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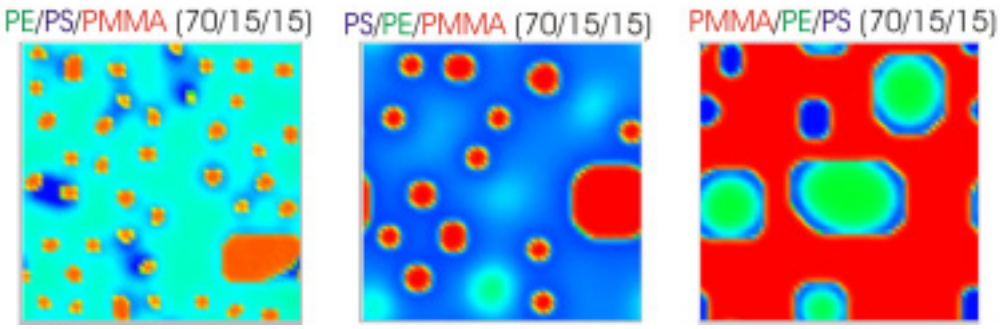
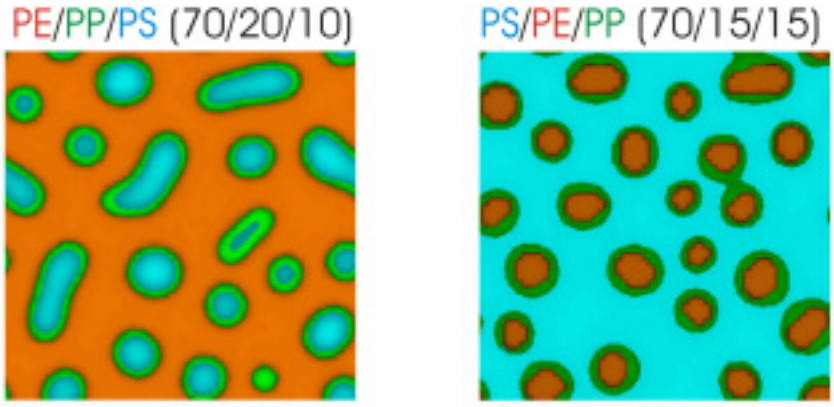
Title	Inspection of the domain structure for actual polymer blends
Researchers	Shinzi Urashita
Purpose of this study	To verify the Scheutjens-Fleer-Fry mean field calculation as the application to the actual polymer system, reproducing the domain structure by using the estimated interaction parameters for actual polymer blends was performed.
System (Material)	Ternary polymer blend Polyethylene / Polystyrene / Poly (methyl methacrylate) blend, Polyethylene / Polypropylene / Polystyrene blend
Program (including analysis)	Mesosimulator Release 981127, Release 990304 Mesosimulator-Viewer (analysis tool)
Method & Some important input parameters	(Method) the Scheutjens-Fleer-Fry mean field theory Hoftyzer & van Krevlen's method, Hoy's method (Input) Interation parameter, chain length, Kuhn length, blend ratio, density
Advance & Problem	Advance: For the estimated system, calculated results were consistent with the experiments. Problem: Verification of the parameters including the interaction parameter is indispensable for quantitative calculation.
Reference	
KeyWord (in English)	Ternary polymer blend, domain morphology, chi-parameter, Hoftyzer & van Krevlen's method, Hoy's method, group contribution method

Results (Remarks)

I estimated the domain structure of the polymer blends by the Scheutjens-Fleer-Fry dynamic mean field simulation with the interaction parameters estimated by van Krevlen's method. The following figures are the results of the polyethylene / polystyrene / poly (methyl methacrylate) for various blend ratio.



In the case that polyethylene or poly (methyl methacrylate) is major part, the minor components make the core-shell structure. In the other case where polystyrene is major part, the minor components make separated droplet.
I also estimated the domain structure of the blends of polyethylene / polypropylene / polystyrene for various blend ratio.



In the case that polyethylene or polystyrene is major part, the minor components make the core-shell structure like the previous figure.
The results are consistent with the experimental results.
(H. F. Guo, S. Packirisamy, N. V. Gvozdic and D. J. Meier *Polymer* **38**, 785 (1997))