

Advanced Modeling & Simulation Seminar Series
NASA Ames Research Center, October 25, 2018

Integrated simulation system
for soft materials

J-OCTA

<http://www.j-octa.com>

JSOL CORPORATION

NTT data Global IT Innovator
NTT DATA Group

About JSOL



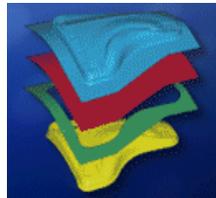
- Tokyo, Osaka, Nagoya office in Japan
- System Integration and CAE, Simulation
- 1,300 employees (150 for Simulation field)
- More than 20 CAE, Simulation Software packages

Structure, Production

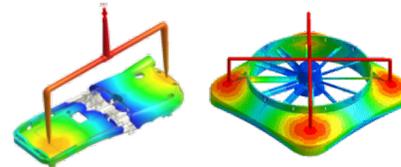
LS-DYNA



JSTAMP

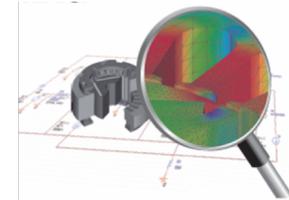


Moldex3D



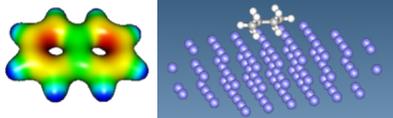
Electro Magnetic

JMAG

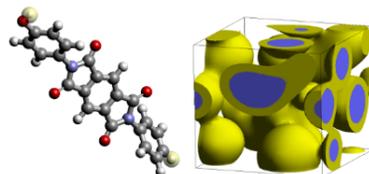


Material Simulation

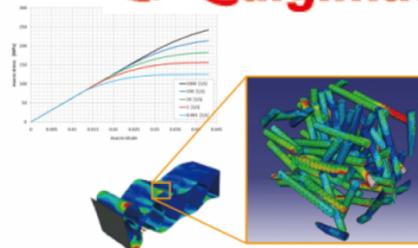
siesta
TM



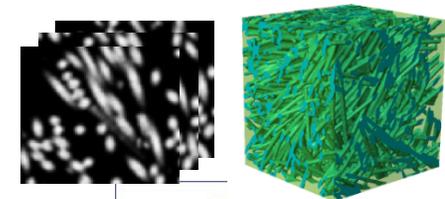
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digimat



Simpleware™ Software



J-OCTA
Integrated simulation system for soft materials

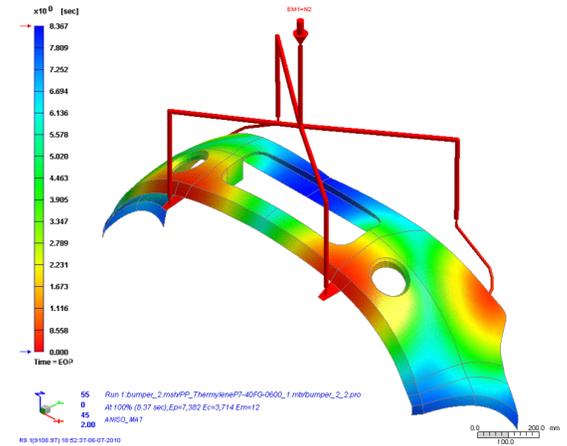
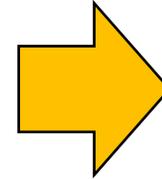
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Motivation, In the case of FRP



Macro-scale

Injection molding



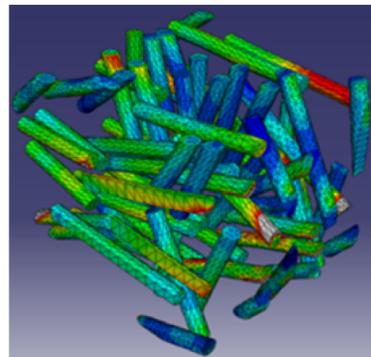
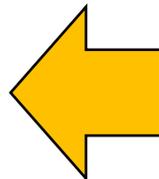
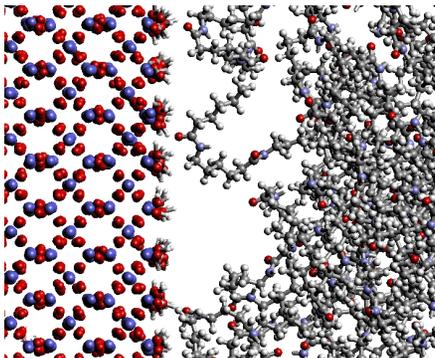
LS-DYNA

Moldex3D

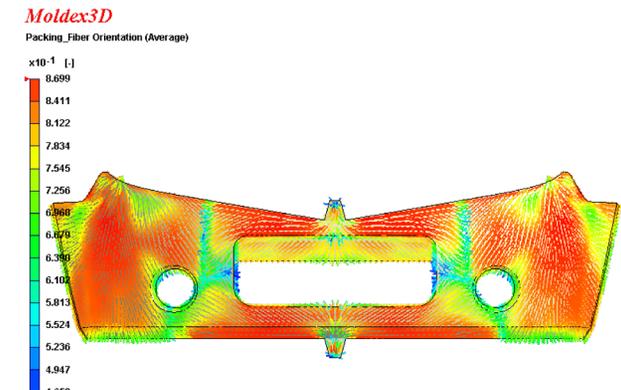
Multi-scale structure

J-OCTA

Interface



Fiber orientation
Filler dispersion



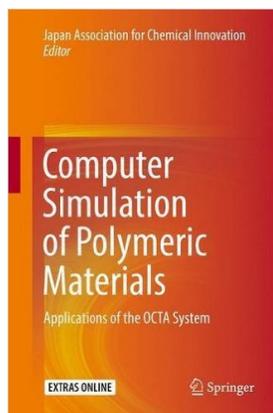
digimat

J-OCTA JSOL
Integrated simulation system for soft materials



Open Computational Tool for Advanced material technology

OCTA



Source :
<http://link.springer.com>

J-OCTA

- Since 2002
- National project in Japan (Leader = Prof. Masao Doi)
- Open source
- Engines, Simple GUI, Python
- Current distributor = AIST
- BBS users > 2600

- Since 2005
- Developed by JSOL
- Commercial version
- Modelers for OCTA Engines
- Parallel MD engine
- Industrial users > 100 sites

Multi-scale Simulation

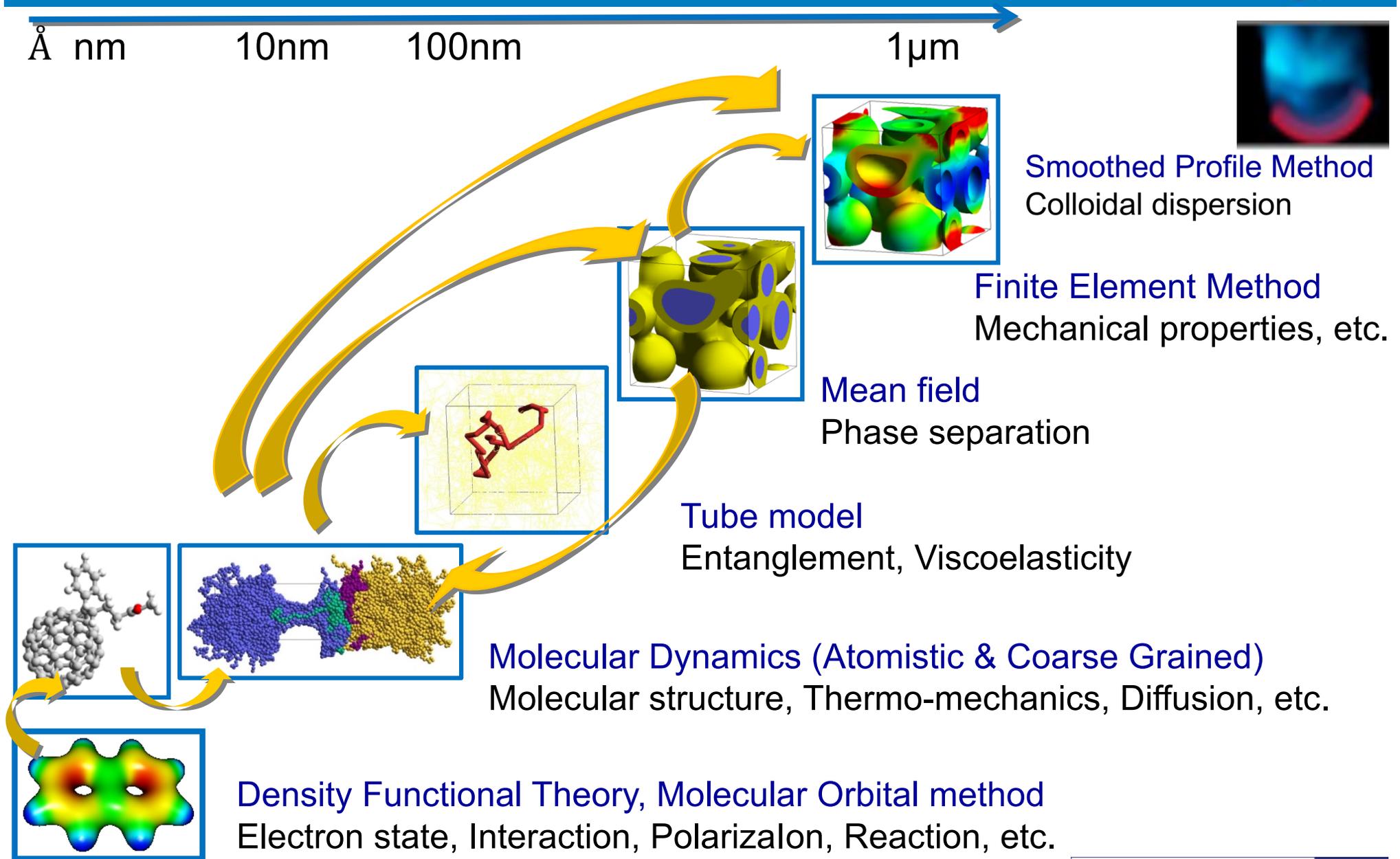


Å nm

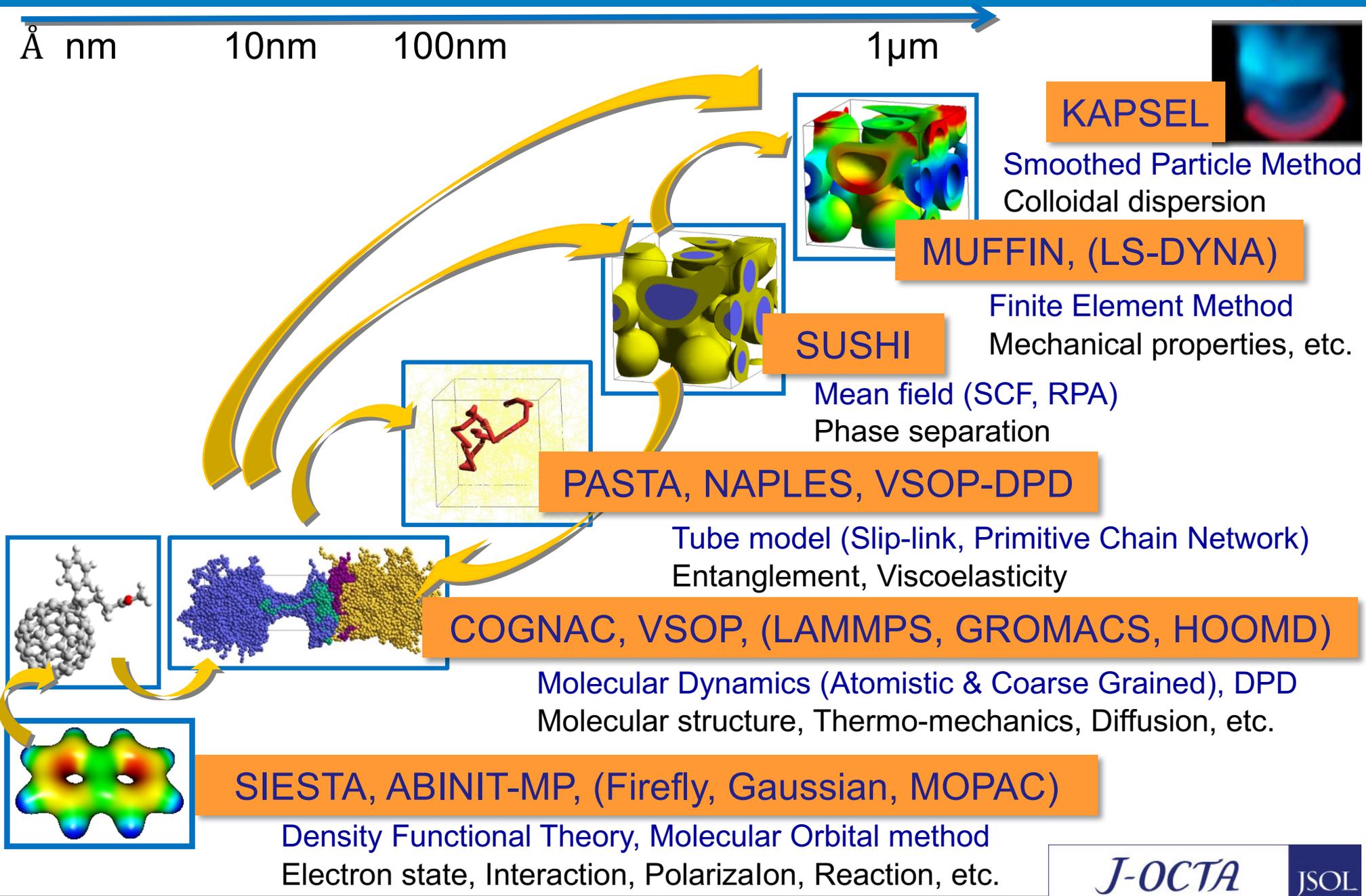
10nm

100nm

1 μ m



Multi-scale Simulation



Multi-scale Simulation



Å nm

10nm

100nm

1μm

Kyoto **A**dvanced **P**article **S**imulator for **E**lectro-hydrodynamics

MU**L**t**I**F**A**rious **F**ield simulator for **N**on-equilibrium system

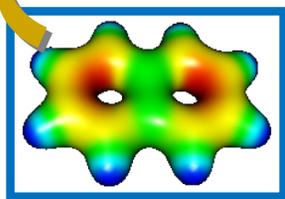
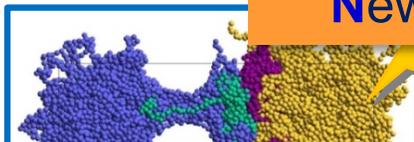
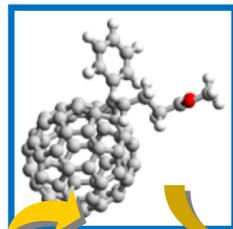
Simulation **U**tilities for **S**oft and **H**ard **I**nterfaces

Polymer rheology **A**nalyzer with **S**lip-link model of en**T**anglement

New **A**lgorithm for **P**olymeric **L**iquids **E**ntangled and **S**trained

CO**A**rse-**G**rained molecular dynamics program by **N**Agoya **C**ooperation

Spanish **I**nitiative for **E**lectronic **S**imulation with **T**housand of **A**toms



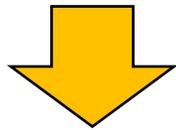
Density Functional Theory



SIMUNE

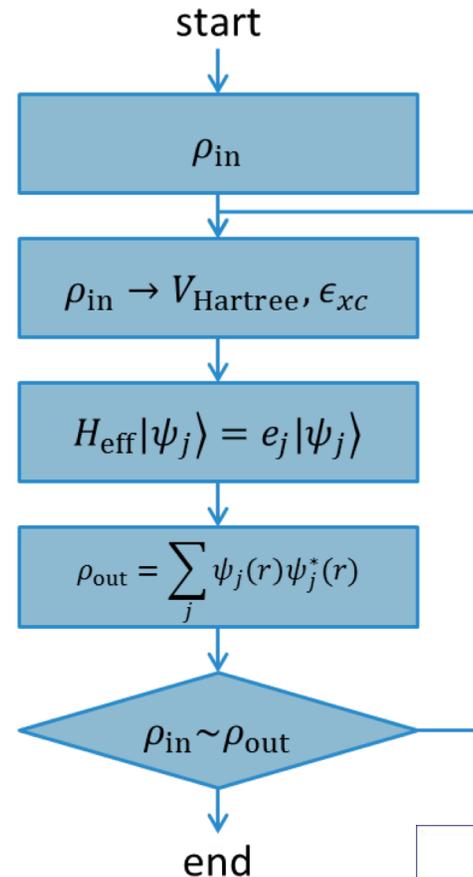
Density Functional Theory (Kohn-Sham)

$$E_{KS}[\rho] = T_s[\rho] + \int dr V_{\text{ext}}(r)\rho(r) + E_{\text{Hartree}}[\rho] + E_{II} + E_{\text{xc}}[\rho]$$



$$H_{\text{eff}} = -\frac{1}{2}\nabla^2 + V_{\text{eff}}$$
$$V_{\text{eff}} = \frac{\delta E_{\text{ext}}}{\delta \rho} + \frac{\delta E_{\text{Hartree}}}{\delta \rho} + \frac{\delta E_{\text{xc}}}{\delta \rho}$$

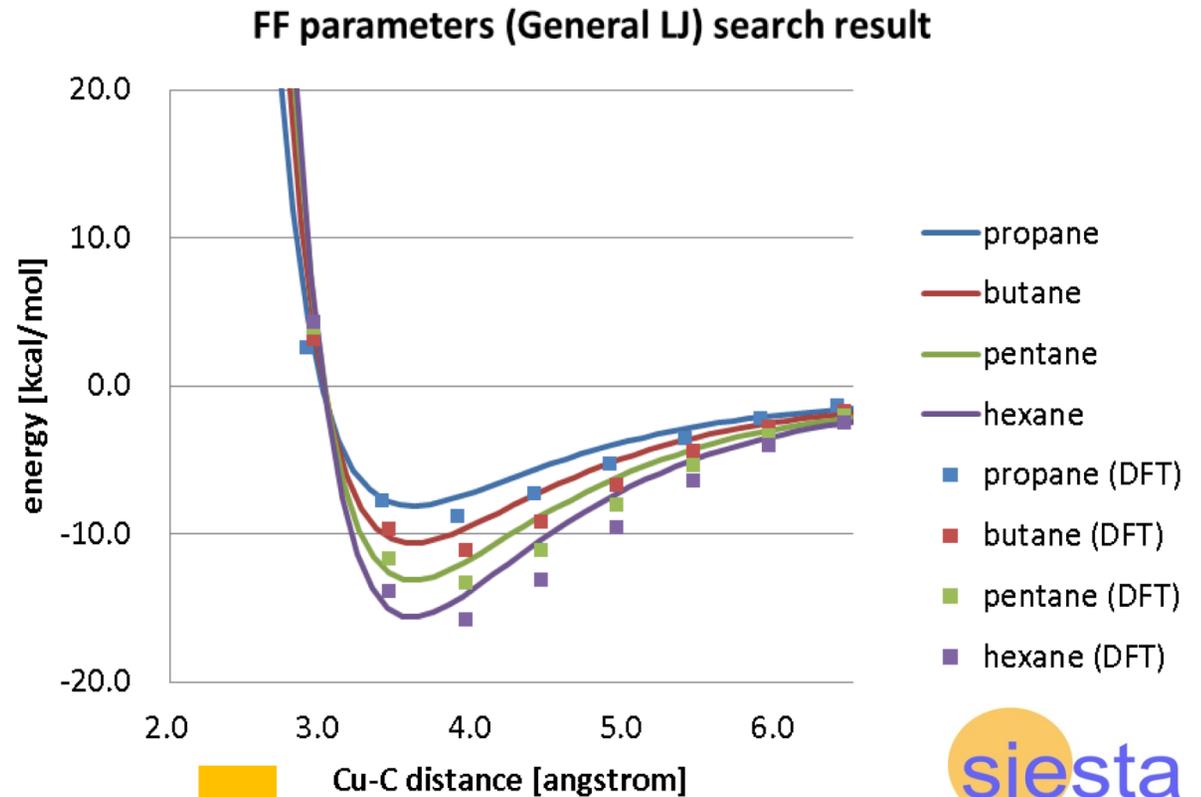
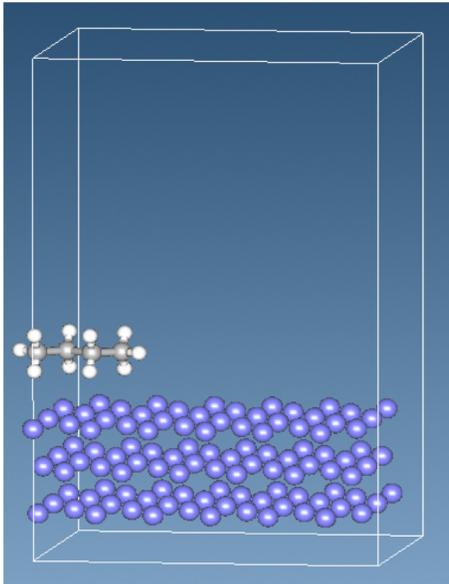
$$H_{\text{eff}}|\psi_j\rangle = e_j|\psi_j\rangle$$



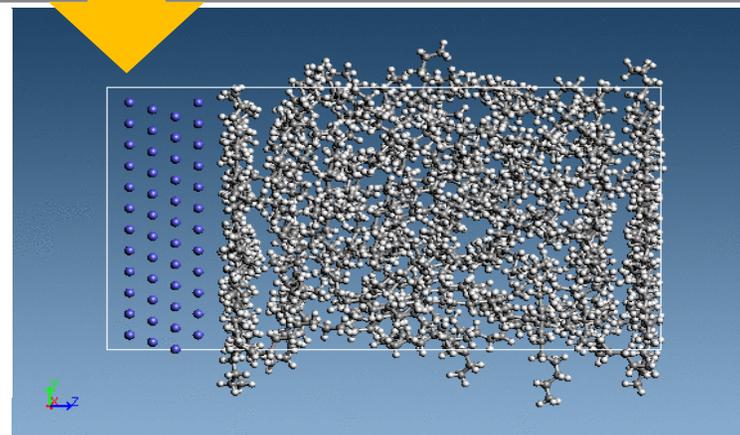
Interfacial energy

Density Functional Theory

Small molecule on Cu(111) surface



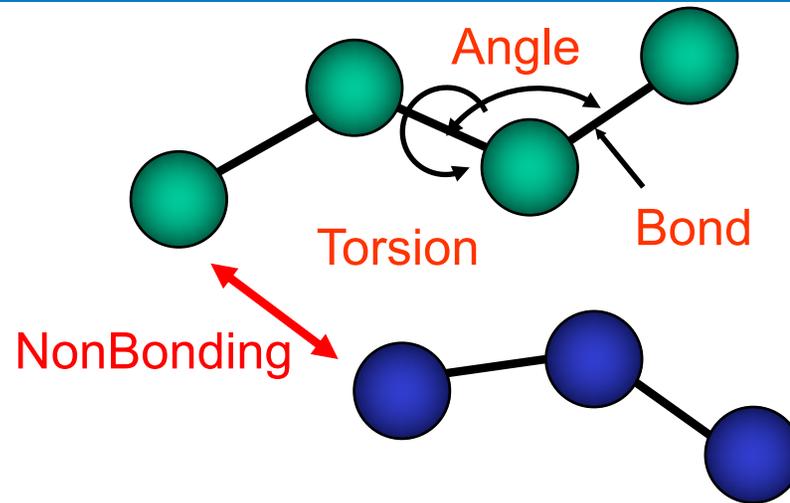
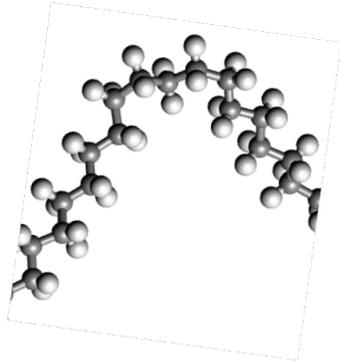
- Adsorption of Alkane molecules onto Cu surface
- Results of DFT was fitted to the Generalized Lennard Jones potential
- Obtained LJ potential was used in the classical MD calculation





Atomistic model

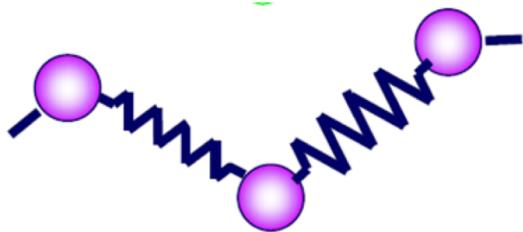
$$m \frac{d^2 \mathbf{r}}{dt^2} = \mathbf{F}$$



Coarse Grained model

$$m \frac{d^2 \mathbf{r}}{dt^2} = \mathbf{F} - \Gamma \frac{d\mathbf{r}}{dt} + \mathbf{W}(t)$$

Γ : Friction constant, \mathbf{W} : Thermal noise



Potential functions

■ Non-Bonding

van der Waals (Lennard-Jones potential)

Coulomb

$$U(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

$$U(r) = \frac{1}{4\pi\varepsilon_0} \frac{Q_1 Q_2}{r}$$

■ Bonding

2 atoms: Bond potential

$$U(l) = \frac{1}{2} k (l - l_0)^2$$

3 atoms: Angle potential

4 atoms: Torsion potential

$$U(\theta) = \frac{1}{2} k (\theta - \theta_0)^2$$

$$U(\varphi) = \frac{V}{2} [1 - \cos(n(\varphi - \varphi_0))]$$

Thermoset resin

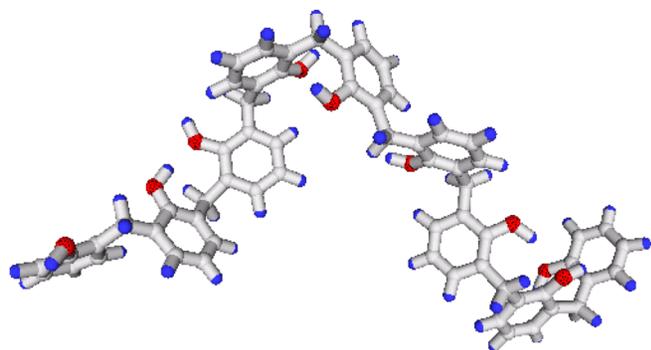


Full Atomistic Molecular Dynamics

■ Modeling of Cross-Linked Phenolic Resins

courtesy of

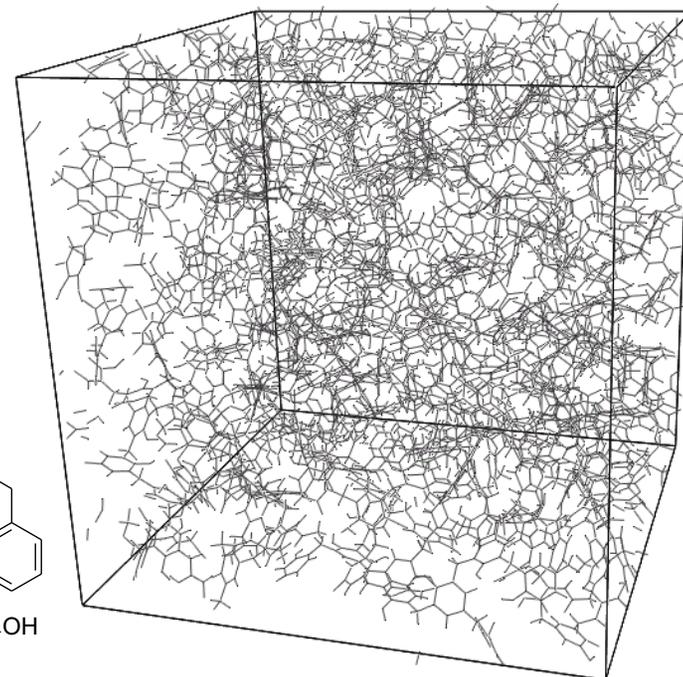
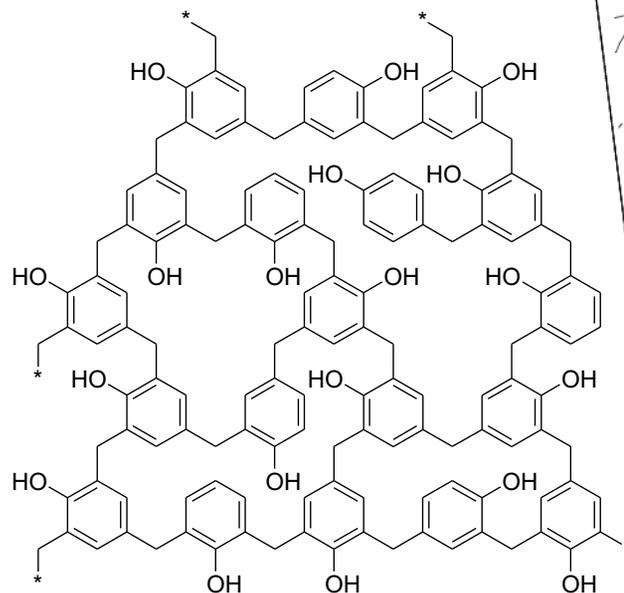
 SUMITOMO BAKELITE CO., LTD.



9-mer x 50 molecules



Cross-Linking Reactions



Cross-linking reactions were repeated until the degrees of cross-linking (D) reached 70%, 82%, and 92%, where D is given by $(2N_{CH_2})/(3N_{PhOH}) \times 100$.

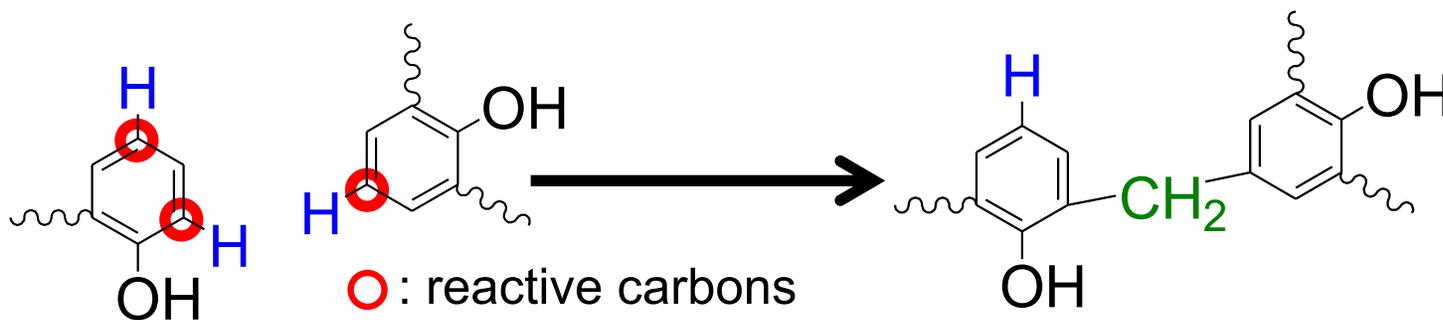
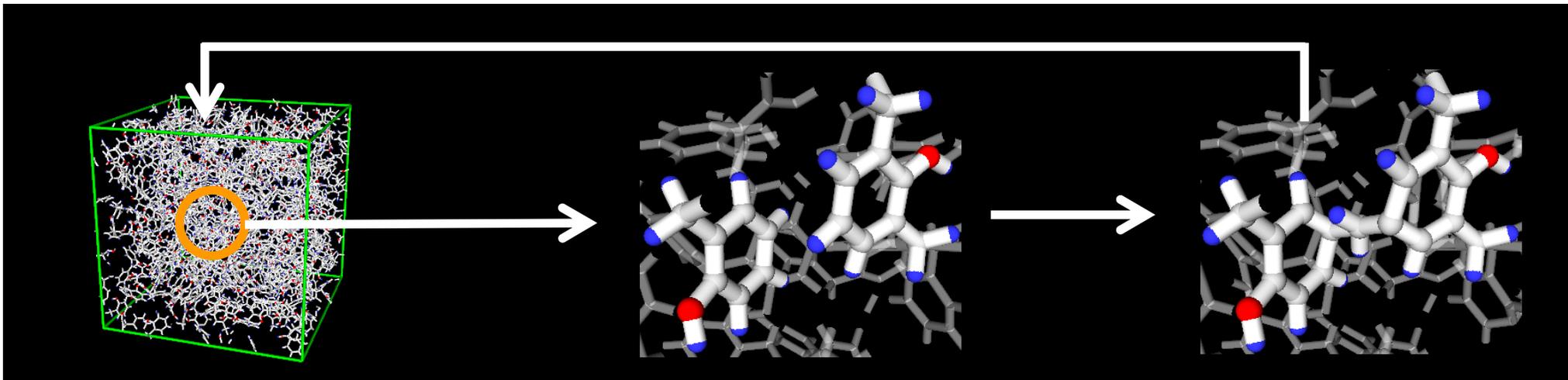
Soft Matter, **8**, 5283 (2012)



Thermoset resin



- Scheme of Cross-Linking Reactions **Full Atomistic Molecular Dynamics** courtesy of **SUMITOMO BAKELITE CO., LTD.**



Two reactive carbons at the first nearest neighbor were selected and attached hydrogens were removed.

Soft Matter, **8**, 5283 (2012)

A methylene was inserted and reactive carbons were connected via the methylene carbon.



Thermoset resin

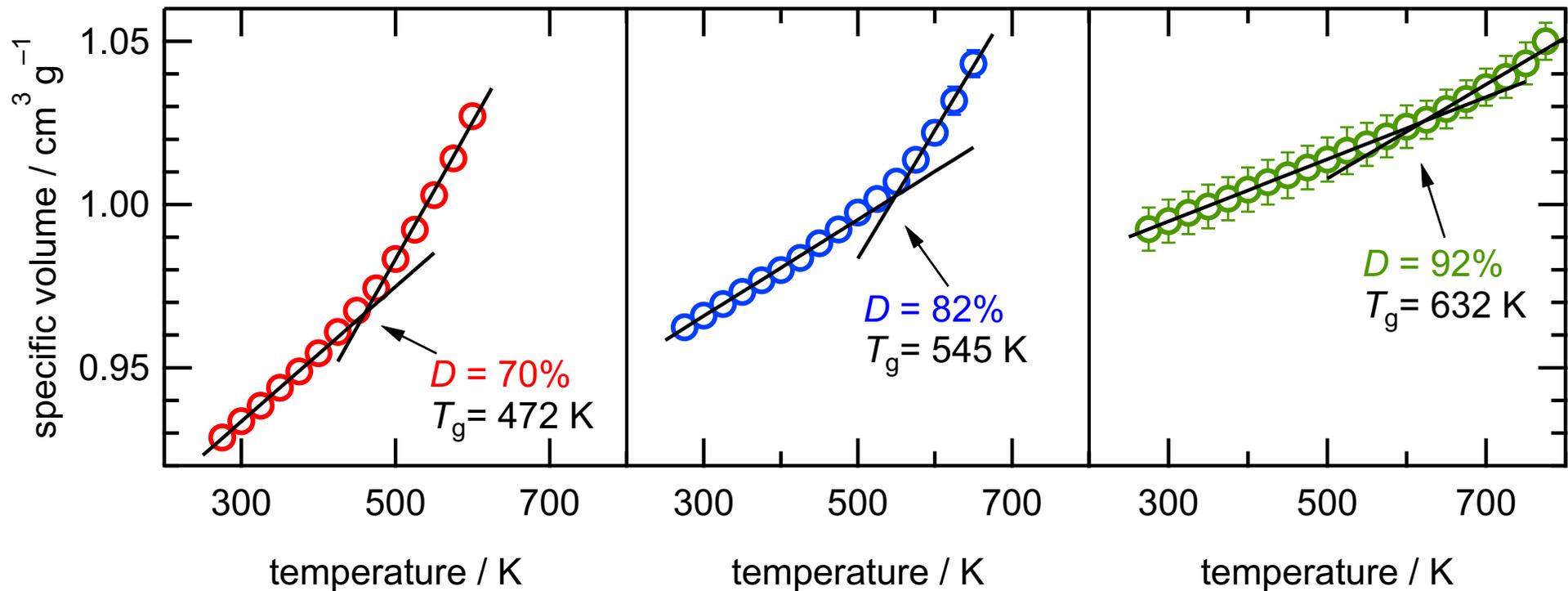


Full Atomistic Molecular Dynamics

■ Glass Transition Temperature (T_g)

courtesy of

 SUMITOMO BAKELITE CO., LTD.



Soft Matter, **8**, 5283 (2012)

Thermoset resin

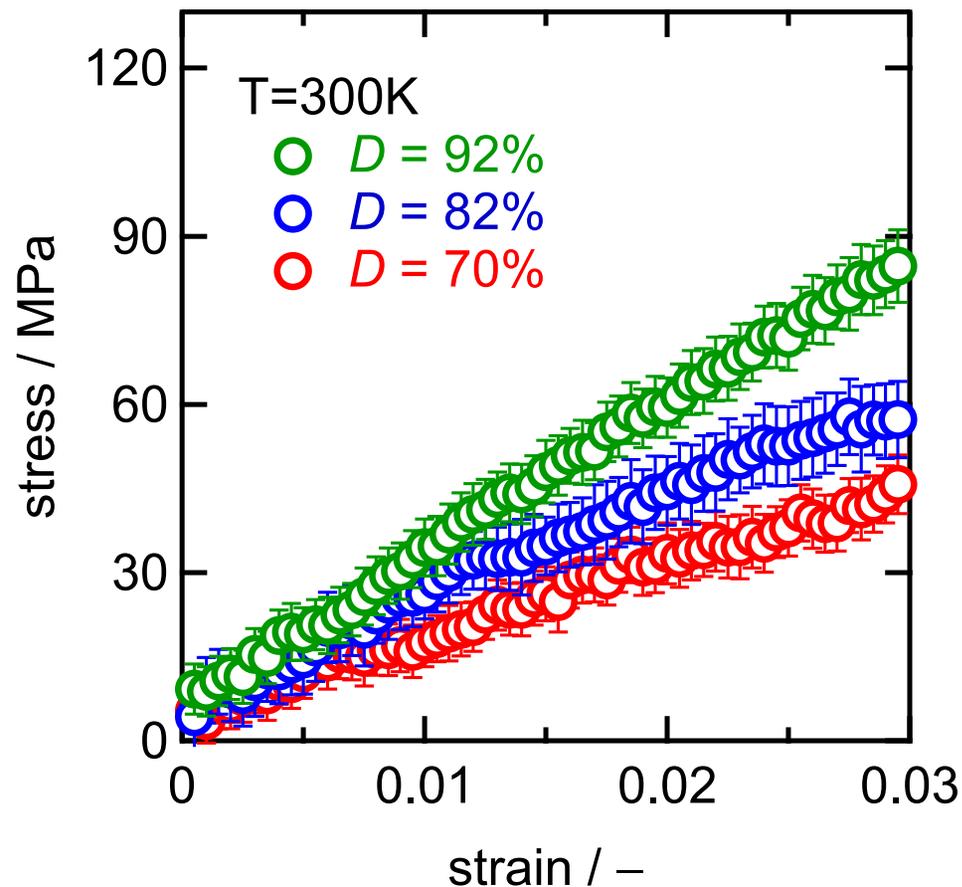


Full Atomistic Molecular Dynamics

■ Uniaxial Elongation: Stress–Strain Curves

courtesy of

 SUMITOMO BAKELITE CO., LTD.

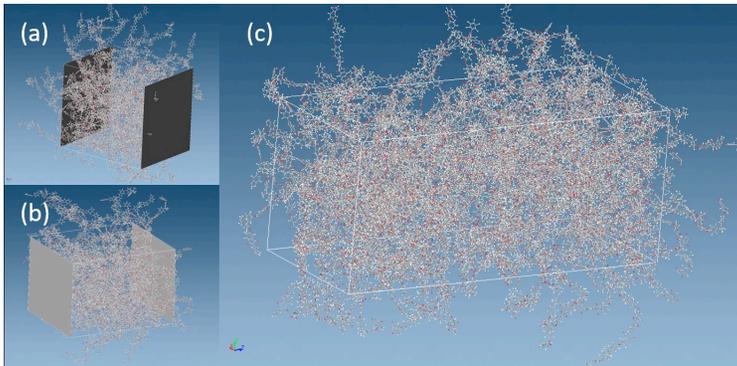


Soft Matter, **8**, 5283 (2012)

Shear Viscosity

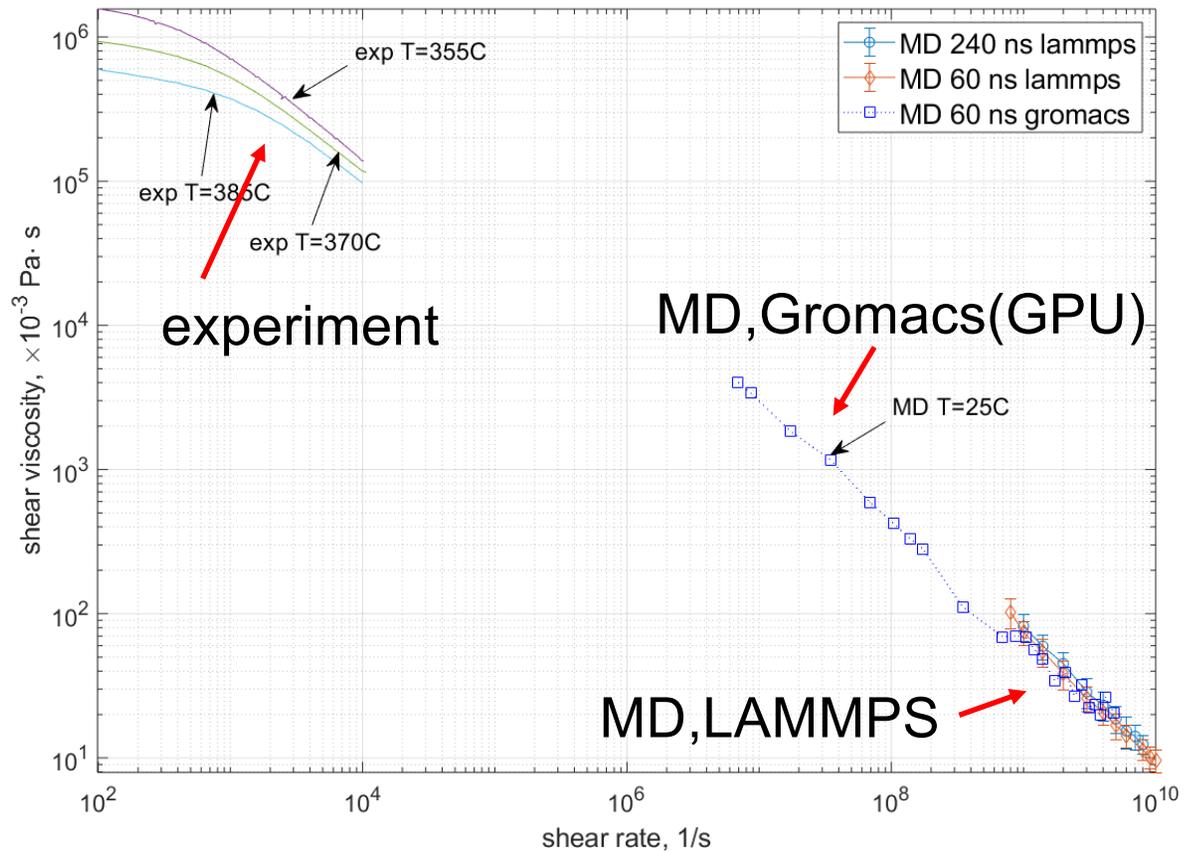


- ✓ Shear Thinning behavior of polymer melt
- ✓ Direct comparison with the experiment by narrowing the gap between MD and experiment from 5 to 2.5 orders of magnitude.
- ✓ Large systems (over 100,000 atoms) can be efficiently analyzed using GPU based cloud computin



Dr.Dmitry Luchinsky, Dr.Halyna Hafiychuk,
Dr.Gabriele Jost, NASA

Collaboration with supercomputing division
at Ames and Amazon cloud computing at
AWS.



Mean field : Self Consistent Field Theory (SCFT)

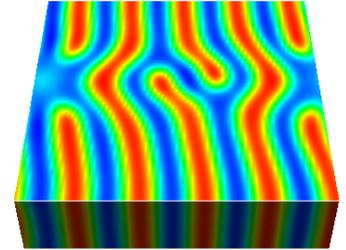


Mean field approximation



$$V_K(r) = \sum_{K'} \chi_{KK'} \phi_{K'}(r) + \gamma(r)$$

Segment density $\phi(r)$



consistent

Potential $V(r)$

Path integral Q
(statistical weight)

Path integral to calculate the conformation of polymer chain.

$$\frac{\partial}{\partial s} Q(s, r) = \left[\frac{b^2}{6} \nabla^2 - \frac{1}{k_B T} V(r) \right] Q(s, r)$$

Calculation of the segment density considering Ensemble.

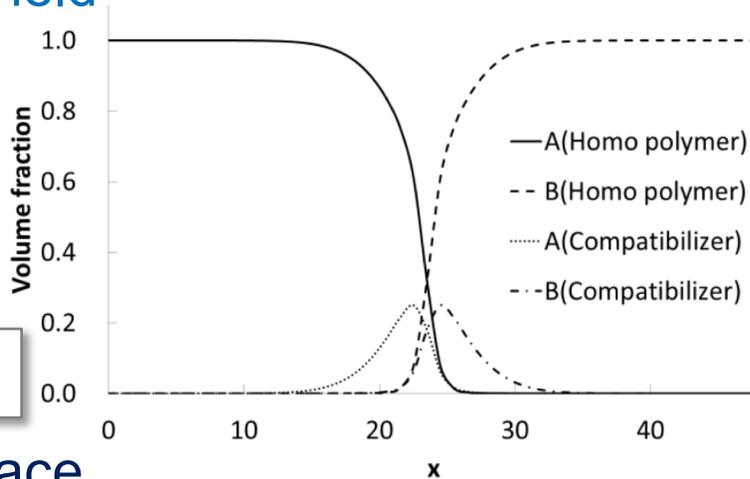
$$\phi_K(r) = M_k \frac{\int_0^N ds \int dr_0 \int dr_N Q_K(0, r_0; s, r) Q_K(s, r; N, r_N)}{\int dr_0 \int dr_N Q_K(0, r_0; N, r_N)}$$

Strength of interface (polymer blend)



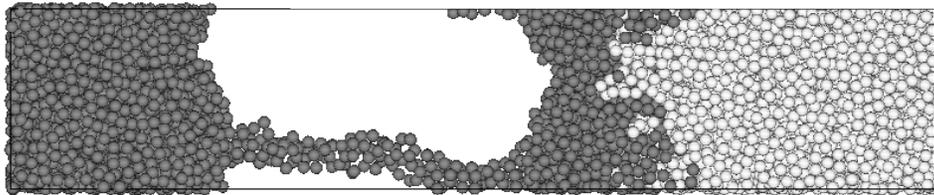
Mean Field -> Coarse grained Molecular Dynamics (CGMD)

1D Mean Field

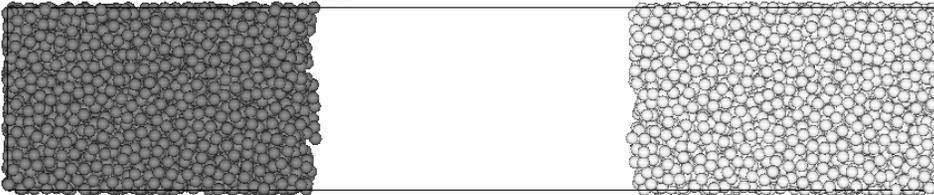


Elongation

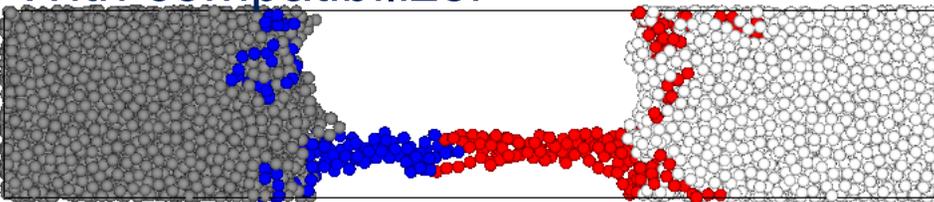
Thick interface



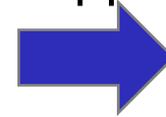
Thin interface



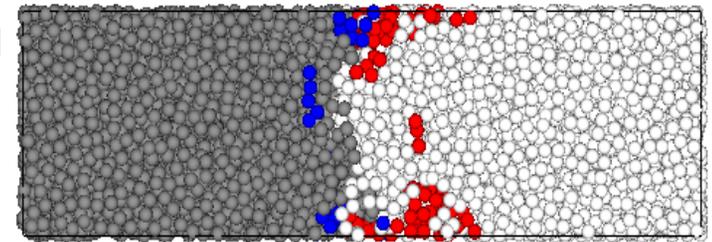
With compatibilizer



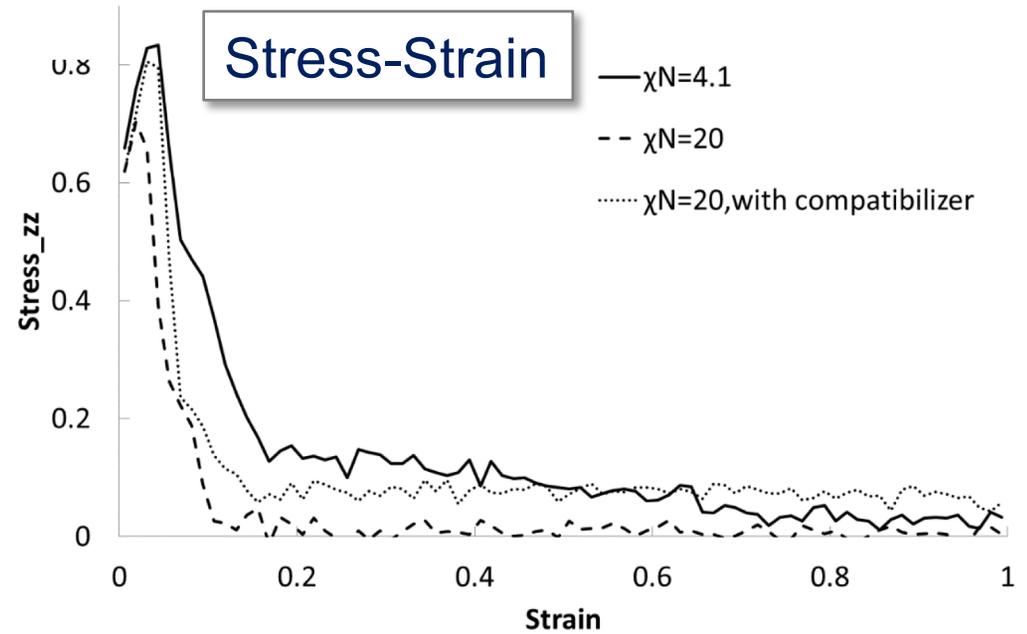
Mapping



Molecular Dynamics



Stress-Strain



J.Soc.Rheol.Jpn, 37,75 (2009)



Filled Rubber

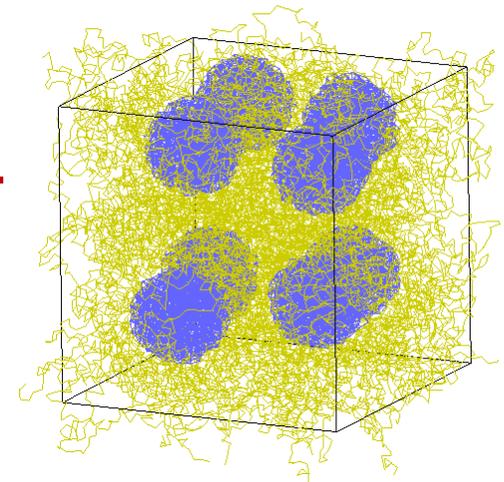
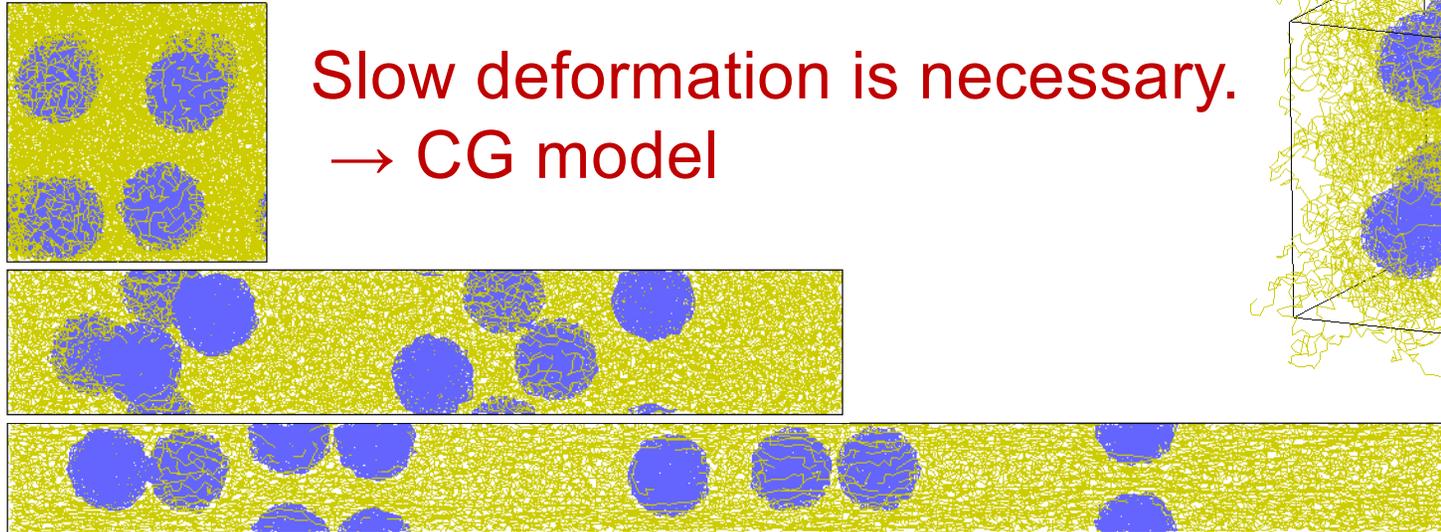
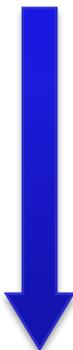


- Cross linked rubber
- Influence of cross link, interaction between filler and polymer

Coarse grained Molecular Dynamics (CGMD)

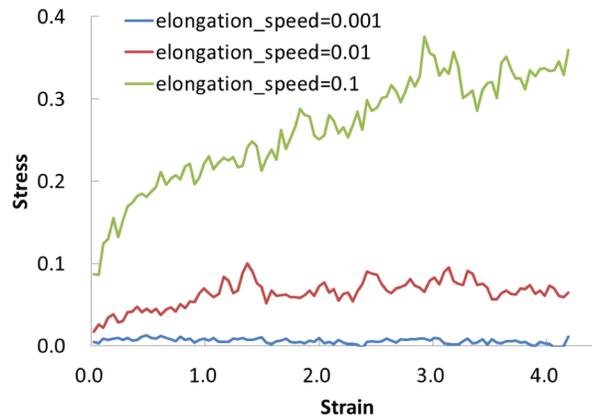
Slow deformation is necessary.
→ CG model

Elongation

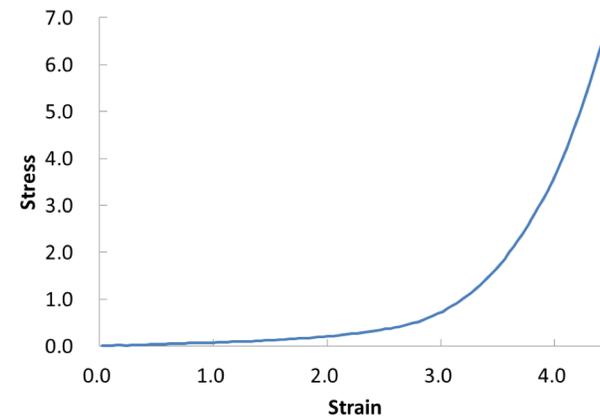


Stress-Strain curve

Non-cross link
Influence of deformation speed



With cross-link (elongation speed is 0.001)



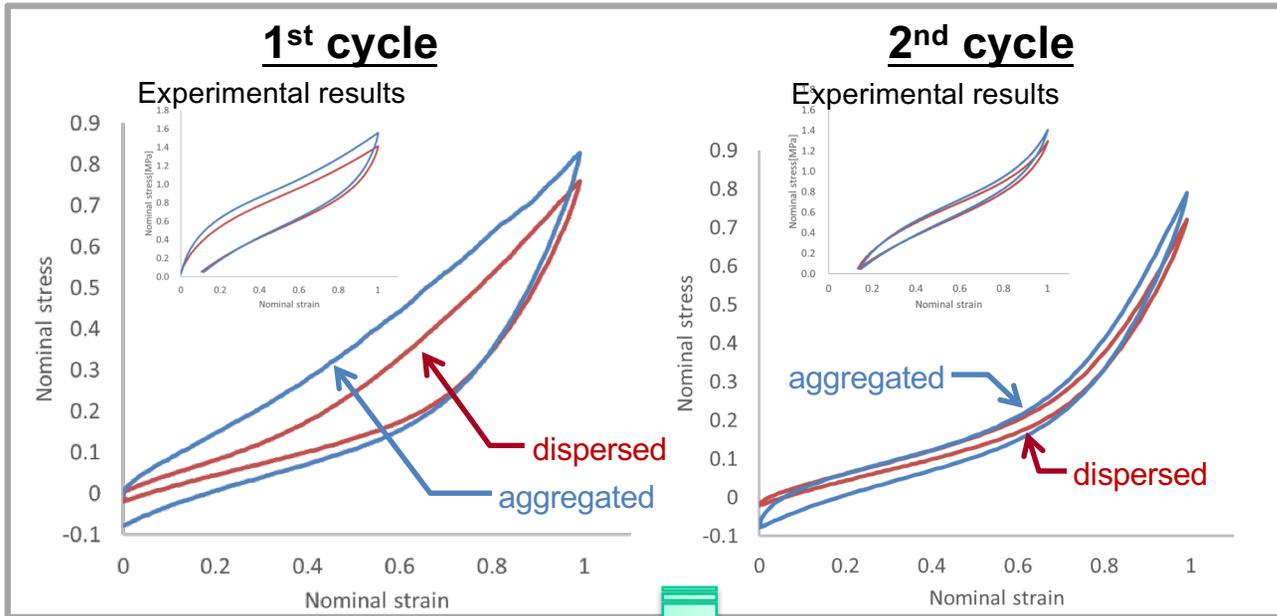
Filled Rubber under Cyclic Tensile Deformation



Courtesy of

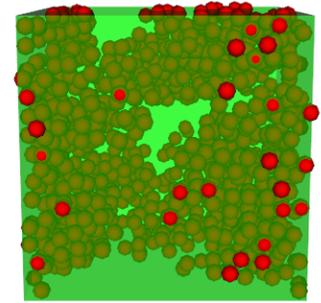
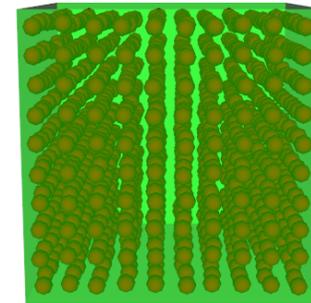


The origin of the difference in dynamic response by Morphology



Dispersed

Aggregated

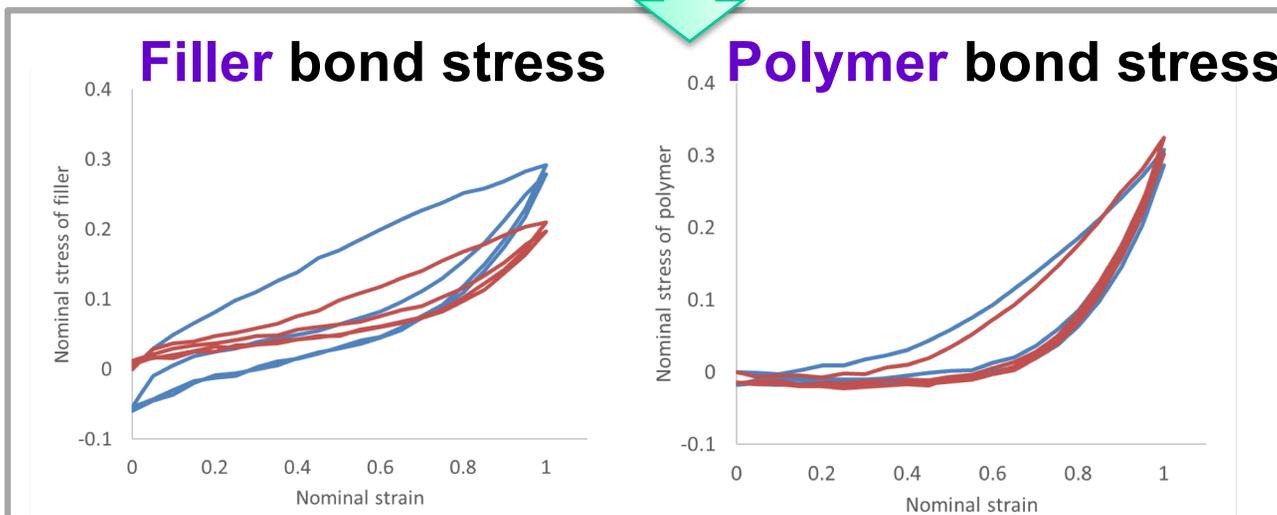


Polymer

- Kremer-Grest model
- Chain length : 20,000
- Chain number : 1,000 (Cross link : 3%)

Filler

- Number 1,000 (15vol%)



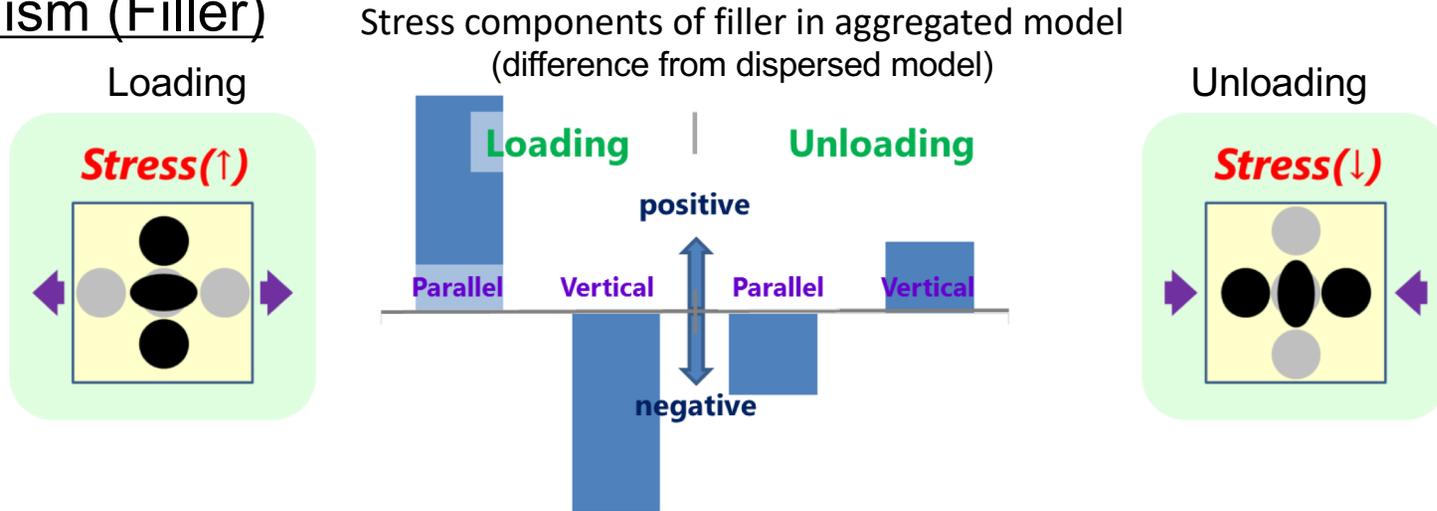
Filled Rubber under Cyclic Tensile Deformation



Courtesy of YOKOHAMA

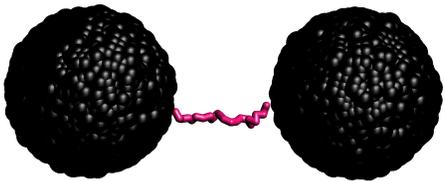
Mechanism of hysteresis

Mechanism (Filler)

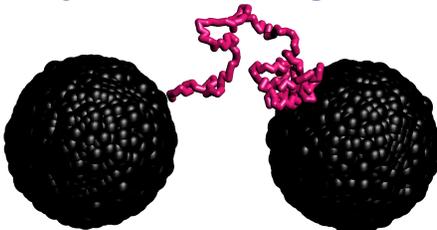


Mechanism (Polymer)

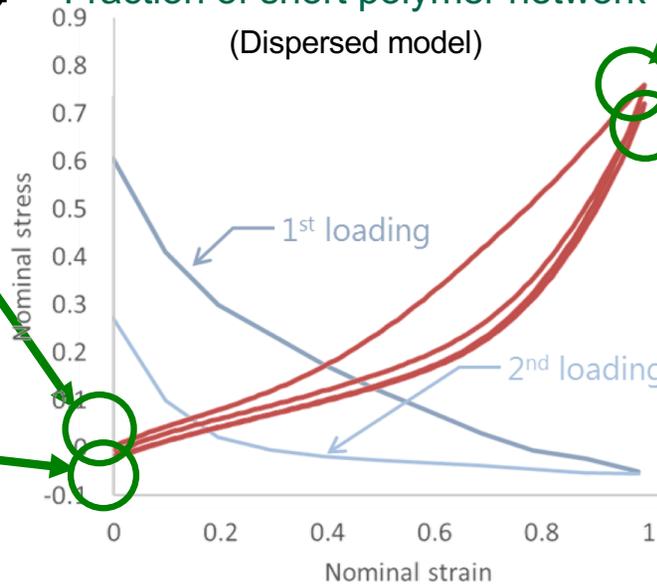
1.



2. Polymer folding



Stress-Strain curve and Fraction of short polymer network (Dispersed model)



3. Polymer stretching



4. Polymer unfolding



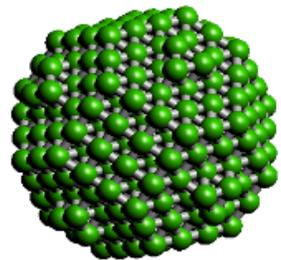
Slurry coating process



TOYOTA

■ Simulation model (Cognac/VSOP)

- Bead-spring model



Particle



Polymer



Solvent

Study of material property

- Interactions between molecules
- Polymer rigidity

Objectives

- ✓ Develop the method to simulate diffusion in materials by CGMD

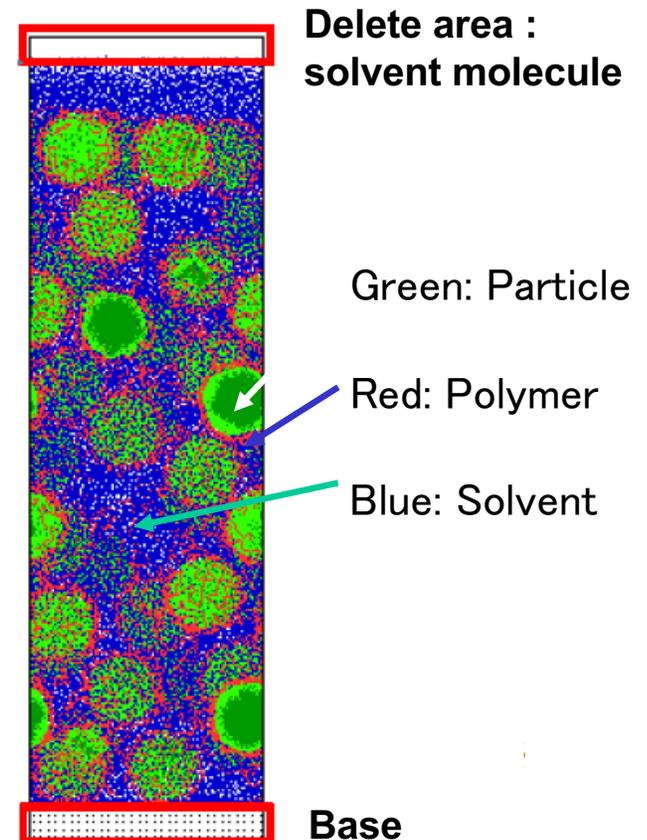


- ✓ Clarify the mechanism of slurry coating process
- ✓ Understand the correlation between battery performance and material properties

- Evaporation of the solvent



Evaporation



Delete area :
solvent molecule

Green: Particle

Red: Polymer

Blue: Solvent

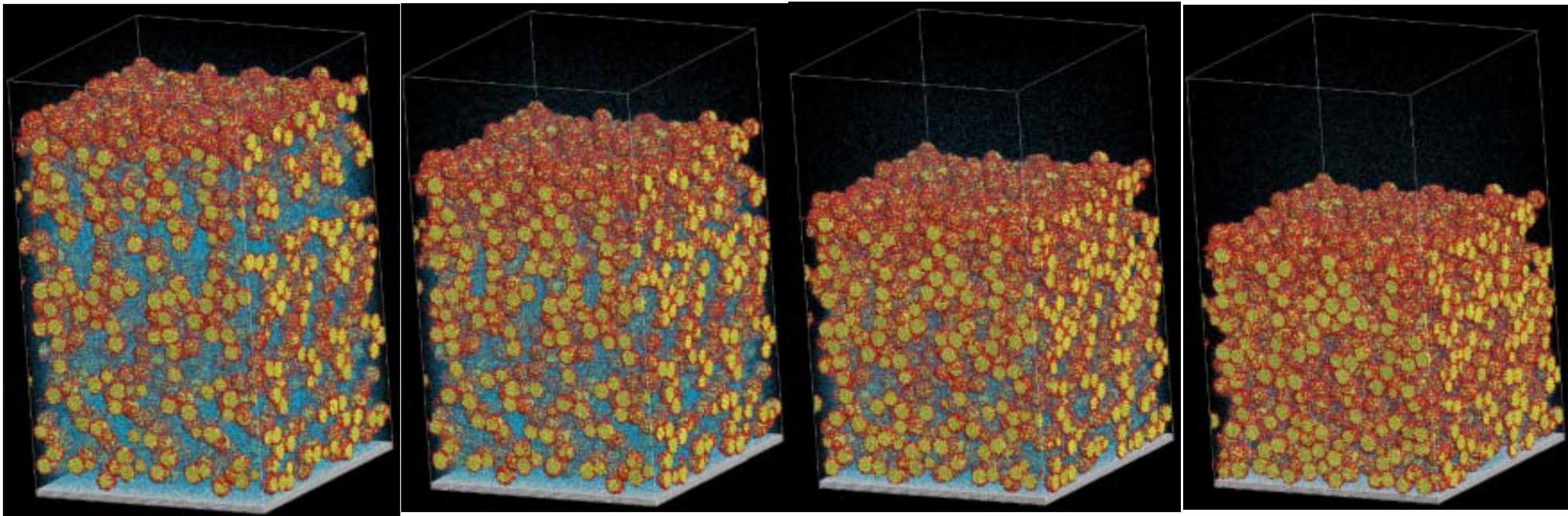
Base

Slurry coating process



TOYOTA

- **【Result】 Molecular Dynamics (Large-scale model)(VSOP)**
 - Evaporating process (4 millions coarse-grained particles)



Initial  Final

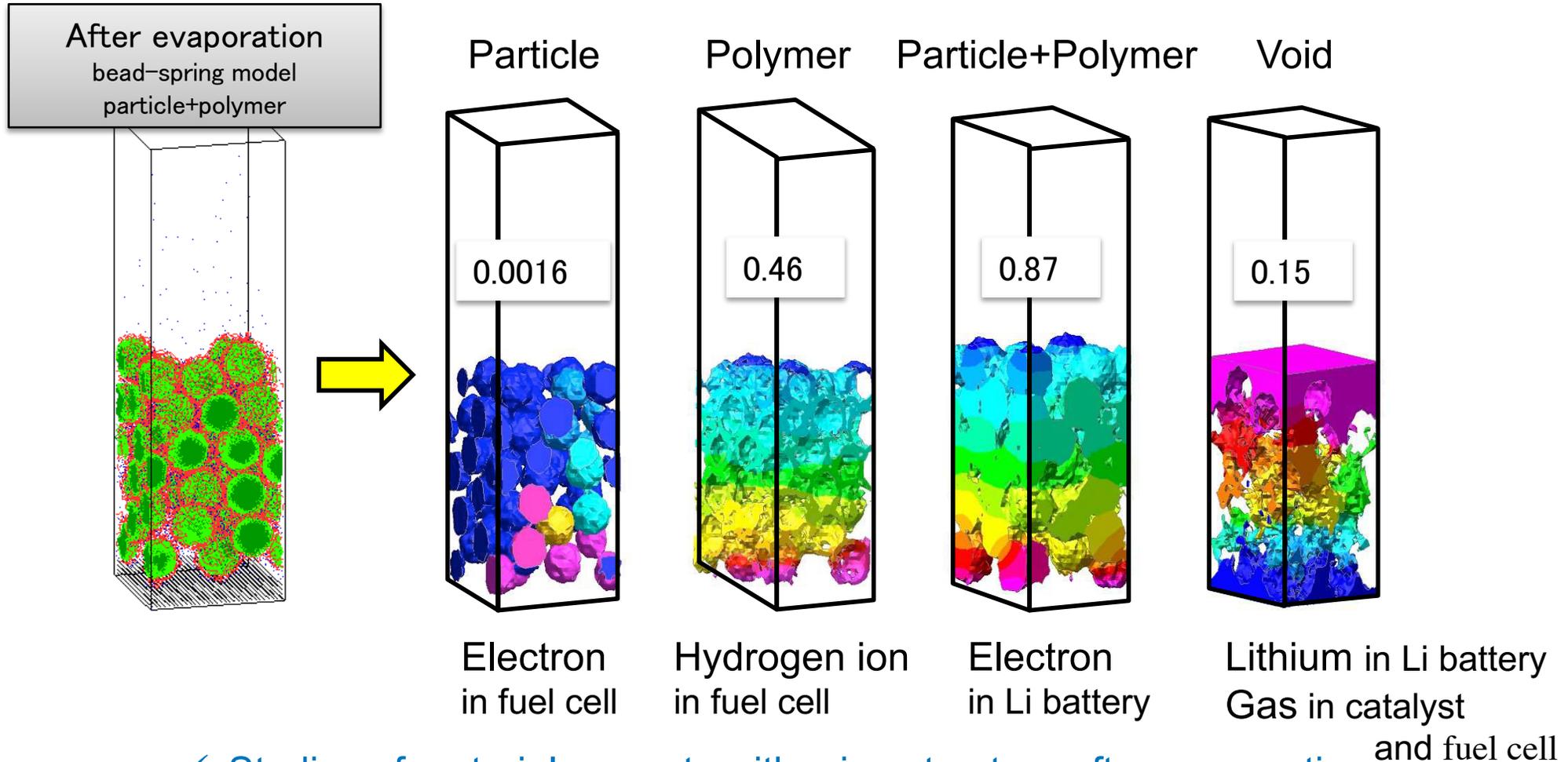
Confirmed that the slurry coating process can be simulated from molecular level

Slurry coating process



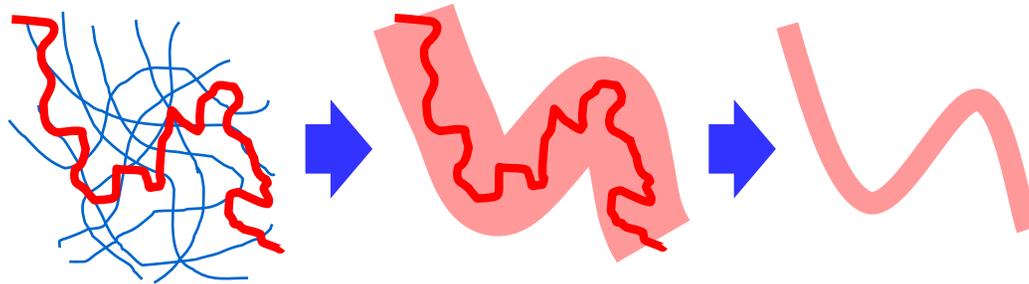
TOYOTA

■ Diffusion coefficient/Conductivity (LS-DYNA/Muffin)



✓ Studies of material property with microstructure after evaporation using molecular dynamics (micro) and FEA (macro)

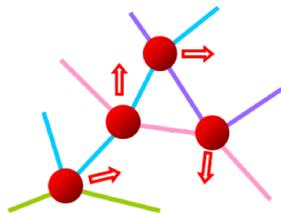
Tube model



Primitive Chain Network Model

Motion of entanglement points

$$\zeta \frac{d\mathbf{R}_i}{dt} = \frac{3kT}{b^2} \sum_j \frac{r_j}{n_j} - n_0 \nabla \mu + \mathbf{f}$$

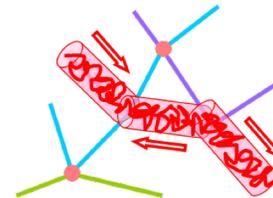


Tension

Osmotic force
(Chemical potential)

Diffusion of monomers in a tube

$$\frac{\zeta}{2\rho} \frac{dn_i}{dt} = \frac{3kT}{b^2} \left(\frac{r_{i+1}}{n_{i+1}} - \frac{r_i}{n_i} \right) - n_0 \nabla \mu + f$$



Tension

$$\rho = \frac{1}{2} \left(\frac{n_{i+1}}{r_{i+1}} + \frac{n_i}{r_i} \right)$$

Osmotic force
(Chemical potential)

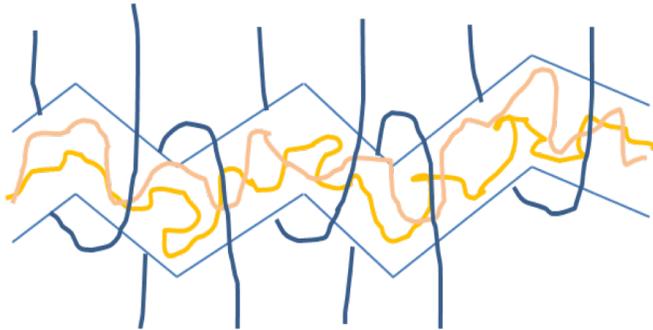
z: friction, b: tube length, n_i : number of monomers in i -th tube segment z: friction, b: tube length, n_i : number of monomers in i -th tube segment

Provided by Prof.Masubuchi

Dynamics of entangled polymer melt

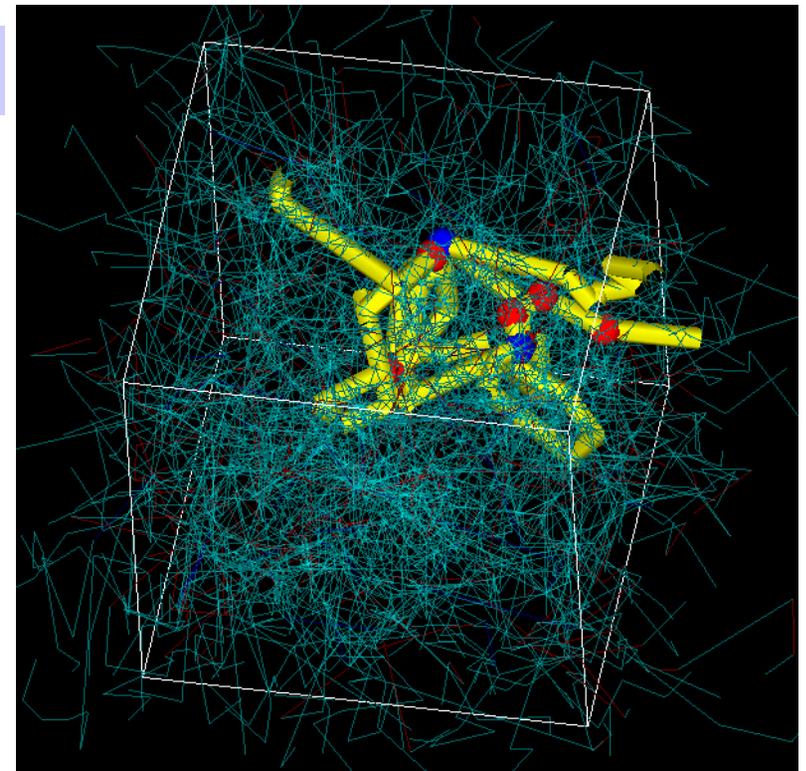
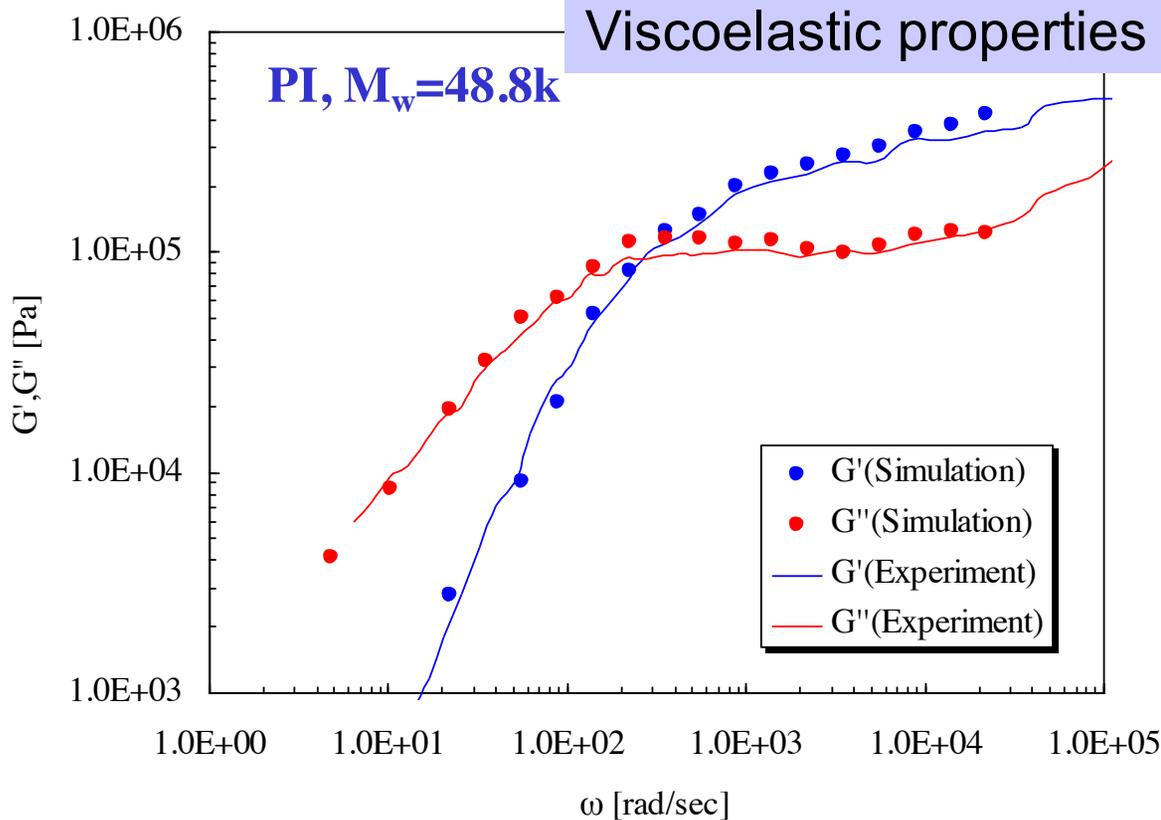


Slip-link model
Primitive chain network model



- Coarse grained unit is based on entanglement
- Entangled polymer chain's long time relaxation
- Shear viscosity, elongation viscosity, etc.

Based on tube model.(Doi-Edwards)





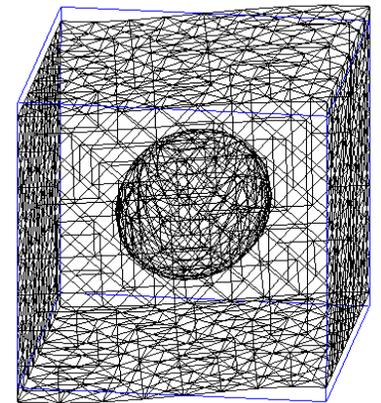
Free energy of the elastic material, Continuum mechanics

$$F\{u_i(\mathbf{x})\} = \int_V d^d x \left\{ G(\mathbf{x}) \left(e_{ij} - \frac{1}{d} \delta_{ij} e_{ll} \right)^2 + \frac{K(\mathbf{x})}{2} (e_{ll})^2 - K(\mathbf{x}) \alpha(\mathbf{x}) e_{ll} \right\}$$

$K(\mathbf{x})$ Bulk Modulus
 $G(\mathbf{x})$ Shear Modulus

$$- \int_V d^d x \rho(\mathbf{x}) g_i u_i(\mathbf{x}) - \int_{S_t} d^{d-1} x T_i(\mathbf{x}) u_i(\mathbf{x})$$

Calculation of distribution of displacement u ,
 under the condition Free energy becomes minimum.



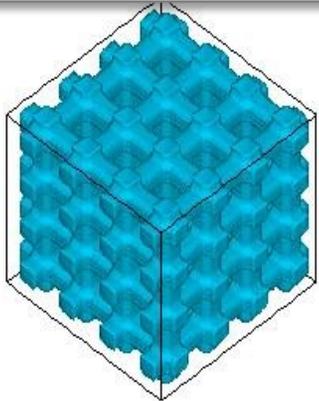
Stress tensor

$$\sigma_{ij} = \frac{\partial F}{\partial e_{ij}} = 2G(\mathbf{x}) \left(e_{ij} - \frac{1}{d} \delta_{ij} e_{ll} \right) + K(\mathbf{x}) \delta_{ij} e_{ll} - K(\mathbf{x}) \alpha(\mathbf{x}) \delta_{ij}$$

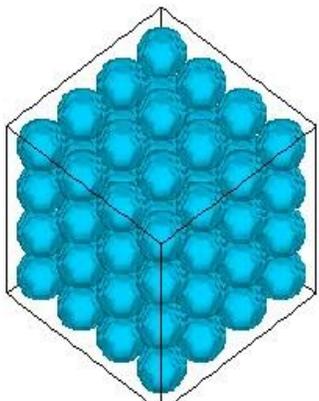
Averaged modulus of PP/Elastomer



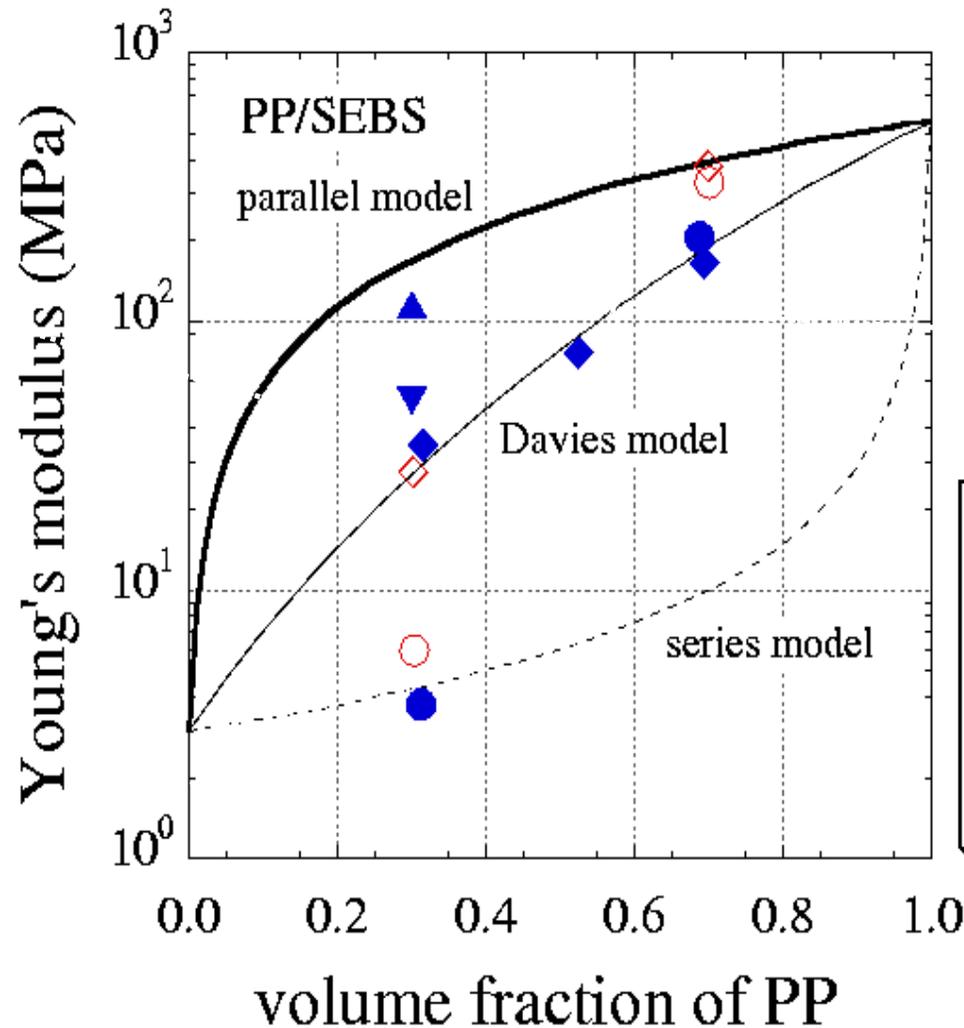
Prediction of average bulk modulus (MUFFIN)



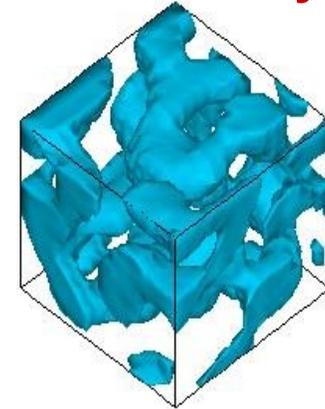
Bicontinuous



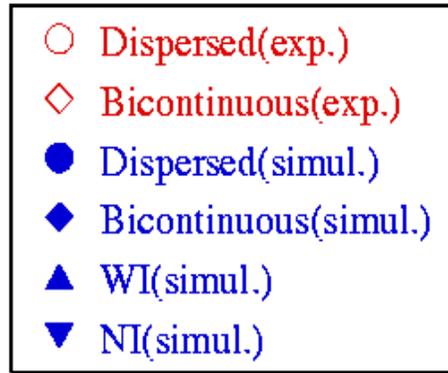
Dispersed



Mean field →
Elastic analysis (FEM)



Mean field



- Elastic analysis based on phase-separated structure.
- Same volume fraction, but different average elastic modulus.

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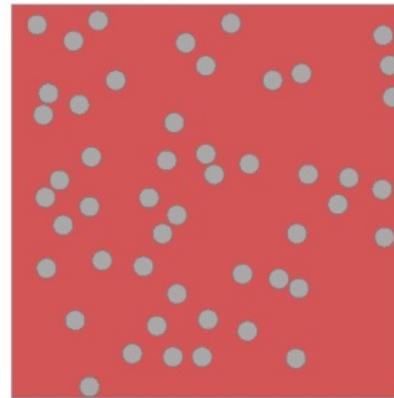
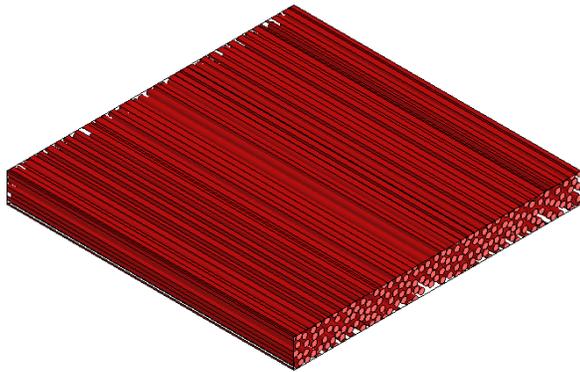
Fracture of CFRTP



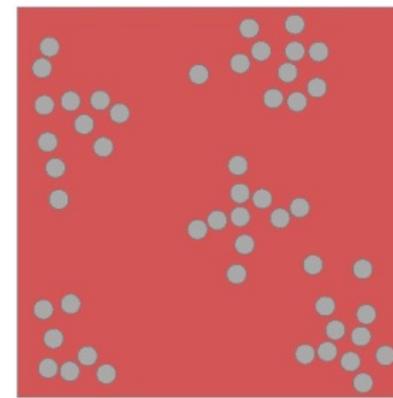
Meso-Structure (UD material)

digimat
LS-DYNA

Sectional view



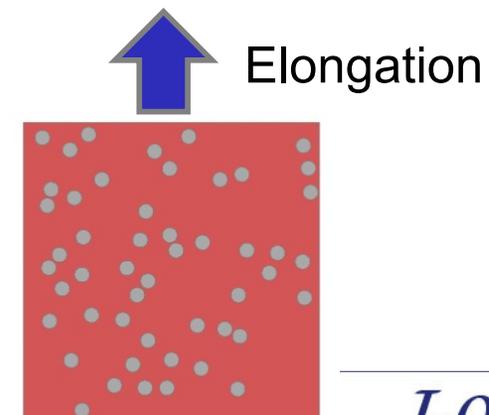
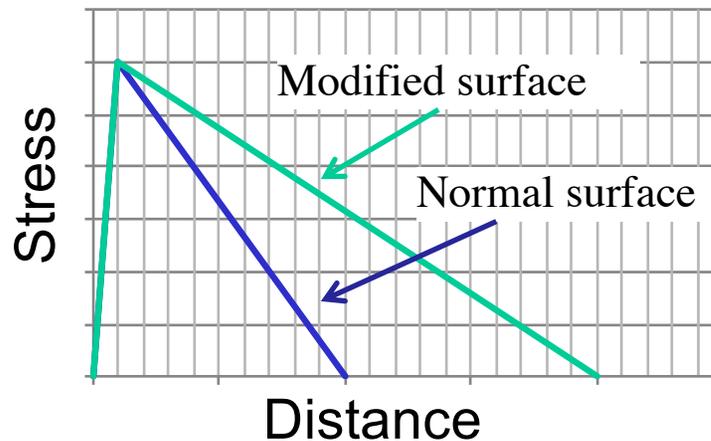
Dispersed



Aggregated

Matrix : PA
Fiber : CF
10 vol%

Cohesive element considering results of CGMD

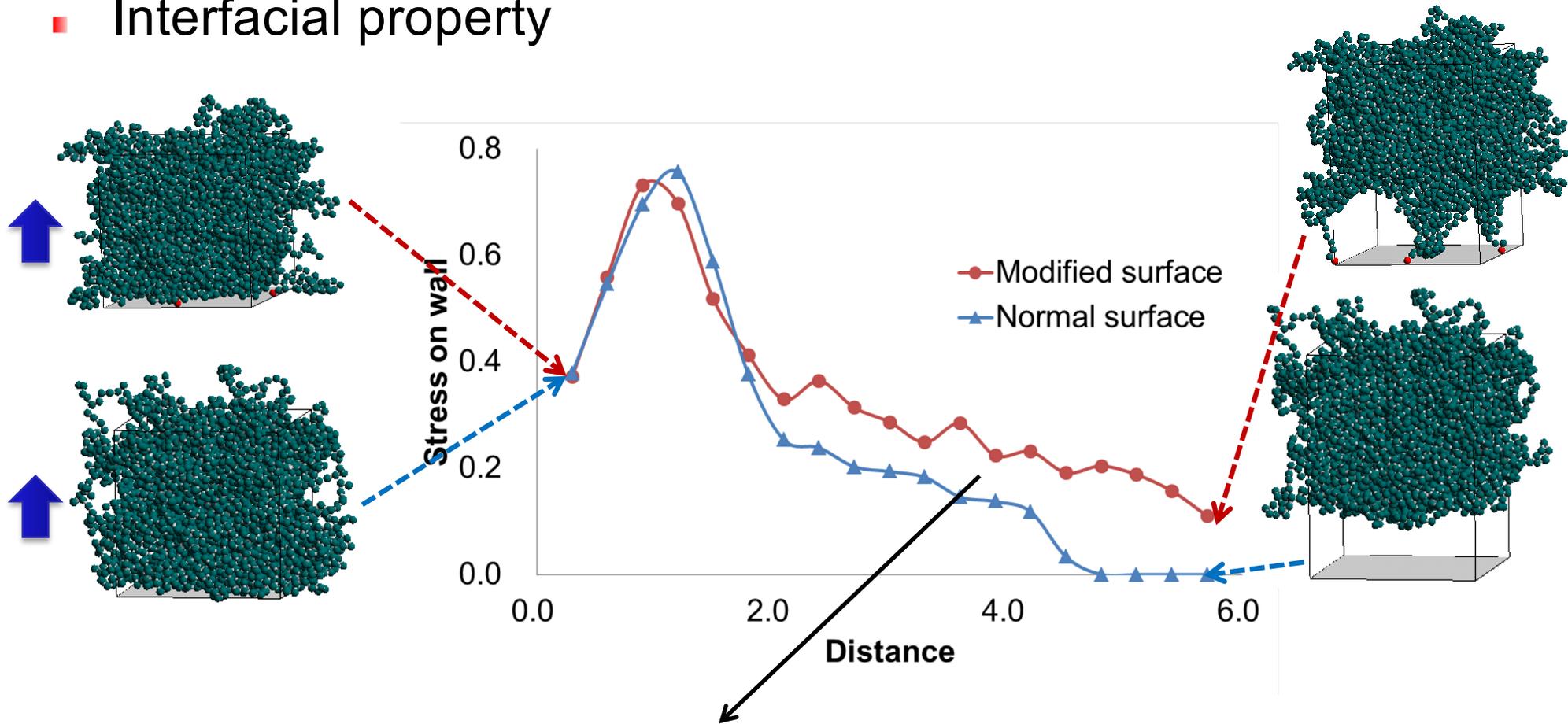


Fracture of CFRTP



Coarse grained Molecular Dynamics (CGMD)

■ Interfacial property

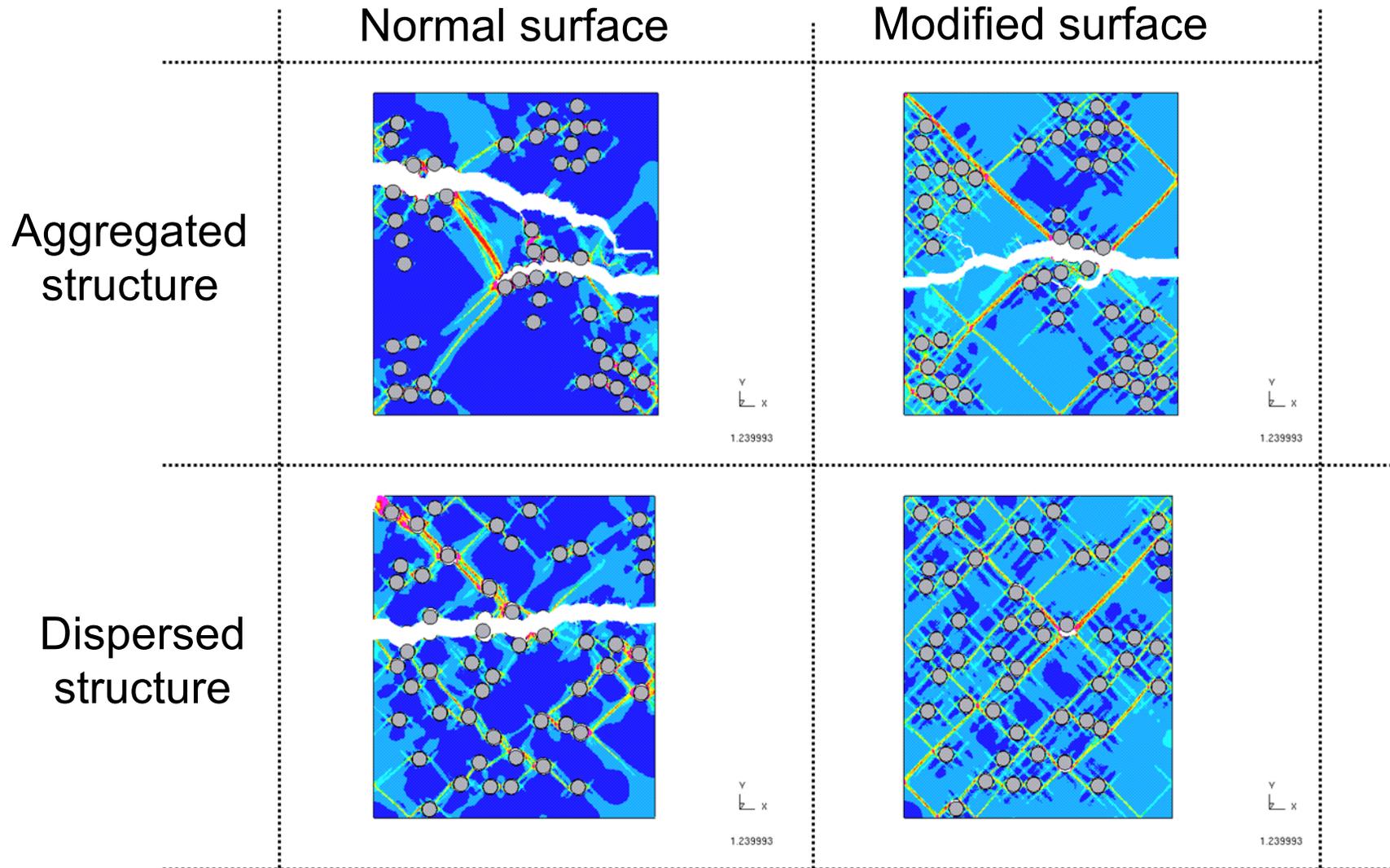


Fracture of CFRTP



digimat
LS-DYNA

Non-linear structure analysis





Thank you for your attention.

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