3. Interaction parameter for bead-spring model
Advance & Problem	(Advance) 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. (Problem) 1. quantitative assessment applying to realistic polymer system. 2. Application to semi crystalline polymer.
References	[Presentation] - 50-th koubunshi toronkai (2001/9) - ICAPP2001 Yonezawa(2001/10) [Manuscript] - 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, (~ Rg), 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 ($\delta\varepsilon N=0.0$) except $-\delta\varepsilon$ 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.

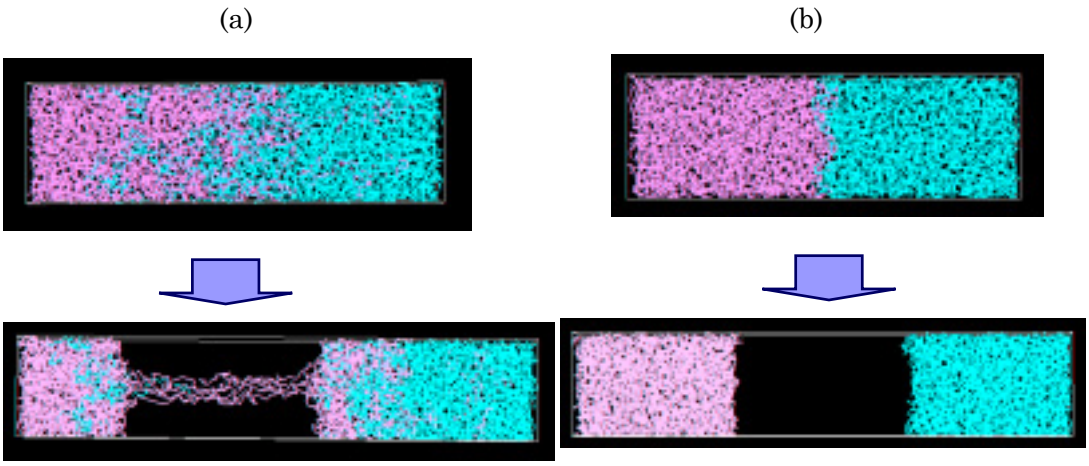

Fig.1 Snapshot structure of polymer blend at interface during elongation,
(a) thick interface ($-\delta\varepsilon N=0.3$), (b) thin interface ($-\delta\varepsilon N=10.0$).

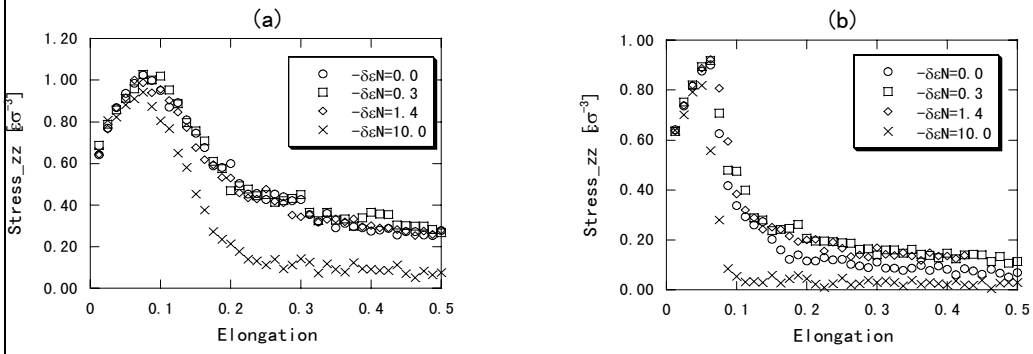

Fig.2 Stress-strain curve of polymer blend at interface.
Initial strain rate, $d\varepsilon/dt$: (a) 2.08×10^{-3} [τ^{-1}] (b) 2.08×10^{-4} [τ^{-1}]