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Multiscale simulation of cellulose composites considering atomistic interfacial properties

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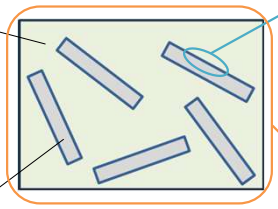
Introduction

Bio composites

Base material・・・ Thermoplastic resin hydrophobic

Interfaces occur
Causes delamination and fiber agglomeration, etc.

Reinforcing fibers・・・ Cellulose nanofibers(CNF) hydrophilic



Analysis of the mechanical properties of interfaces requires atomistic analysis using first-principles calculations.

Analysis of macroscopic properties requires multi-scale analysis based on homogenization methods.

Integration

The properties of the composite, including the interfaces

Interfacial treatment methods
- Silane coupling agent
- Maleic anhydride-modified
- etc.

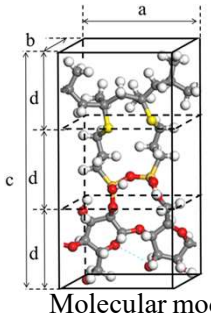
Computational methods

First-principles calculations

SCA
Silane coupling agent

APS (Amino Propyl trimethoxysilane)

MPS (Mercapto Propyl trimethoxysilane)

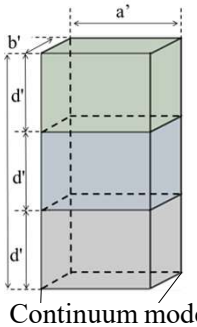


Molecular model

➢ Virtual loading tests on interfacial molecular models.

➢ Create interfaces in microstructures based on molecular models of interfaces.

Multiscale simulation



Continuum model

PP Already known

Silane coupling agent Unknown

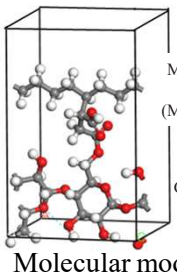
CNF Already known

➢ Define the elastic modulus ratio k of the interface and obtain it from first-principles calculations and tensile test results.

Material	Young's modulus [MPa]
PP	$E_m = 493$
Interfacial layer	$E_{if} = E_m \times k$ $\{k = 0.1, 0.2, 0.3, 0.4, 0.5, 1, 2, 5\}$
CNF	$E_f = 1.4e+05$

➢ Assign the obtained ratio k to the interfacial properties of the microscale fiber dispersion model considering the interface.

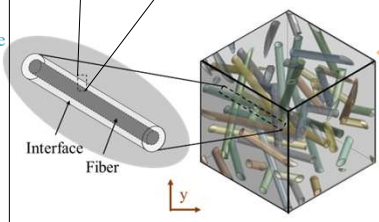
MAPE + MAPP
Maleic anhydride-modified polyethylene and polypropylene



MA-polymer binds to the hydroxy group linked to one of the C2,3,6 of the CNF.

➢ Compare the binding stability at several binding points from the cohesive energy.

Molecular model

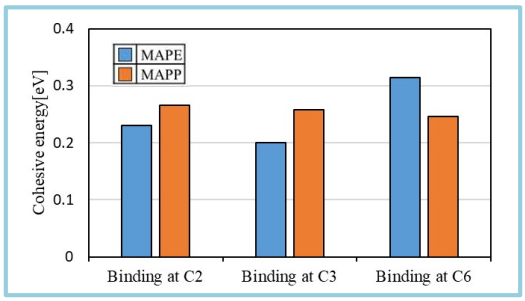


Microstructure

Analysis Solver
・Finite Element Analysis(FEA)
Model Generation
・Random Sampling Algorithms(RSA)

➢ Obtain macroscopic mechanical properties of fiber-dispersed composites considering interfacial properties.

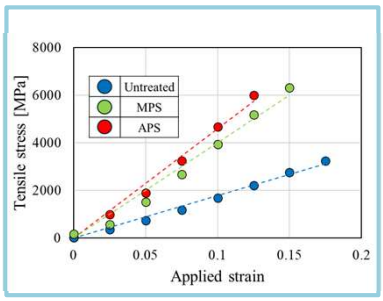
Results of MA-polymer



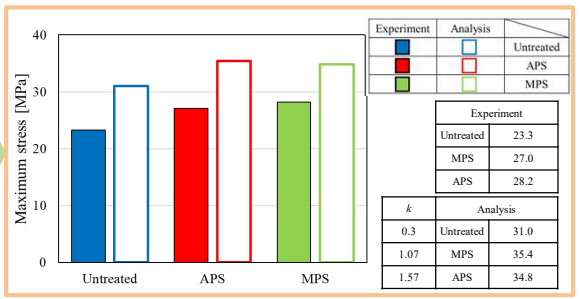
Binding stability by cohesive energy based on First-principles calculations.

➢ The stability of binding was higher for MAPE in the order of C6, C2, and C3, while no difference in stability by binding site was observed for MAPP.

Results of SCA



Virtual loading test of interfacial phases based on first-principles calculations.



Multiscale simulation of composite materials considering interfacial phases.

➢ The mechanical properties of the fiber dispersion model considering the interfacial characteristics obtained from the virtual loading test were evaluated by multiscale analysis and were generally correct, although slightly overestimated compared to the experimental values.

Conclusions

- Comparison of binding stability by cohesive energy shows that C6 is the most stable at the MAPE/CNF interface and that there is no difference in stability at the MAPP/CNF interface. For the most reactive C6, MAPE was found to be more stable in binding to CNF than MAPP.
- Virtual loading test show that at the PP/CNF interface the silane coupling agent improves the properties by 203% for APS and 204% for MPS.
- The results of first-principles calculations on the mechanical properties of the interface were incorporated into a multiscale analysis of a fiber dispersion model that takes the interface into account.
- The method relies on the results of first-principles calculations and requires a discussion of the molecular modelling setup and bonding modes.
- The thickness of the interface is still difficult to measure, so setting the interface thickness in a microscale model is one of the issues to be addressed in the future.

[1] Uetsuji Y, Fukui N, Yagi T, et al. The effect of number of chemical bonds on intrinsic adhesive strength of a silane coupling agent with metals: A first-principles study[J].Journal of Materials Research, 2022, 37(4): 923-932.

[2] H. Demir, et al., The effect of fiber surface treatments on the tensile and water sorption properties of polypropylene–luffa fiber composites[J]. Composites Part A:Applied Science and Manufacturing, 2006, 37(3): 447-456.