

No. EAR2-017-02

First registration: 2000/ 5/18 New: 2001/ 11/21

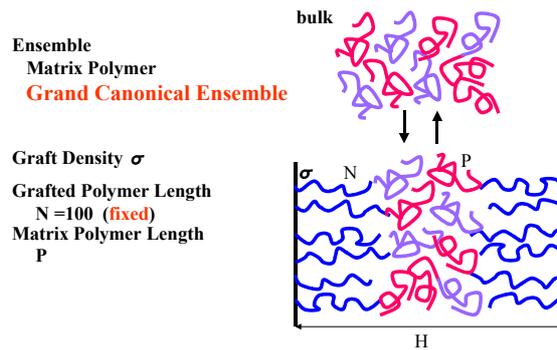
Title	Interaction between polymer grafted walls
Researchers	Takashi Honda, Hiroya Kodama, Toshihiro Kawakatsu
Purpose of this study	Calculate the interaction between colloidal particles and predict the dispersity of the particles.
System (Material)	Polymer solutions with polymer grafted particles.
Program (including analysis)	InterfaceSimulator-branch-SurfaceVer. 1.0 / SUSHI Ver. 3.0
Method & Some important input parameters	(Method) Static SCF(Self-consistent field) method (Inputs) Grafting density, Chain length of grafted chain, Composition of the polymer solution
Advance & Problem	(Advance) We can estimate the interaction whether it is attractive or repulsive between polymer grafted particles in the polymer solution. (Problem) We assume that the radius of the particle is large enough than the polymer length and the surface grafted by polymers is assumed as the plane surface. It is need to consider different model to calculate the system with small particles.
References	[Manuscript] Submitted/Accepted(/) [Presentation at conferences (Meetings)] ACS National Meeting(at San Francisco 2000 Mar.), Computers in Chemistry #148
KeyWords (in English)	SCF, graft, free energy, excess free energy, brush

Results (Remarks)

Simulation model: One dimensional model

The two walls grafted by polymers were dipped into the polymer solutions. The length of the grafting chain and the chain in the solution were N and P .

We set the $N=100$ and vary the P . The interaction between the segments are set to zero (good solvent solution)



Output: Excess free energy (It can be considered as the interaction energy.)

The concentration of the polymer solution set to 50 %. The result is follows.

The condition of attractive interaction can be seen with large P .

The large grafting density enhances the effect.

