Atomistically Driven Computational Framework to Predict the Behavior of CNT-Embedded Nanocomposites

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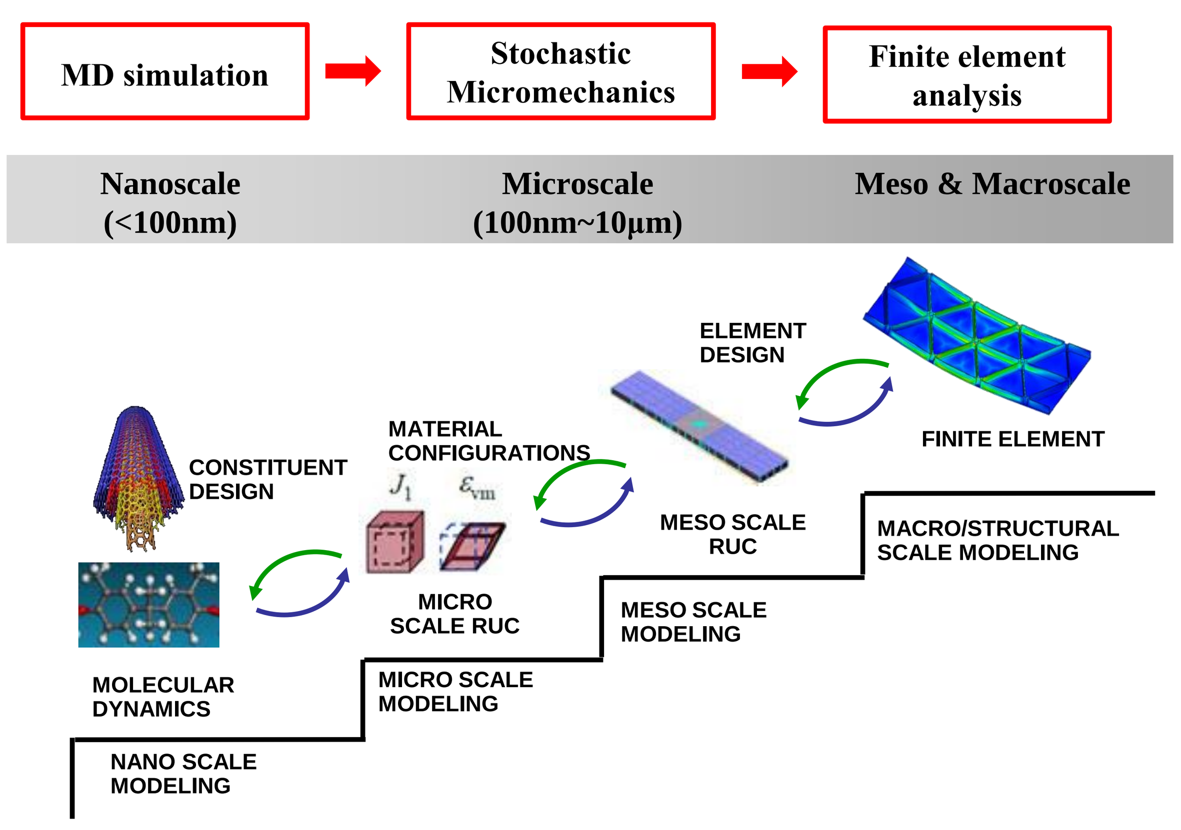
Objectives:

- Construct a computationally efficient multiscale modeling framework for CNT-enhanced nanocomposites
- Understand material response of CNT nanocomposites from the molecular level to the continuum scale
- Integrate damage initiation and evolution mechanisms caused by molecular events to system level information

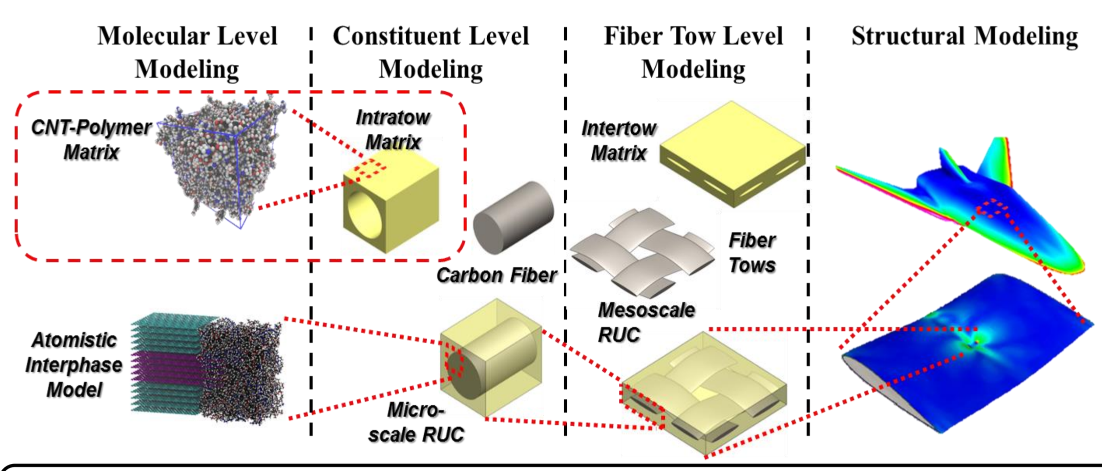
Proposed Approach



Multiscale Modeling Motivation

Motivation:

- Global constitutive response affected by properties at nanoscale
  - Distribution of nanoparticles, cross-linking degree, local interfaces
- Capturing damage evolution requires information exchange through length scales
- Computational traceability requires a multiscale framework



A framework to enhance existing knowledge-base on material properties and response of complex CNT-enhanced composites; help promote use of nanomaterials

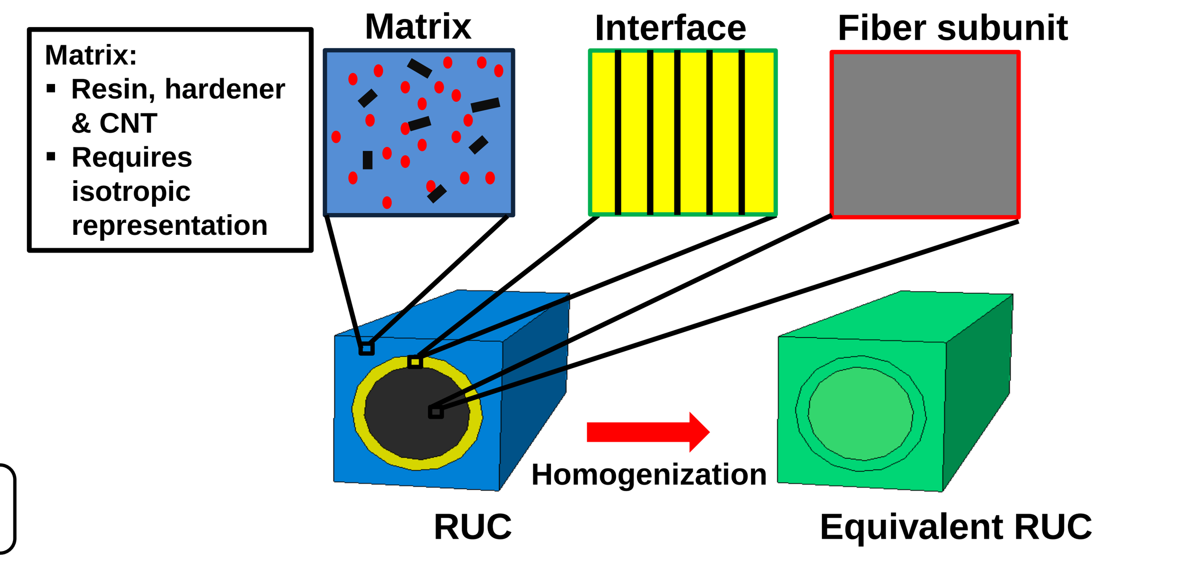
Challenges: Local Material Modeling

Different models required for typical subregions

Interface:
- CNT-dispersed matrix & fiber
- Requires anisotropic representation

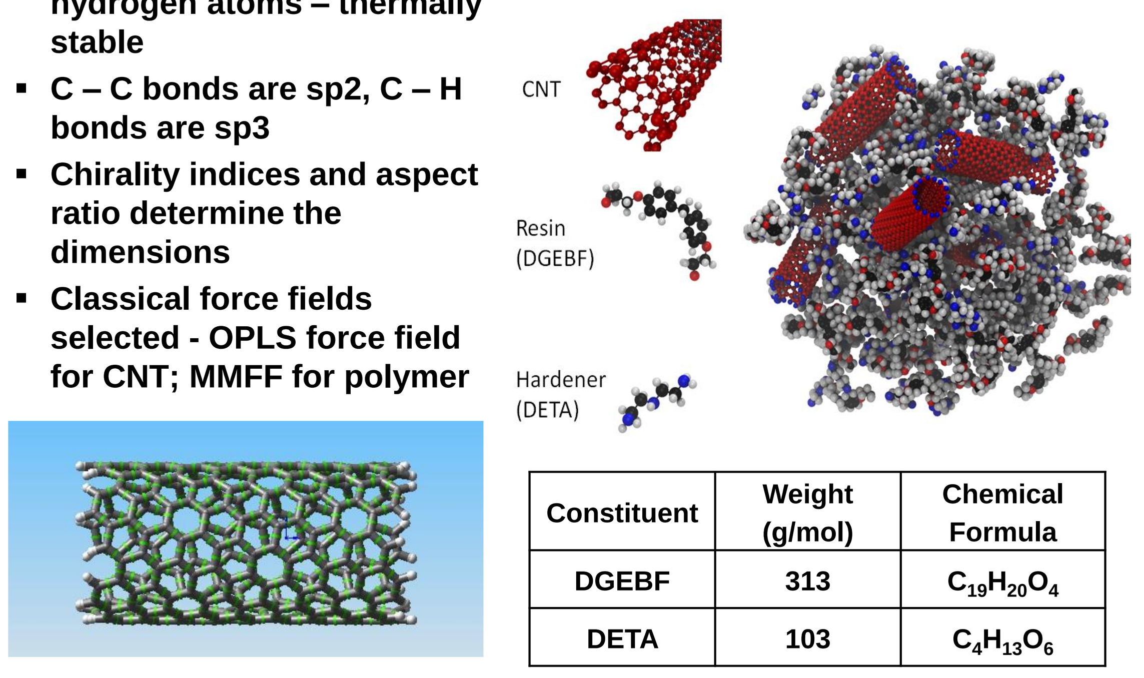
Fiber:
- Unidirectional carbon fibers
- Requires orthotropic representation

Matrix:
- Resin, hardener & CNT
- Requires isotropic representation



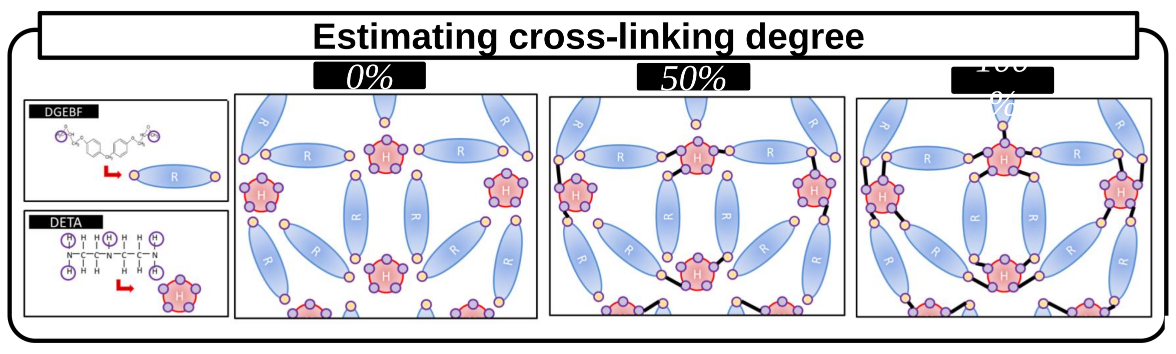
CNT & Polymer Modeling

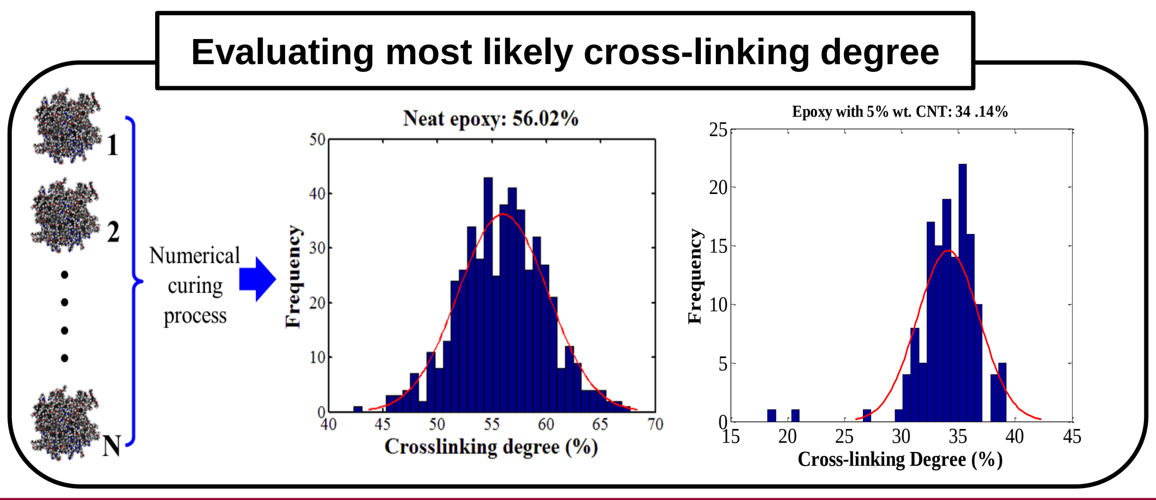
- SWNT with terminal hydrogen atoms – thermally stable
- C – C bonds are sp2, C – H bonds are sp3
- Chirality indices and aspect ratio determine the dimensions
- Classical force fields selected - OPLS force field for CNT; MMFF for polymer
- Epoxy-based polymers are amorphous



Constituent	Weight (g/mol)	Chemical Formula
DGEBF	313	$C_{19}H_{20}O_4$
DETA	103	$C_4H_{13}O_6$

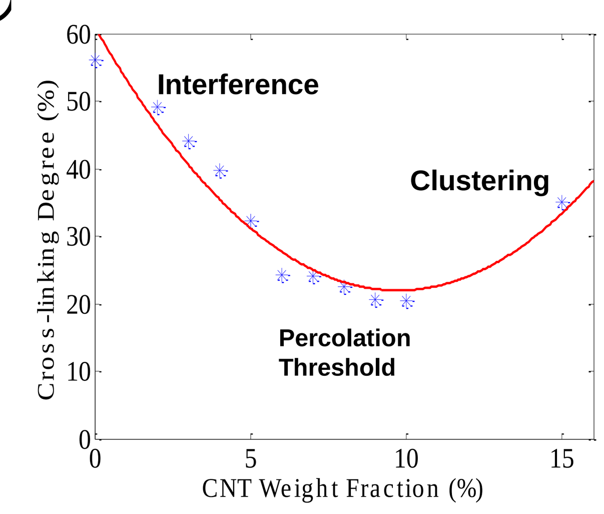
Cross-linking Degree Estimation





Correlation: Crosslinking Degree & CNT Weight Fraction

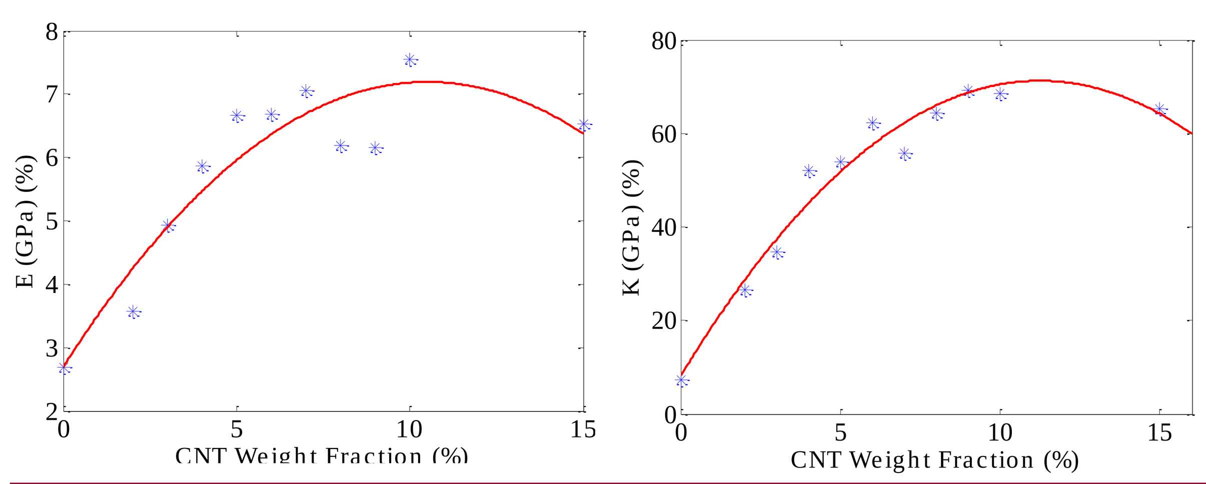
- RUCs contain different CNT weight fractions; distribution of CNTs in the simulation volume is random
- Investigated resulting CL degree from the numerical curing process for a constant value of cut-off distance (4.5 Å)



- Interference: Inclusion of CNT molecules in RUC interferes with crosslinks formed between resin & hardener molecules
- Clustering: With higher number of CNT molecules in RUC, intermolecular attractive force draws CNTs to RUC center

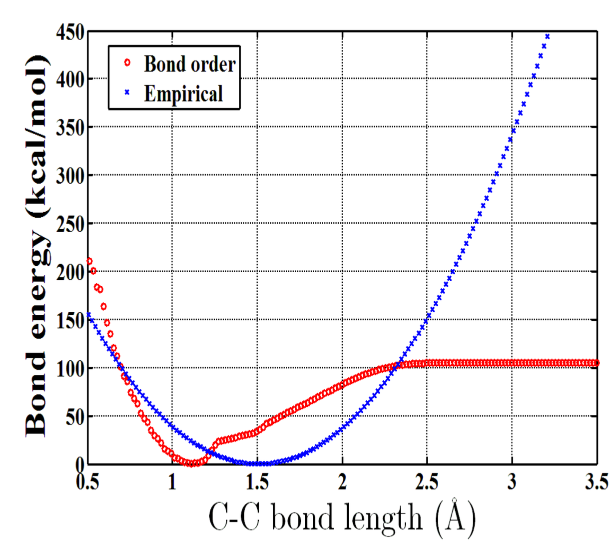
Effect of CNT Weight Fraction, CNT Distribution

- Each data point obtained as an average from multiple MD simulations
- Improvement in mechanical properties of nanopolymer observed until CNT weight fraction of ~ 7%
- Properties remain mostly invariant at higher weight fractions
- CNT clustering effects could result in inefficient load transfer through the matrix



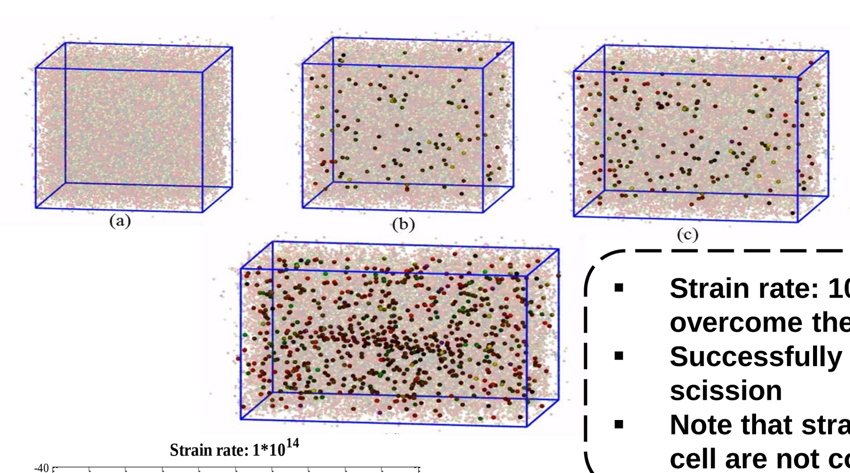
Damage Initiation Modeling

- Harmonic (classical) bond potential in MD valid only for processes occurring about equilibrium bond length (e.g. cross-link formation); does not simulate bond dissipation
- Accurate simulation requires a combination of classical and bond-order based force fields

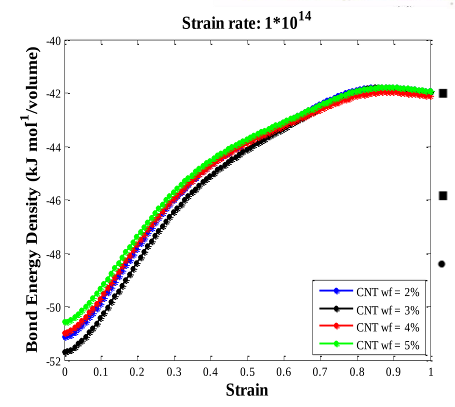


- Deformation tests stretch bonds & require recalculation of bond order at each time step
- Bond order-based force field captures bond dissociation as a function of bond length

Simulation of Bond Scission Events



- Strain rate: 10^{14} s^{-1} used to overcome thermal vibrations
- Successfully captures bond scission
- Note that strains of the unit cell are not continuum strains

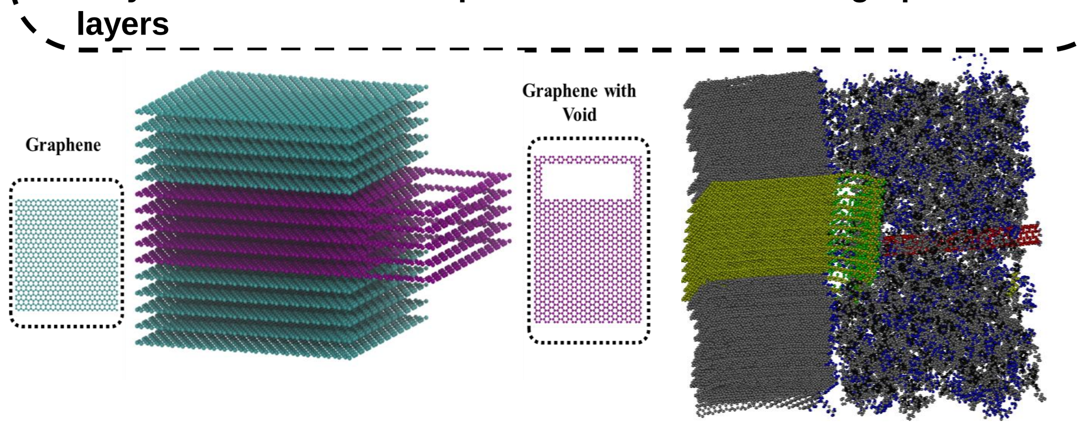


- Continuum Damage Mechanics (CDM) framework developed from atomistic Bond Dissociation Energy Density
- BDE Density obtained as a continuous function of strain and CNT weight fraction
- Anisotropic damage tensor defined in the principal directions

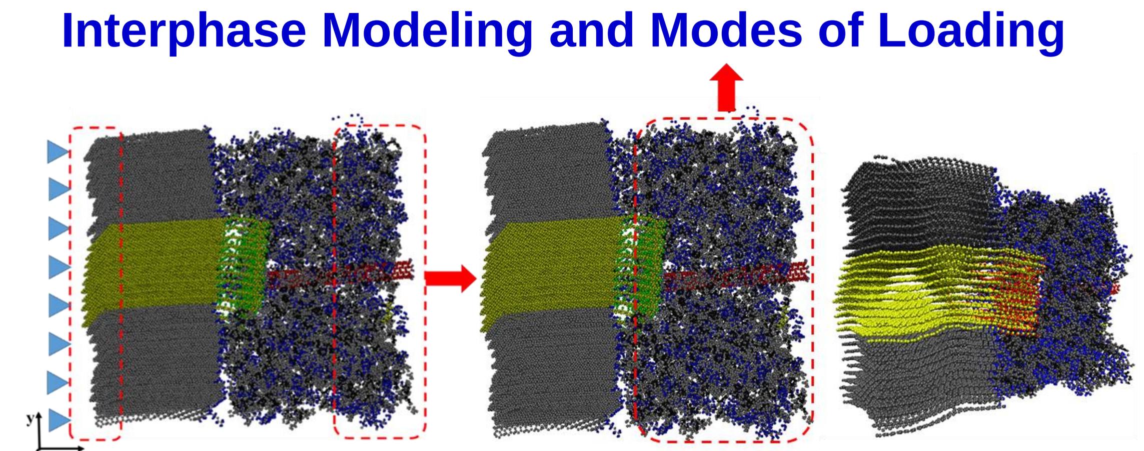
$$d = \frac{B(\epsilon,\rho) - B_{ip}}{B_c - B_{ip}} \qquad D_{ij} = \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix}$$

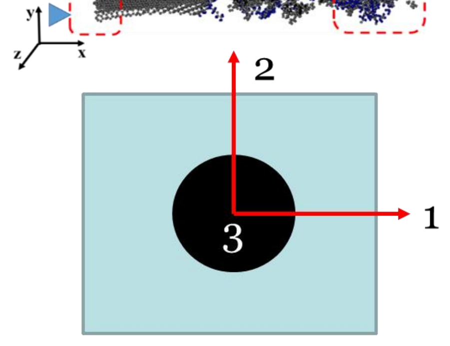
Nanoscale Fiber/Matrix Interphase

- Fiber outer surface modeled with irregularly stacked graphene layers
- Voids induced by selectively removing carbon atoms; hydrogenating active sites by stochastic cutoff based bond formation
- Graphene with induced voids simulates surface roughness, physical mechanical entanglement & chemical interactions from covalent bonds
- Polymer network chains penetrate defect induced graphene layers



Interphase Modeling and Modes of Loading

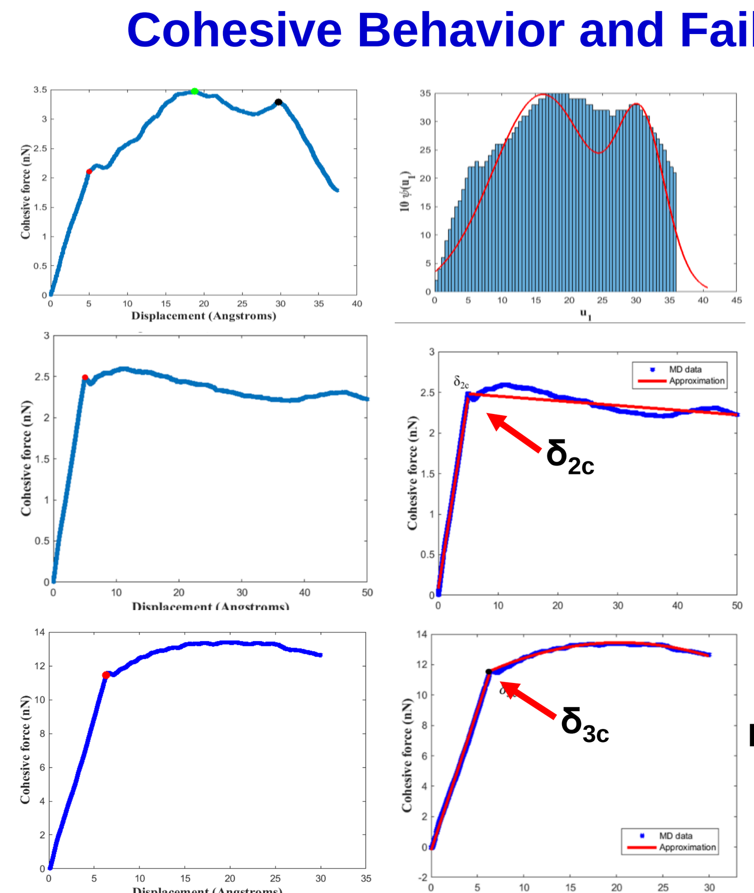




- Loading along 1 simulates ***matrix debond***
- Relative loading along 3: ***fiber pullout***
- Relative shear along 2 among graphene layers and polymer simulates ***fiber rotation***
- ***Stress-strain response, pair & bond energy variations*** obtained for each case

$T_1 = \frac{u_1}{\delta_{c1}} T_{1\,max}\, \phi\left(\frac{u_1}{\delta_{c1}}, \frac{u_3}{\delta_{c3}}, \alpha\right)$ similarly for T_2 and T_3; Critical displacements $(\delta_{c1}, \delta_{c2}, \delta_{c3})$ will be obtained from MD simulation output files

Cohesive Behavior and Failure Modes



Matrix Debond: Bimodal cohesive law

Fiber Rotation: Trapezoidal cohesive law

Fiber Pullout: Trapezoidal cohesive law

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