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Title	Calculation of elastic modulus of polymer blend
Researchers	Masahiro Noda, Makoto Sasaki, Takashi Taniguchi, and Masao Doi
Purpose of this study	Calculation of elastic modulus of polymer blend with phase separated structure
System (Material)	Polymer blend system (PP/SEBS)
Program (including analysis)	MUFFIN ver.2 (MSPD)
Method & Some important input parameters	(Method) Calculation and analysis of strain and strain energy by linear elastic theory (Inputs) elastic modulus of each blend component(bulk modulus and shear modulus), density field
Advance & Problem	(Advance) - We can calculate the elastic modulus of the system with phase separated structure. These values are in good agreement with the value predicted theoretically. - We can use SUSHI or MUFFIN_MSPD data as an input of the density field required for this calculation.
References	[Manuscript] Application report “AMUSE”
KeyWords (in English)	polymer blend, PP, SEBS, linear elasticity, phase separation, bulk modulus, shear modulus, Young’s modulus, strain energy

Results (Remarks)

Output: strain, strain energy etc.
Analysis: total elastic modulus

[Example of analysis]

Input parameter

-Elastic modulus
<PP>
G=1.0(MPa), K=833.333(MPa)
<SEBS>
G=0.50(MPa), K=2000(MPa)

Method

-Simulation of independent displacements, at least two or more kinds
-Total strain energy *f* and distortion is plotted based on the following equation (Fig.1-b)).

$$\sum f = G_{ave} \sum \left(e_{ij} - \frac{1}{d} \delta_{ij} e_{II} \right)^2 + K_{ave} \sum \frac{(e_{II})^2}{2}$$

-The cross point is averaged elastic modulus to be calculated.

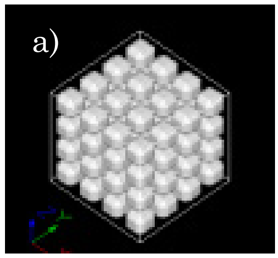
Results

As a result of this technique applied to sphere (dispersed), bicontinuous structure, the modulus was described by the following simple models. (Fig. 2).

$E = \phi_1 E_1 + \phi_2 E_2$ … parallel model

$E^{1/5} = \phi_1 E_1^{1/5} + \phi_2 E_2^{1/5}$ … Davies model

$\frac{1}{E} = \frac{\phi_1}{E_1} + \frac{\phi_2}{E_2}$ … series model



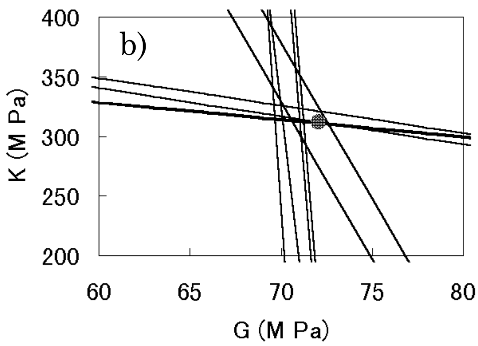


Fig.1a) Example of dispersed structure (white: SEBS).
b) Example of analysis of the simulation using the structure shown in Fig.1-a).

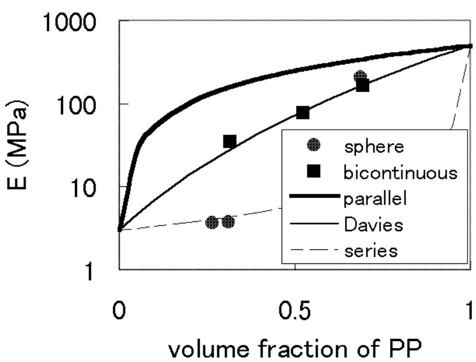


Fig.2
Comparison with the simulation and the theoretical equations. Symbols are for the simulation and lines are for the theory.