Prototype of virtual experiments

AMUSE

(Advanced Materials design Using Simulation Engines)

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JCII, Doi project

Outline

- Introduction
- Lamella structure of semi-crystalline polymers
- Bulk elasticity of PP/elastomer blends
- Interfacial strength of PP/elastomer blends
- Summary

Introduction

AMUSE is an exploratory project conducting a virtual experiments by cooperating two or more simulation programs and the platform.

Test material : Polypropylene(PP) materials (PP/elastomer blend)

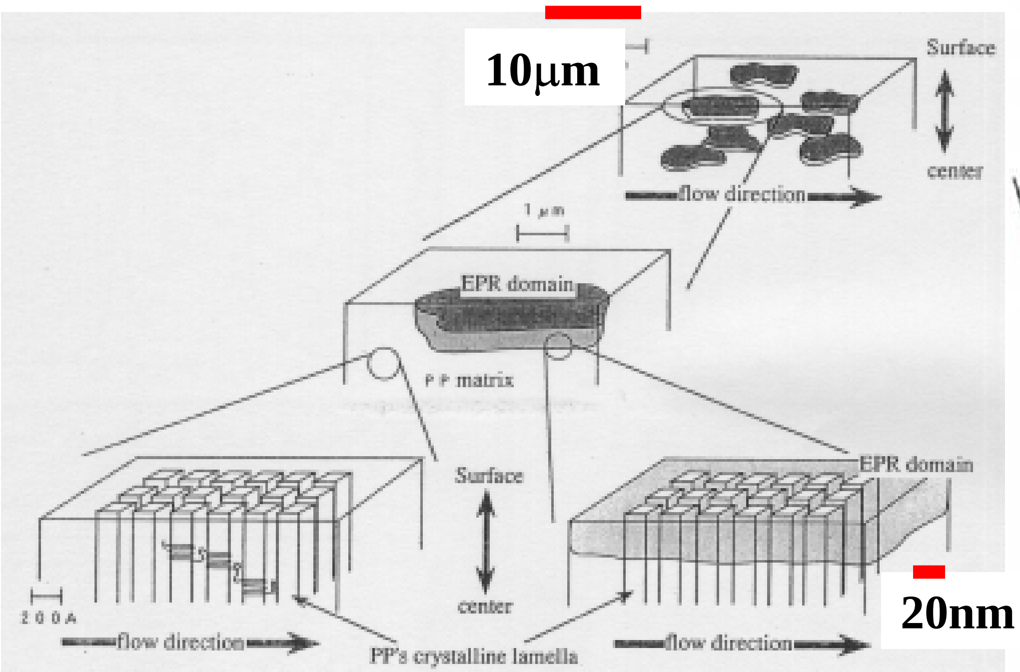
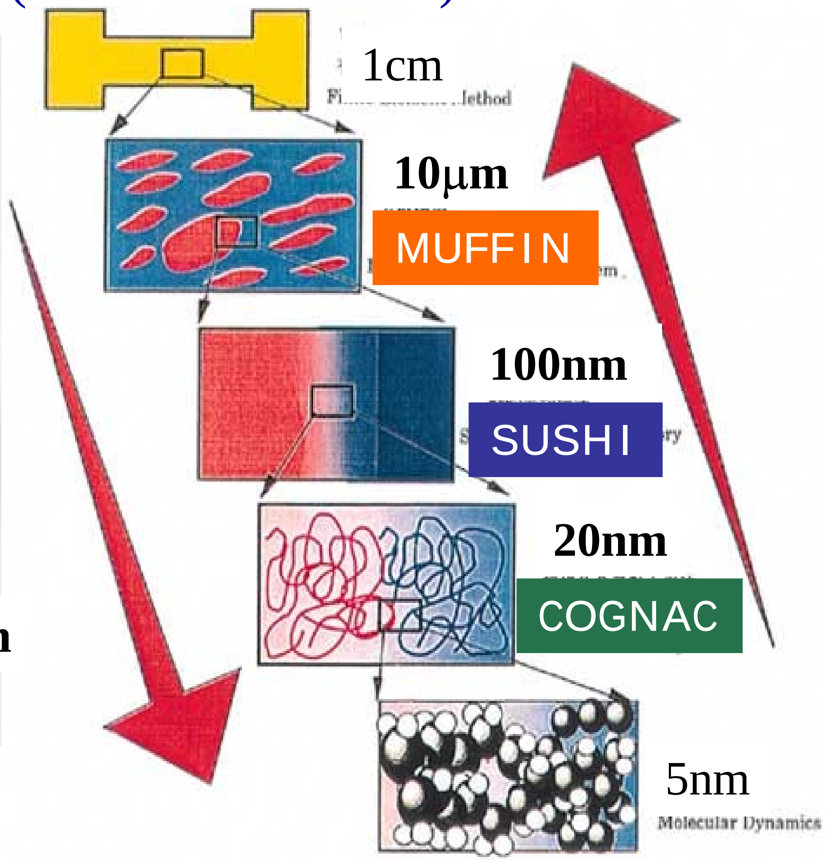


Fig. 8. The model of SOP's highly ordered structure.

T. Nomura, T. Nishio, H. Tanaka, K. Mori,
Japanese Journal of Polymer Science and Technology,
vol.52, N0.2, pp.90-96 (1995))



Ultimate Goal : Seamless Zooming !!

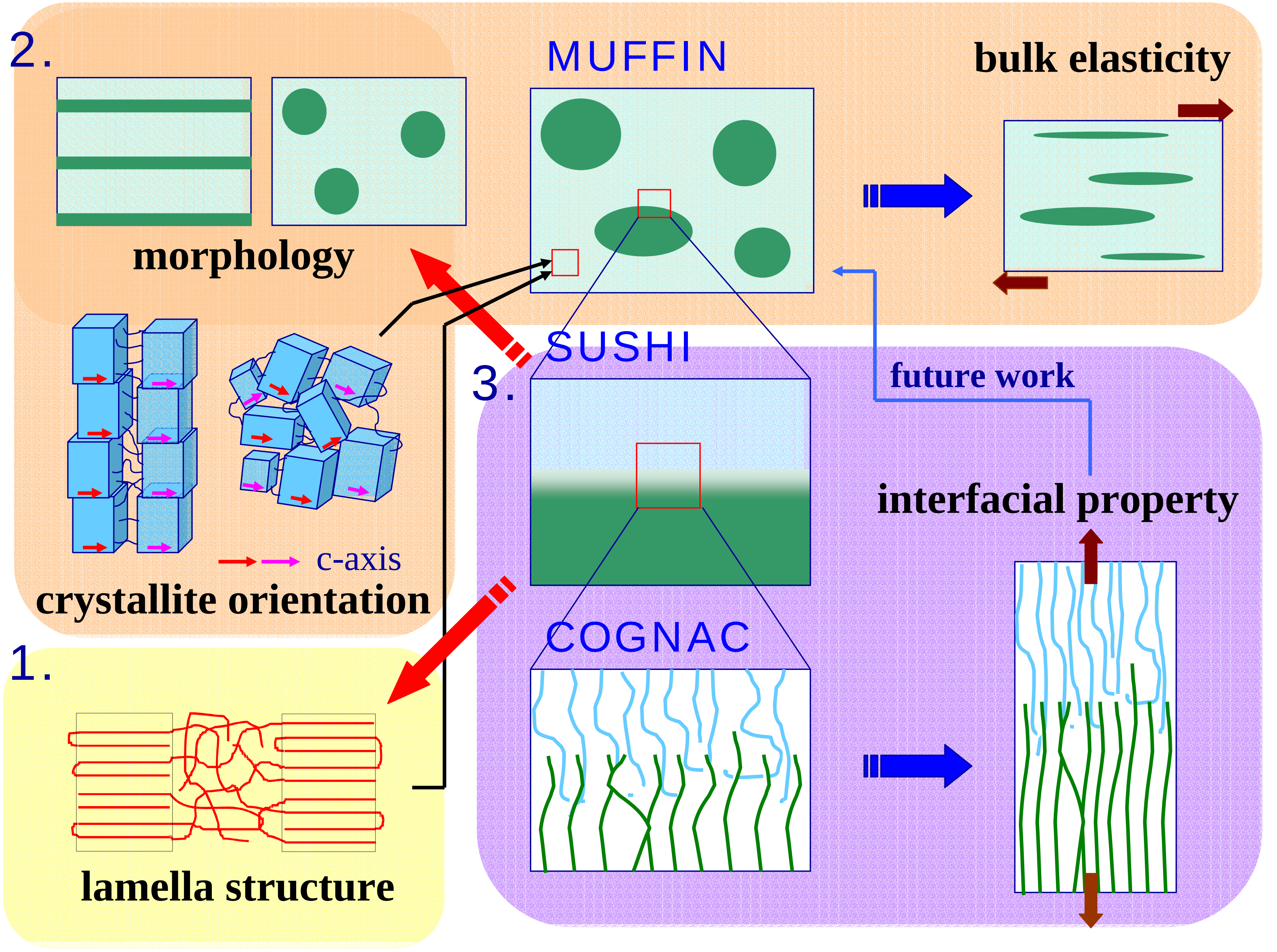
Important properties of PP materials

PP material design

stiffness

toughness

- Lamella structures of alternating crystalline and amorphous phases.
- Tie molecules related to the molecular weight and tacticity of polypropylene.
- Orientation of the polypropylene crystallite.
- Morphology of a polypropylene/elastomer blend.
- Conformation at a polypropylene/elastomer interface.


2.
MUFFIN
bulk elasticity
morphology
c-axis
crystallite orientation
SUSHI
3.
future work
interfacial property
COGNAC
1.
lamella structure

AMUSE

1. Lamella structure of semi-crystalline polymers.
 - Generate the initial semi-crystalline lamella structure by zooming from SUSHI to COGNAC.
 - Predict the elasticity of the PP crystal using the model of amorphous layer.

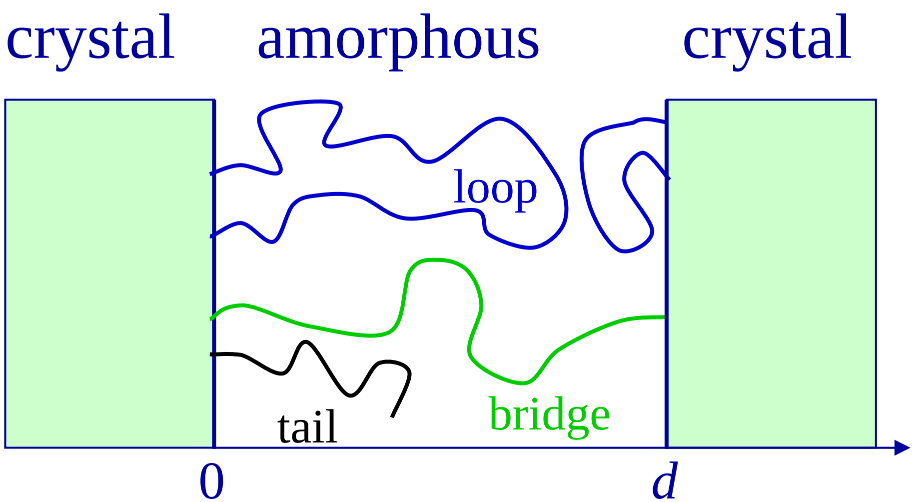
2. Bulk elasticity of PP/elastomer blends.
 - Predict the elastic modulus of PP materials by zooming from SUSHI to MUFFIN.

3. Interfacial strength of PP/elastomer blends.
 - Generate the initial structure of polymer chain at an interface by zooming from SUSHI to COGNAC.
 - Study the interfacial properties of PP/elastomer blends.
 - Predict the mechanical properties of bulk materials using the physical properties at the interface (future work).

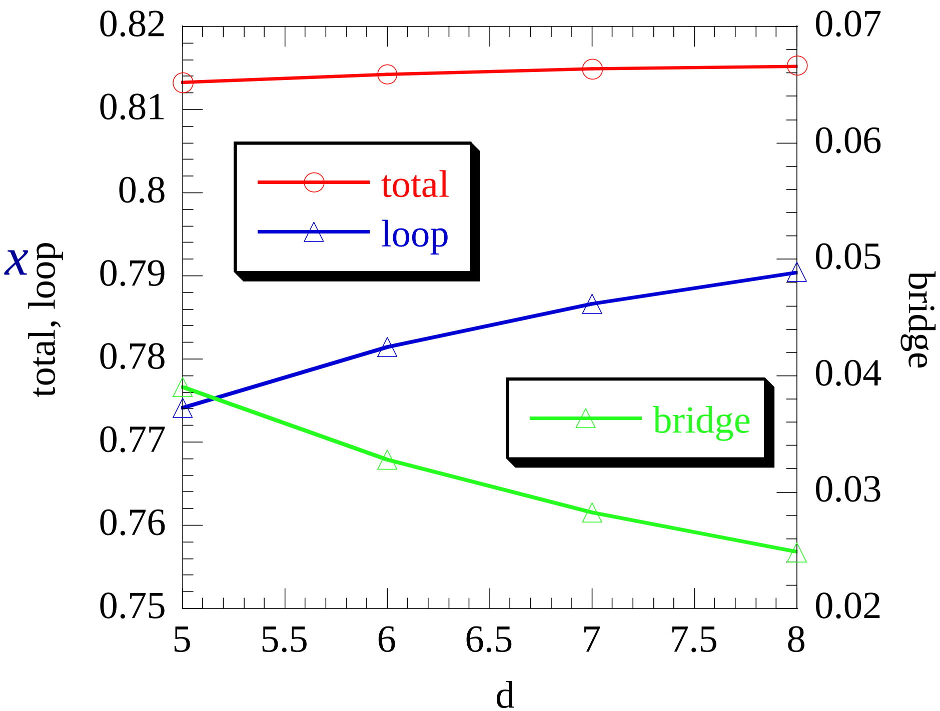
Lamella structure of semi-crystalline polymers

Kodama

Calculation of the chain conformation in an amorphous layer (SUSHI).



Loop bridge fraction for infinite chain.



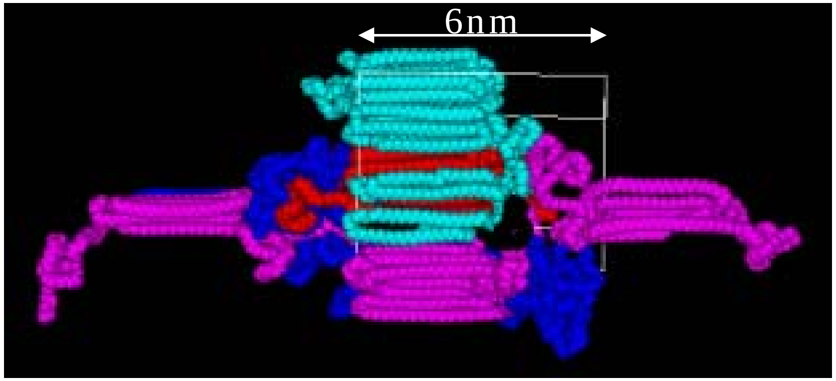
Parameters :
Long period, Crystallinity,
Molecular weight,
Molecular weight distribution,
Branching ...

Lamella structure of semi-crystalline polymers

Shoji & Aoyagi

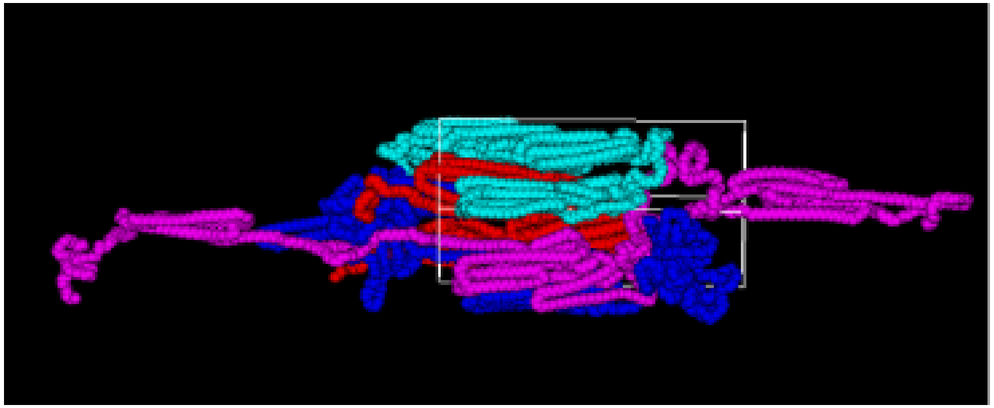
Generating lamella structure by using a method of COGNAC.

COGNAC can generate a lamella structure of semi-crystalline polymer using the conformation distribution of loop and bridge obtained by SUSHI,.



elongation

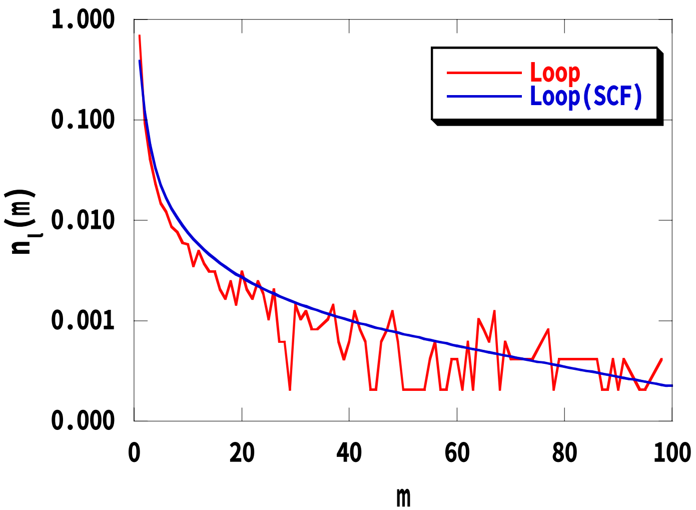
Molecular dynamics simulation of the stretching of the lamella structure.



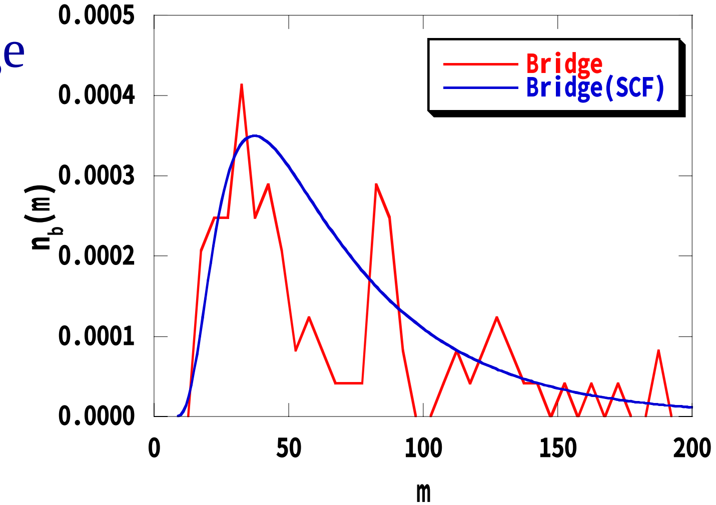
Lamella structure of semi-crystalline polymers

Aoyagi

Loop



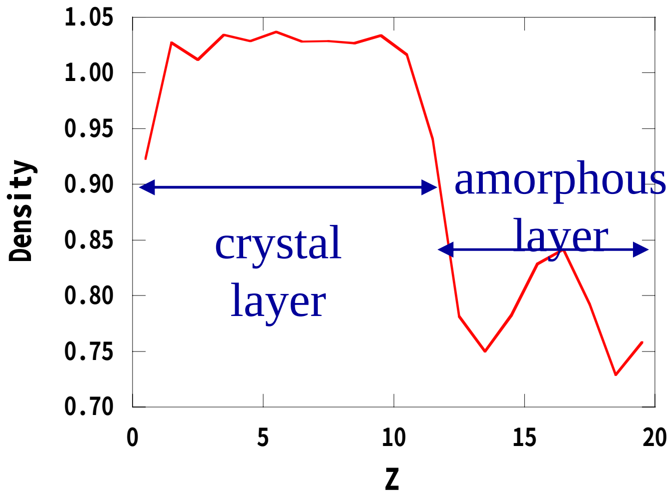
Bridge



bead-spring model

4 chains with 1200 beads

Density profile

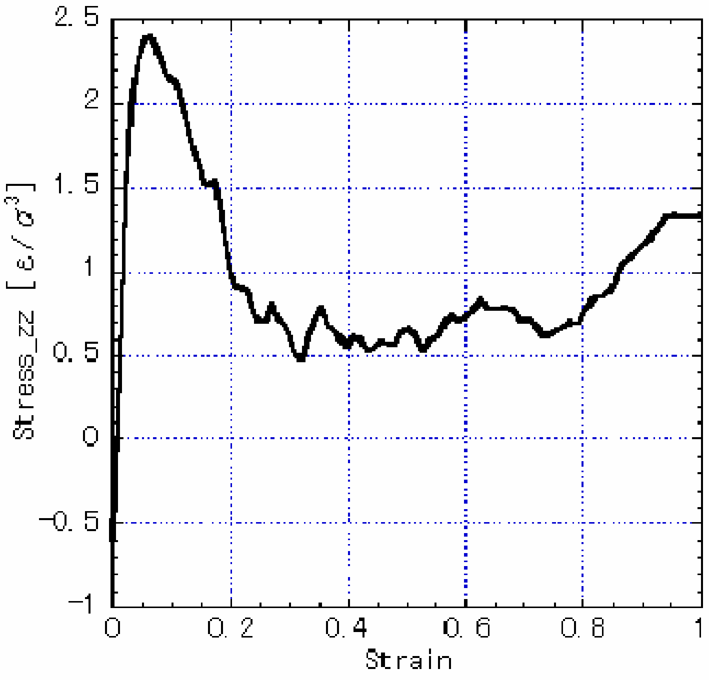


Lamella structure of semi-crystalline polymers

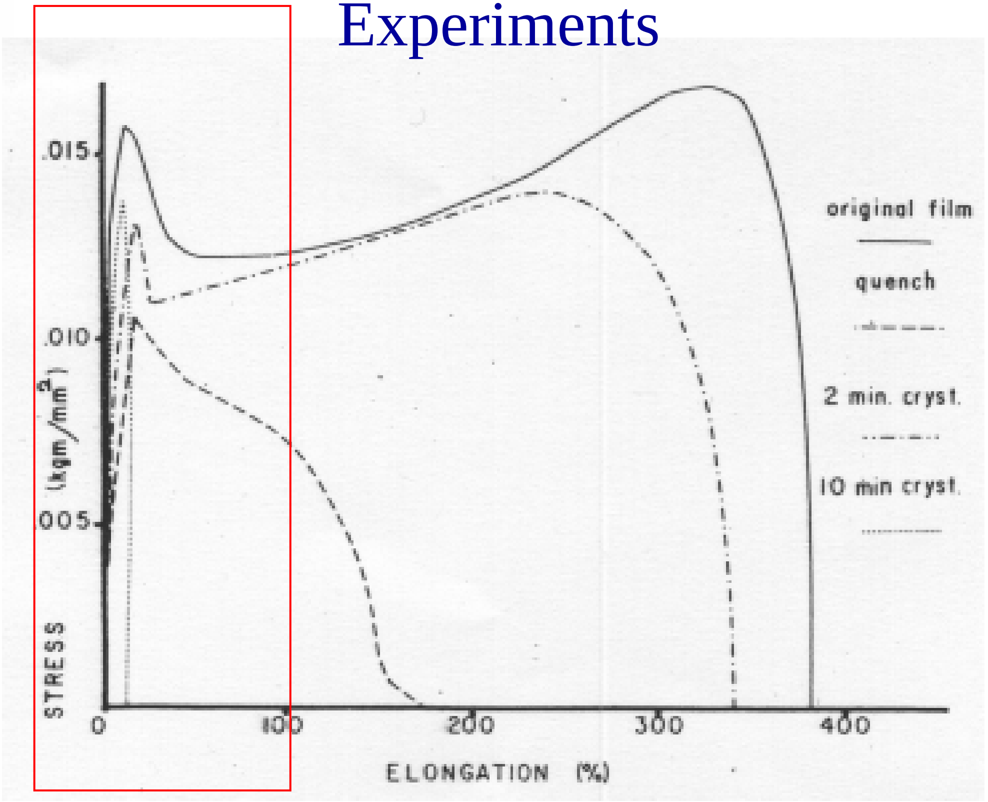
Shoji

Stress-strain curve

Simulation



Experiments



L. Barish, J. Appl. Polymer Sci., 6, 617 (1962)

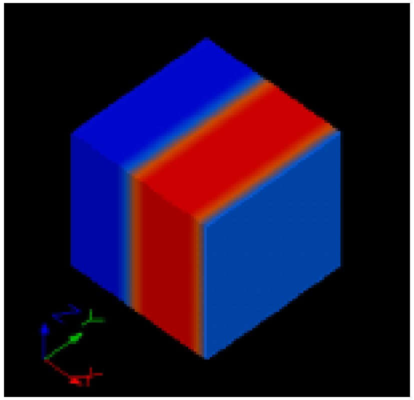
Bulk elasticity of PP/elastomer blends

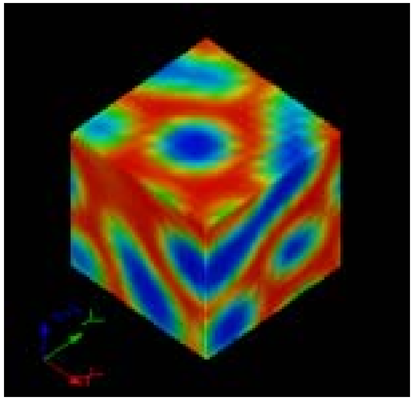
Noda & Sasaki

Zooming from SUSHI to MUFFIN.

SUSHI

Morphology of PP/elastomer blends

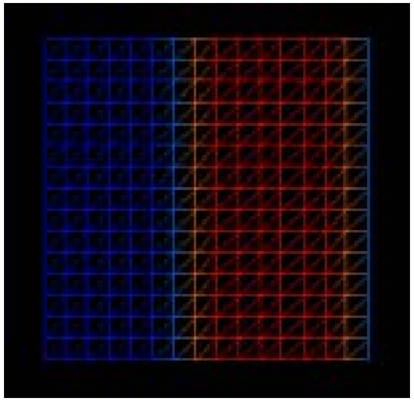




volume fraction of component A

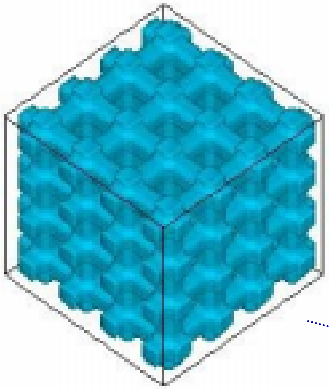
MUFFIN

Elastic modulus of the material having some morphology

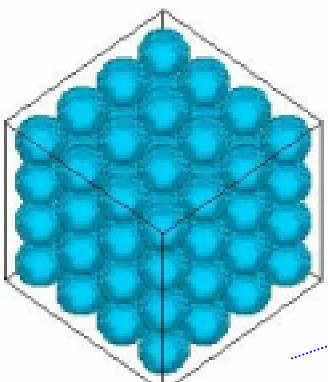


Bulk elasticity of PP/elastomer blends

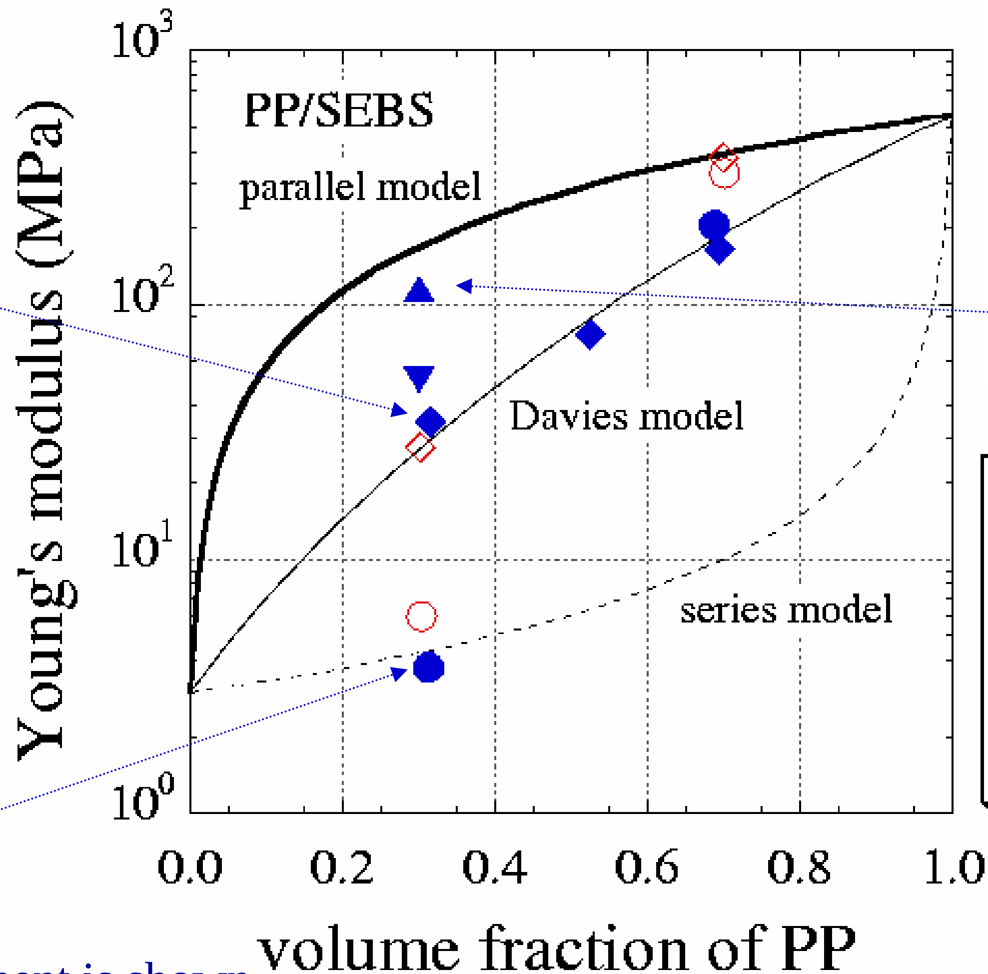
Noda

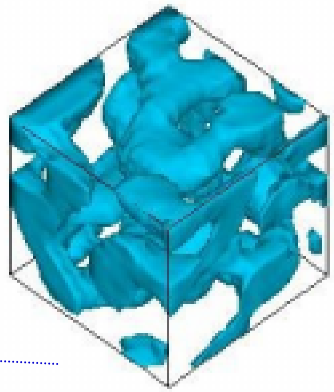


Bicontinuous



Dispersed





WI & NI

The only minor component is shown.

Veenstra, H., et al., Polymer, 41, 1817 (2000)

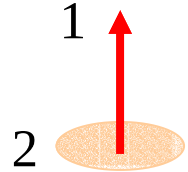
Bulk elasticity of PP/elastomer blends

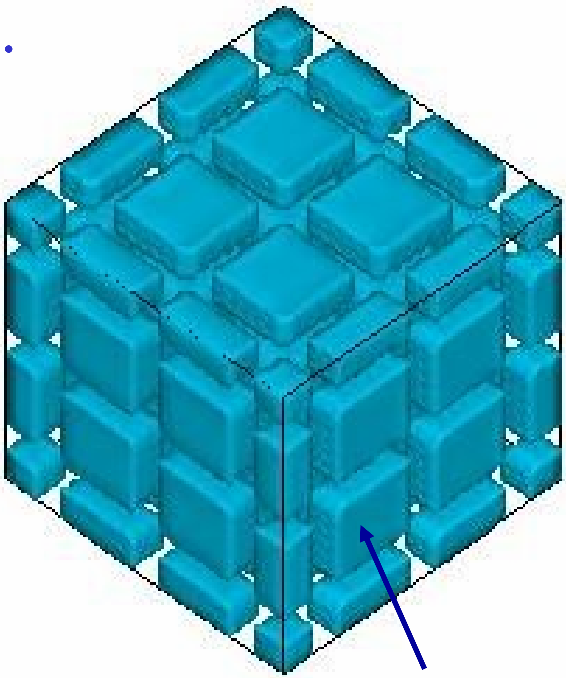
Noda

Calculation of elasticity of oriented crystallite.

Anisotropic elastic moduli used for the calculation are obtained by COGNAC.

c-axis
(molecular axis)





crystallite

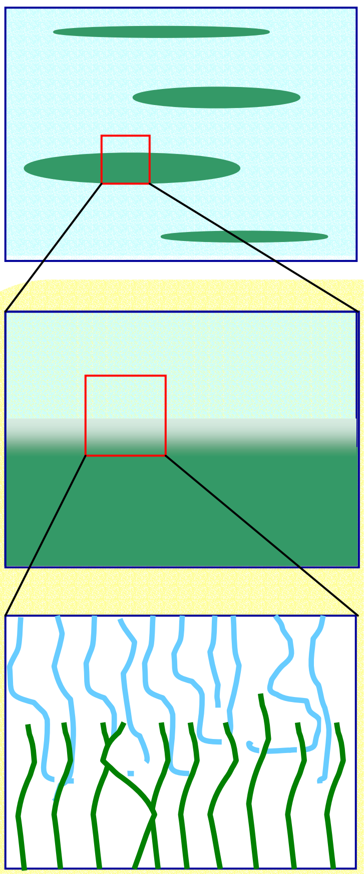
High orientational case (anisotropic) $E_{1,ave}$:1100 (MPa)

$E_{2,ave}$: 58 (MPa)

Random case(isotropic) E_{ave} : 550 (MPa)

Interfacial strength of PP/elastomer blends

Yokomizo & Aoyagi



MUFFIN — Structure formation under shear

Predict PP/elastomer morphology under shear.

SUSHI — Interfacial thickness, Chain conformation

Calculate the chain conformation at the interface.

COGNAC — Stress-Strain curve

Calculate the interfacial strength at the interface

MUFFIN — Toughness etc. (Future work)

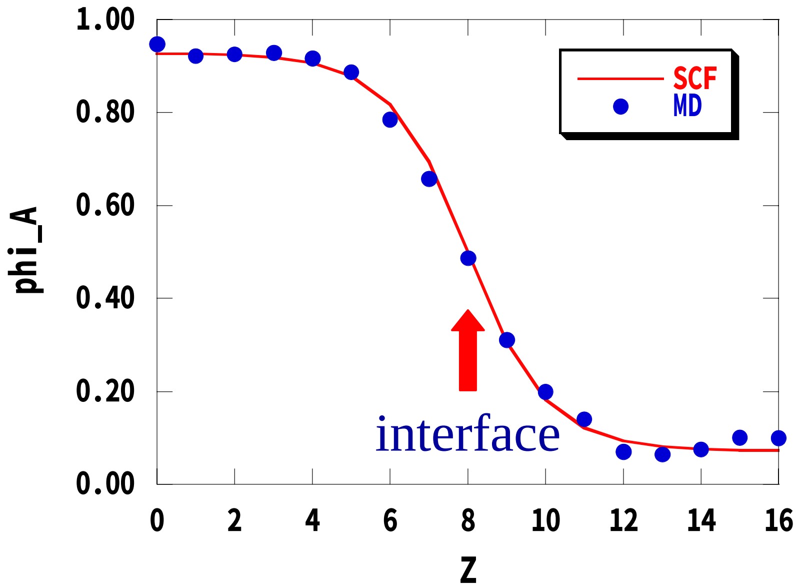
Predict the mechanical properties of bulk material reflecting the physical properties at an interface.

Interfacial strength of PP/elastomer blends

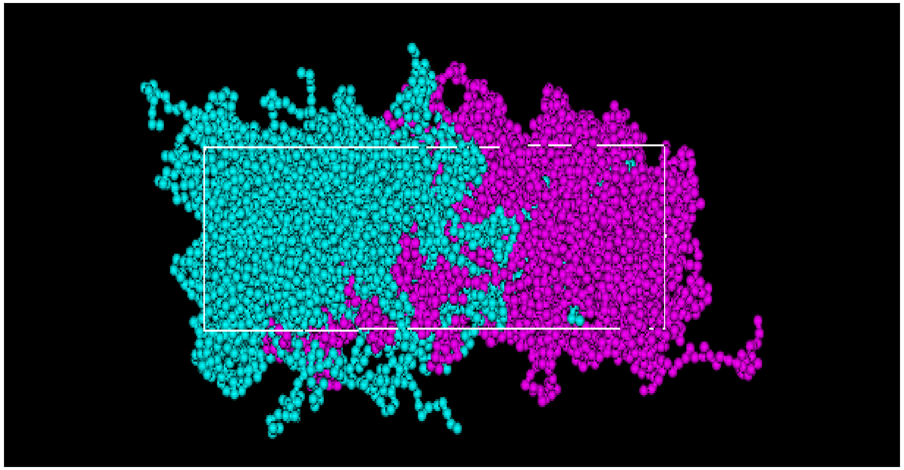
Aoyagi

A method of generating the initial structure of polymer chains at an interface by zooming from SUSHI to COGNAC.

SUSHI
1D calculation
Neuman boundary condition



COGNAC
bead-spring model(1bead=1SCF segment)
Staggered reflective boundary condition



Interfacial strength of PP/elastomer blends

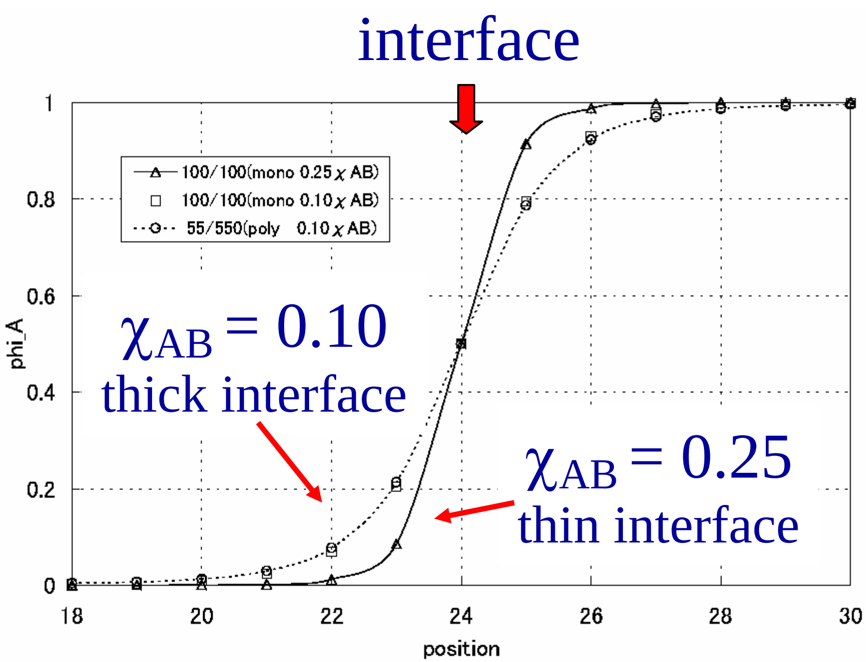
Yokomizo

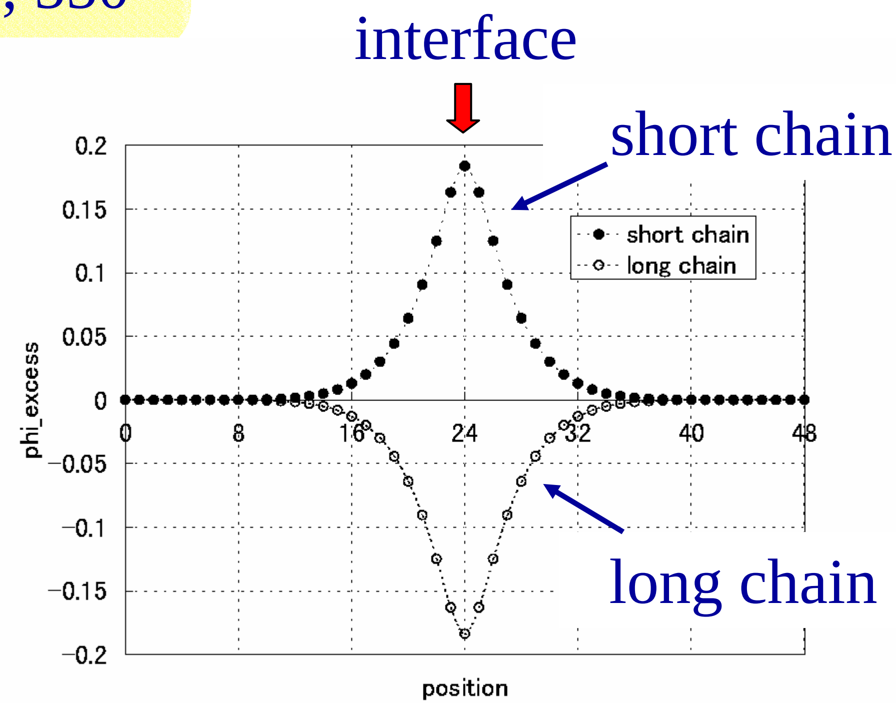
Effects of polydispersity on the interfacial properties.

AB polymer blends

monodisperse : A100 / B100

polydisperse : A55, 550 / B55, 550



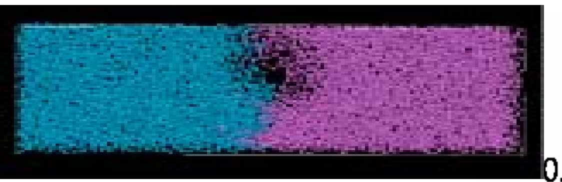


Interfacial strength of PP/elastomer blends

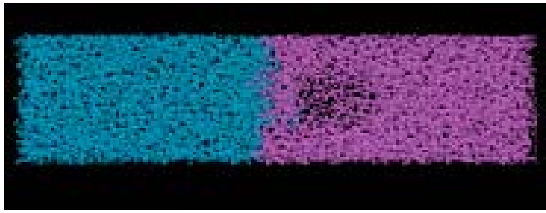
Yokomizo

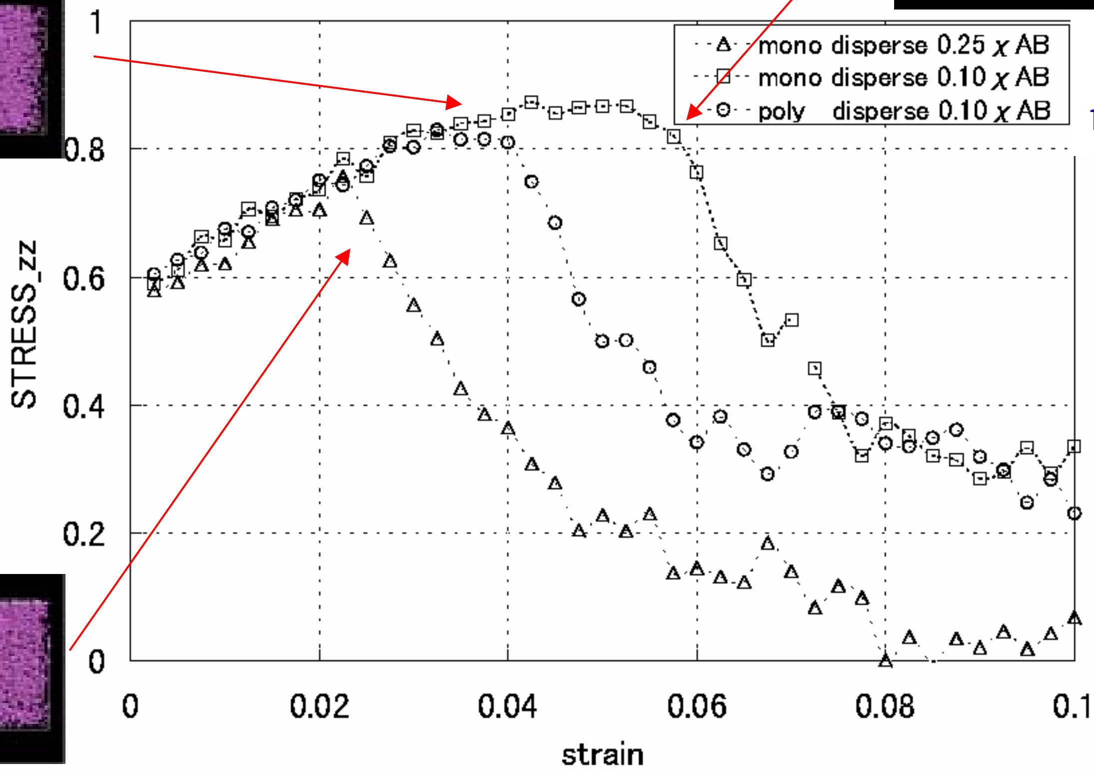
Effects of polydispersity on the stress-strain behavior.

polydisperse thick interface

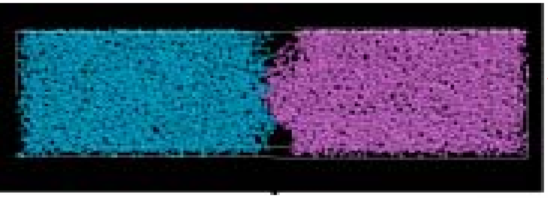


monodisperse thick interface





monodisperse thin interface

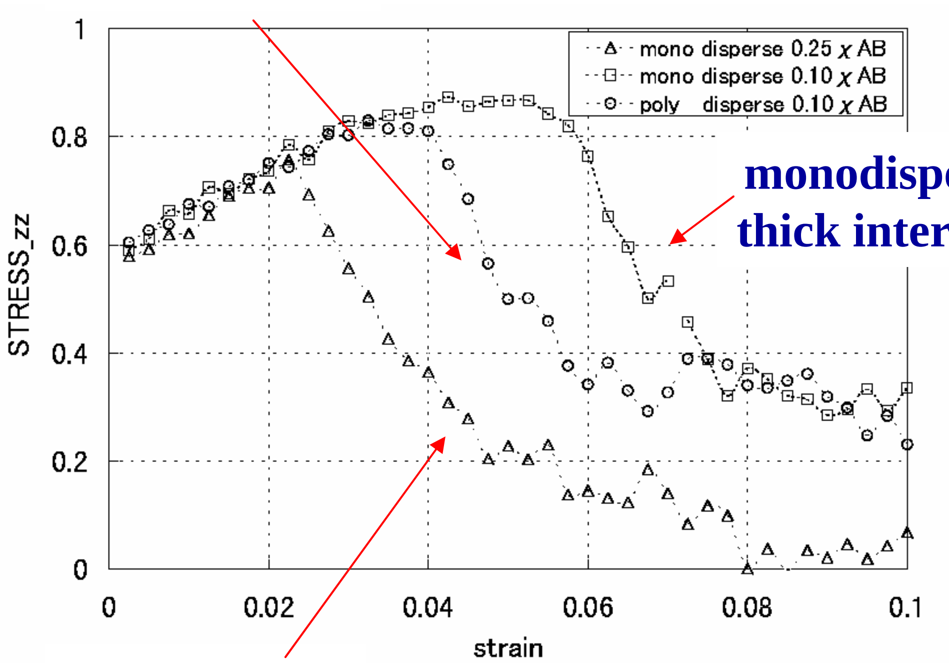


Interfacial strength of PP/elastomer blends

Yokomizo

Simulations

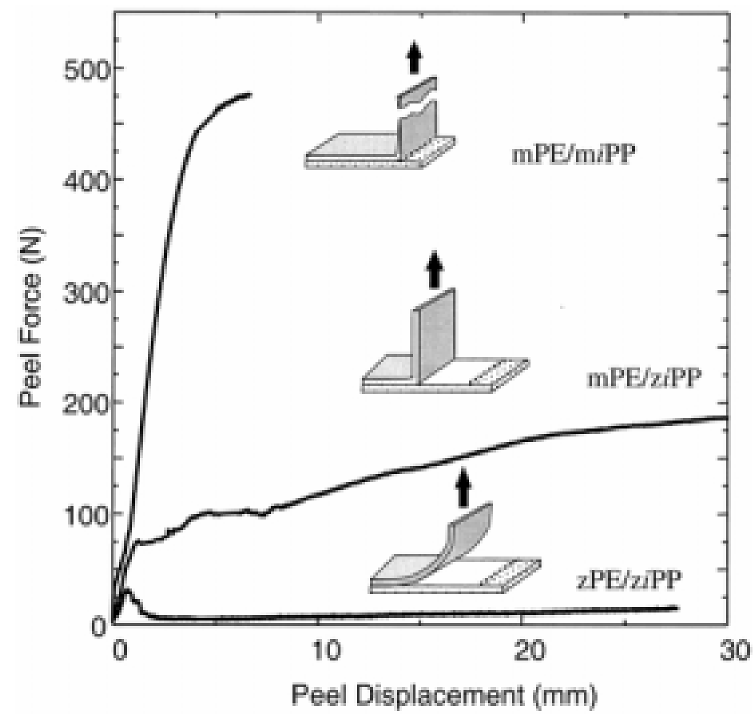
polydisperse thick interface



monodisperse thick interface

monodisperse thin interface

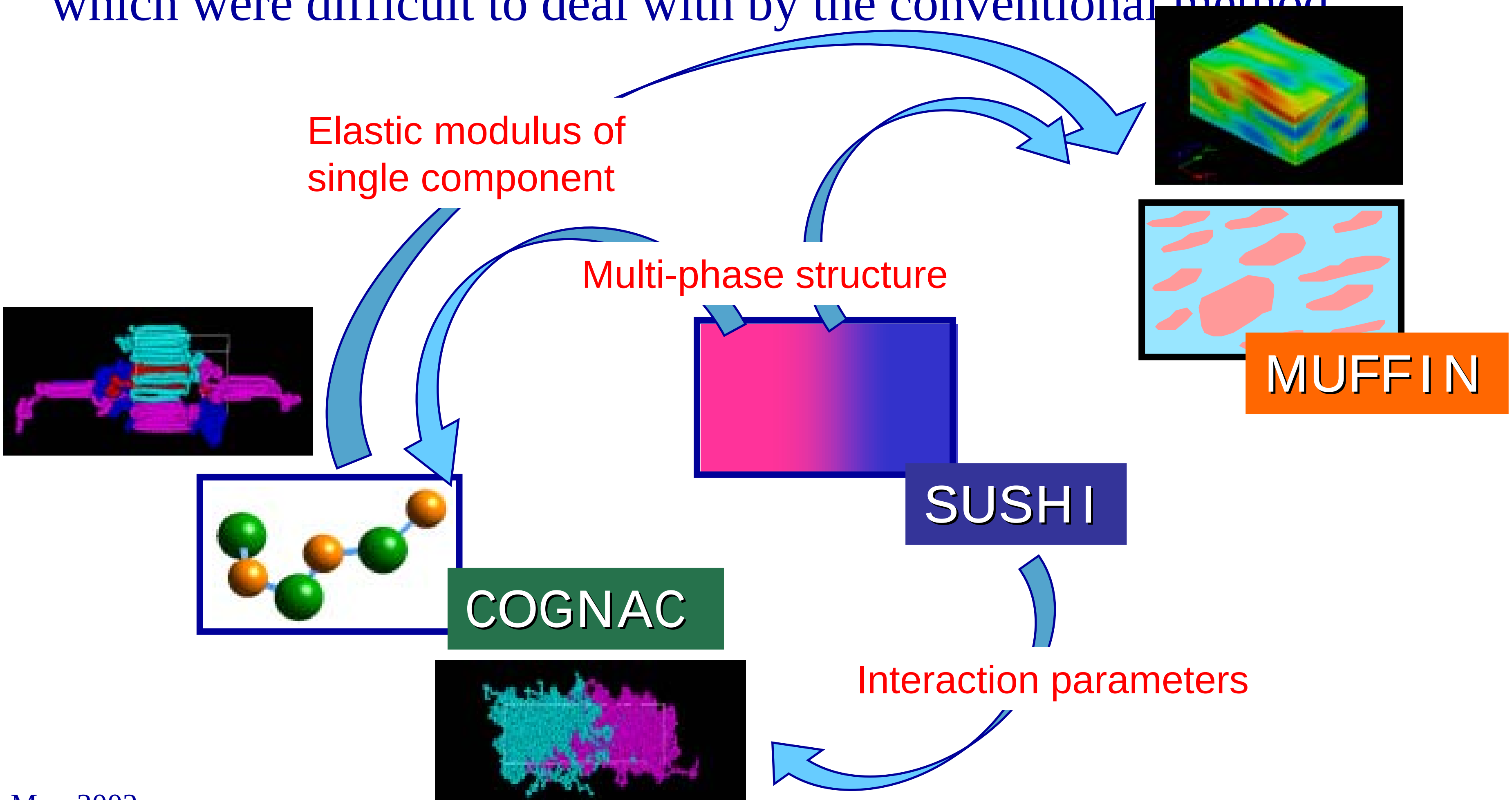
Experiments



Kimberly A. Chaffin, Frank S. Bates, et al., Science 2000, 288, 2187-2190.

Summary

By combining the simulation programs on a platform, practical simulation has become possible to study many phenomena which were difficult to deal with by the conventional method.



End

Acknowledgements:

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