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Title	Study of interface strength of polymer blend with polydispersity
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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	(Method) 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 (Inputs) 1. Polymer architecture, i.e. A55/A550/B55/B550 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, polydispersity in chain length on the stress and strain behavior of interfaces are clarified. (Problem) 1. A 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, 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 Mn but have different values of the interaction parameter. The model-3 is a polydisperse system with the same values of Mn 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.

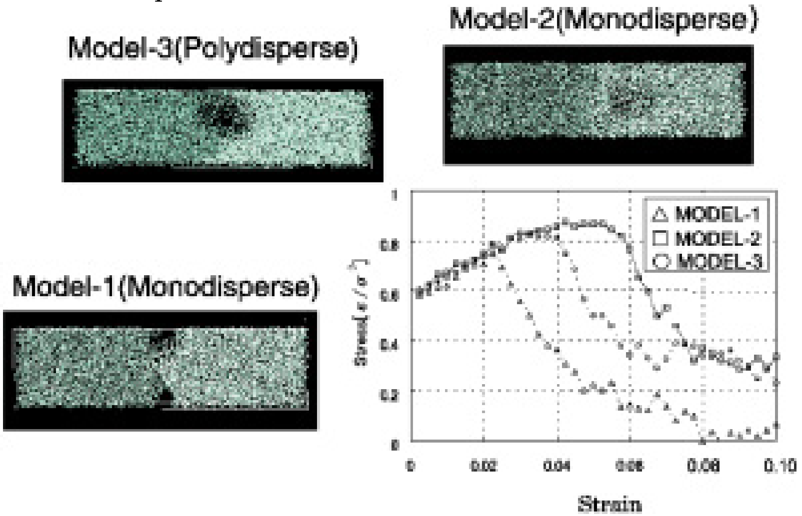

Fig.1 Stress - strain curves and snapshots of the interfacial structure after elongation.
Model-1 : $N_s=N_l=100$, $\chi_{AB}=0.25$. Model-2 : $N_s=N_l=100$, $\chi_{AB}=0.10$. Model-1: $N_s=55$, $N_l=550$, $\chi_{AB}=0.10$

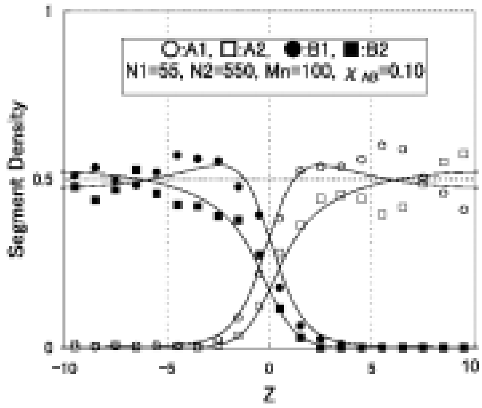

Fig.2 Density plofiles of the segments belonging to each type of chains obtained from COGNAC (symbols) and from SUSHI (curves).