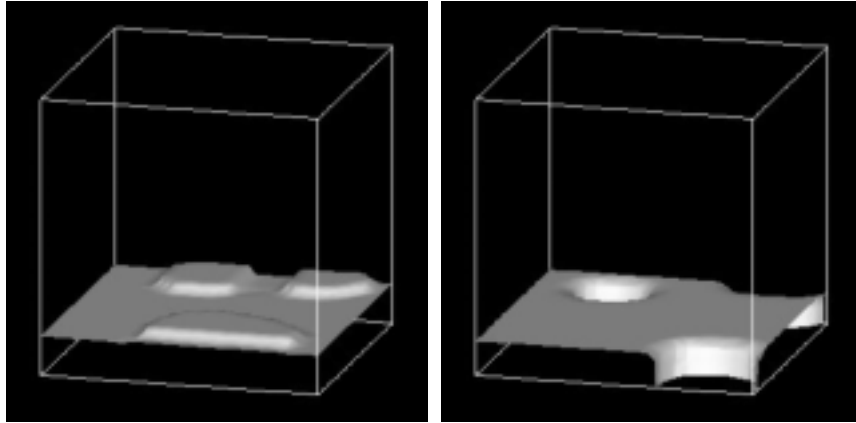| Title	Analysis of the interfaces of the phase separated structures in ultra thin polymer films
Researchers	Hiroshi Morita, Toshihiro Kawakatsu, and Masao Doi
Purpose of this study	Development and research of the method to analyze the phase separated structures of ultra thin polymer films which would be constructed by spin cast.
System (Material)	Homopolymer blend system (target : PS/PVME)
Program (including analysis)	MesoSimulator990827 version

Method & Some important input parameters	(Method)
	 Dynamic mean field density functional method
	 (Scheutjens-Fleer model + Cahn-Hilliard eq.)
	(Inputs)
	    Polymer Polymer A (corresponds to PS), polymer B (corresponds to PVME), Void(for air layer). volume fraction, length, and species for each polymer must be set.
	    Parameters of interactions
	            Potential from wall (like χ parameter)
	            Segment-segment interaction parameter(χ)

Advance & Problem	(Advance) - We can simulate the surface roughening structure at free surface of thin films consistently with experiments. (Experimental: Macromolecules, 28, 934, (1995)) - We can simulate the cylindrical phase separated structure in thin films under the surface roughening conditions. (Experimental: Macromolecules, 29, 3232, (1996)) - Construction of the phase diagrams of surface roughening conditions using the equilibrium of interfacial tension was succeeded. - The obtained film thickness by our simulation was from 10 nm to 20 nm.(using $(Rg)^2 = Nb^2$) (Problem) - Quantitative correspondence between the simulation and experiments. (including χ parameters)
References	[Manuscript] [Presentation at conferences (Meetings)] International Polymer Conference99(at Yokohama 1999.10)
KeyWords (in English)	Thin film, surface roughening, interfacial tension, phase diagram, cylindrical structure, mean field, dynamic density functional method, neumann triangle

Results (Remarks)

Output : Density field and it's time dependent.
Analysis : Phase separation dynamics.

Figures: Interfacial structures of thin polymer blend films
Left Figure: Computational results of the surface roughening structure at free surface (at the case of roughening) .
Right Figure: Computational results of the cylindrical phase separated structure. (interfacial structure of polymer A)

[Example of analysis]
Phase diagram for the surface roughening at free surface.