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Title	Prediction of interfacial tension of an A/B polymer blend
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Purpose of this study	Analysis of polydispersity effects on the interfacial tension of an A/B homo polymer blend
System (Material)	Polymer blends with polydispersity
Program (including analysis)	SUSHI, FluidSimulator
Method & Some important input parameters	(Method) 1-dimensional canonical SCF (statics) (Inputs) Flory-Huggins segment interaction parameter Volume fraction and segment numbers of each polymer
Advance & Problem	(Advance) - FluidSimulator equilibrates the system and calculates the volume fraction profiles of all components and the interfacial excess free energy (interfacial tension). - Components can be polymers (homo-polymers, block- or graft-copolymers, etc) or solvents. (Problem) - Molecular design of compatibilizer
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)]
KeyWords (in English)	interfacial excess free energy, polymer architecture, polydispersity, equilibrium interfaces,

Results (Remarks)

Output: interfacial excess free energy, etc.
Analysis:polydispersity effects on the interfacial tension

[Example of analysis]
- The effects of polydispersity on the polymer interfaces are investigated for A/B binary homopolymer mixtures where both polymers have molecular weight distributions. The equilibrium structure of the polymer blend is obtained by the 1-dimensional static SCF calculation under the Neumann boundary condition. Let us denote the segment density of the i type chains as $\phi^{\alpha}{}_{i}$ where α specifies each of the coexisting equilibrium phase. Using $\phi^{\alpha}{}_{i}$ and the equilibrium free energy F, one can calculate the free energy of the bulk phase f^{bulk} and the equilibrium chemical potential of each component μ_i.
- Then, the excess free energy F^{excess} is calculated as follows. The volume fraction ,segment numbers and system size are expressed as $\phi^{0}{}_{i}$, N_i and L.

$$f^{bulk} = \sum_i \frac{\phi_i^{\alpha}}{N_i} \ln \frac{\phi_i^{\alpha}}{N_i} + \frac{1}{2} \sum_{ij} \chi_{ij} \phi_i^{\alpha} \phi_j^{\alpha}$$

$$\mu_i = 1 + \ln \frac{\phi_i^{\alpha}}{N_i} + N_i \sum_j \left(\chi_{ij} \phi_j^{\alpha} - \frac{\phi_j^{\alpha}}{N_j} \right) - \frac{1}{2} N_i \sum_{ij} \chi_{ij} \phi_i^{\alpha} \phi_j^{\alpha}$$

$$F^{excess} = LF - Lf^{bulk} - L \sum_i \frac{\mu_i \left(\phi_i^{0} - \phi_i^{\alpha} \right)}{N_i}$$

Results

- We investigated molecular weight dependence of the excess free energy by changing the chain length and the volume fraction
- Each system shows almost the same behavior, which resembles to that of the molecular weight dependence of a mono disperse polymer blend system.
- It asymptotically approaches the theoretical value of the interfacial tension obtained by Helfand and Tagami[1] in the limit of infinite molecular weight.

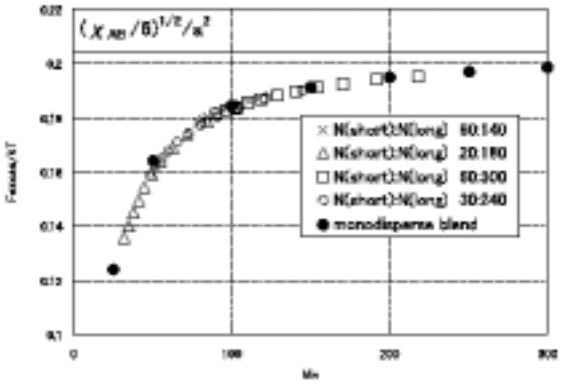

Fig.1 Molecular weight dependence of the excess free energy.(χ_{AB}: 0.25)

(1) Helfand,E. and Tagami, Y. :J.Chem.Phys.,62,1327(1975)