

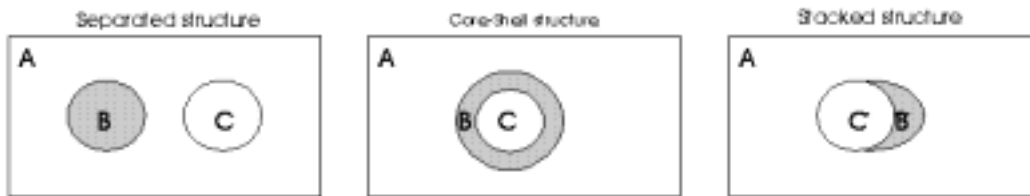
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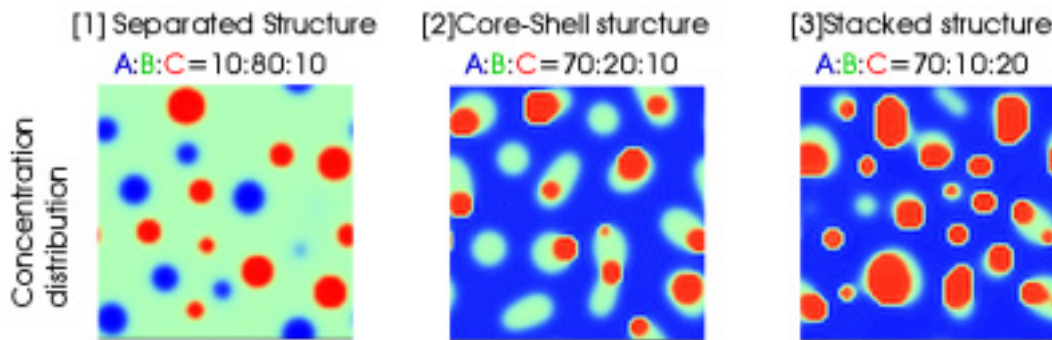
<b>Title</b>	Analysis of the structure of polymer blend system
<b>Researchers</b>	Shinji Urashita
<b>Purpose of this study</b>	To predict and estimate physical properties of polymer alloy, it is expected that we recognize the domain structure identification. Therefore, the methods for objective classification of each type of domain structures are useful.
<b>System (Material)</b>	Ternary polymer blend system
<b>Program (including analysis)</b>	MesoSimulator Release990304, dynamic mean fields simulation program Geoman: calculation tool for the Euler characteristic Conturn: generation tool for the colored contour
<b>Method &amp; Some important input parameters</b>	(Method) the Scheutjens-Fleer-Fry mean field theory, labeling algorithm, bi-cubic spline interpolation  (Inputs) Interaction parameter, chain length, blend ratio, concentration field
<b>Advance &amp; Problem</b>	(Advance) - By using Euler characteristic plot, the domain identification for ternary polymer blend is successful.  - Typical example for the domain identification is shown for the separated, core-shell, and stacked structures.
<b>References</b>	[Presentation at conferences (Meetings)] "The prediction of the domain morphology of polymer blend by using dynamic mean field simulation", S.Urashita and T.Kawakatsu, 14 <sup>th</sup> Molecular Simulation Symposium of Japan, 2P06 (2001)
<b>KeyWords (in English)</b>	Minkowski functionals, Euler characteristic, Domain morphology, Ternary polymer blend

## Results (Remarks)

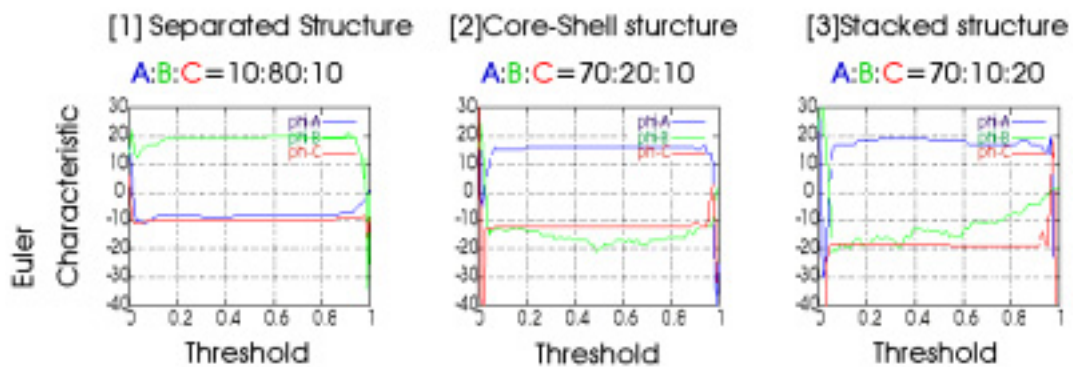
Typical domain structures for ternary polymer blend are following:



The simulation based on the Scheutjens-Fleer-Fry dynamic mean field theory generates the corresponding structures and the colored contours for each structure are given.



It is difficult to distinguish the structure [2] and [3] by eyes, thus method the Euler characteristic, it is one of Minkowski functionals and is defined as  $\chi(\rho) = N_{\rho}^{(7)} - N_{\rho}^{(t)}$ , is adopted for the guidepost of the domain identification. By using the colored contours, the plots for the Euler characteristic and threshold concentration are shown in the below.



It is clearly distinguished for each domain structures by the plots.