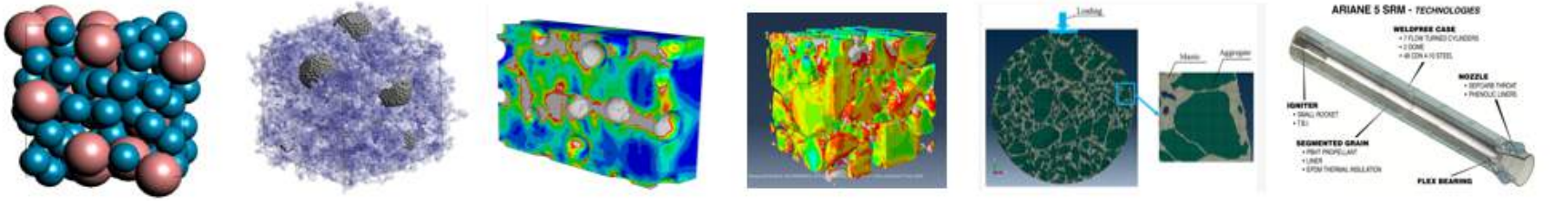
Beijing University of Technology
JSOL Corporation
ANSCOS Technology
MSC Corporation

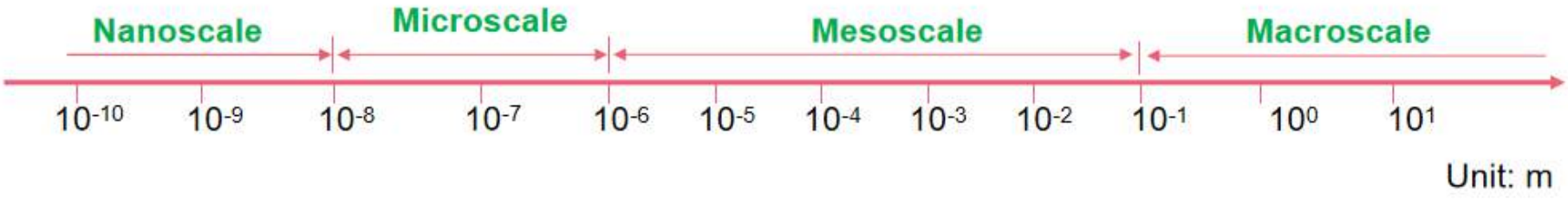
Multiscale Mechanics in Polymer Composite

Speaker: Cao Peng

Associate Researcher

株式会社JSOL ANSCOS MSC Software





Some Challenges for Polymer composite

- Electrification
  - Battery, Motor, Inverter, etc.
    - Electrode (Active materials, Binder), Separator, Elect
    - Magnet
    - Power devices (SiC, etc), Sealing
    - Heat resistance, Thermal conductivity, Low thermal e
      Adhesiveness
- Lightweight
  - Fiber Reinforced Plastics（CFRP, GFRP)
  - Thermoplastic elastomer
    - Stiffness, Fracture
- Low rolling resistance tire
  - Rubber composite (Carbon black, Silica)
    - Viscoelasticity
- High speed communication
  - 5G
    - Low dielectric constant & tanδ, Heat resistance, Moisture resistance

2020 美国 500 强（化工行业榜）		
今年排名	公司名称	收入（百万美元）
78	陶氏	42951
103	3M	32136
152	杜邦	21512
180	宣伟（Sherwin-Williams）	17900
209	PPG 工业公司	15146
213	艺康（Ecolab）	14906
343	伊士曼化学公司（Eastman Chemical）	9273
355	空气化工产品公司（Air Products & Chemicals）	8919
356	美盛（Mosaic）	8906
382	亨斯迈（Huntsman）	8342
391	西湖化学（Westlake Chemical）	8118
470	塞拉尼斯公司（Celanese）	6297
481	奥林（Olin）	6110

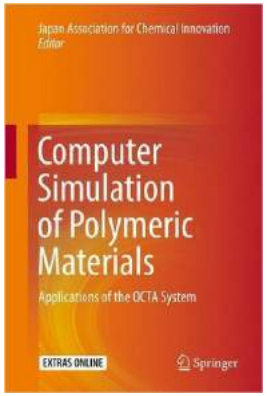
Cost–Effective

Basic material properties are targets.

OCTA and J-OCTA

Open **C**omputational **T**ool for **A**dvanced material technology

OCTA



Source : http://link.springer.com

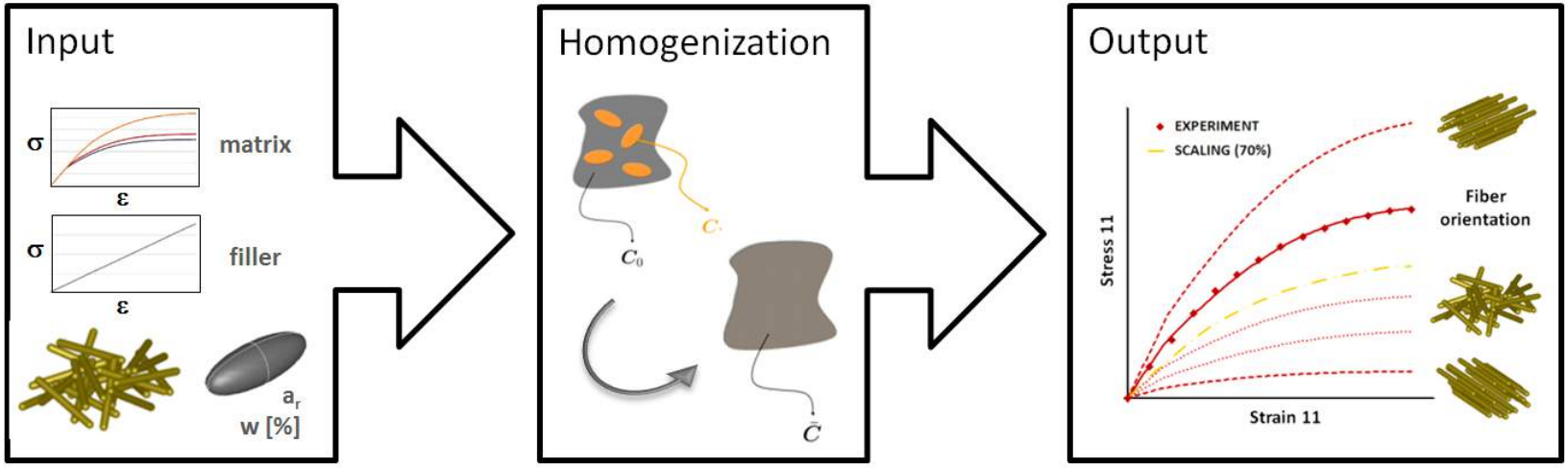
J-OCTA®

- Since 2002
- National project in Japan
- Open source
- Engines, Simple GUI, Python
- Current distributor = AIST
- BBS users > 3000

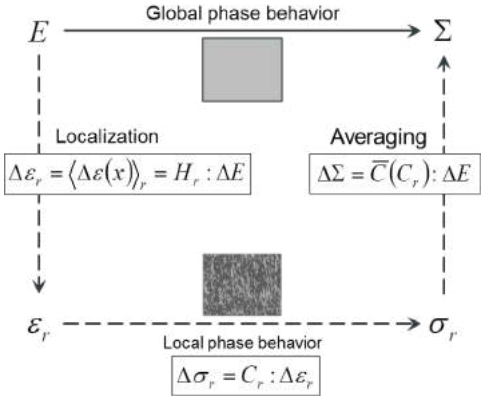
- Since 2005
- Developed by JSOL
- Commercial version
- Modelers for OCTA Engines
- Parallel MD engine
- Industrial users > 100 sites

http://octa.jp/references/publications/

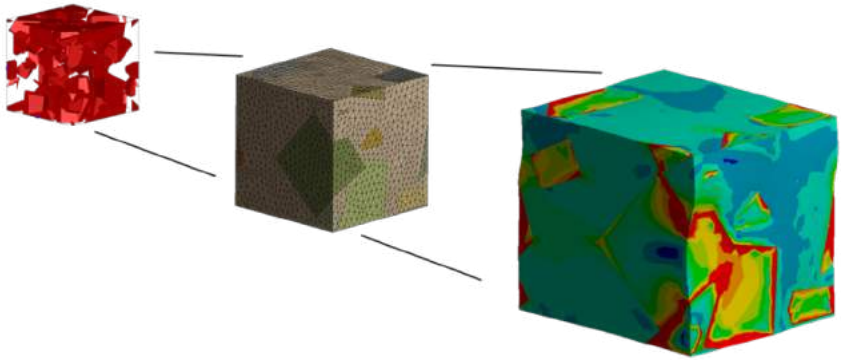
MFH and FEM



Mean-Field Homogenization



Finite Element Homogenization



Simulation Engines

Å nm 10nm 100nm 1μm

KAPSEL

Smoothed Profile Method
Colloidal dispersion

MUFFIN, (LS-DYNA)

Finite Element Method
Mechanical properties, etc.

SUSHI

Mean field (SCF, RPA)
Phase separation, DPD can be applied.

PASTA, NAPLES, VSOP-DPD

Tube model (Slip-link, Primitive Chain Network)
Entanglement, Viscoelasticity

COGNAC, VSOP, (LAMMPS, GROMACS, HOOMD)

(Atomistic & Coarse Grained) Molecular Dynamics, DPD
Molecular structure, Thermo-mechanics, Diffusion, etc.

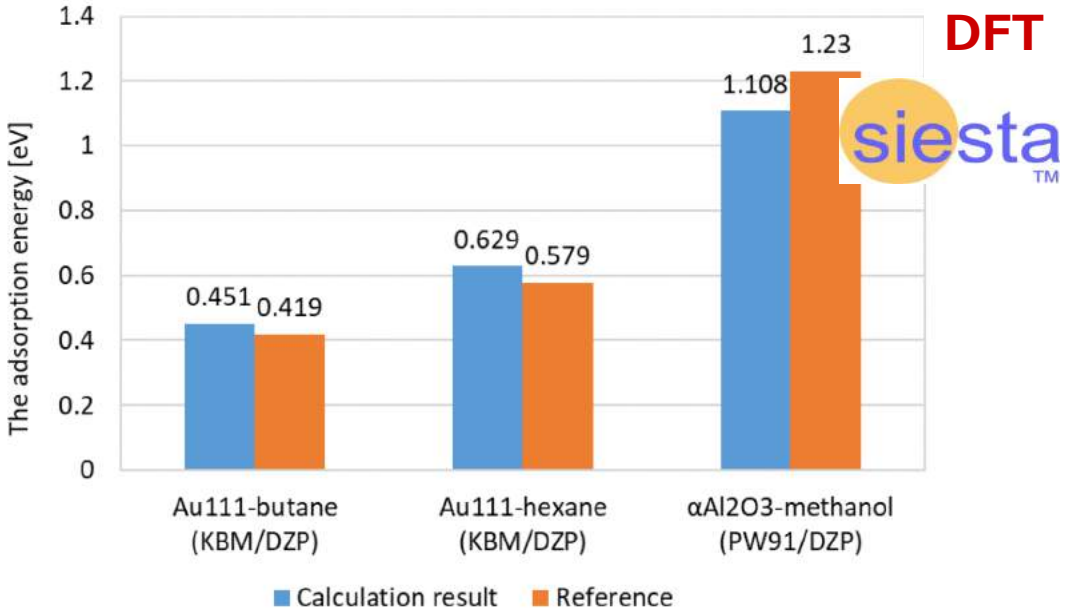
SIESTA, ABINIT-MP, (Firefly, Gaussian, MOPAC)

Density Functional Theory, Molecular Orbital
Electron state, Interaction, Polarization, Reaction, etc.

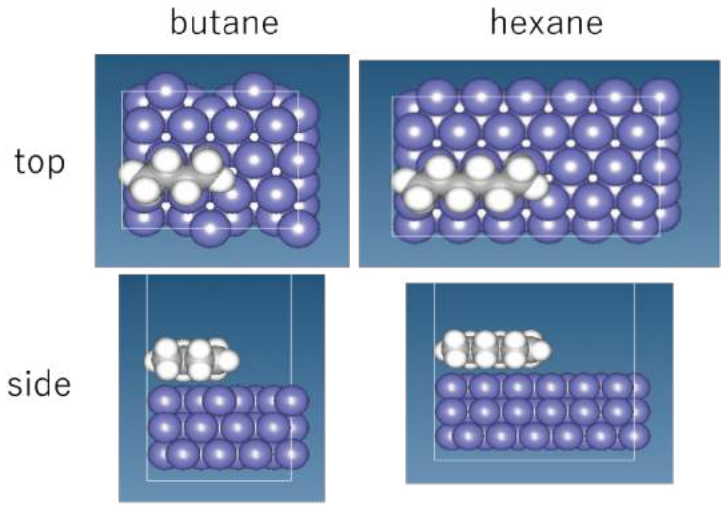
Case studies

Adhesion (Intermolecular force)

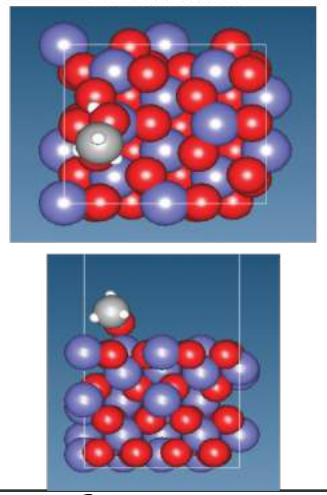
- ✓ Adhesion of molecules on Au/Alumina surfaces
- ✓ Density Functional Theory(DFT) calculation
- ✓ Structure optimization and the evaluation of the adsorption energy



Molecular adsorption on Au (111) surface



Molecular adsorption on α -alumina surface



APPLICATION:
Aeronautics and Astronautics

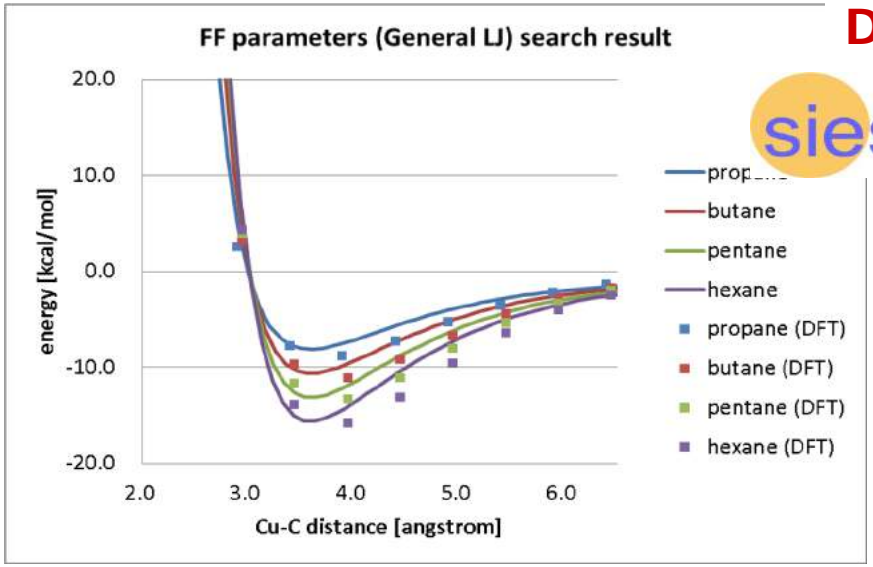
joint Sealing equipment

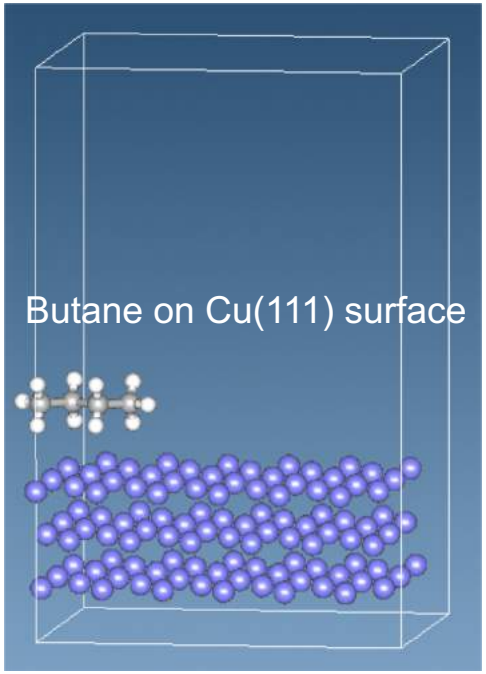
Adhesion (Intermolecular force)

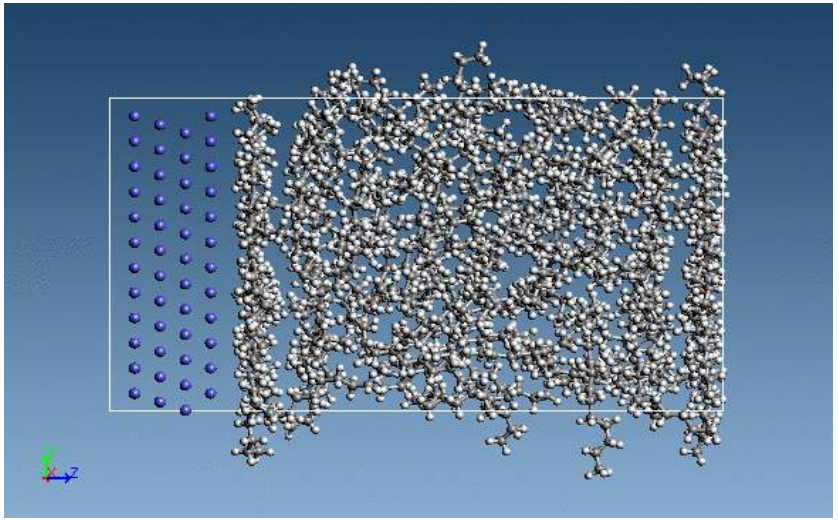
- SIESTA Interfacial Energy Tool
- Adsorption of Alkane molecules onto Cu surface
- Results of DFT was fitted to the Generalized Lennard Jones potential
- Obtained LJ potential was used in the classical MD calculation
- Composite materials, Adhesive, Electrode, etc.

DFT

siesta™



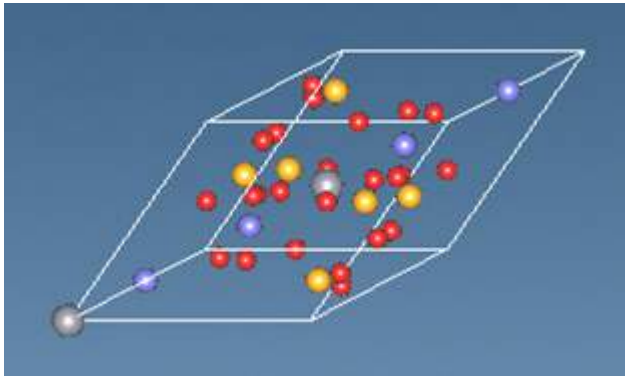


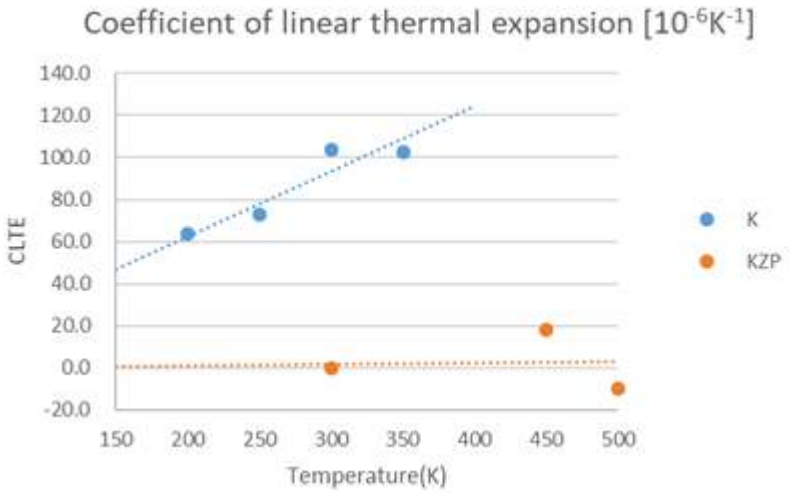


Thermal expansion of ceramics

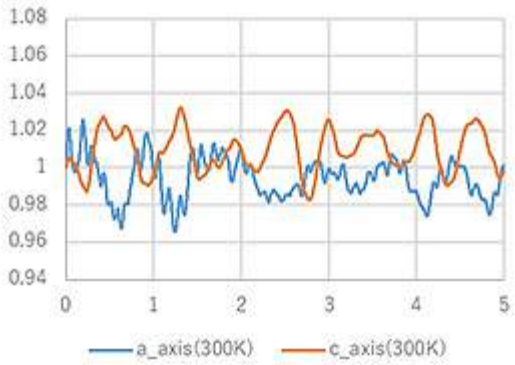
DFT

- The temperature variation in the crystal cell volumes of K and KZP ($KZr_2(PO_4)_3$) were studied with SIESTA.
- KZP shows low expansion.
- Anisotropic expansion is shown.

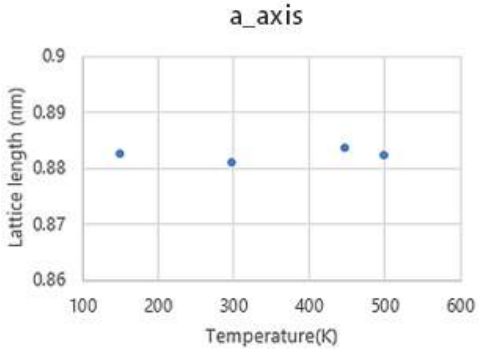


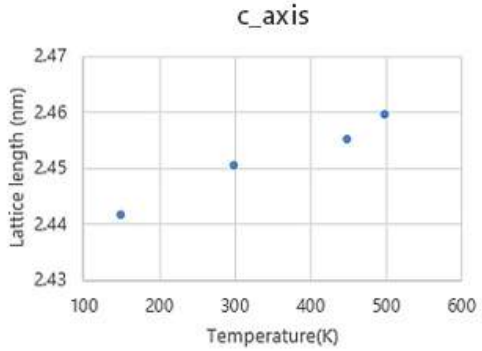


Cell volume changes



Anisotropy of thermal expansion of KZP

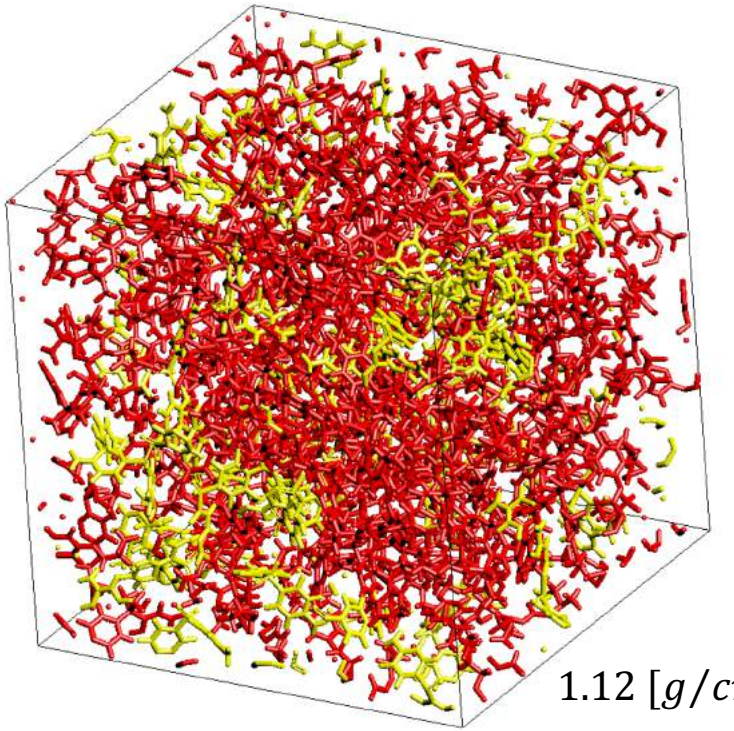




Cross-Linked Epoxy Resin

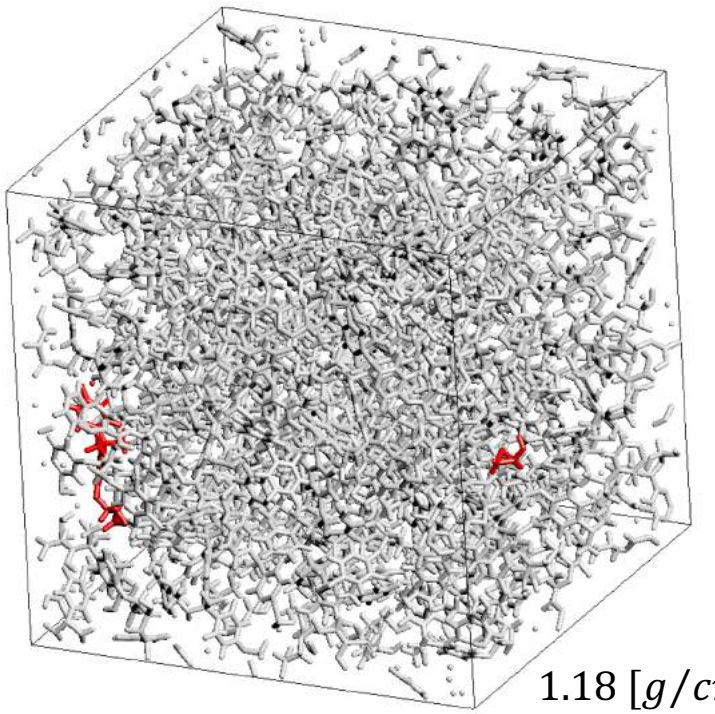
Full Atomistic Molecular Dynamics

- Modeling of Epoxy Resin



$1.12\ [g/cm^3]$

Cross-linking



$1.18\ [g/cm^3]$

DGEBA 双酚A环氧甘油醚

44DDS 氨苯砜

Epoxy Resin

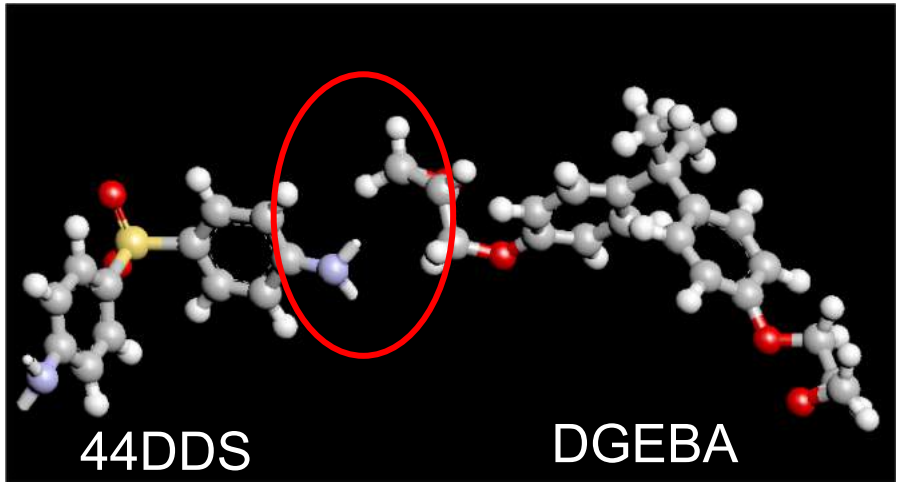
Cross-linking of DGEBA and 44DDS simulated by J-OCTA / VSOP [1]

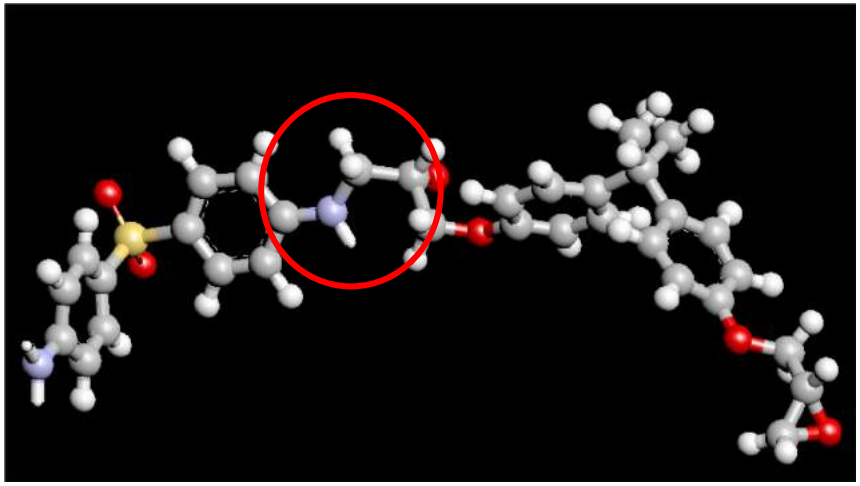
[1] T. Okabe, “Atomistic simulation of curing and mechanical properties of Epoxy resin”, J-OCTA Users Conference 2014

Cross-Linked Epoxy Resin

Full Atomistic Molecular Dynamics

- Process of Cross-Linking Reactions





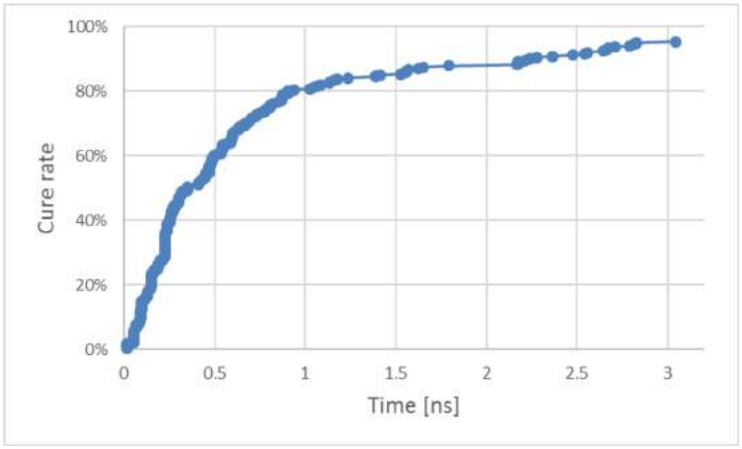
Distance Criterion of reactive atoms

↓

Judge of reaction occurrences
by Monte Carlo using activation energy

↓

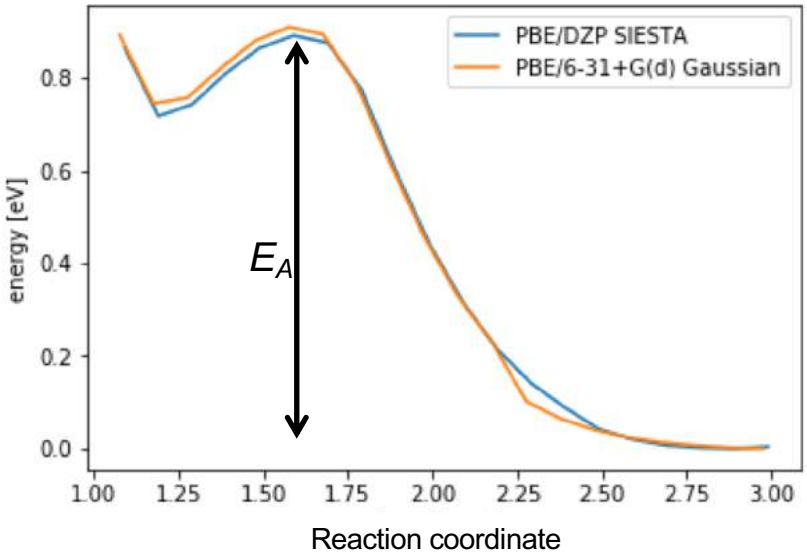
Accelerations by heat of formation

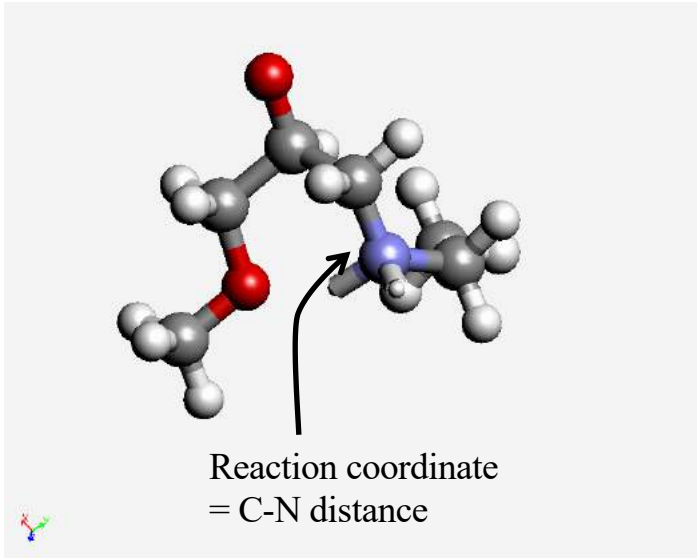


Curing curve

Reaction path analysis

- Relaxed Potential Energy Surface
  - Bond formation between epoxy and amine

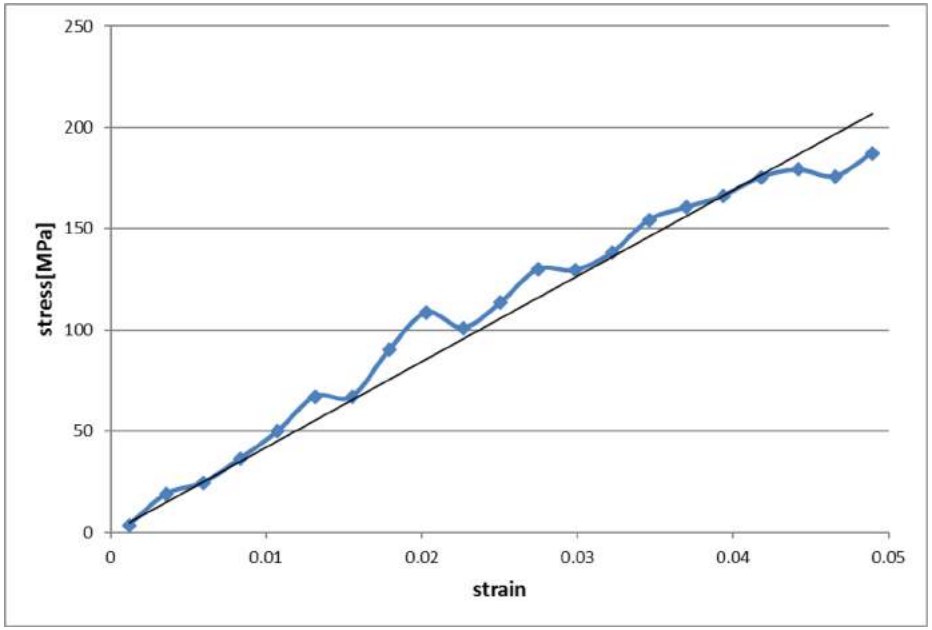




Cross-Linked Epoxy Resin

Full Atomistic Molecular Dynamics

Evaluation of Elastic Modulus

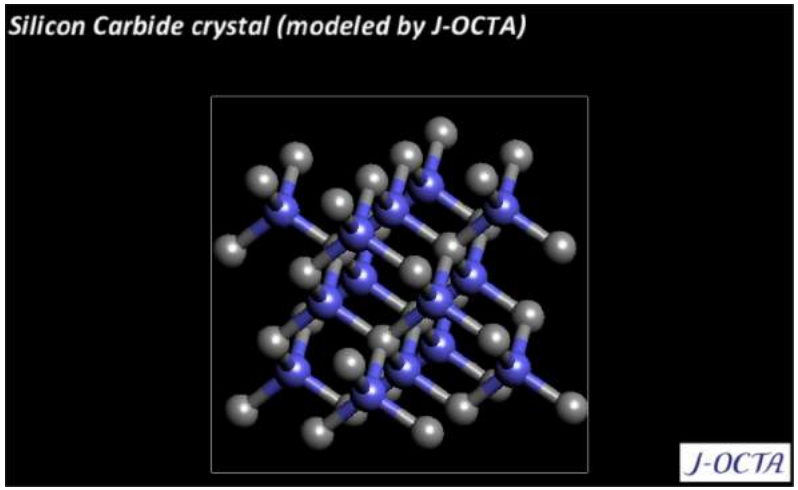


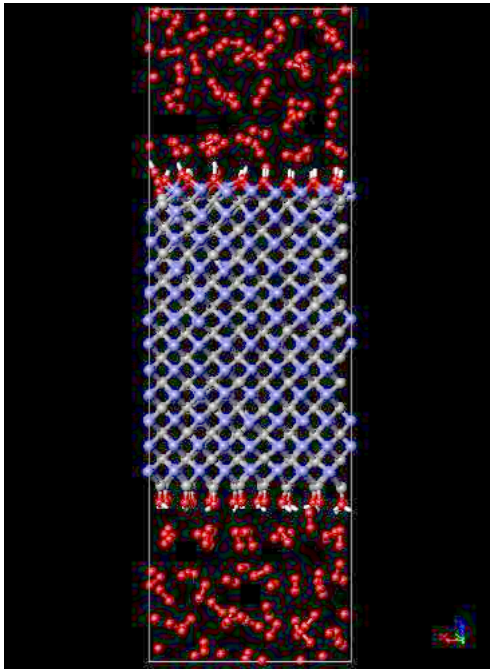
- Cell deformation with elongation rate 10.22 [m/s] under NPT ensemble.
- Young's modulus is evaluated with SS curve fitting of 5% strain.
- Evaluated Young's modulus : 4.22 [GPa] (Experiment [2] : 3.76 [GPa])

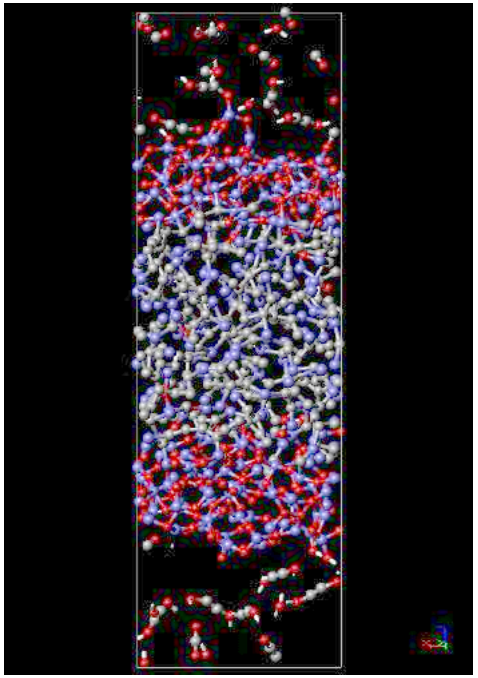
[2] V. Sundararaghavan, A. Kumar, International Journal of Plasticity, 47, 111 (2013)

Complex MD Calculation

- Example of ReaxFF, I/F with LAMMPS
  - Example : Oxidation of SiC







D. Newsome, D. Sengupta, H. Foroutan, M. F. Russo and Adrianus C van Duin, 2012, "Oxidation of silicon carbide by O2 and H2O: A ReaxFF reactive molecular dynamics study: Part I", Journal of Physical Chemistry, **116**, pp. 16111-16121

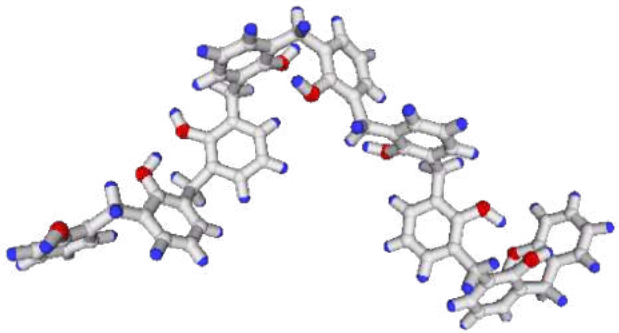
Cross-Linked Phenolic Resins

Full Atomistic Molecular Dynamics

- Modeling of Cross-Linked Phenolic Resins

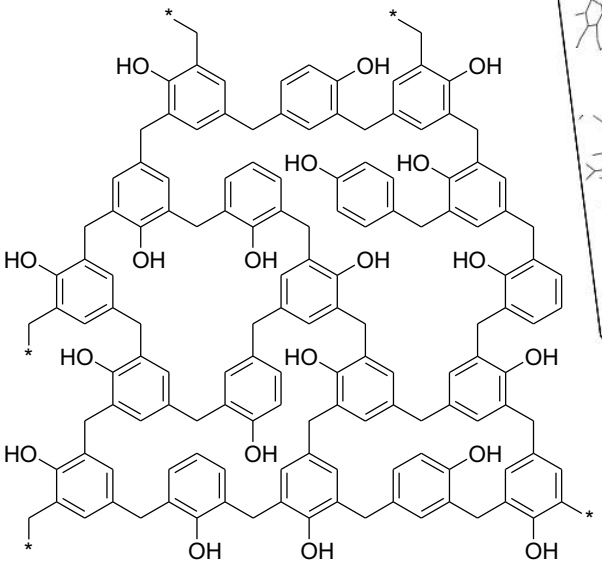
courtesy of

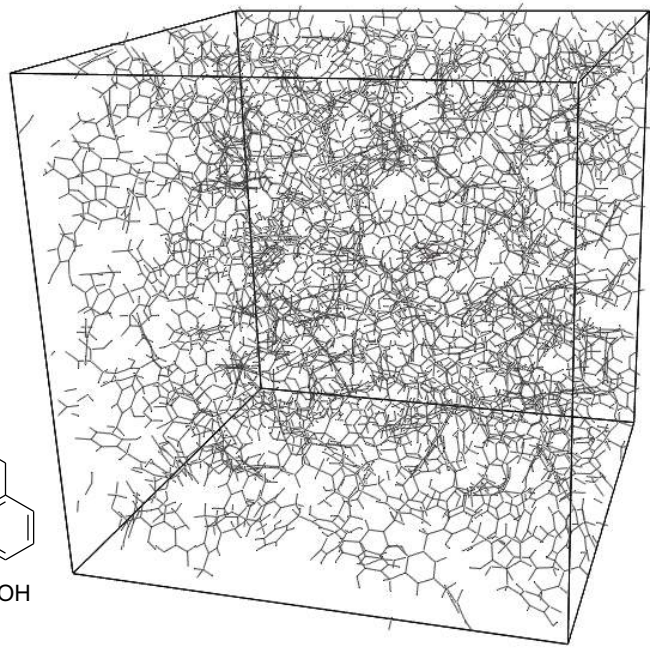
SUMITOMO BAKELITE CO., LTD.



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 $(2N_{CH2})/(3N_{PhOH})$x100.

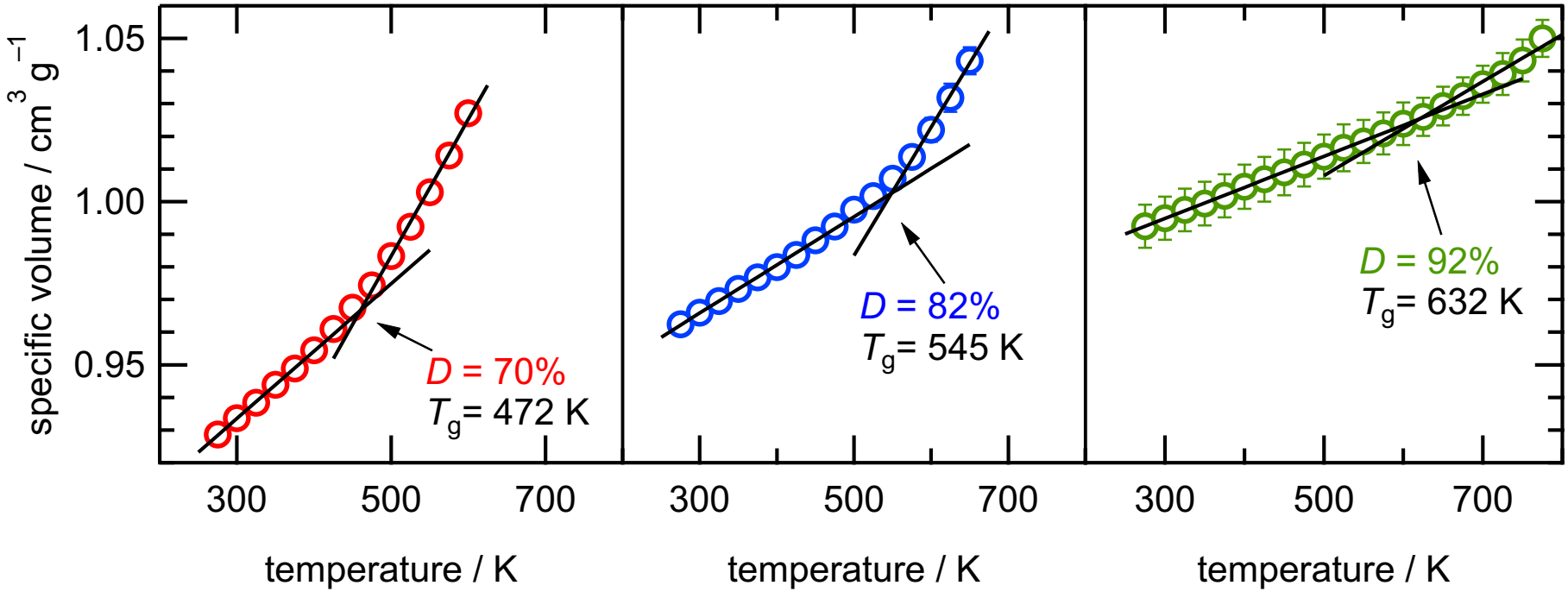
Soft Matter, **8**, 5283 (2012)

Cross-Linked Phenolic Resins

Full Atomistic Molecular Dynamics

- Glass Transition Temperature (T_g)

courtesy of SUMITOMO BAKELITE CO., LTD.



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

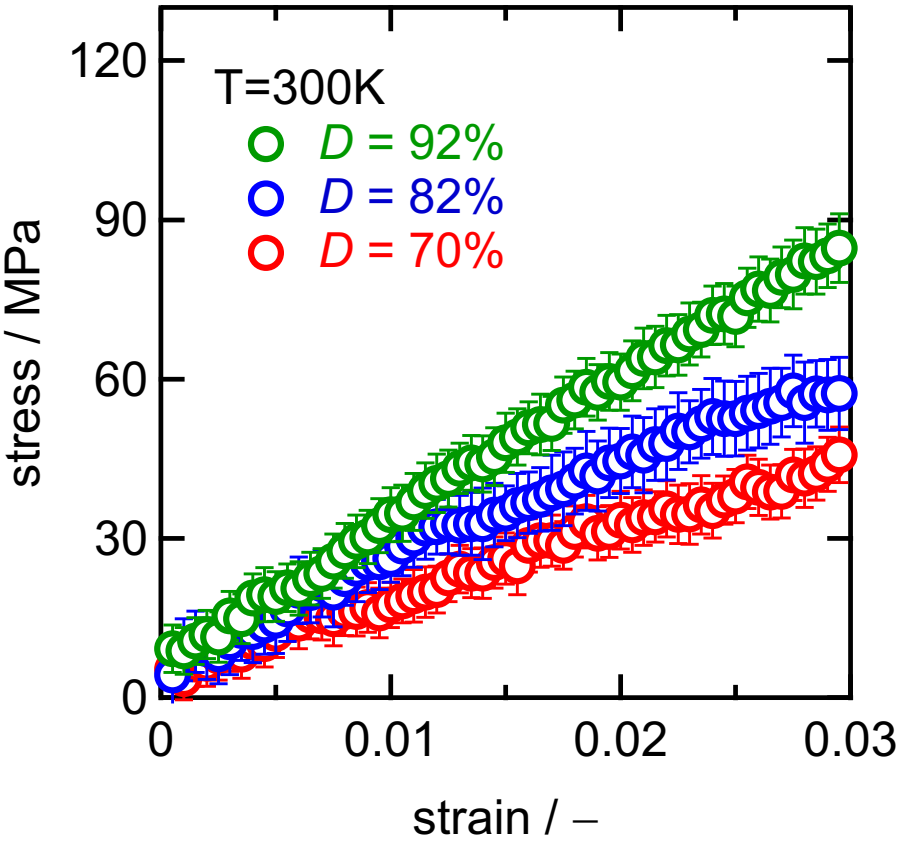
Cross-Linked Phenolic Resins

Full Atomistic Molecular Dynamics

- Uniaxial Elongation: Stress–Strain Curves

courtesy of

SUMITOMO BAKELITE CO., LTD.

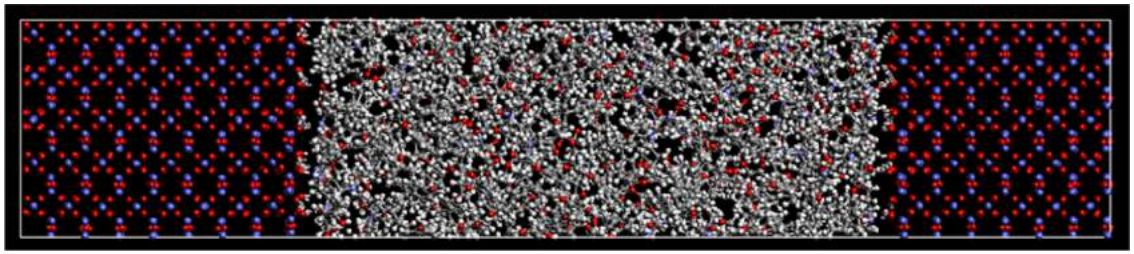


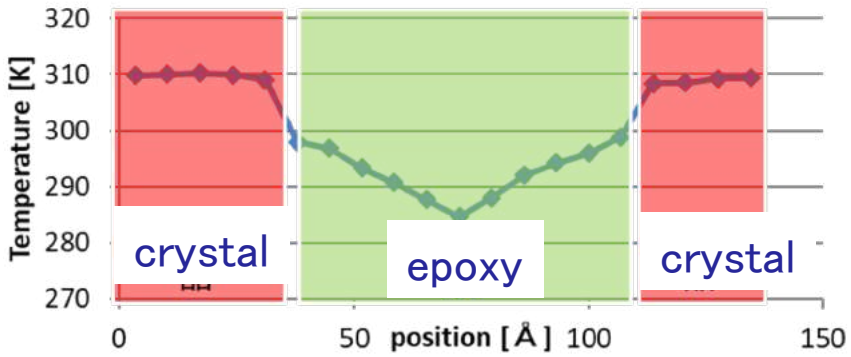
Soft Matter, **8**, 5283 (2012)

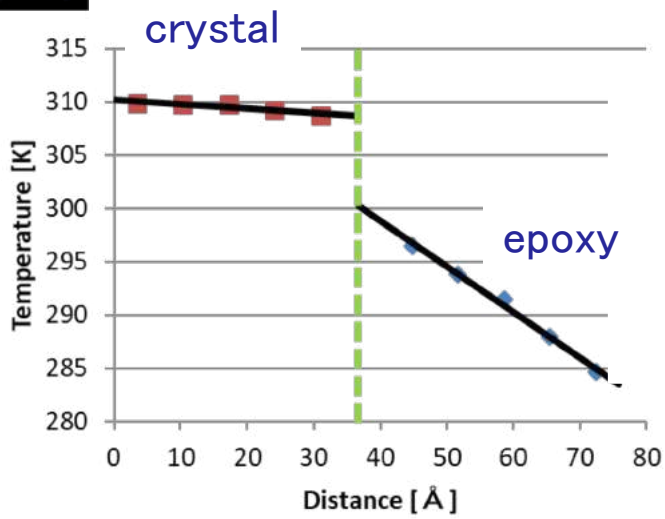
Thermal conduction

Full Atomistic Molecular Dynamics

- High and low temperature regions are set (RNEMD).
- Not only one component, but also the interface between inorganic crystal and the epoxy resin.
- Effects of the interfacial modification.







Solubility

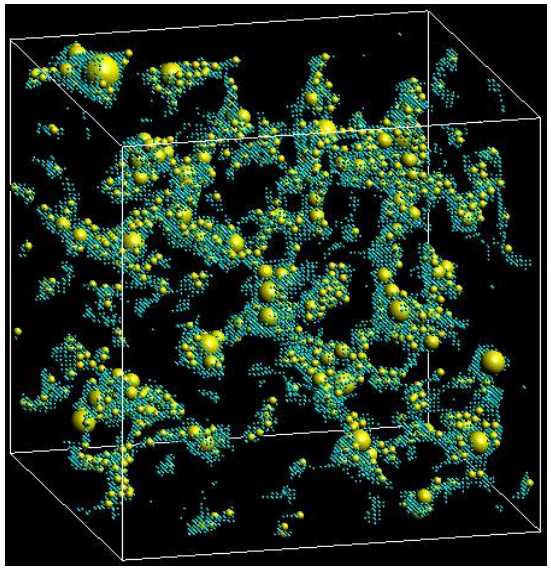
Full Atomistic Molecular Dynamics

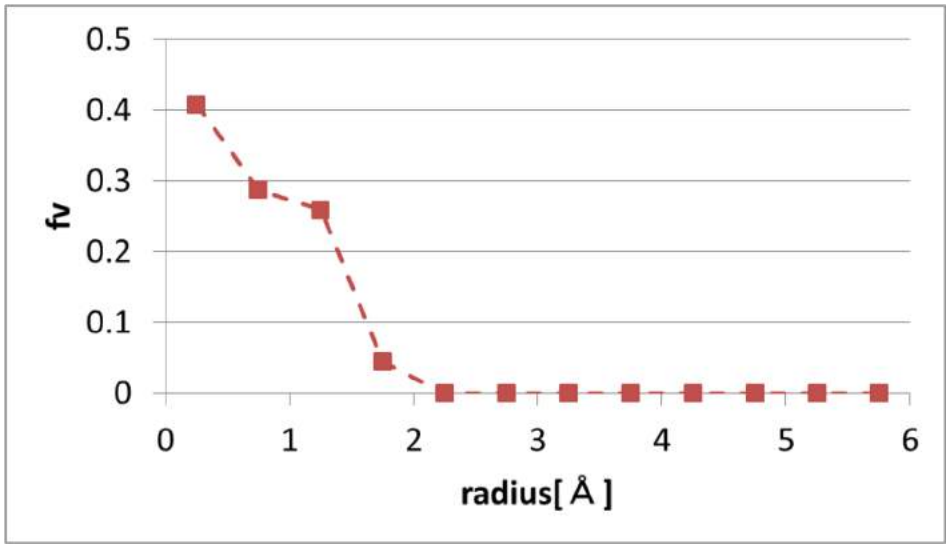
Diffusion D, Solubility S, Permeability P

$$P = D \times S$$

S is calculated by using EVMS (Excluded Volume Map Sampling)

(Ex) CO_2 in *cis* Polyisoprene（聚异戊二烯，橡胶）
S = 4.23E-06 [cm^3(STP)/(cm^3 Pa)]





Distribution of free volume in bulk polymer system

Diffusion of small molecules in polymers

Full Atomistic Molecular Dynamics

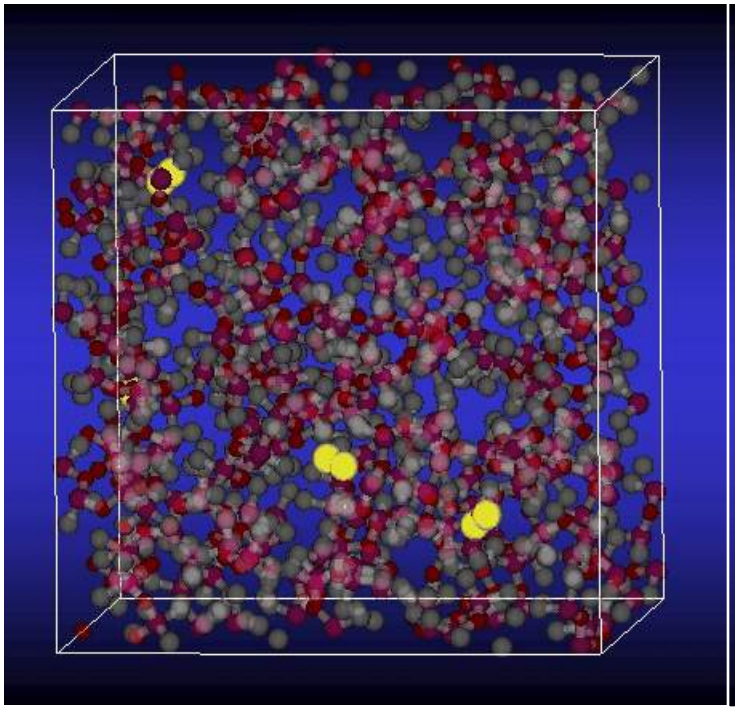
Diffusion of small molecules in PDMS

Diffusion coefficients

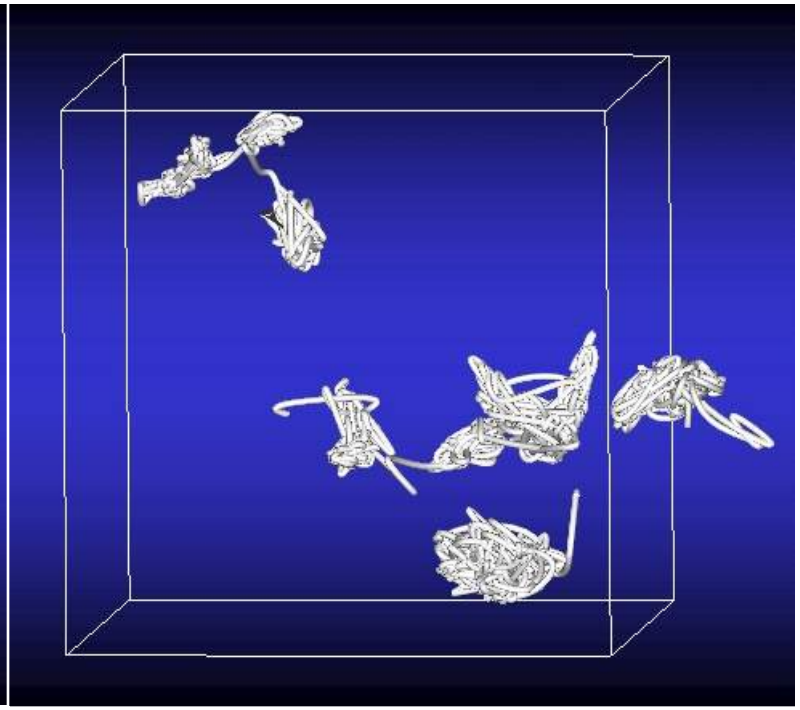
聚二甲基硅氧烷

[cm^2/sec]

Molecule	Calc. (300[K])	Exp. (308[K])
CO_2	2.65E-05	2.63E-05
O_2	5.61E-05	3.96E-05



Dynamics of O_2 (Yellow molecule)

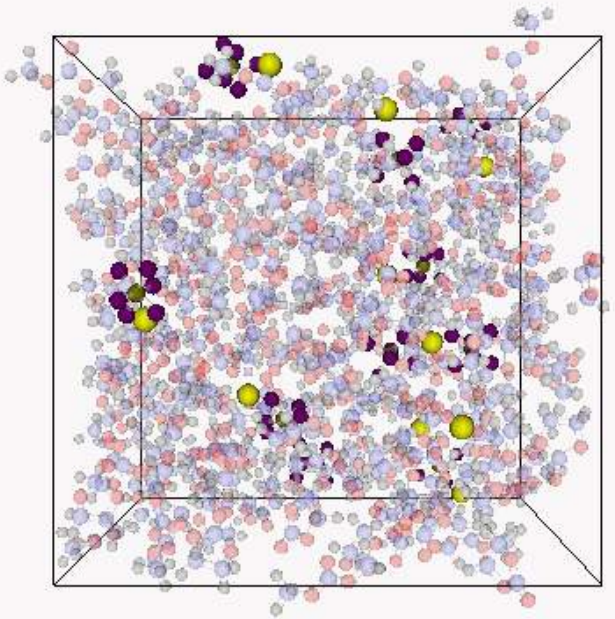


Trajectory of O_2

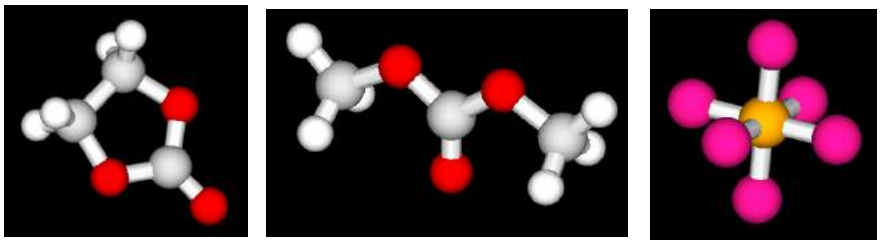
Electrolyte (Li+ ion)

Full Atomistic Molecular Dynamics

- Diffusion of Li+ ion in the electrolyte solution
- Effect of molecular structures
- Evaluation of ionic conductivity from diffusion coefficient



Li+ ion (yellow particle) in electrolyte



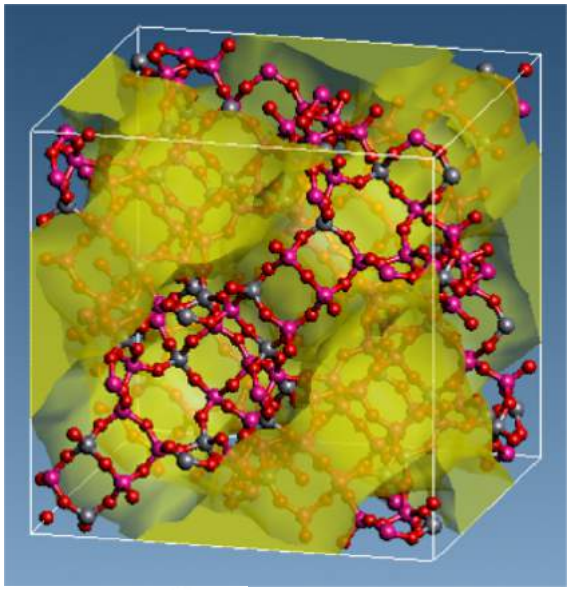
EC DMC PF6

乙基纤维素
碳酸二甲酯
聚酰胺（尼龙材料）

Gas adsorption on zeolite

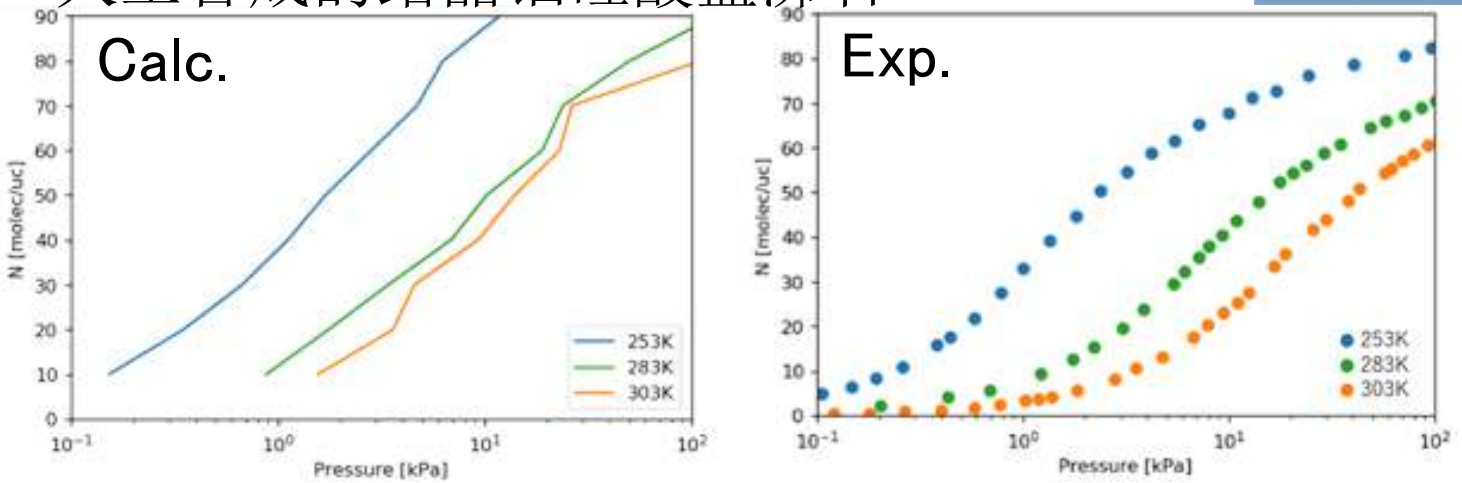
Full Atomistic Molecular Dynamics

- NaY zeolite
  (CO_2 is adsorbed in yellow region)
- Evaluation of adsorption isotherms of gas molecules by free energy calculations



$Na_{56}[(AlO_2)_{56}\ (SiO_2)_{136}]\cdot 250H_2O$

人工合成的结晶铝硅酸盐沸石

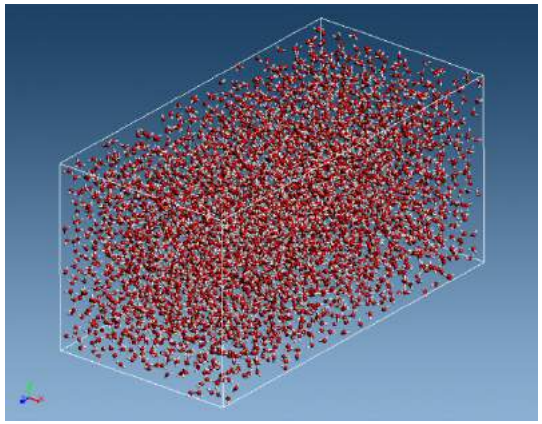


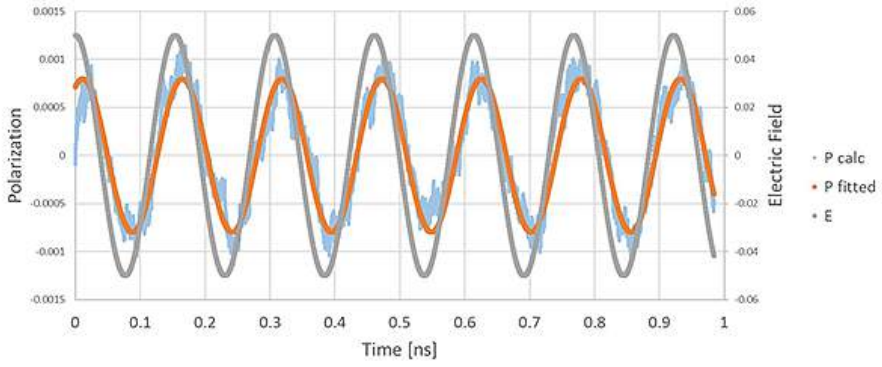
Adsorption isotherms of gas molecules

Dielectric dispersion in the GHz frequency range

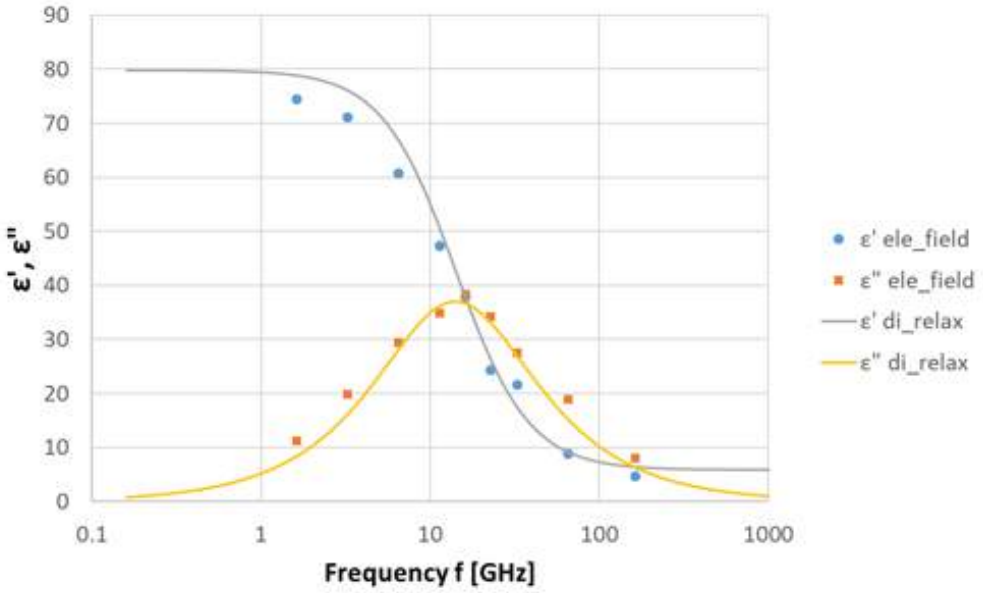
Full Atomistic Molecular Dynamics

- Evaluate the response of the polarization at each time by applying a periodic electric field
- Evaluation of the complex permittivity

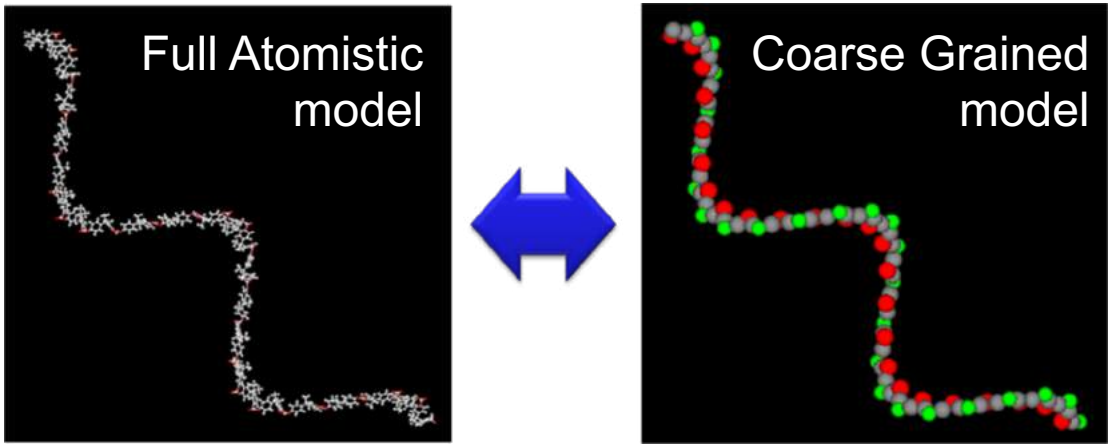


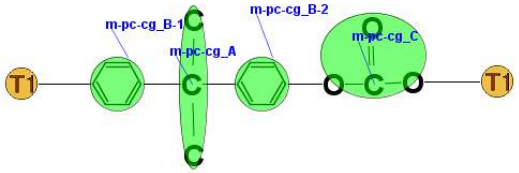


response of the polarization



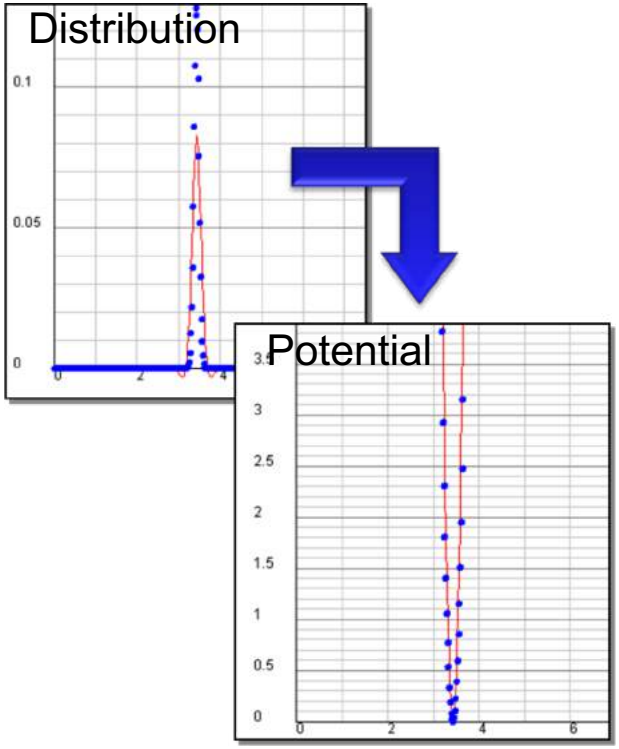
Coarse Grained potential





Bond potential

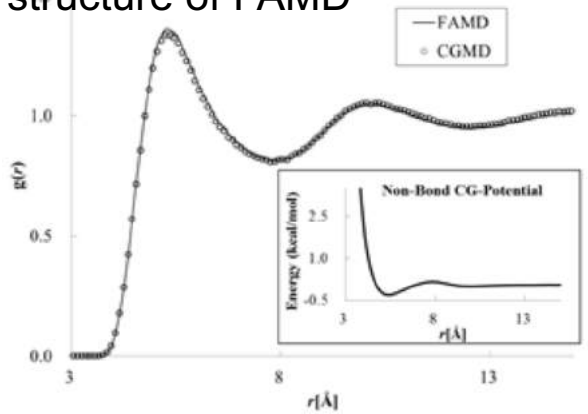
Distribution obtained by FAMD for isolated system



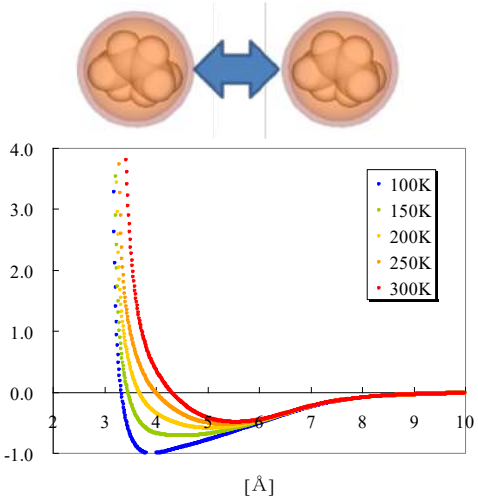
Non-Bond potential

1. Iterative Boltzmann Inversion

Reproduction of amorphous structure of FAMD



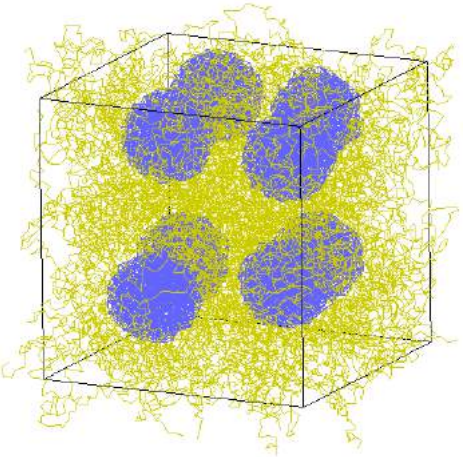
2. Direct estimation

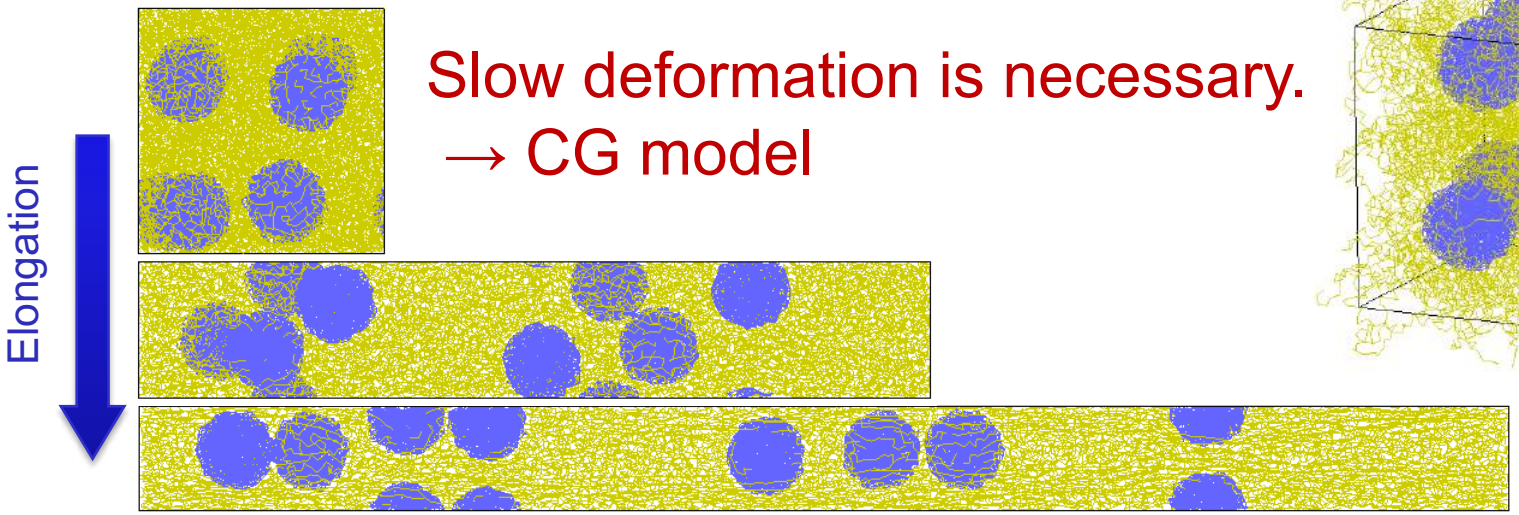


Typical case study of CG model

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

Coarse grained Molecular Dynamics (CGMD)

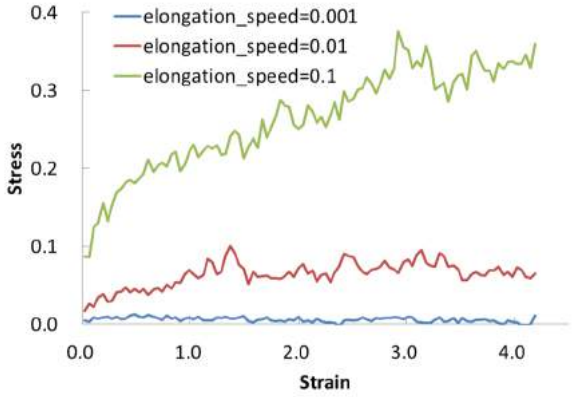




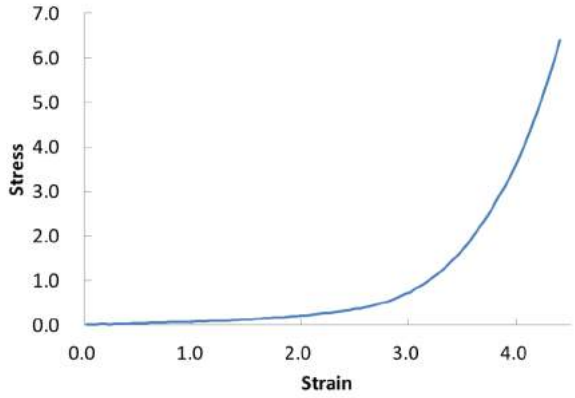
Slow deformation is necessary.
→ CG model

Stress-Strain curve

Non-cross link
Influence of deformation speed



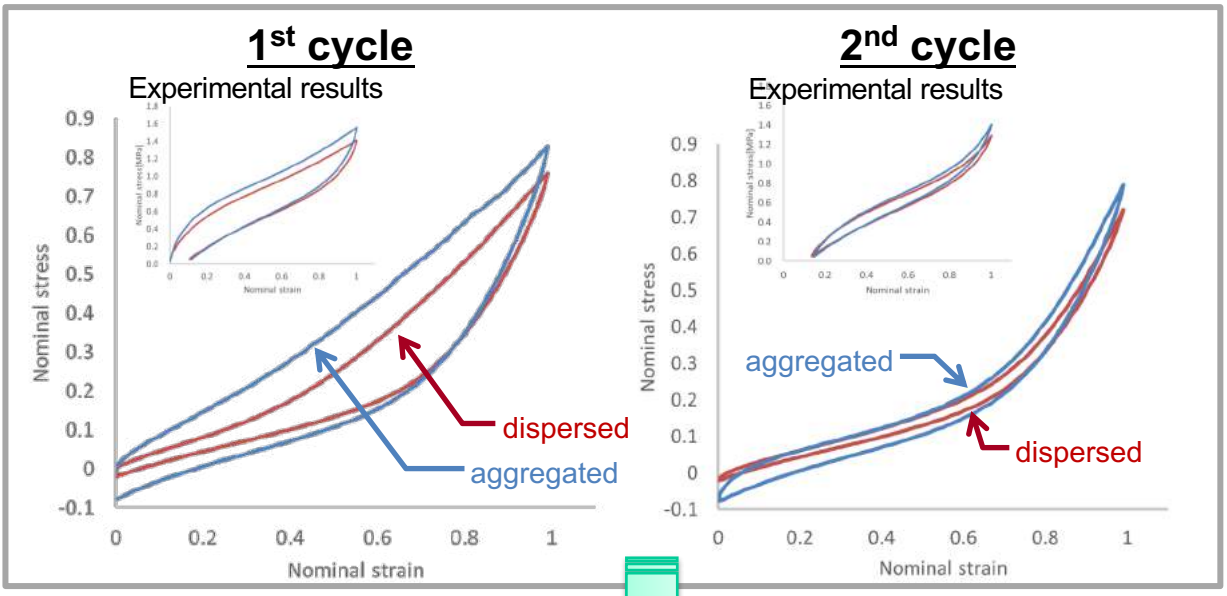
With cross-link (elongation speed is 0.001)

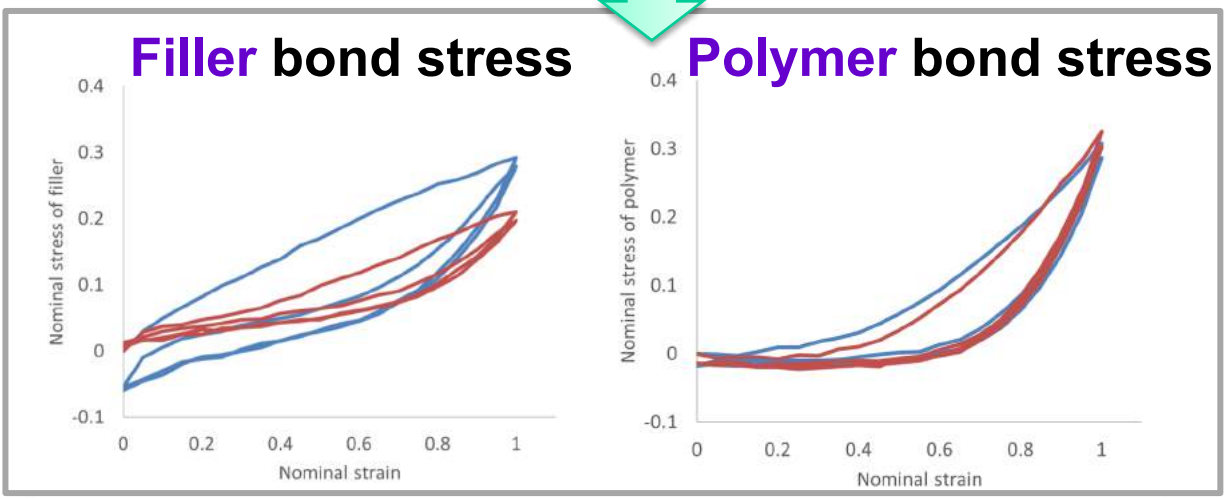


Filled Rubber under Cyclic Tensile Deformation

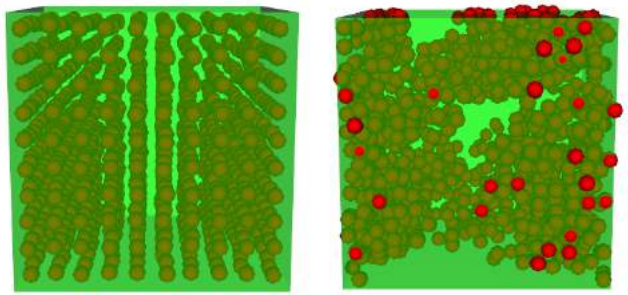
Courtesy of YOKOHAMA

- **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%）

- **MULLION EFFECT**

Filled Rubber under Cyclic Tensile Deformation

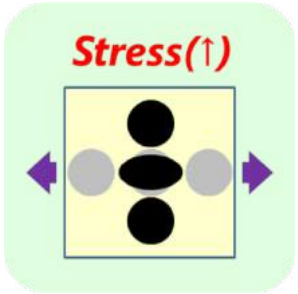
Courtesy of YOKOHAMA

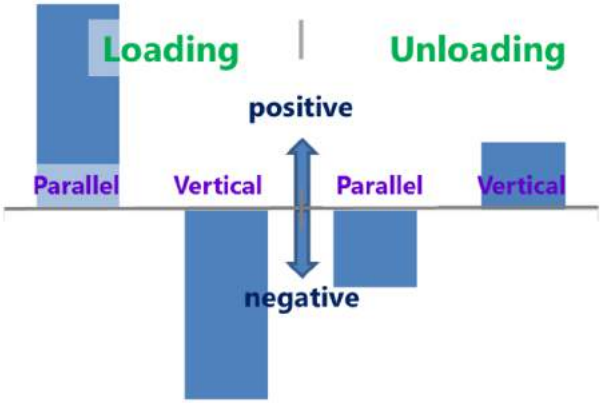
Mechanism of hysteresis

- Mechanism (Filler)

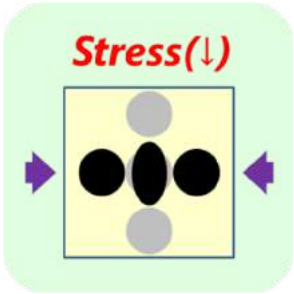
Stress components of filler in aggregated model
(difference from dispersed model)

Loading



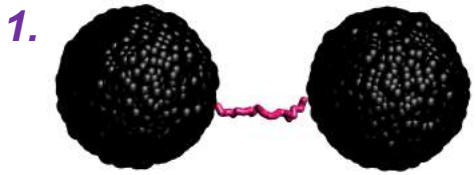


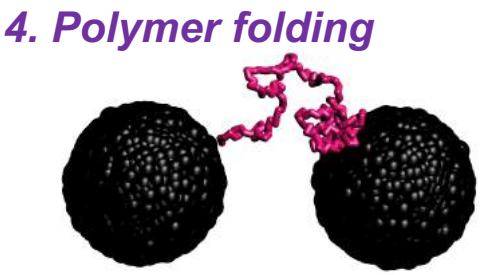
Unloading

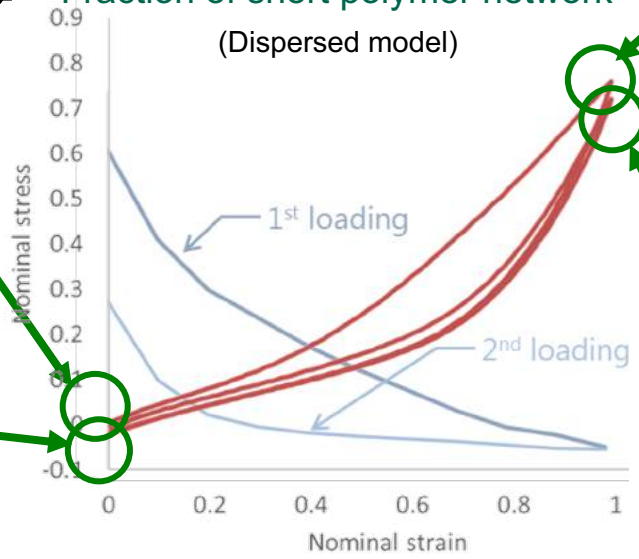


- Mechanism (Polymer)

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





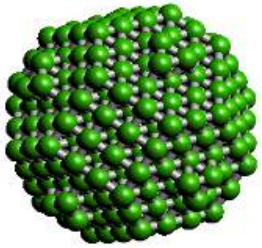


Slurry coating process

TOYOTA

- **Simulation model (Cognac/VSOP)**

- Bead-spring model



Particle

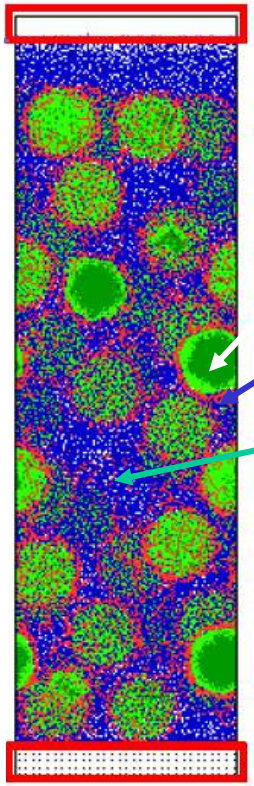
Polymer

Solvent

Study of material property
- Interactions between molecules
- Polymer rigidity

- Evaporation of the solvent

Evaporation



Delete area : solvent molecule

Green: Particle

Red: Polymer

Blue: Solvent

Base

Objectives

✓ Develop the method to simulate diffusion in materials by CGMD

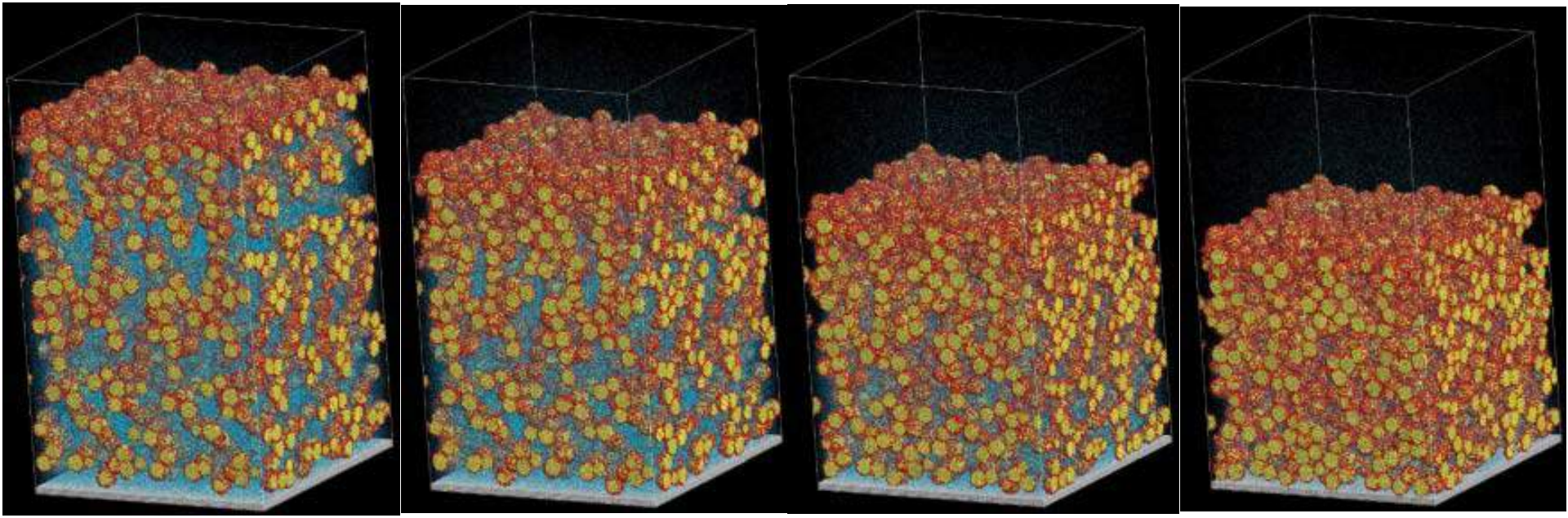
✓ Clarify the mechanism of slurry coating process

✓ Understand the correlation between battery performance and material properties

Slurry coating process

TOYOTA

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



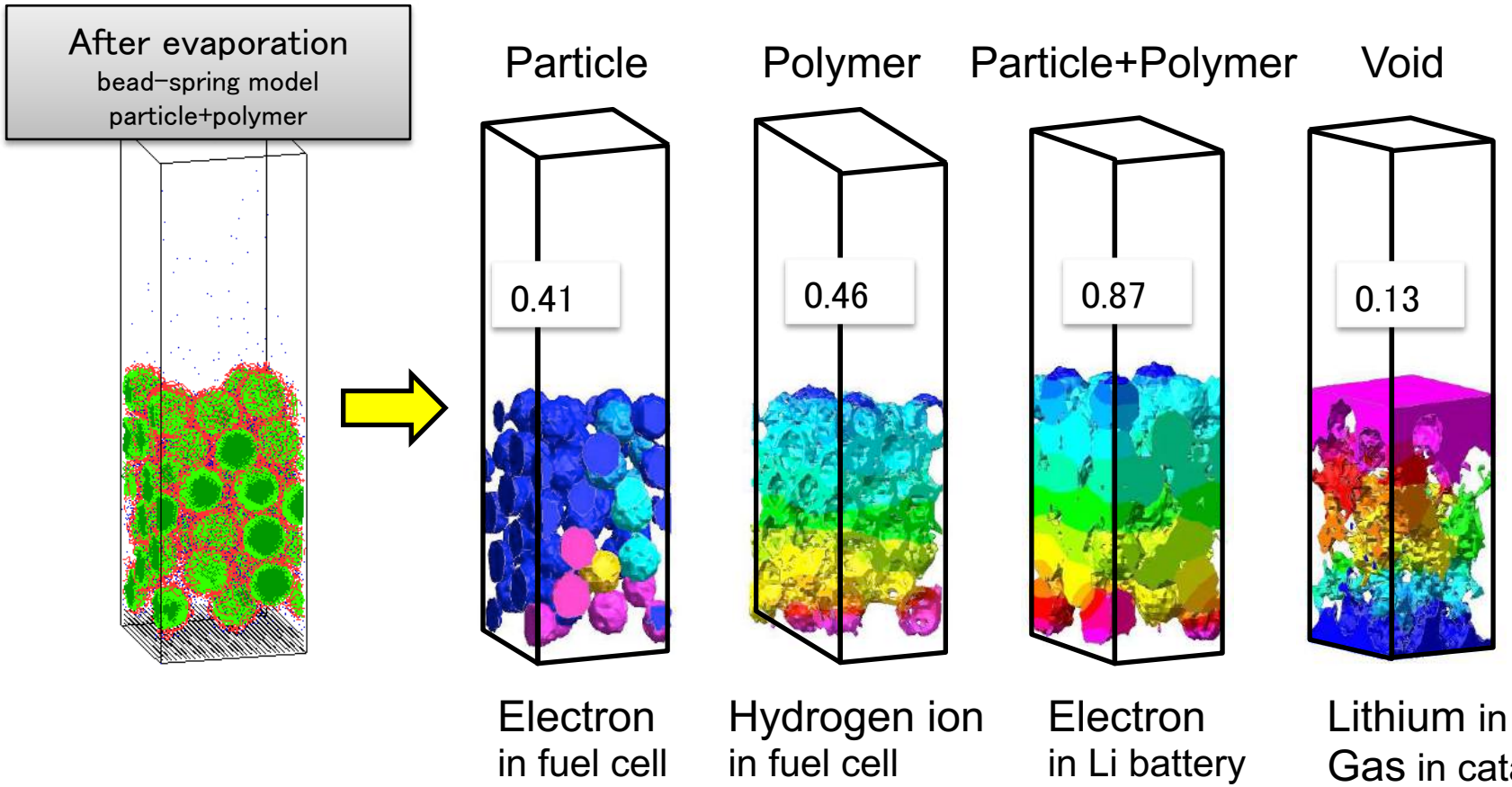
Initial → Final

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

Slurry coating process

TOYOTA

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



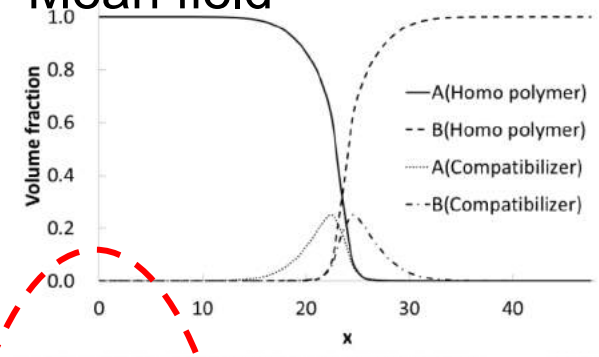
✓ Studies of material property with microstructure after evaporation using molecular dynamics (micro) and FEA (macro)

Strength of interface (polymer blend)

Mean Field -> Coarse grained Molecular Dynamics (CGMD)

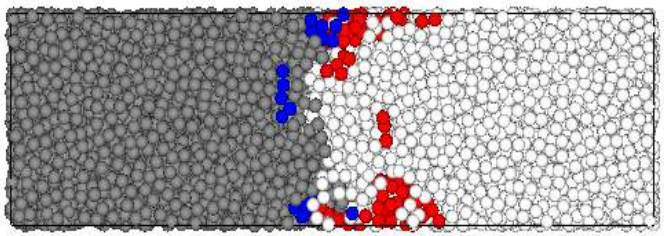
For polymer blend, strength and structure of interface is important.

Mean field



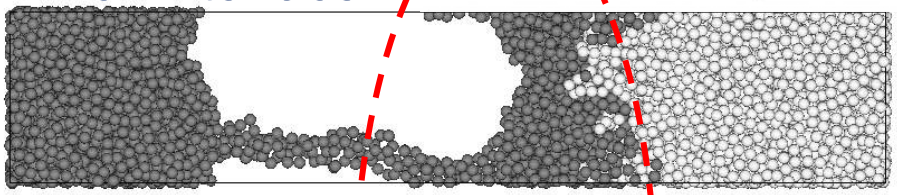
Mapping

CGMD



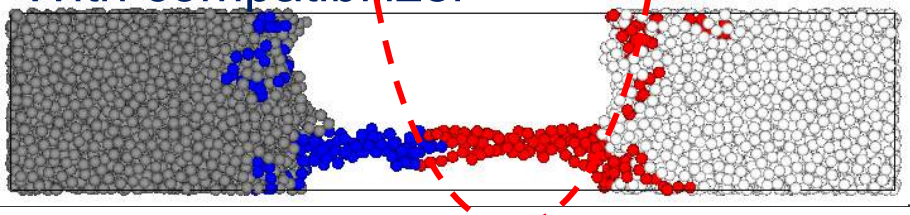
Elongation

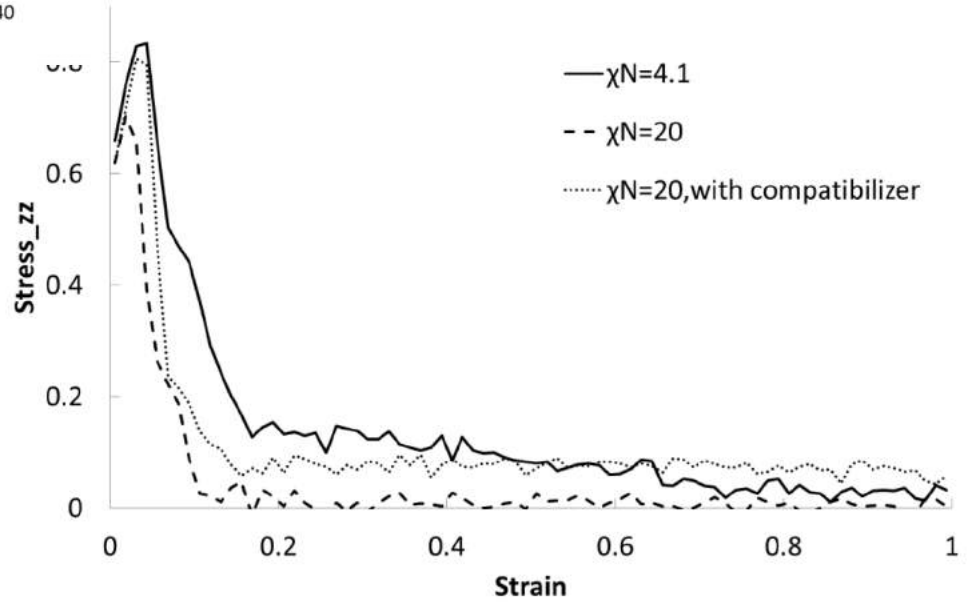
Thick interface



Thin interface

With compatibilizer



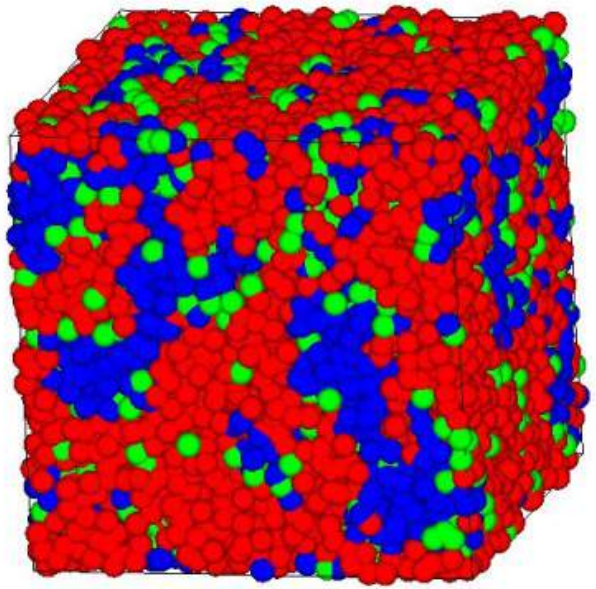


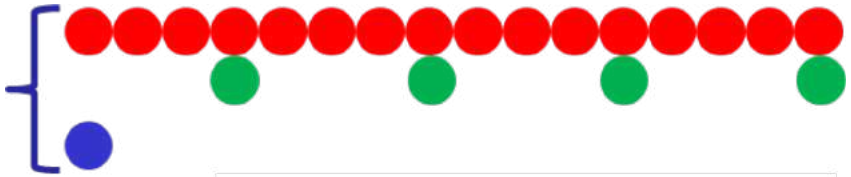
J.Soc.Rheol.Jpn, **37**,75 (2009)

Polymer electrolyte for Fuel Cell

DPD

- Phase separation of polymer electrolyte and water
- Proton moves in the channel of water
- Estimation of the interaction parameter is possible on J-OCTA.
- Phase separation near Pt is calculated as well.



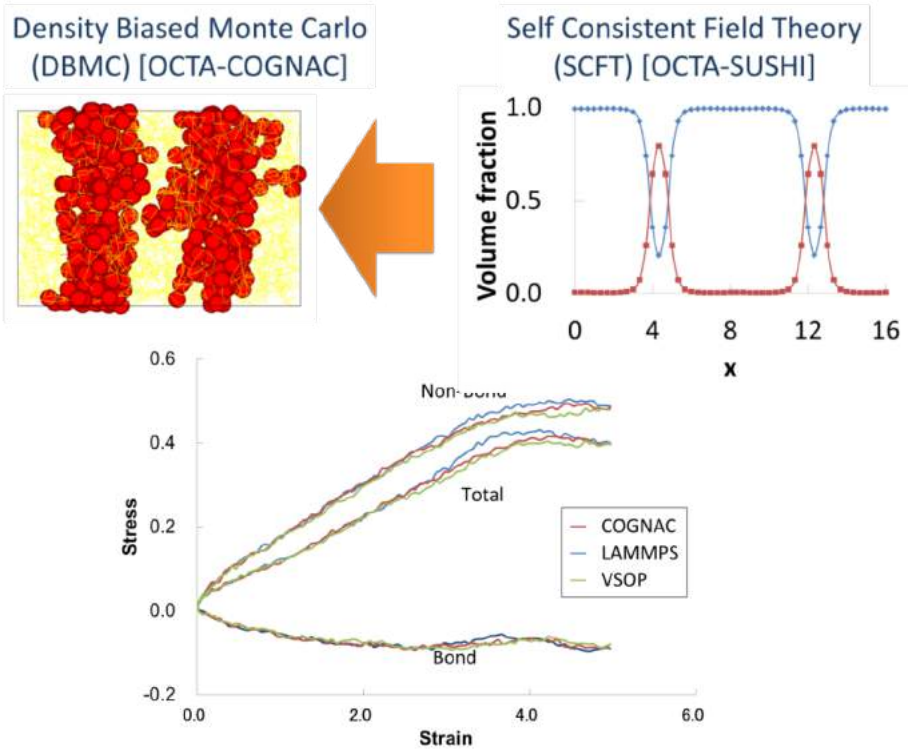


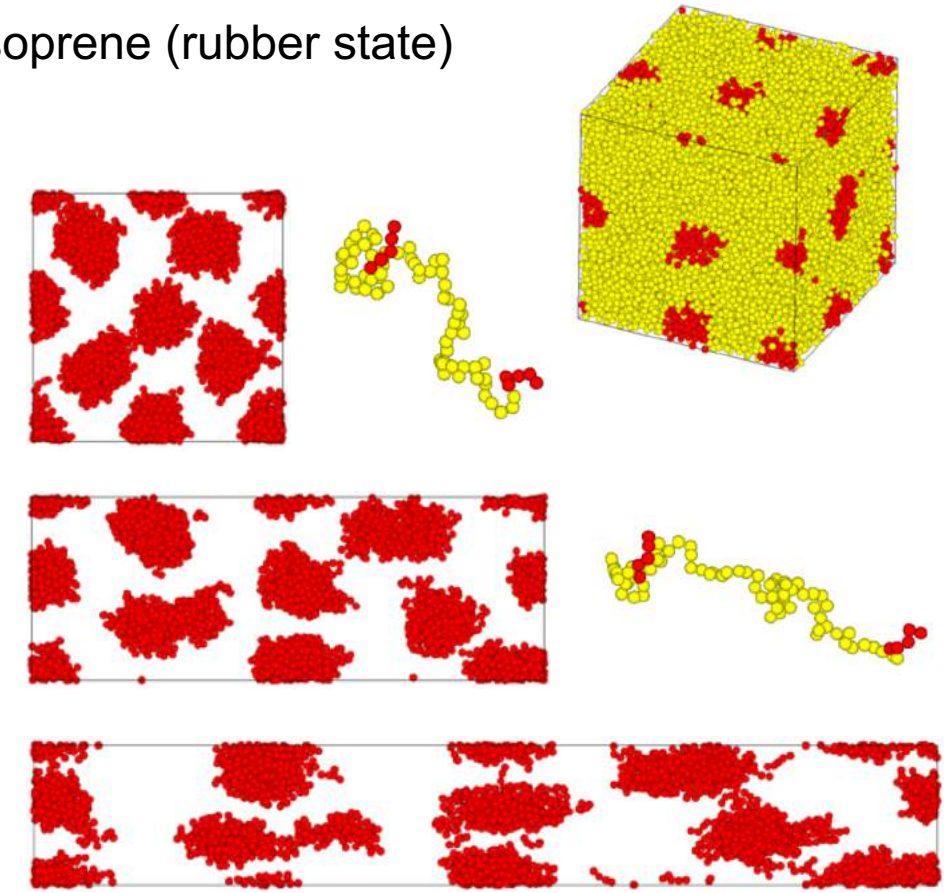
$$-[(CF_2\text{-}CF_2)_n\text{-}CF\text{-}CF_2]_m-$$
$$O\text{-}CF_2\text{-}CF\text{-}O\text{-}CF_2\text{-}CF_2\text{-}SO_3H$$
$$CF_3$$

Thermoplastic elastomer

Mean Field -> Coarse grained Molecular Dynamics (CGMD)

- Phase separated structure of ABA triblock copolymer is calculated by using SCFT (SUSHI). Initial structure of Coarse Grained MD is created by using volume fraction distribution obtained by SCFT (Density Biased Monte Carlo method).
- Red; A=Styrene(glass state), Yellow; Isoprene (rubber state)
- Elongation simulation is conducted.

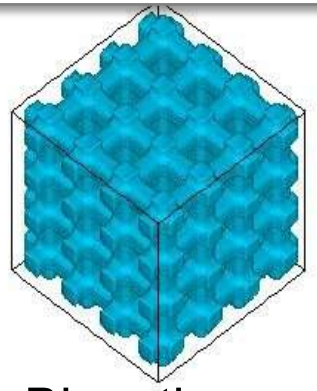




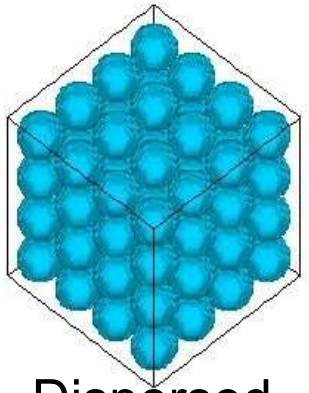
T.Aoyagi and T.Honda, J.Chem.Phys.,117, 8153 (2002)

Polymer blend PP/Elastomer

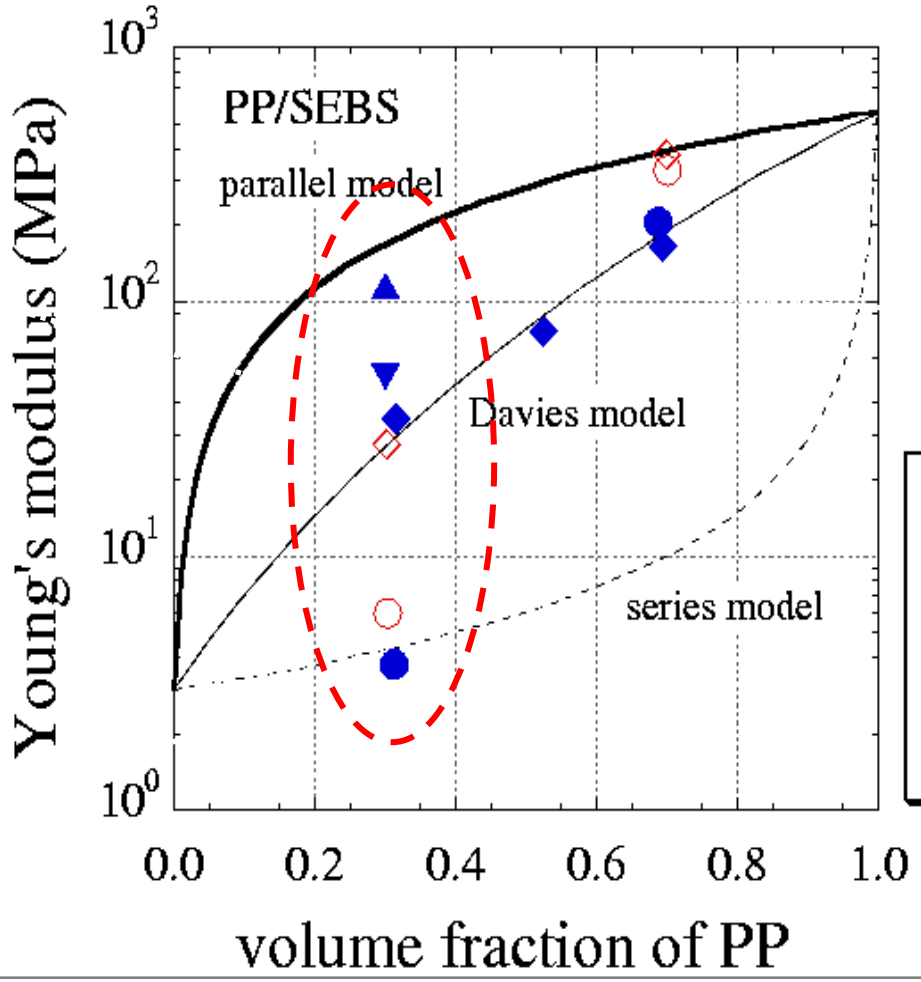
Prediction of average bulk modulus (MUFFIN)



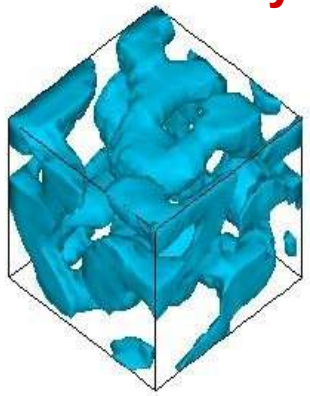
Bicontinuous



Dispersed



Mean field ⟶
Elastic analysis (FEM)



Mean field

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

Polymer blend PP/SEBS

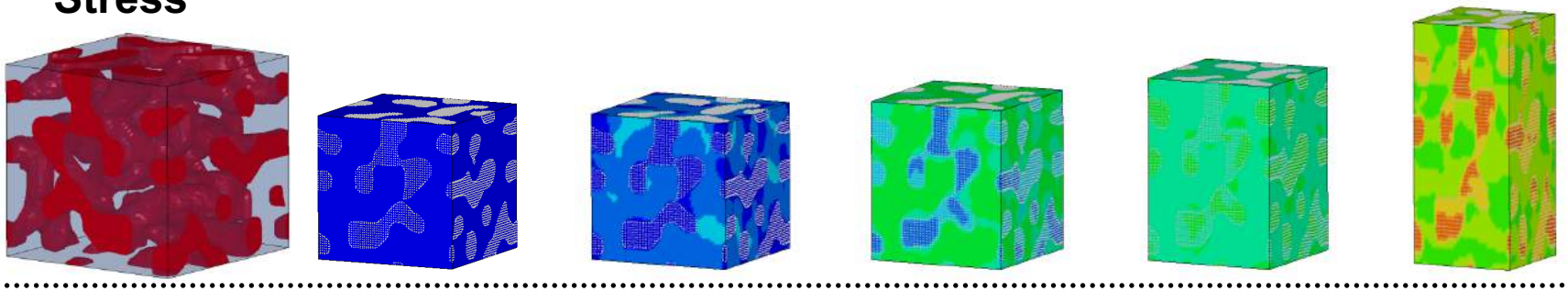
LS-DYNA

Mean field ⟶
Elastic analysis (FEM)

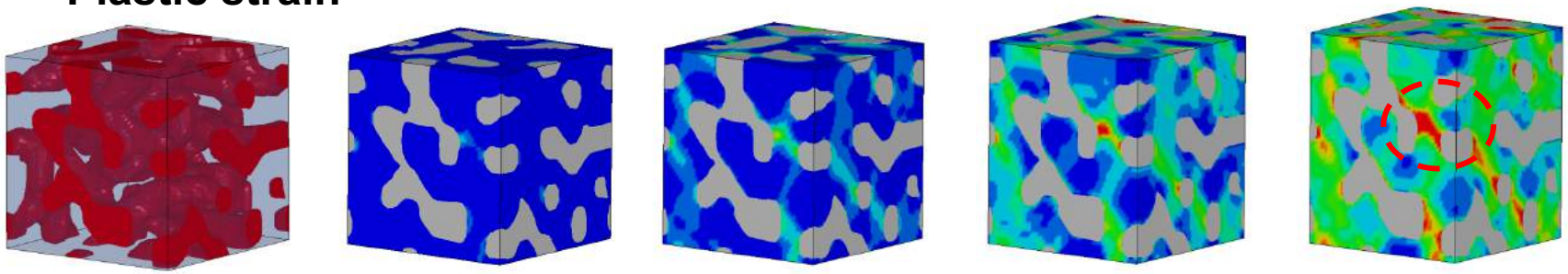
Non-linear structure analysis using LS-DYNA

Direct calculation from J-OCTA is possible.

Stress

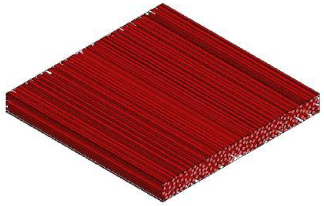


Plastic strain



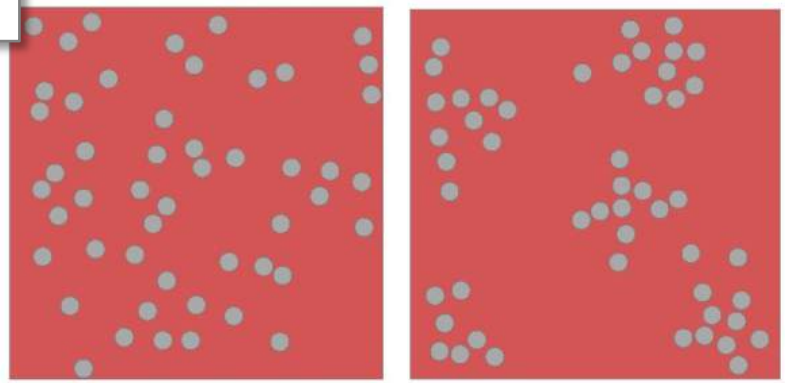
Fracture of CFRTP

Meso-Structure (UD material)



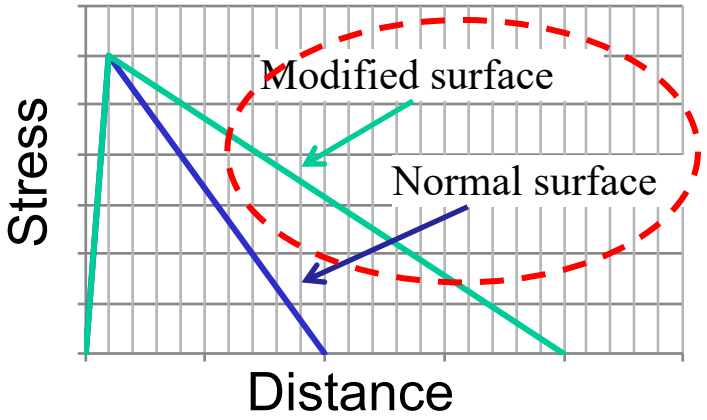
digimat
LS-DYNA

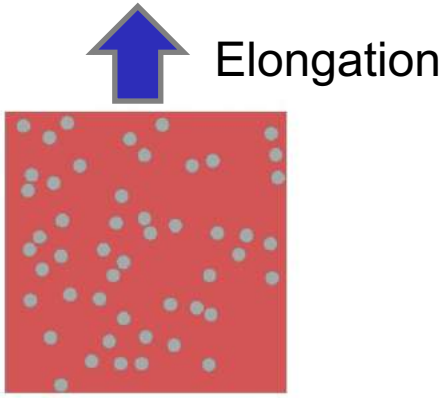
Sectional view



Matrix : PA
Fiber : CF
10 vol%

Cohesive element considering results of CGMD

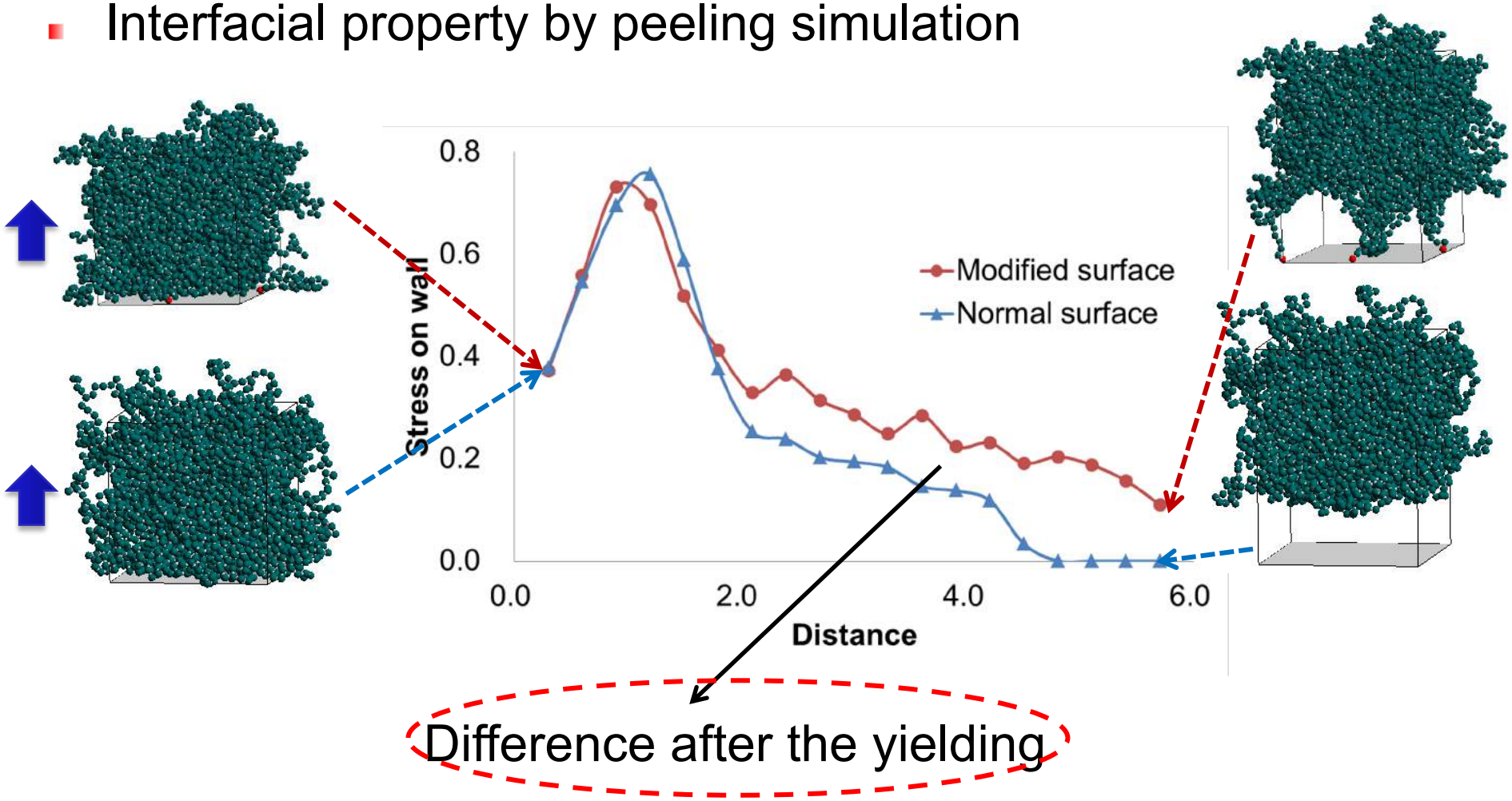




Fracture of CFRTP

Coarse grained Molecular Dynamics (CGMD)

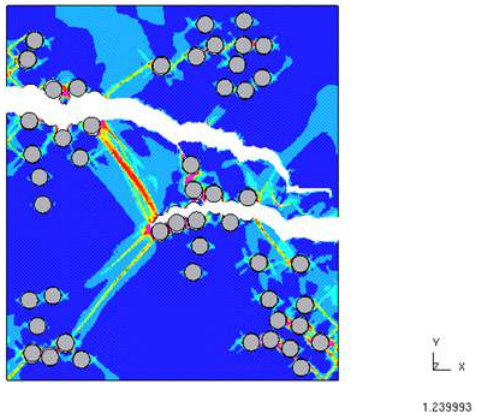
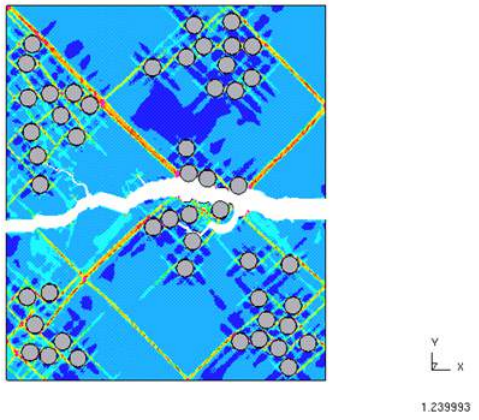
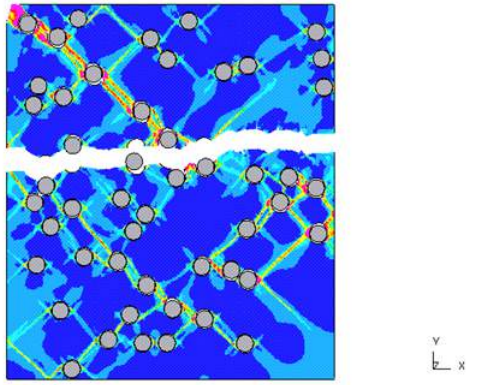
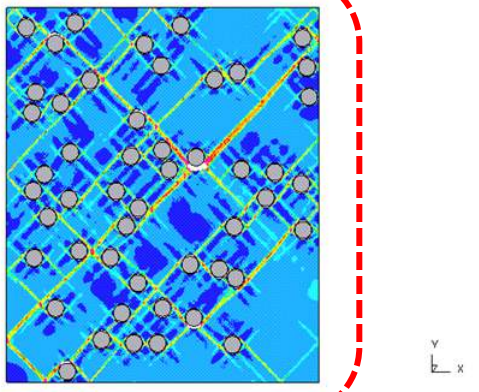
- Interfacial property by peeling simulation



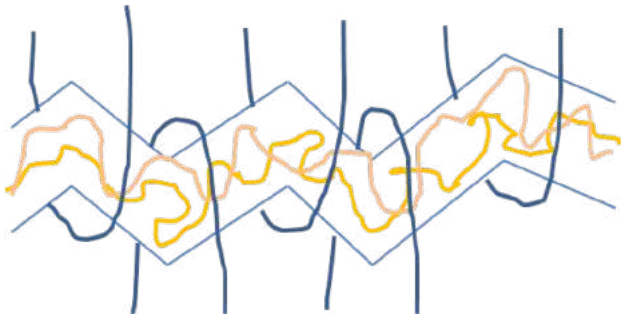
Fracture of CFRTP

Non-linear structure analysis using LS-DYNA

digimat
LS-DYNA

	Normal surface	Modified surface
Aggregated structure		
Dispersed structure		

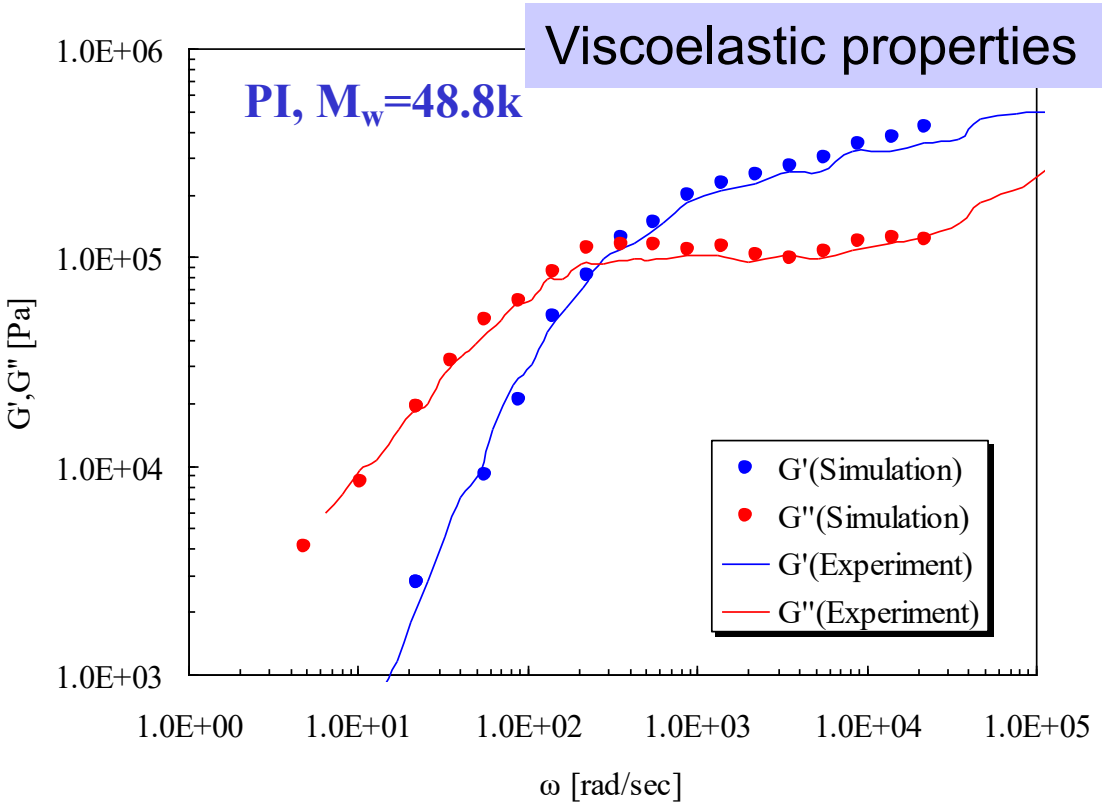
Dynamics of entangled polymer melt

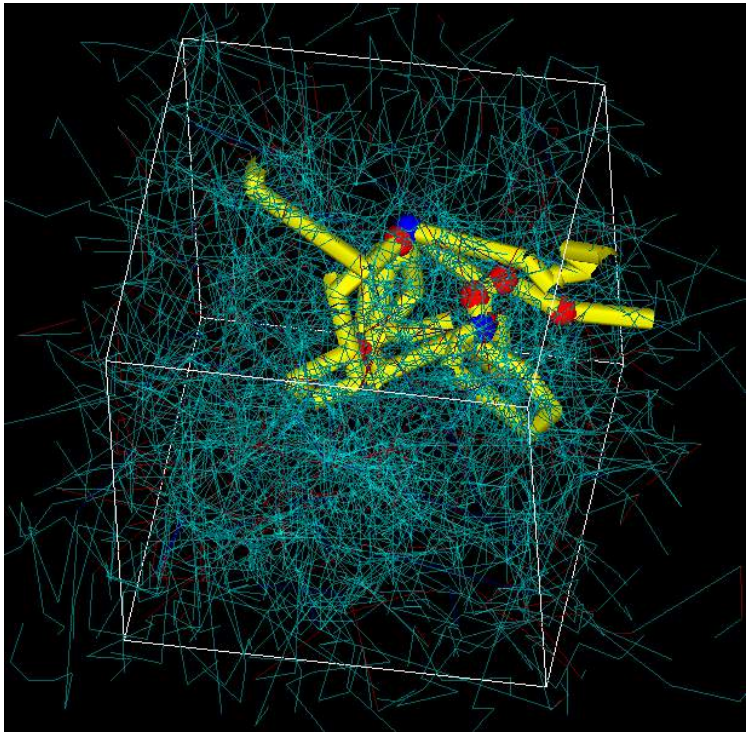


Slip-link model
Primitive chain network model

- 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)



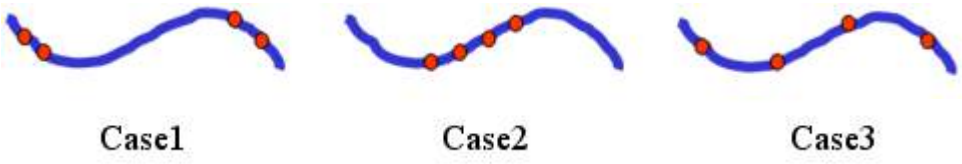


Rolling resistance of tire

courtesy of SUMITOMO RUBBER INDUSTRIES, LTD.

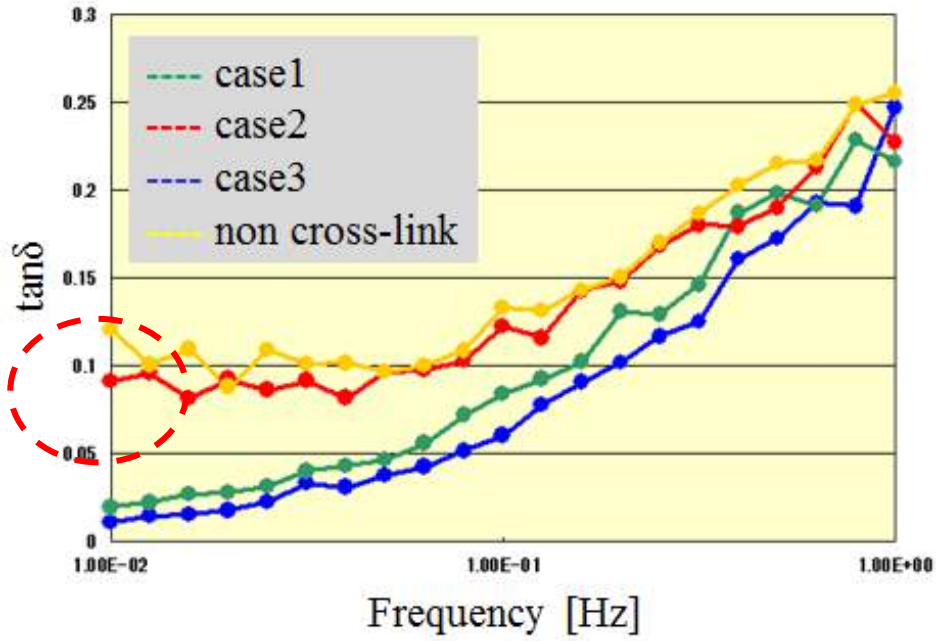
Slip-link model
(Primitive chain network model)

Dynamic viscoelastic properties of cross-linked poly-isoprene was calculated by using Primitive Chain Network model (NAPLES of OCTA). Effects of distribution of cross-linked positions (Fig.1) was evaluated. Molar mass of each molecule is about 300k.



Rolling resistance of tire is related with tanδ (= G''/G'). In case1 and 3, tanδ shows low value at low frequency(Fig.2).

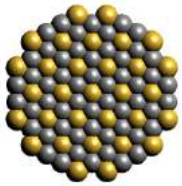
This means that chain end should be cross-linked to get low rolling resistance property.



Nano Composite for CFRTP

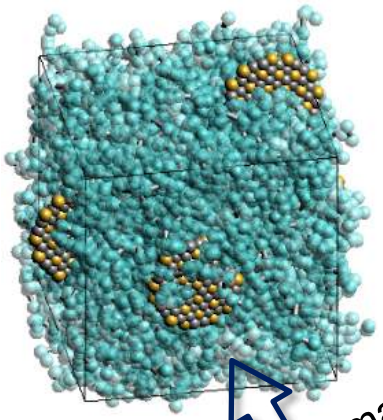
Molecule

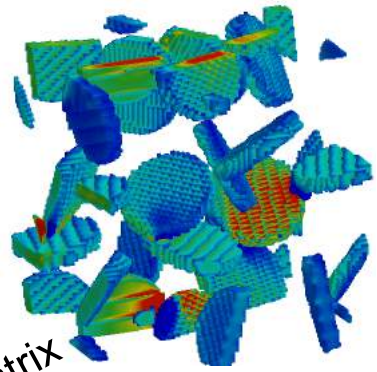
SP values of each component



Micro Structure

DPD and FEA
Graphene sheets in Polymer (PEEK)
Averaged property of polymer matrix

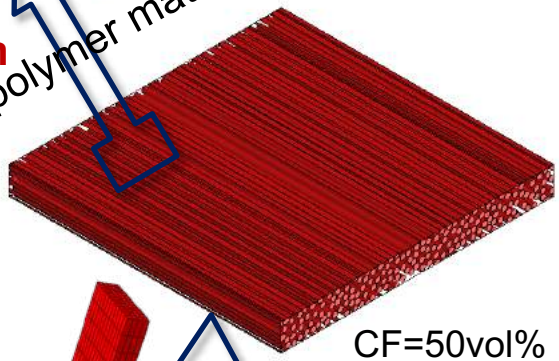




Meso Structure

Equivalent inclusion theory
CFRTP
Averaged property

polymer matrix



CF=50vol%

digimat

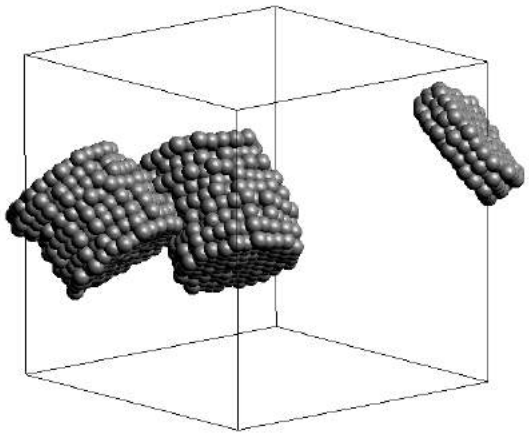
Macro Part

FEA
Composite part

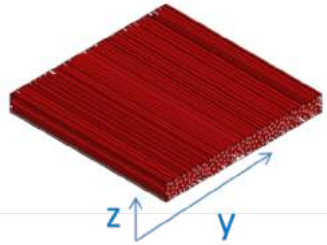
Direction of carbon fiber

T.Ozawa, T.Nakayama, M.Watanabe, G.Goldbeck, V.Regnier, MOLMOD2015

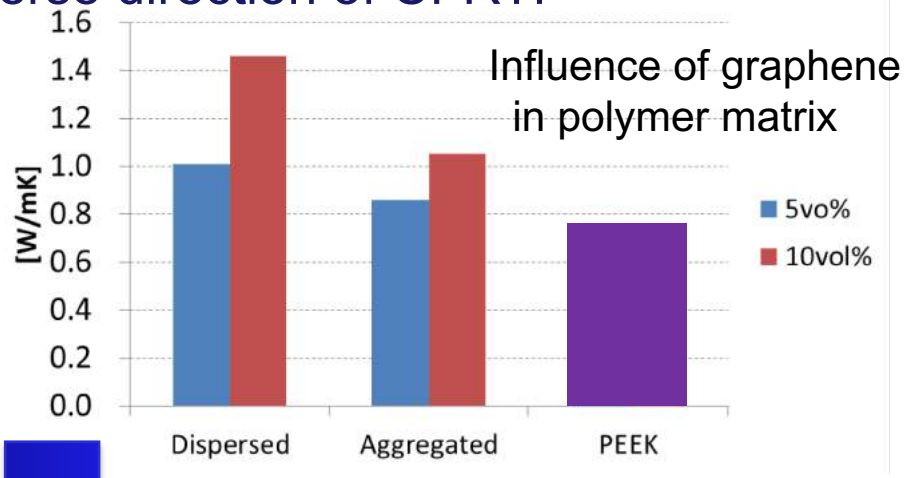
Nano Composite for CFRTP



Aggregated



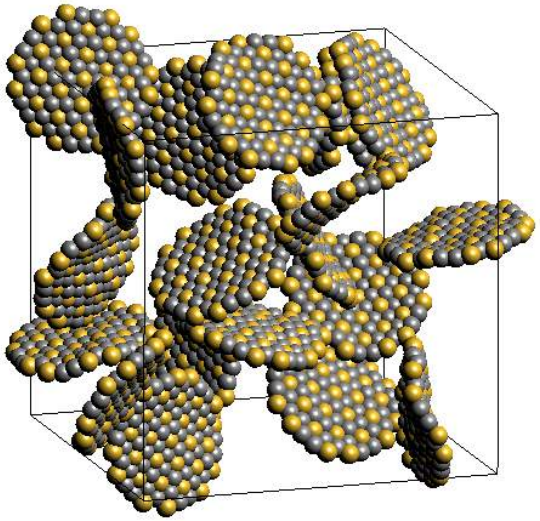
Mean value of thermal conductivity
in transverse direction of CFRTP



Influence of graphene
in polymer matrix

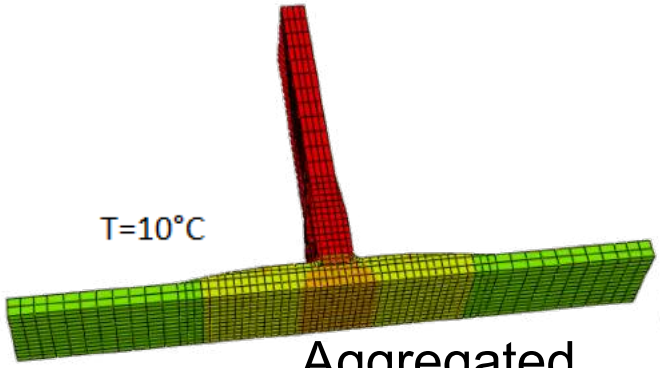
digimat

polymer matrix

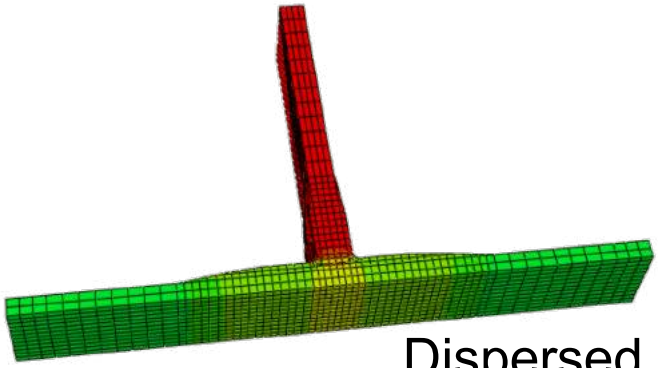


Dispersed

FEA for macro Part (Heat Flux)



Aggregated



Dispersed

*Green is high, red is zero.

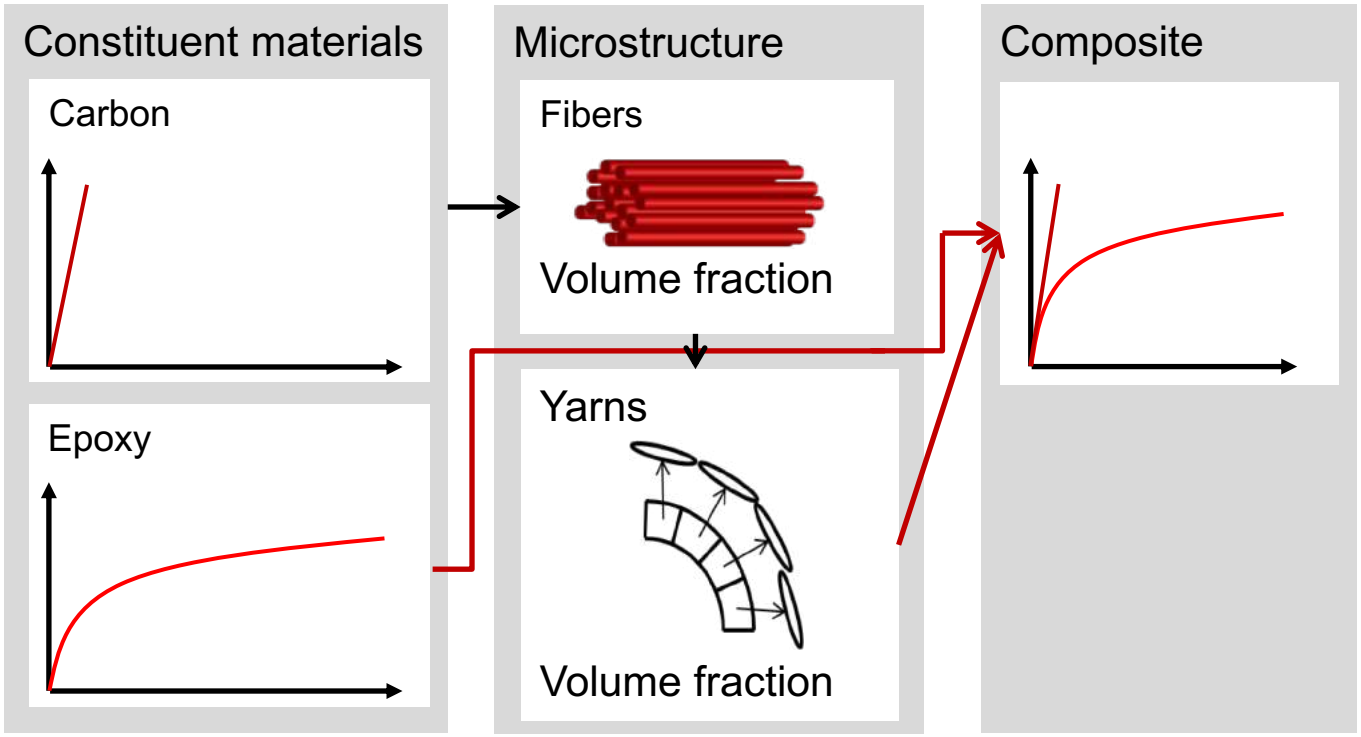
Multiscale studies in Rubber

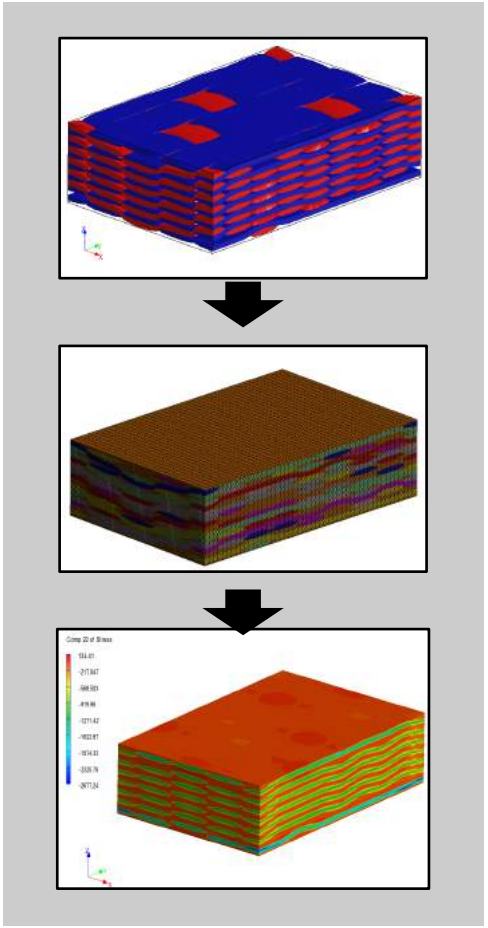
Finite element based homogenization for rubber composites

- Dedicated rubber material model
  - Hyperelastic
  - Thermo-hyperelastic
  - Visco-hyperelastic
- Large set of inclusion shapes (spherical, cylindrical , platelets, …)
  - Including custom CAD
- In-house mesher
  - Conformal tetrahedral mesh
  - Non-conformal hexahedral mesh
  - Conforming extruded hexahedral dominated mesh
- In-house FE solver
  - Direct and iterative solver
  - With dedicated elements for rubber composites
- In-house post-processing

Multi-scale Simulation with Homogeneous Theory

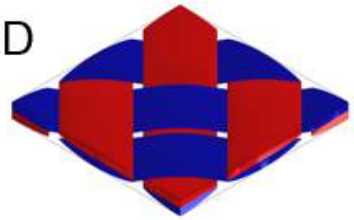
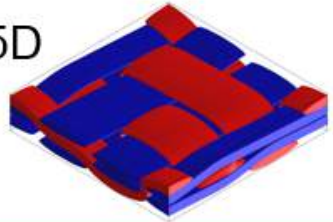
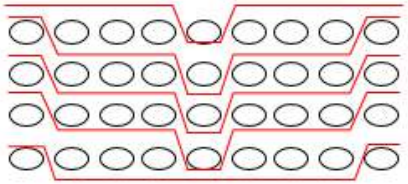
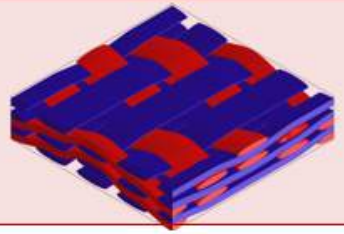
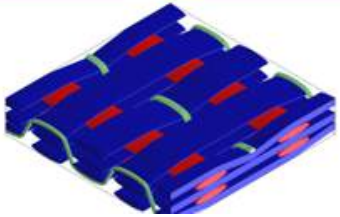
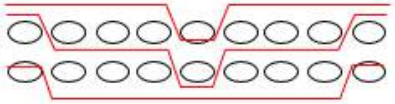
- Two scales simulation for Woven
  - Mean-field homogenization for yarn
  - Full-field homogenization for woven





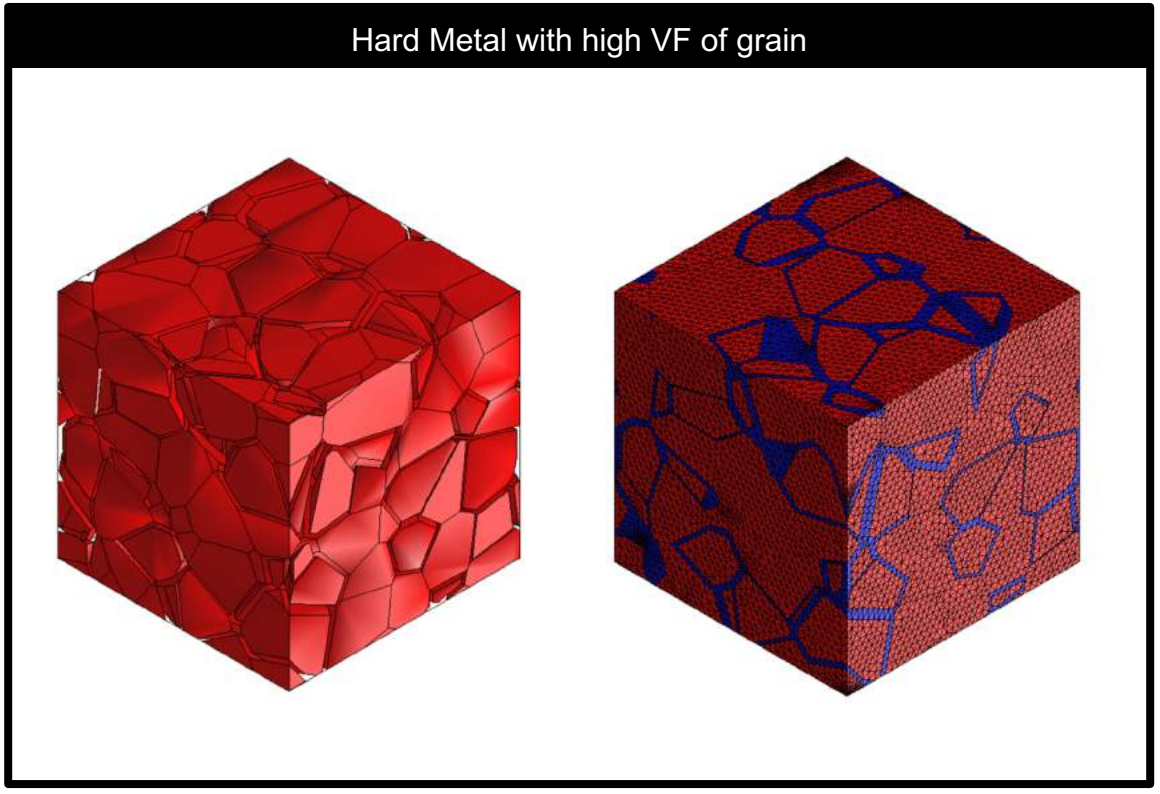
Digimat offers 3D Woven capabilities

3D Woven from Template to User defined

Fabric type	Weave definition	
Woven 2D 	User defined	
Woven 2.5D 	User defined	
Woven 3D interlock 	Template	Additional templates become accessible for woven 3D interlock
Woven 3D orthogonal 	Template	 Many more…

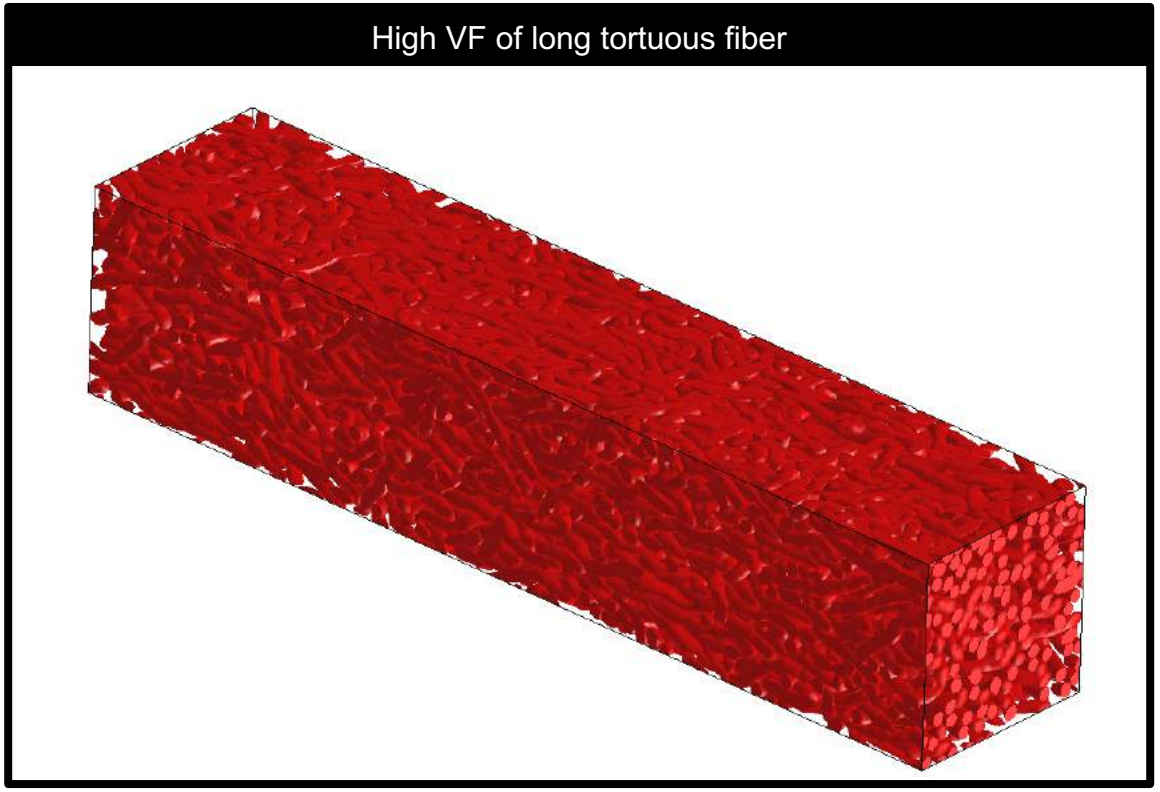
Complex RVE generation with FEM

- For various type of microstructures
  - SFRP
  - LFRP
  - Hard metals
  - Woven



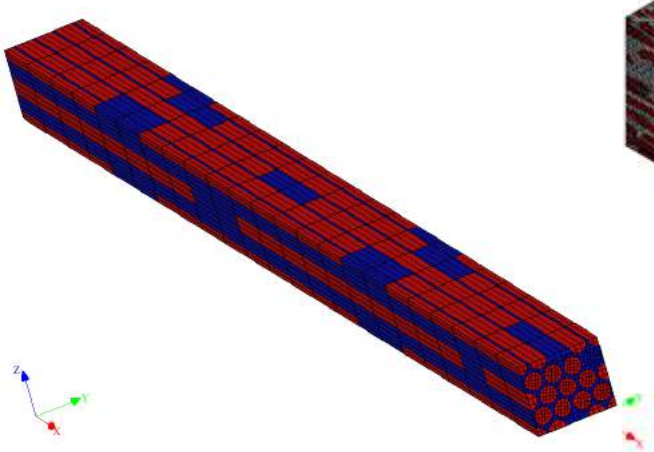
Complex RVE generation with FEM

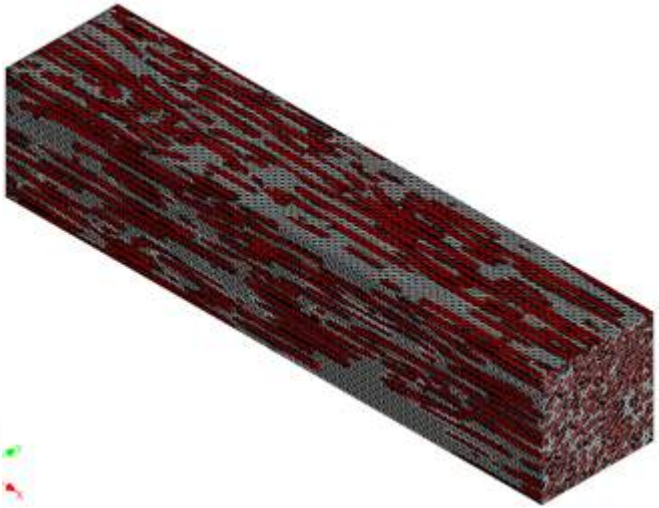
- For various type of microstructures
  - SFRP
  - LFRP
  - Hard metals
  - Woven

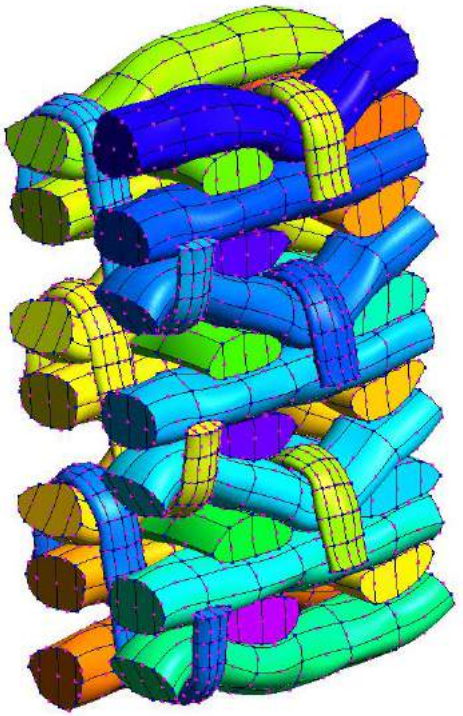


The expertise in advanced meshing

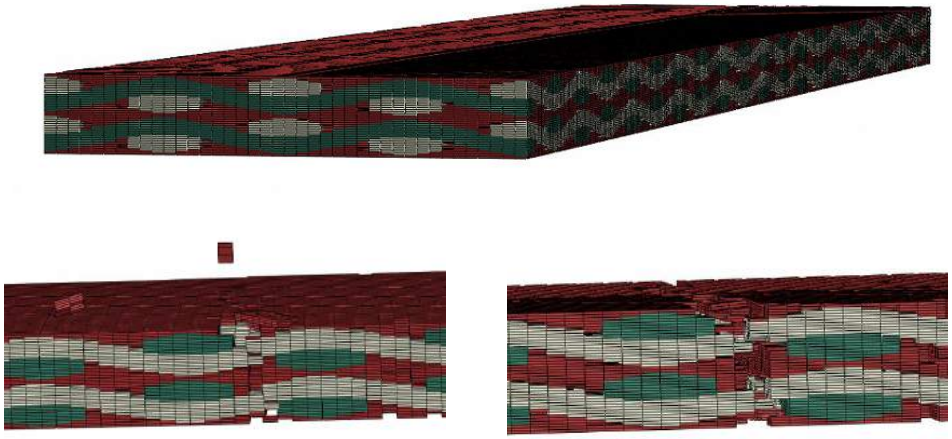
- Conforming extruded hexahedral dominated mesh
- Mesh cutting algorithm

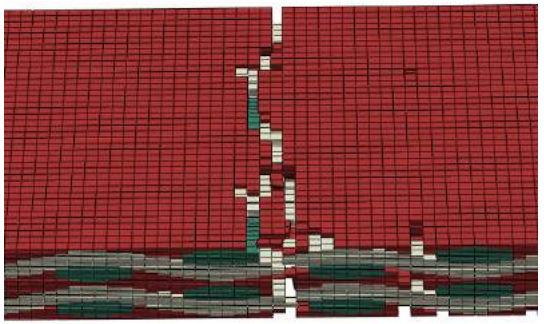


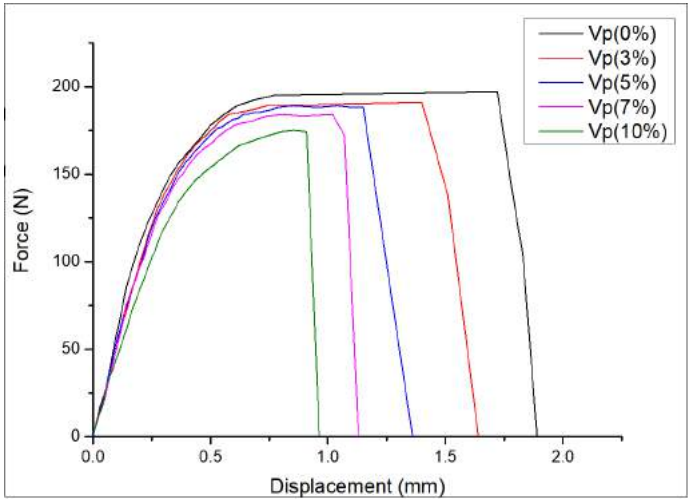


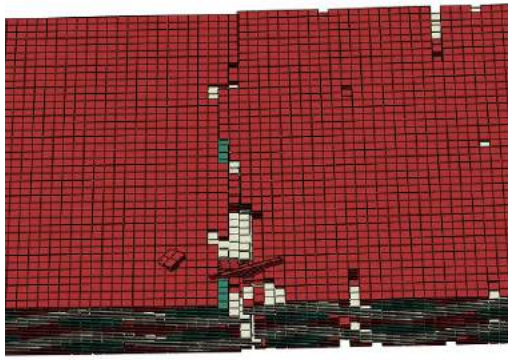


Failure modeling capabilities



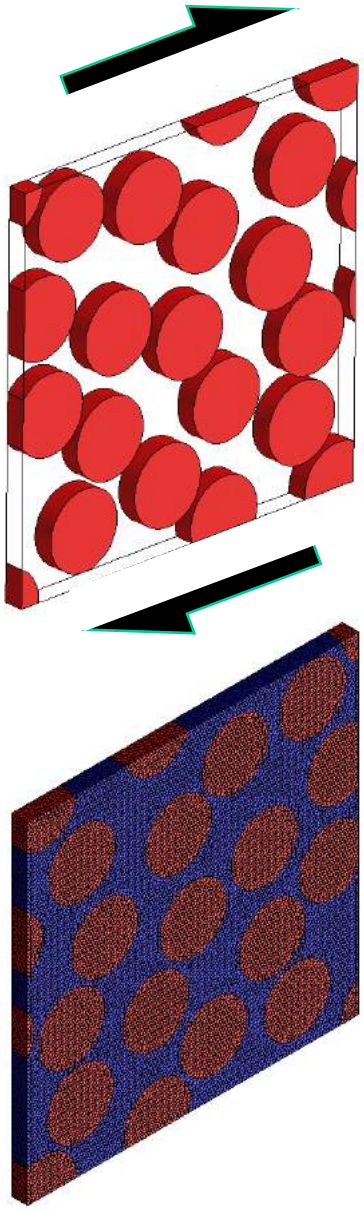




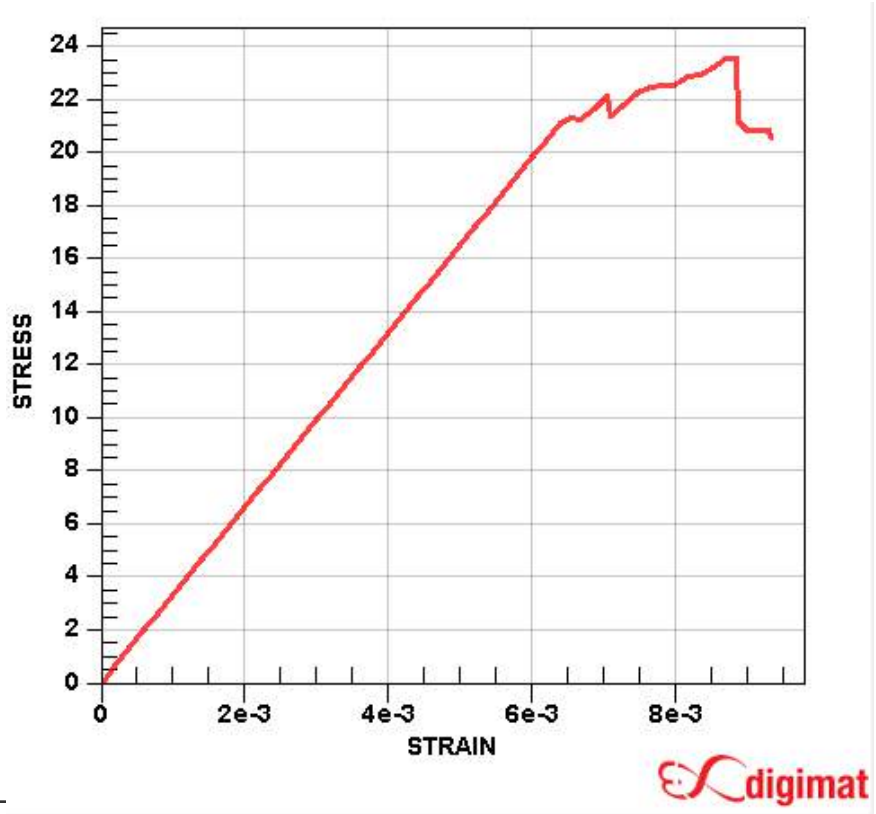


Damage due to different void contents

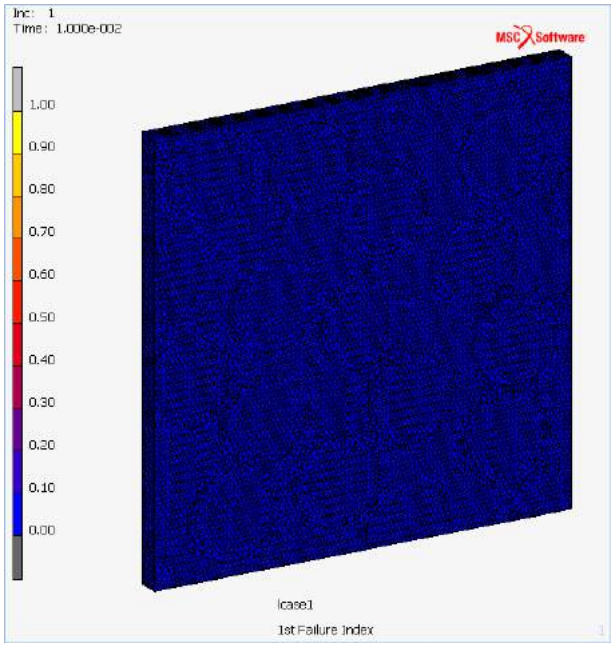
Failure modeling capabilities



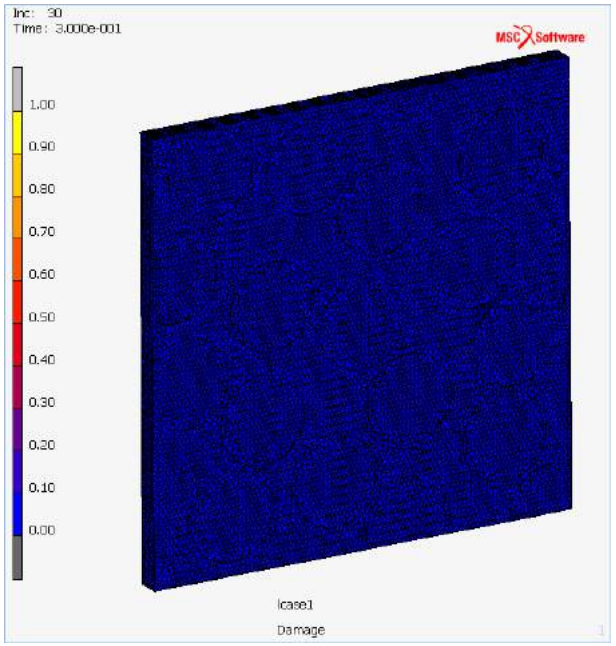
- 3D slice of unidirectional carbon-epoxy composite
- Transverse shear loading
- Elastic with damage resin behavior
- Fiber-matrix debonding using cohesive surfaces



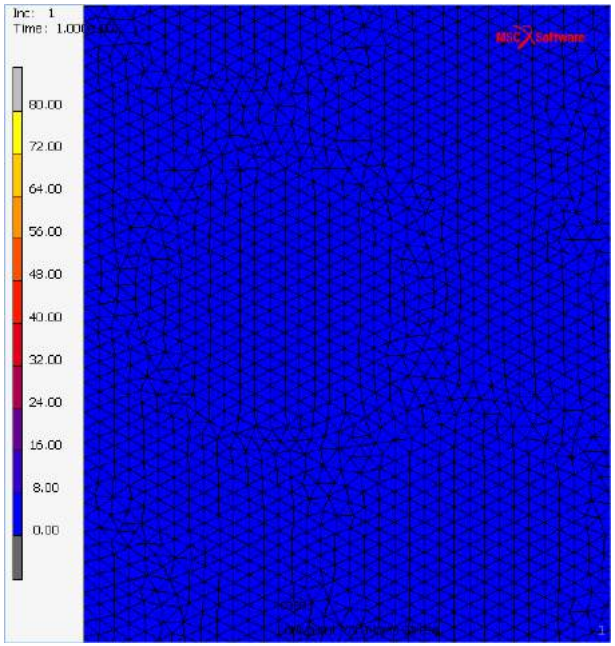
Failure modeling capabilities



Failure criterion



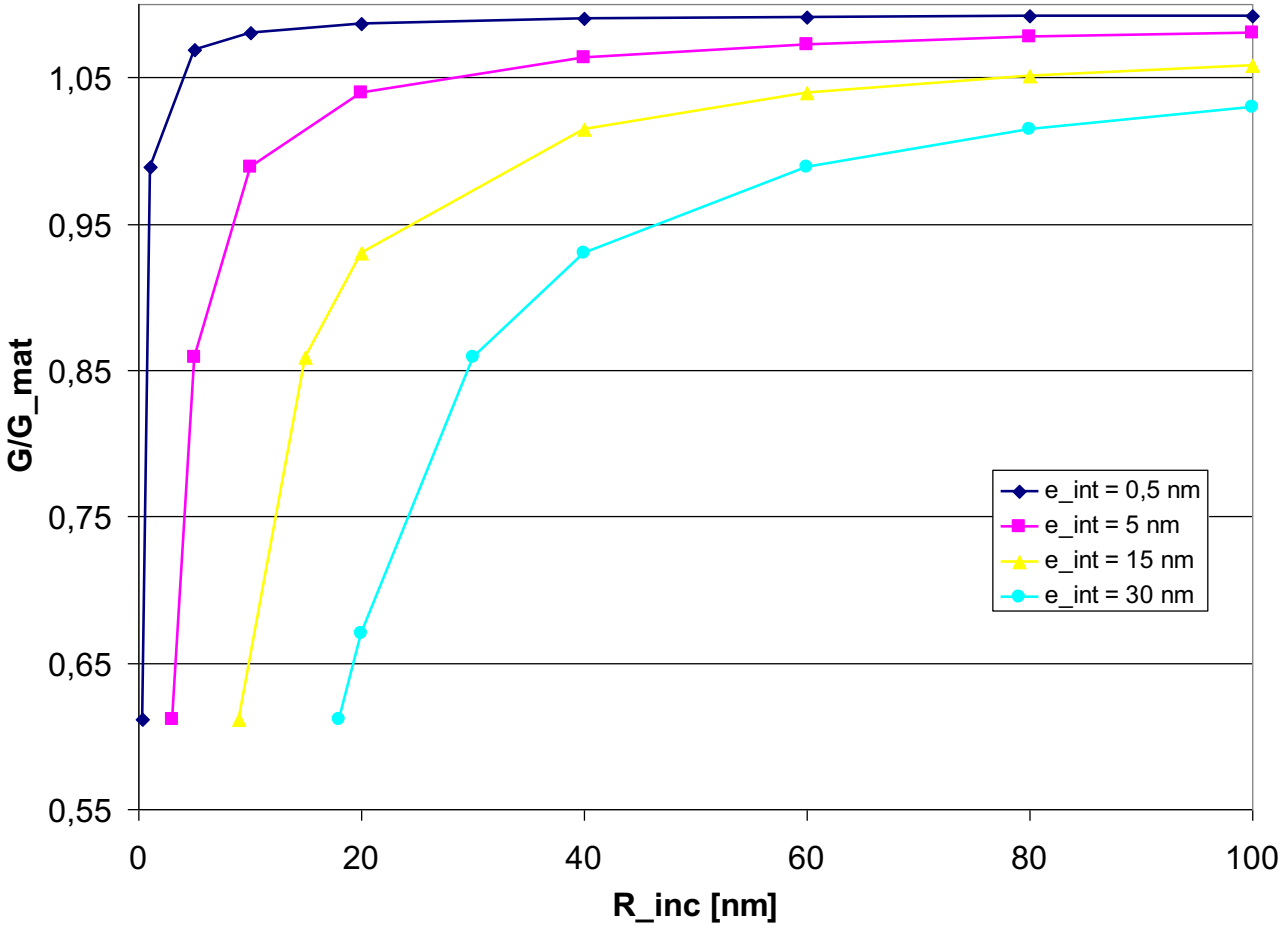
Damage leading to stiffness reduction



Zoom over fiber-matrix debonding
(deformation scale factor of 5)

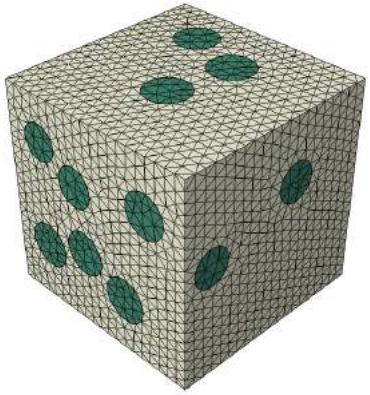
To model matrix-filler interface

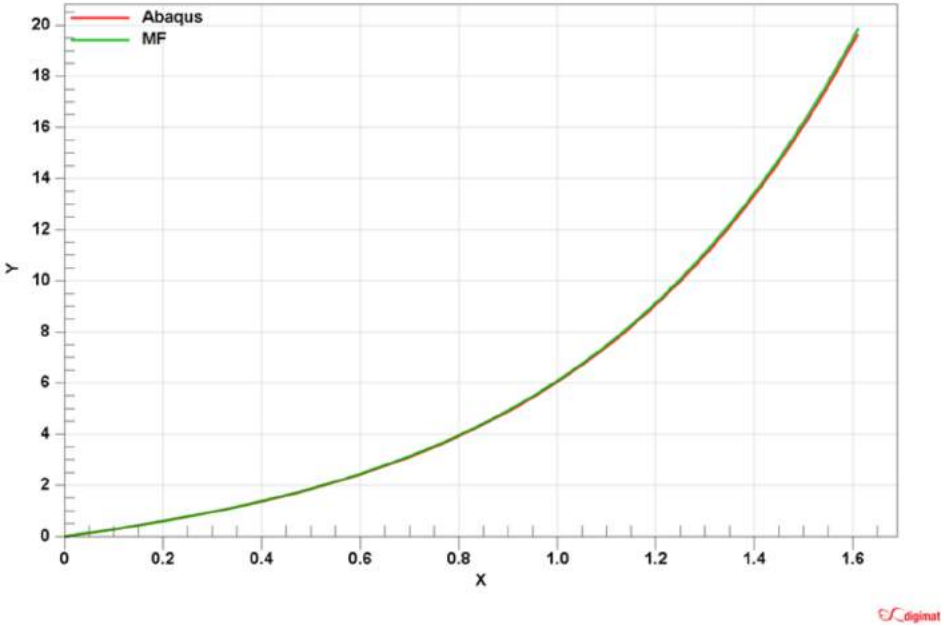
- Coating is a way to model the influence of the filler on the rubber properties at the rubber-filler interface

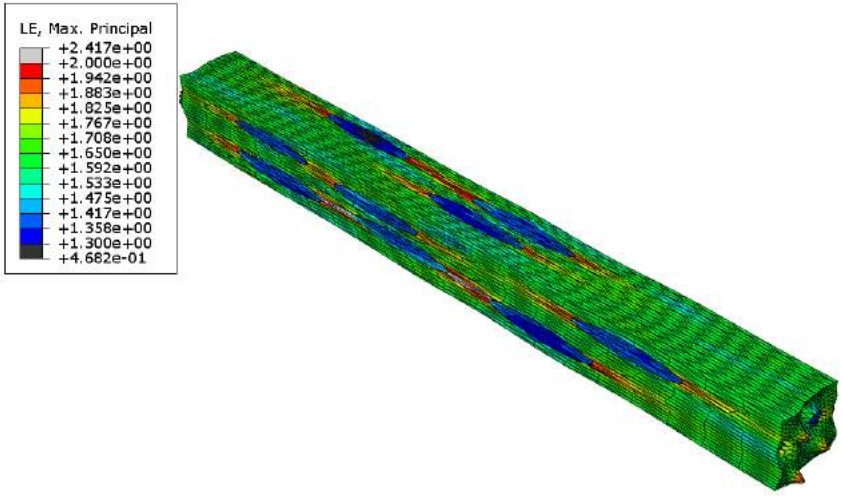


160% deformation in large strain

- For rubber blend

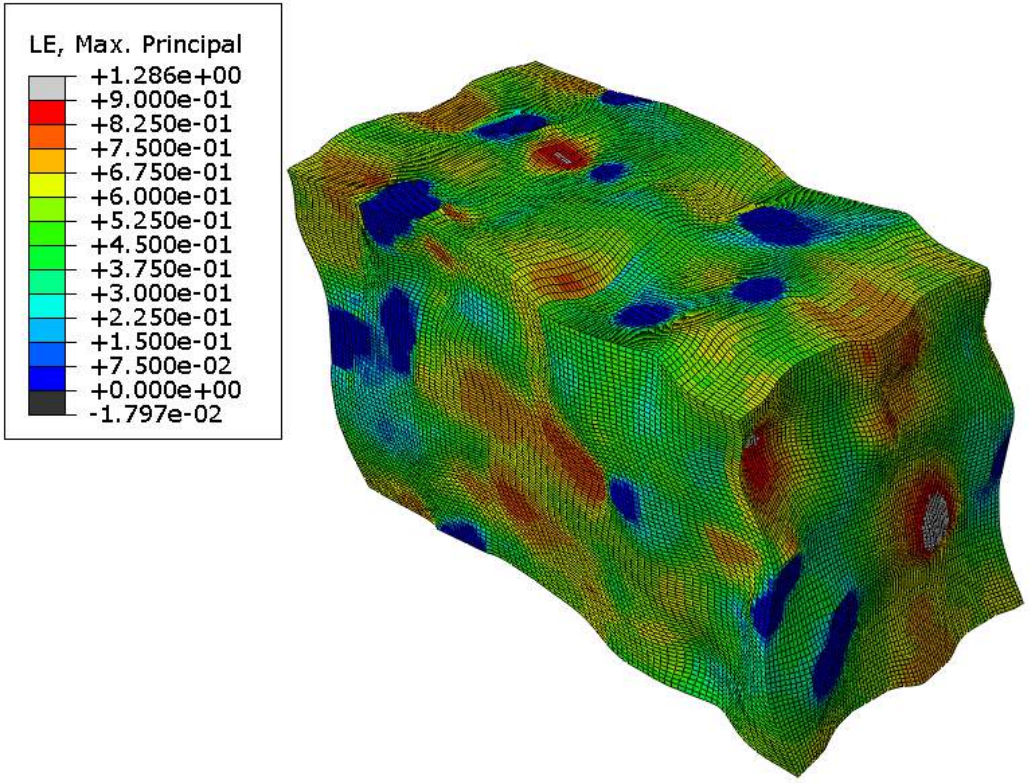






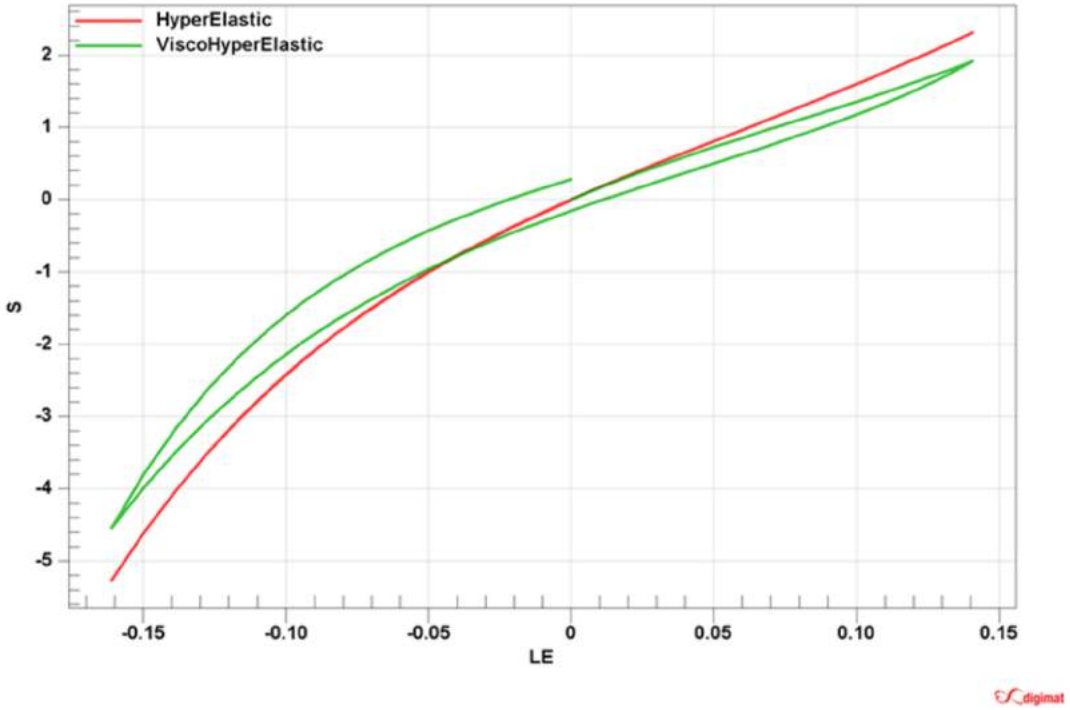
100% deformation in the matrix in large strain

- For silica with silane
  - Reduced integrated elements allow to reach the highest strain but requires large number of elements to reduce hourglassing
  - Fully integrated elements allow accurate predictions for a low number of elements but final strain is lower



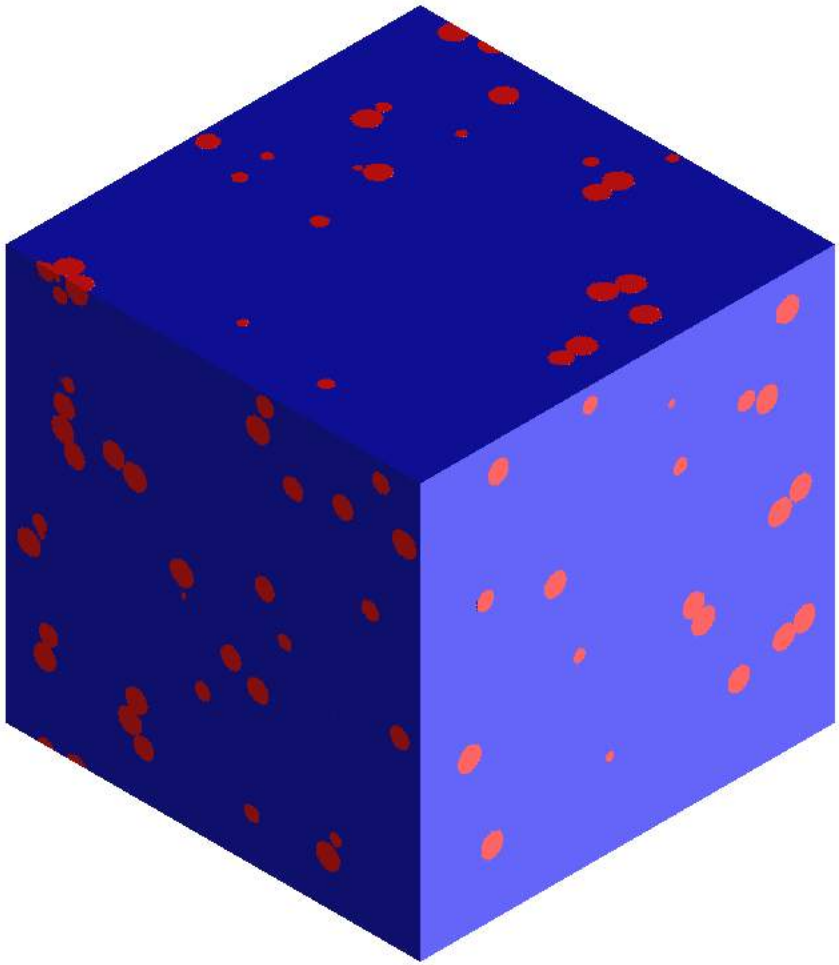
Extend its material library to advanced hyper-elastic model

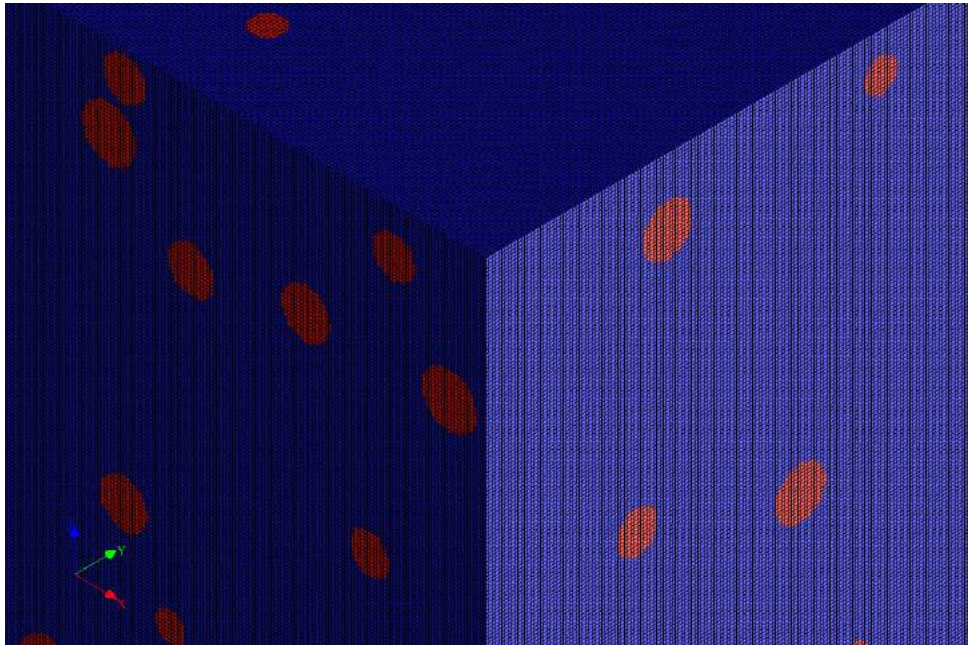
- Visco-hyperelastic model has been tested
  - In FE-Solver
  - In Abaqus
- Other models could be added
  - Thermo-visco-hyperelastic



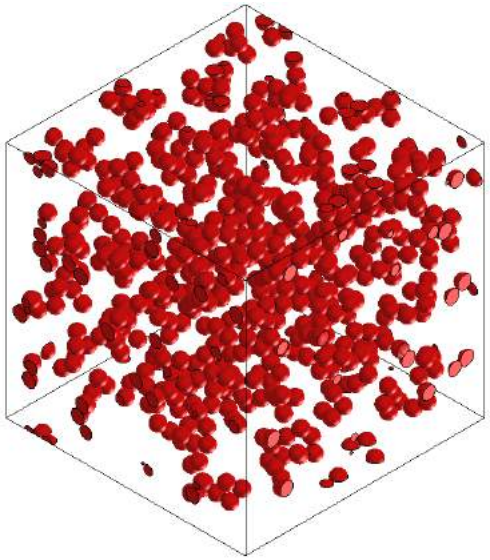
Digimat can generate very large RVE

- Illustration with 640 inclusions and 30M voxels



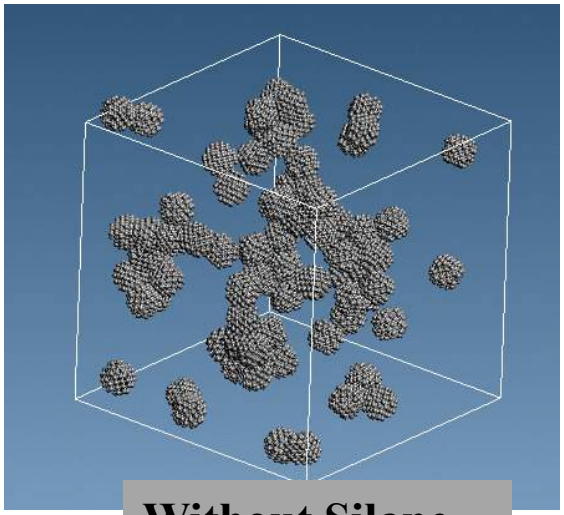


- Connection to Molecular Dynamics

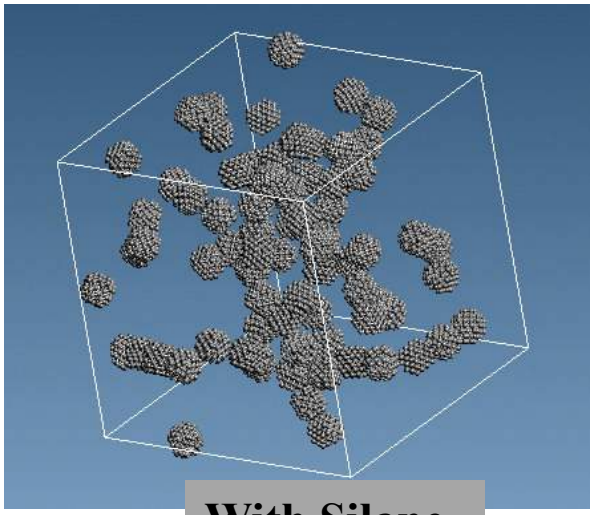


Molecular Dynamics predict dispersion of nano-fillers based on Dissipative Particle Dynamics (DPD)

- Dispersion of silica particles in rubber
  Solubility parameters of silane modified silica particle from reference
  M.Khayet&al, Polymer 46 (2005) 9881-9891



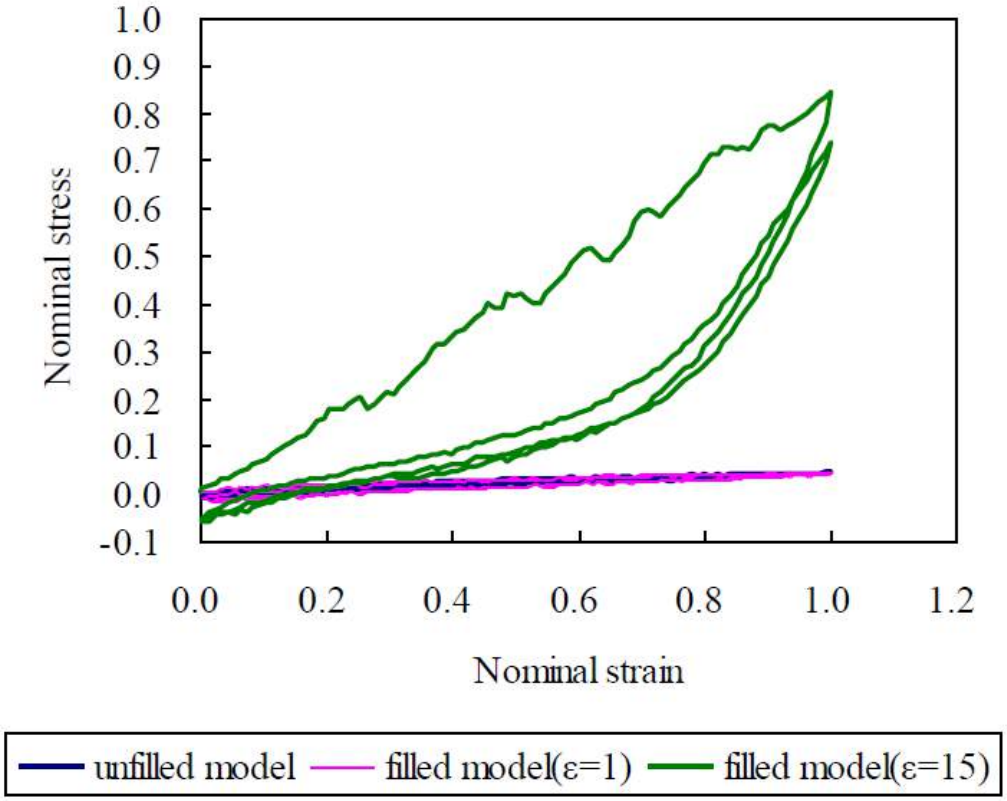
Without Silane



With Silane

Molecular Dynamics predict the influence of fillers on the rubber composite based on CGMD

- Yokohama Rubber (JSME 2015)
  - Influence of bridging polymer chains between fillers
  - Elongation and compression, hysteresis curve.
  - Small system (under 0.1M beads), using J-OCTA.

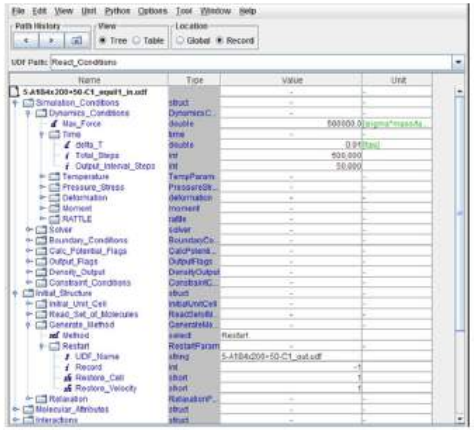


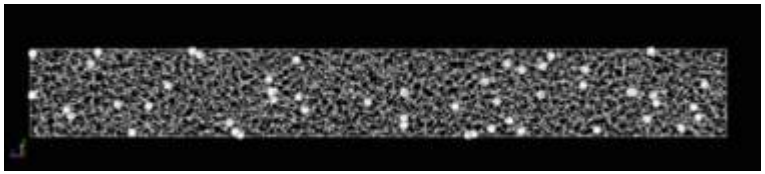
Molecular Dynamics predict the influence of fillers on the rubber composite based on CGMD

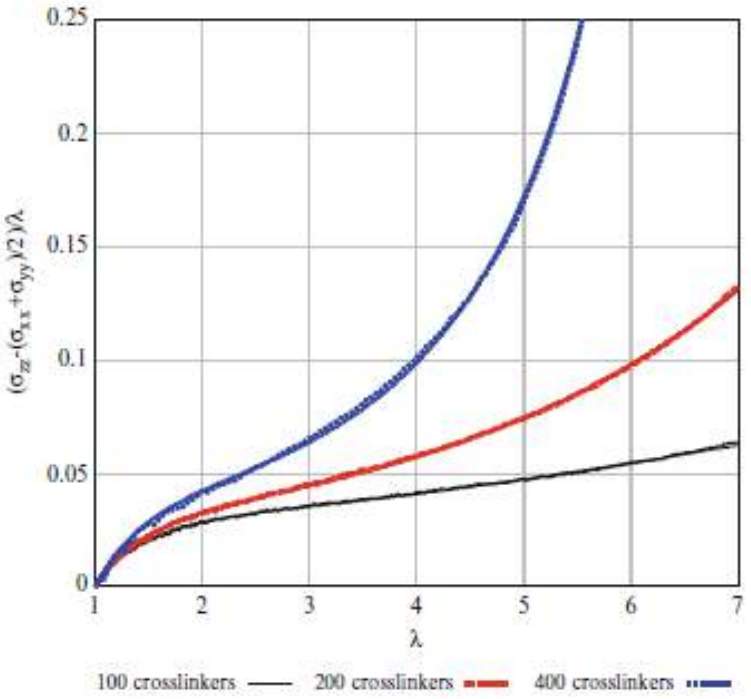
- **Cross-Linked Rubber**

  Hiroshi Shima, BRIDGESTONE Corporation, Tokyo, Japan
  Chapter 15, Computer Simulation of Polymeric Materials
  Applications of the OCTA System, Springer, 2016

- **Formation of cross-linked structures and elongational physical properties using OCTA**

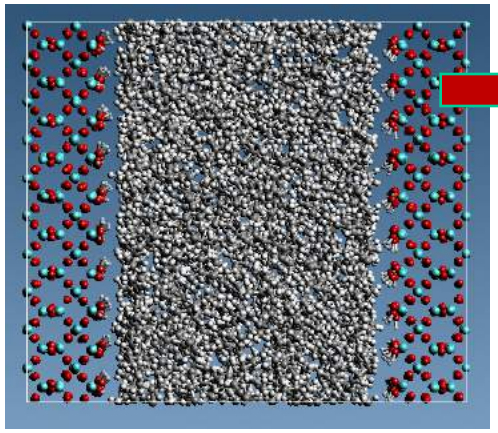




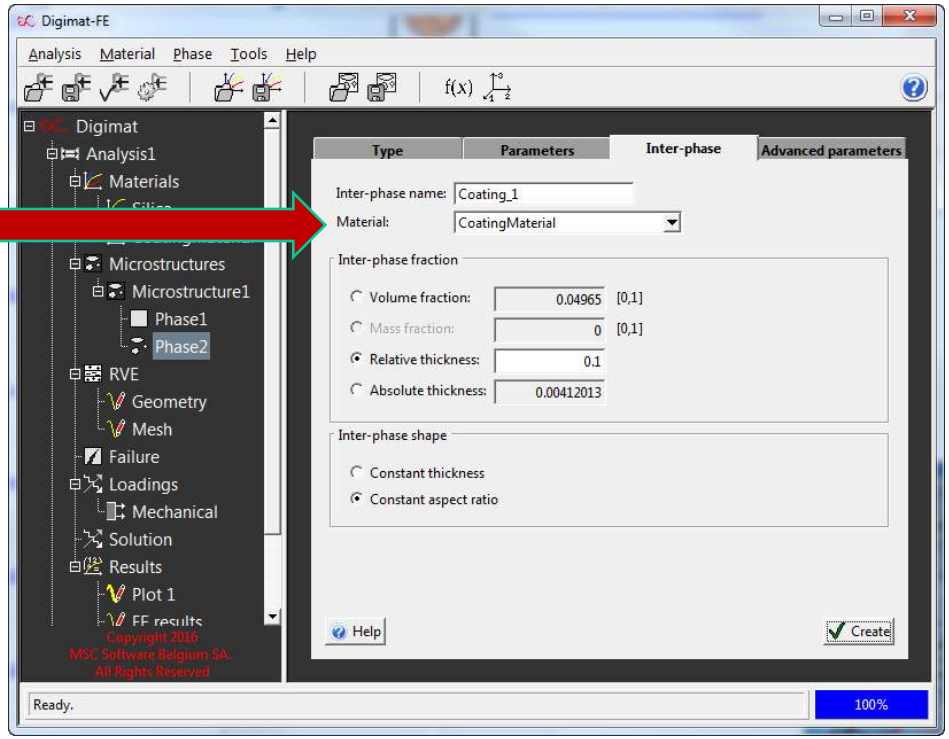


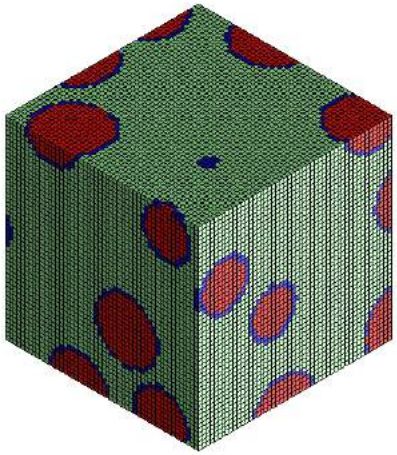
Digimat-FE/J-OCTA Inclusion-Matrix Coupling

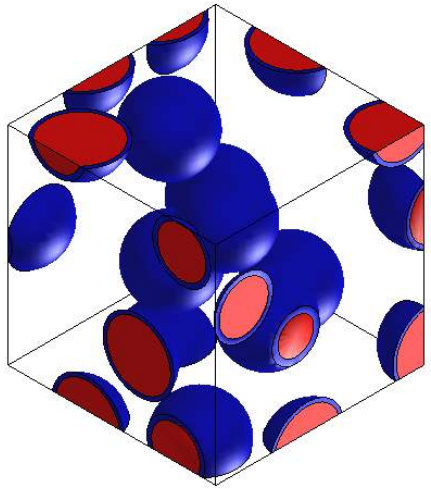
J-OCTA



Silica-Rubber interaction

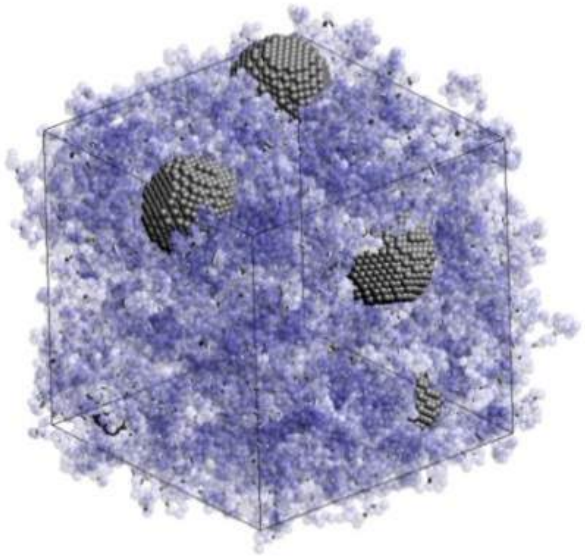




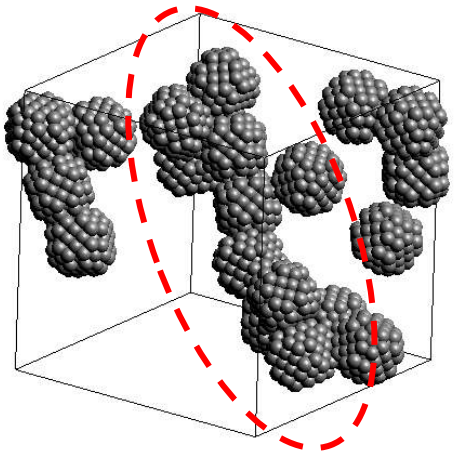


Estimation of the dispersion of nano-fillers

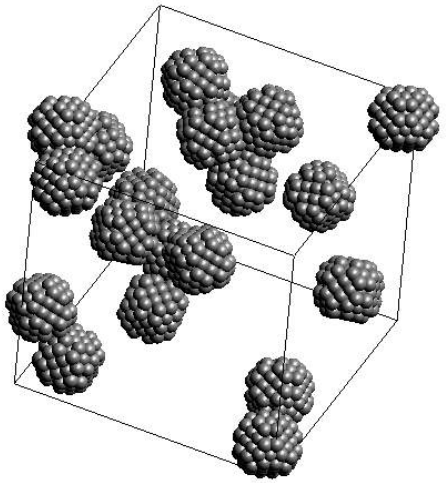
Dispersion of silica particles in polyisoprene (Natural Rubber).
Interaction parameters are decided by using SP values from reference.



aggregation



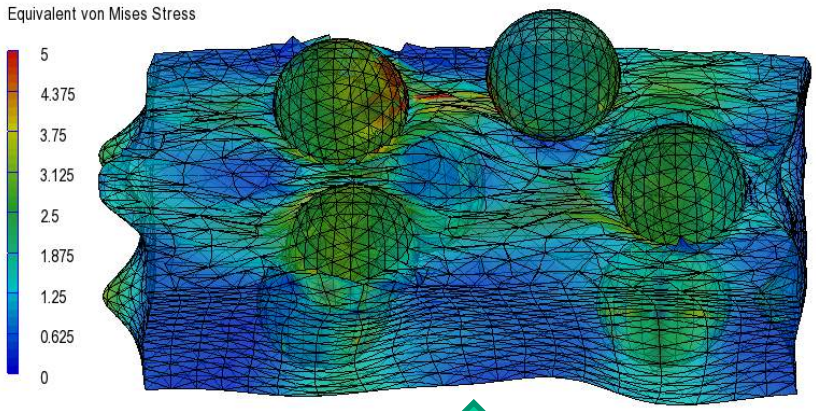
Without Silane coupling

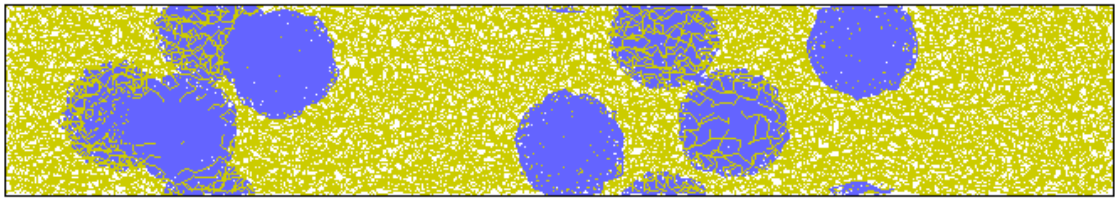


With Silane coupling

Mechanical property using meso-scale simulation

- Just an idea.
- By using the results of CGMD for small system, is it possible to decide parameters of each region(part)'s constitutive eq.?
- Same scale simulation are conducted and compared each others.
- Decided parameters are used for large scale FEA. This region is difficult for CGMD as described before.
- JSOL has interest in this technology.

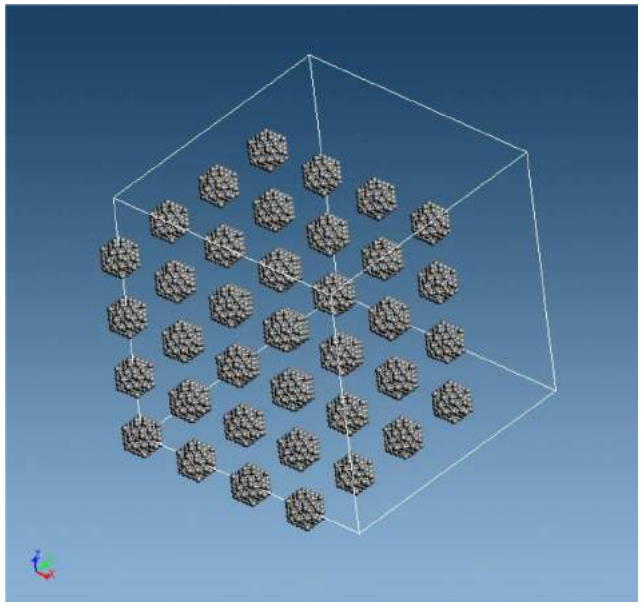


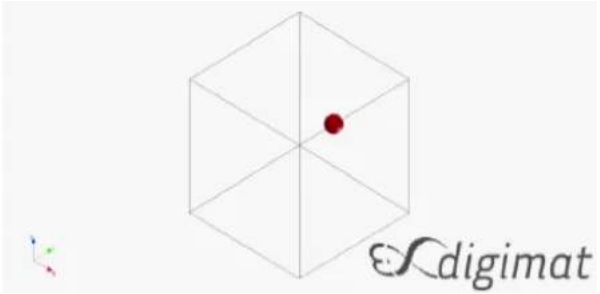


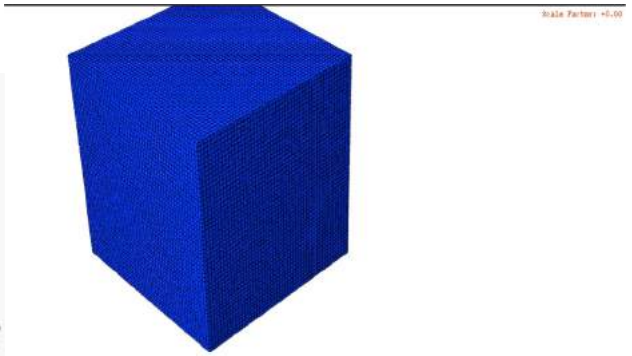
Stress distribution in CGMD can be compared with FEA.

Digimat proposes an interface to Molecular Dynamics

- RVE generation based on inclusion position obtained through DPD

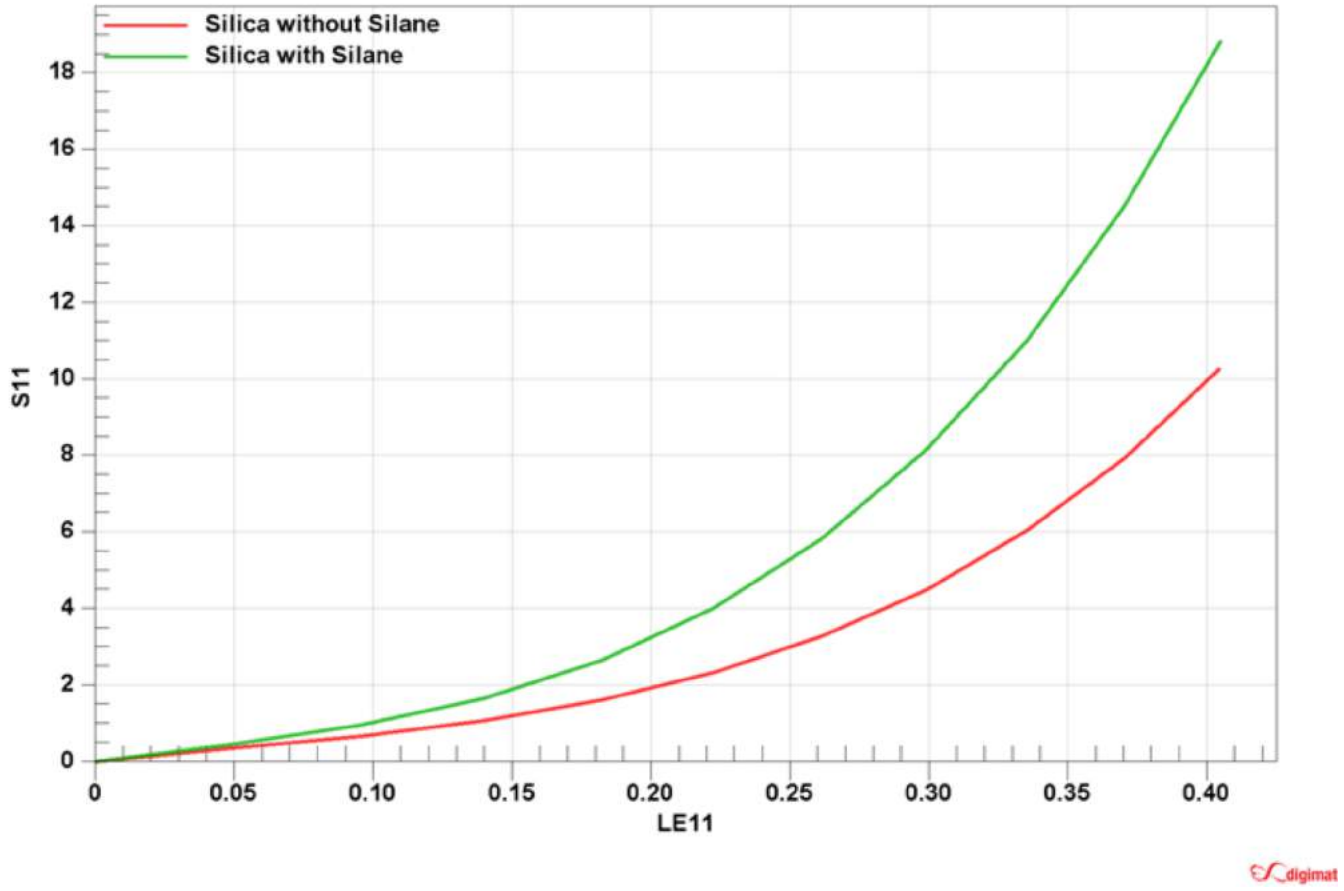






Molecular dynamics coupled with Digimat predict the influence of the nano-fillers dispersion on the composite properties

- The influence of the Silane on the fiber dispersion has a direct influence on the stress-strain curve
  - Hence probably also on the rolling resistance

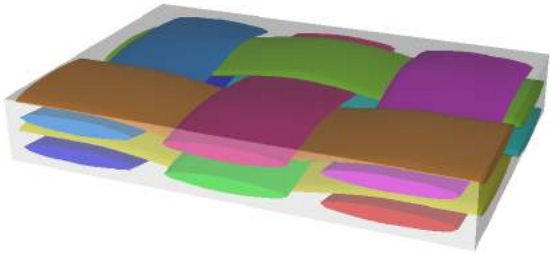


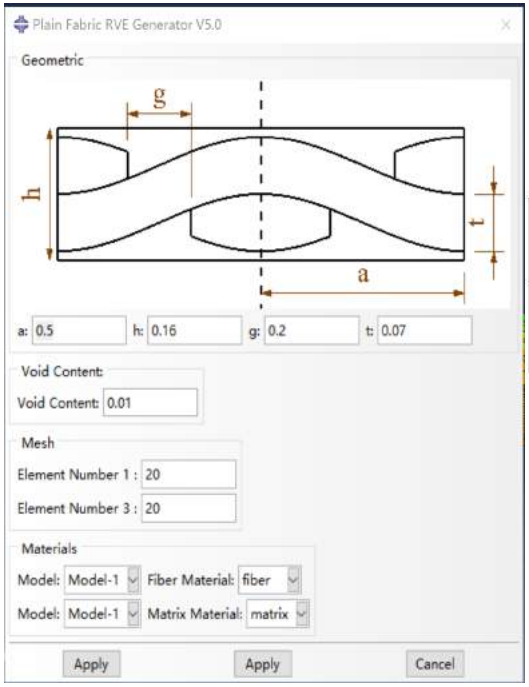
Digimat has the expertise to identify an hyper-elastic model based on CGMD predictions

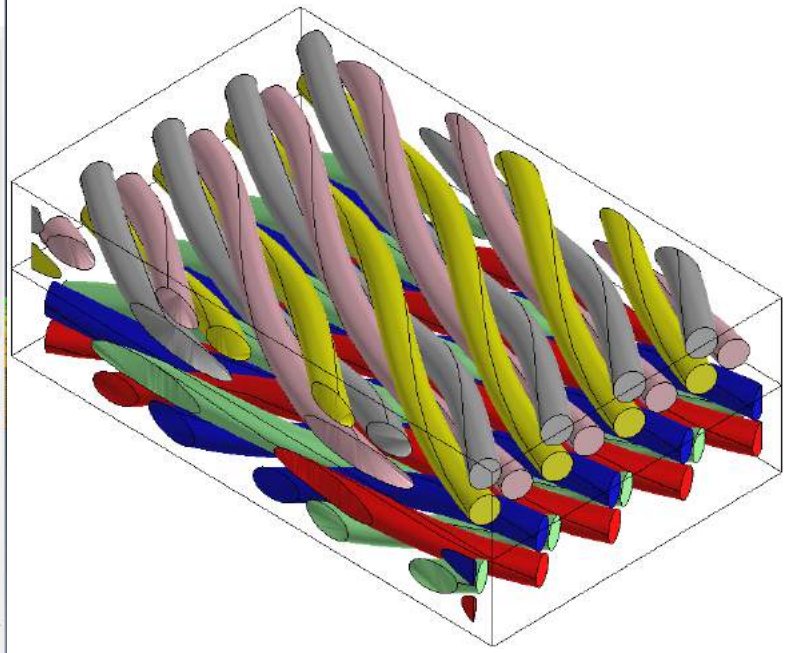
Molecular dynamics → Macro hyper-elastic model

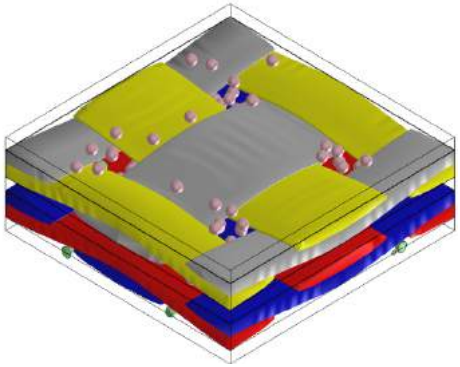
To define a parametrizable cord and meso-structure

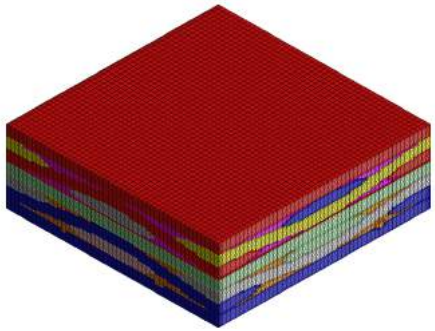
- Define amount of twist per cord length
- Define cord
  - structure
  - material properties
- Computation of homogenized cord properties











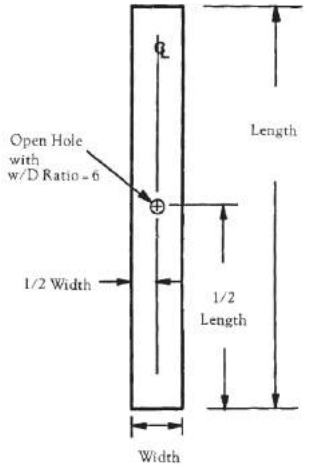
To link virtual testing with full-field homogenization

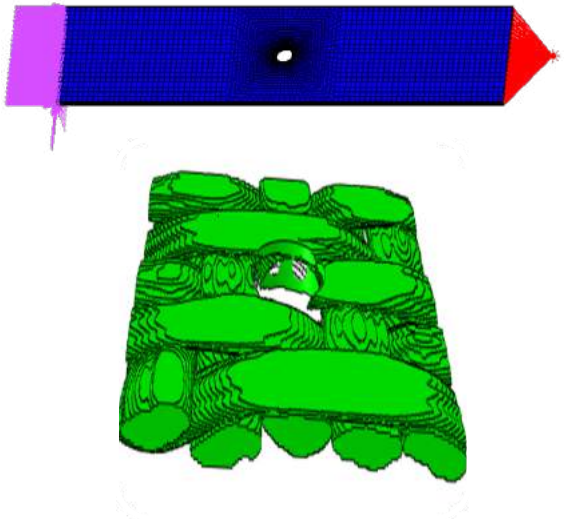
- Design your coupon
- Digimat fill it with fine cord discretization

Test definition
OHT, OHC, UNT…
Materials
Layups

→

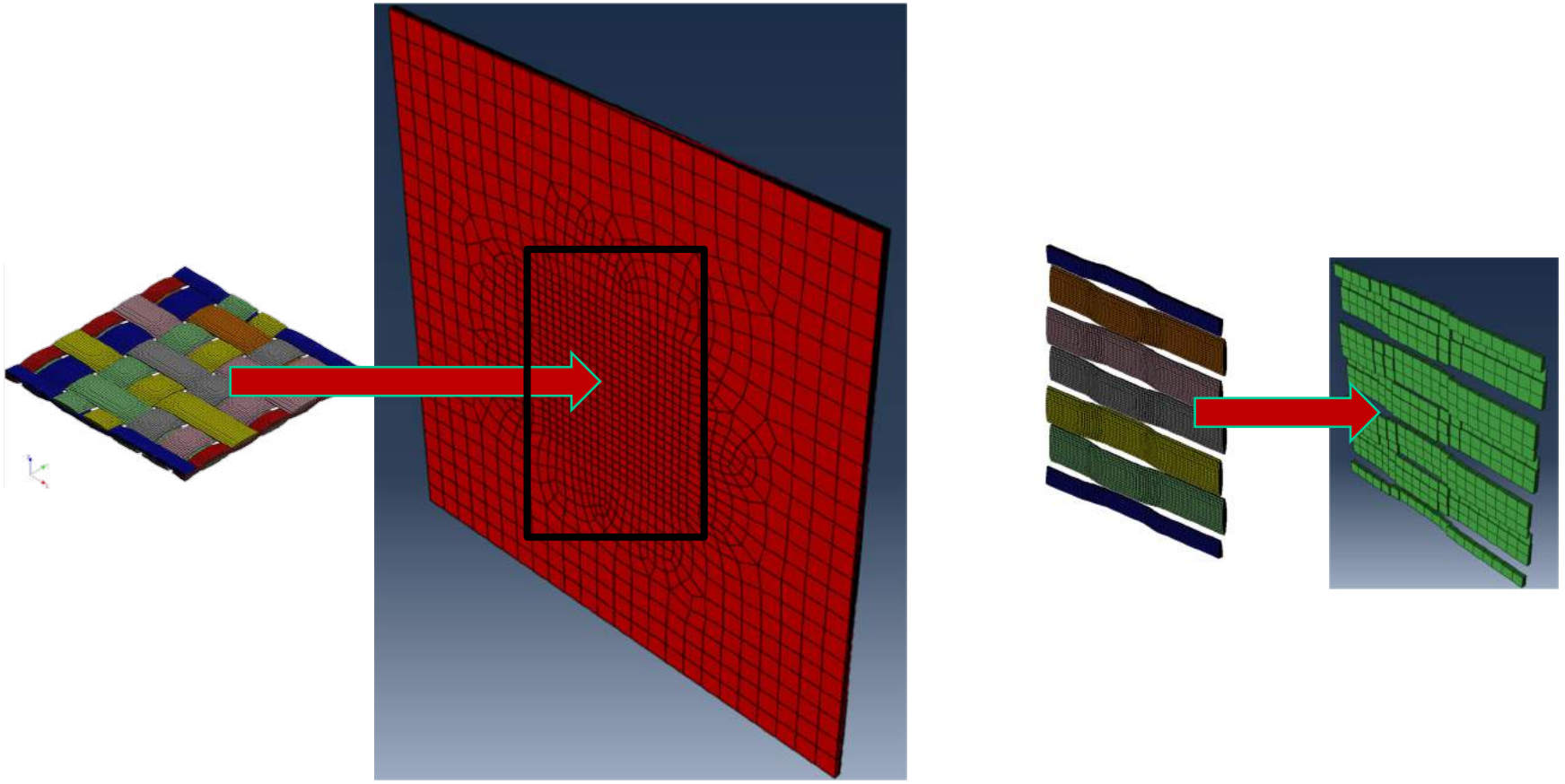
Test simulation
FEA + Progressive Failure





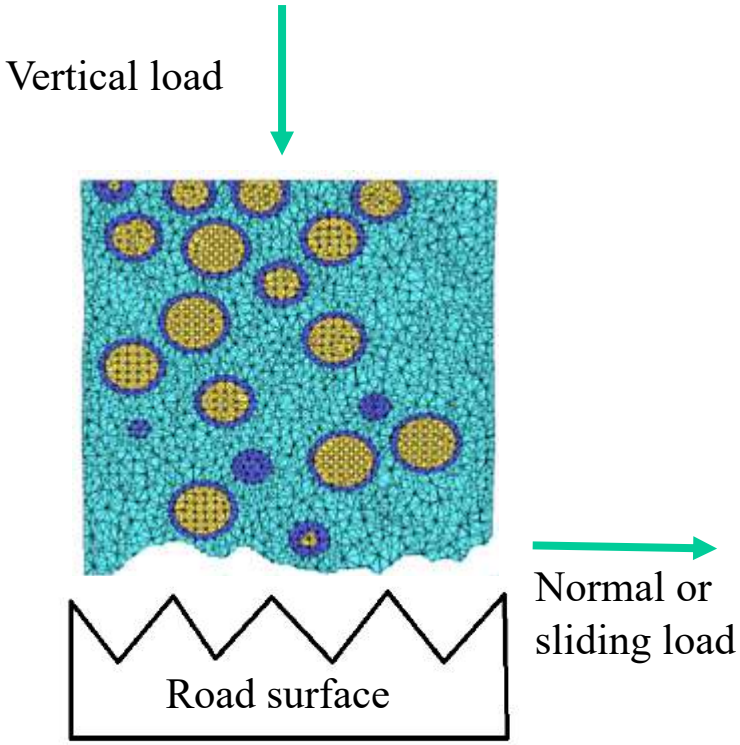
Developping workflow to mix macro and micro modeling

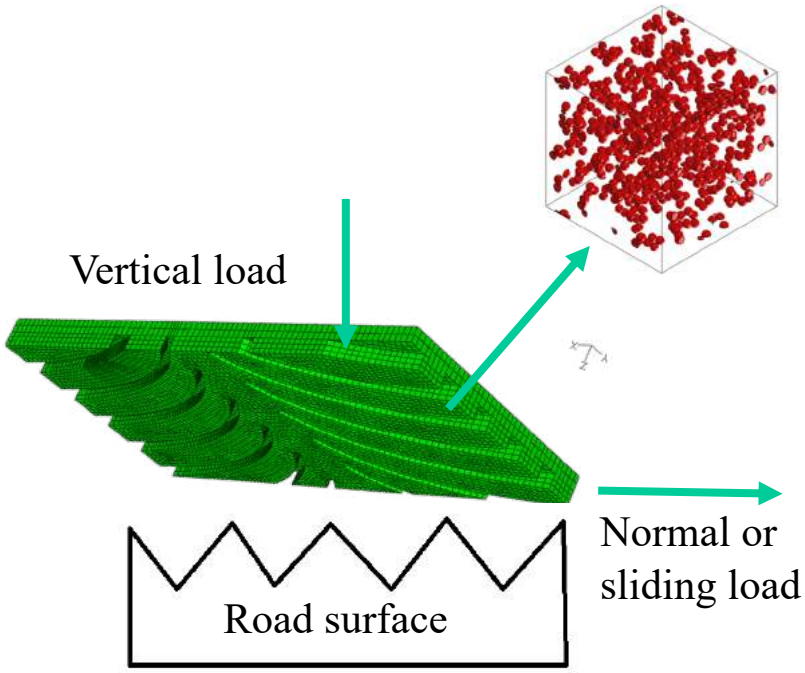
- Mapping of RVE definition onto structural applications
  - Composite behaviour out of the zone of interest
  - Per-phase behaviour in the zone of interest



To predict the friction coefficient of a tyre

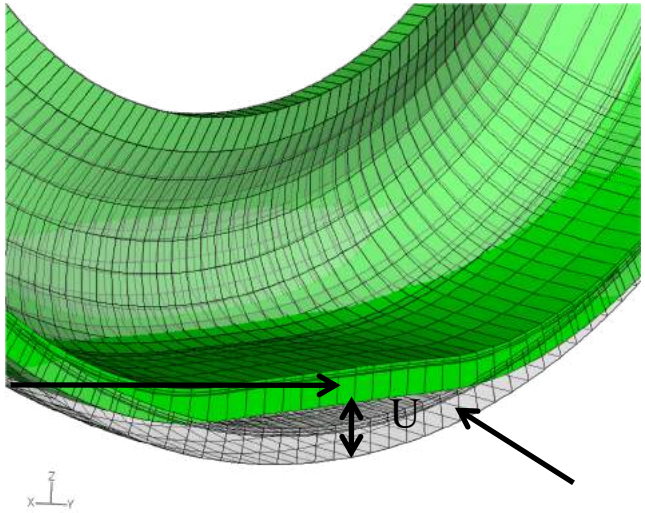
- Performing simulation at various scale
  - Rubber vs road
  - Thread vs road
  - Tire vs road

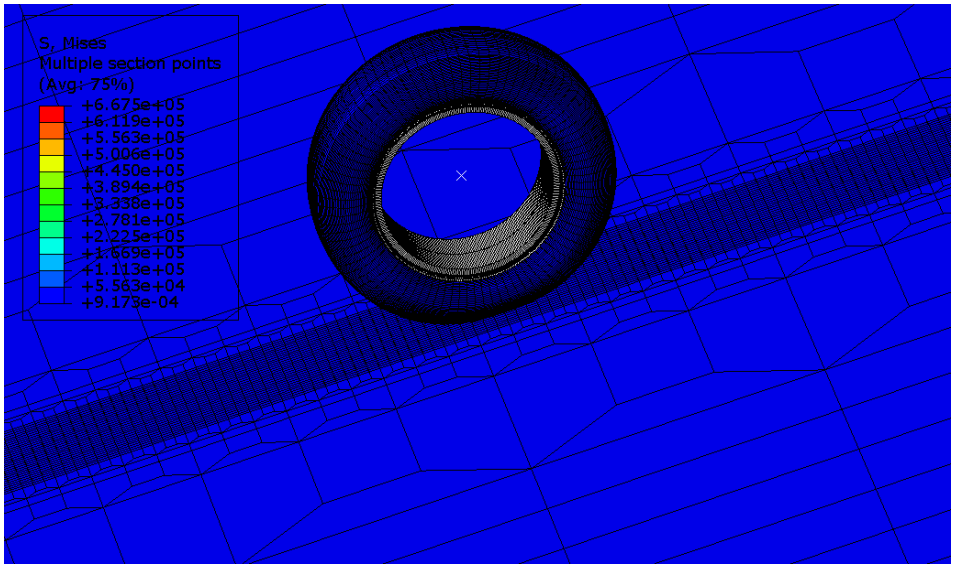


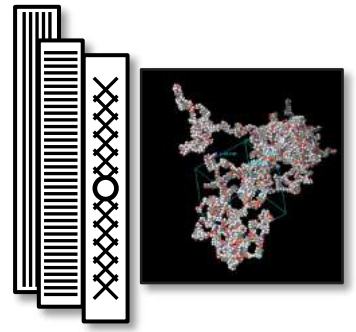


To predict the tire foot print and dynamic simulation

- Predict the tire foot print with various material model based on Digimat
  - Filled rubber
  - Rubber with cords







Simple Coupon Tests or Molecular Dynamics (MD) Simulation

material

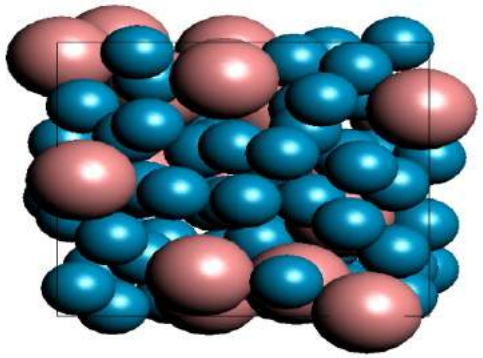
speciman

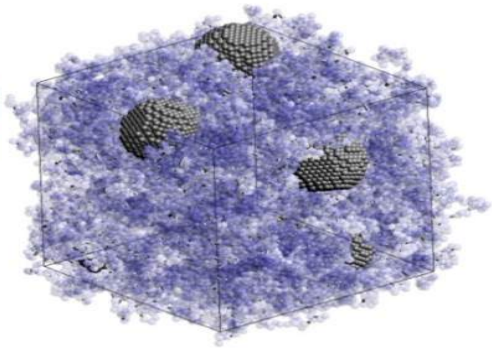
component

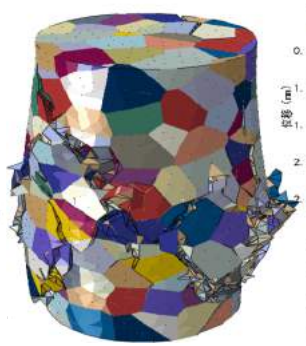
Subsystem

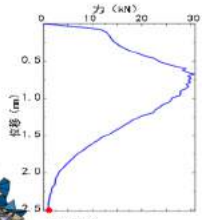
System

Thanks for your attention









Failure