Distinct Element Method for Fibrous Composites: Toward Computational Guided Manufacturing

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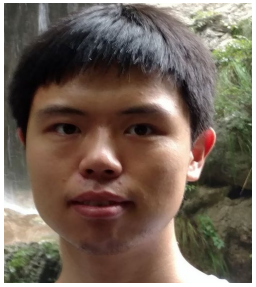

Dr. Hao Xu
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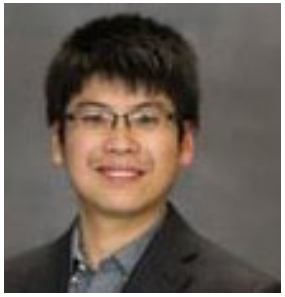

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US COMP
National Aeronautics and Space Administration
FULBRIGHT
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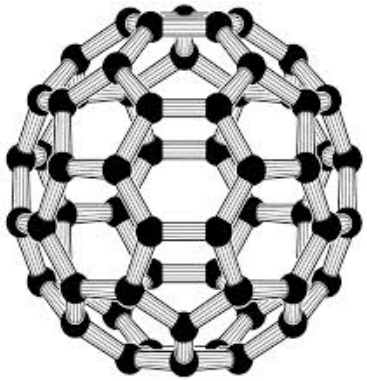
Overview

- **Context**
  - **Carbon Nanotubes – Interest in Developing Lightweight Composites for Space Applications**
  - **Missing Computational Method for the Mesoscale**
- **The Mesoscopic Distinct Element Method for Carbon Nanotube Systems – Contacts and Calibration**
- **Example Application: Stretching of a Carbon Nanotube Network**

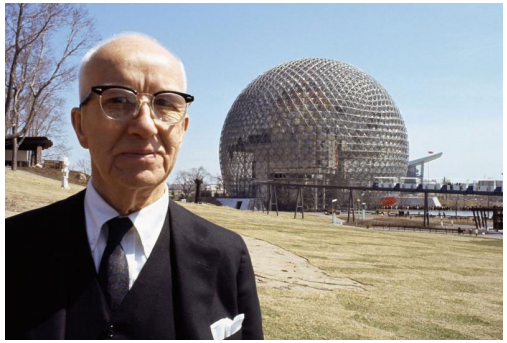
Professor Richard E. Smalley
Nobel Prize in Chemistry 1996



C60

Buckminster fullerene:

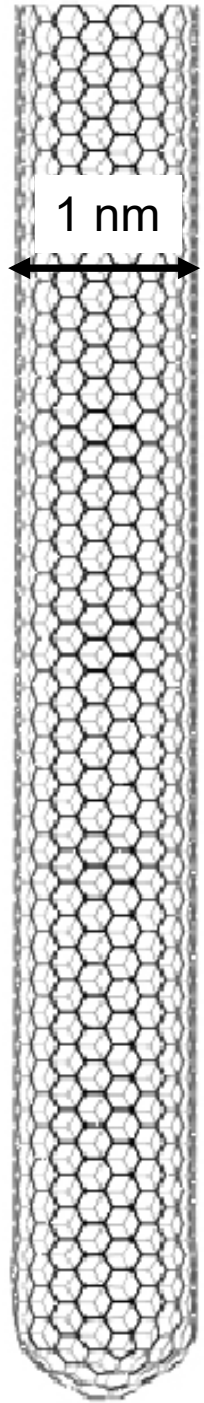
Buckyballs



2 – page paper in Nature

1985

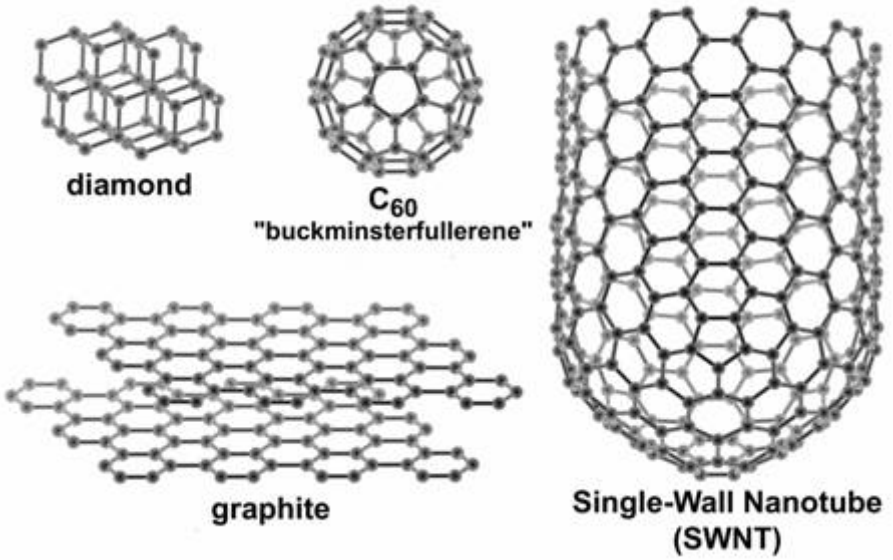
with Robert F. Curl and Harold Kroto

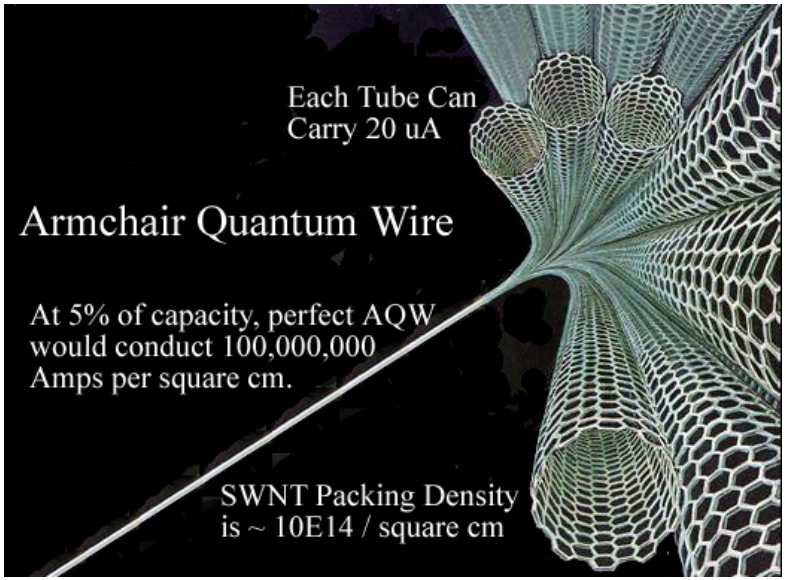


Why Single Wall Carbon Nanotubes?

MOLECULAR PERFECTION & EXTREME PERFORMANCE

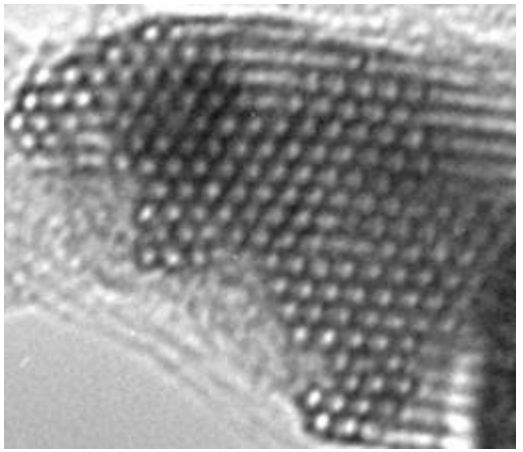
- **The Strongest Fiber Possible.**
- Selectable Electrical Properties
  - Metallic Tubes Better Than Copper
  - Semiconductors Better Than InSb or GaAs
- Thermal Conductivity of Diamond.
- The Unique Chemistry of Carbon.
- The Scale and Perfection of DNA.
- The Ultimately Versatile Engineering Material.

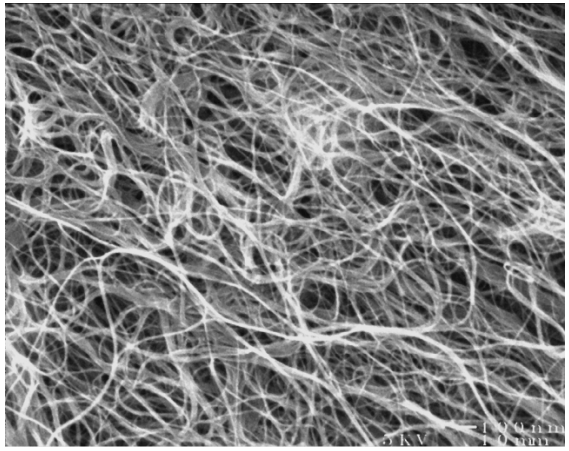


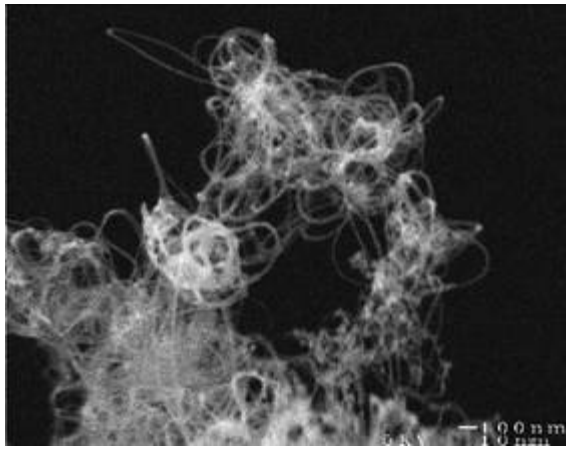


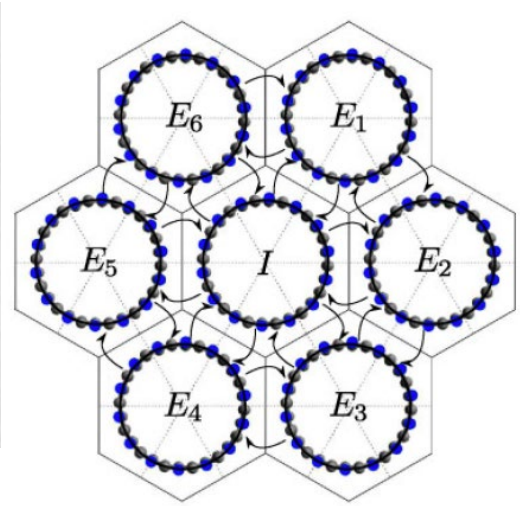
Forming SWNT Single Wall Carbon Nanotubes Wires

- Need macro-crystalline SWNT fiber/wire
- Starting material is tangled at several scales
- Starting material has variety of diameters and types
- Enormous Van der Waals forces make it hard to separate SWNT bundles

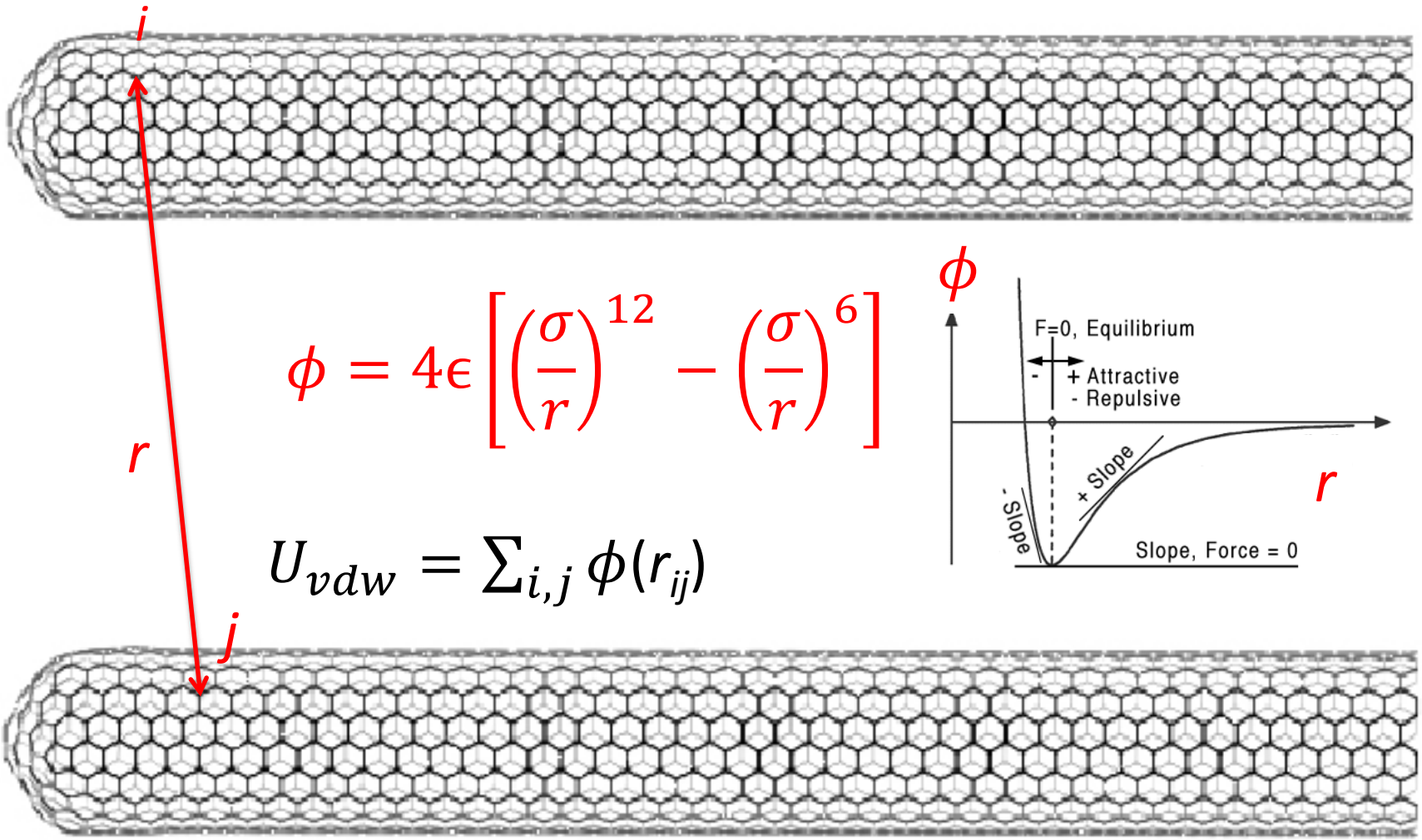








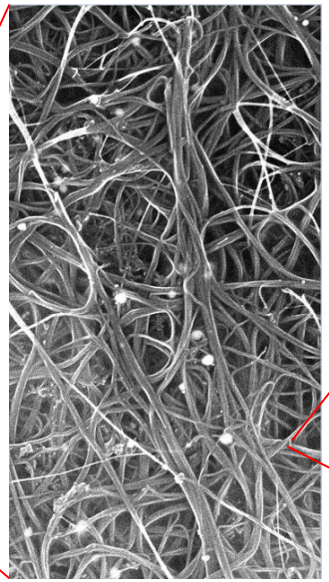
The Van der Waals Forces

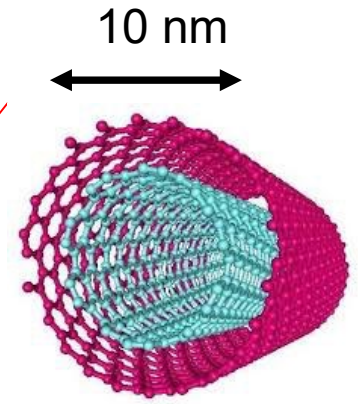


$$\phi = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$U_{vdw} = \sum_{i,j} \phi(r_{ij})$$

Miralon®
Multi-walled carbon nanotube-based advanced materials



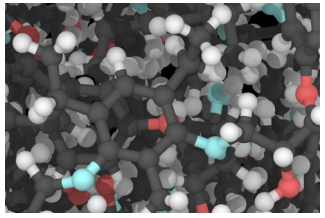


nanocomp TECHNOLOGIES, INC.
A Huntsman Company

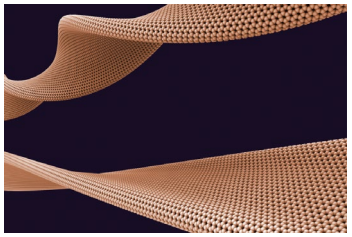
TORTECH nano fibers

Computational:

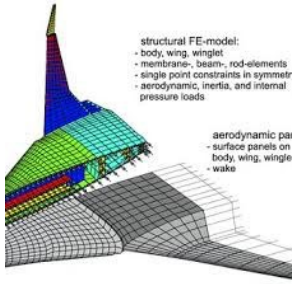
- Molecular modeling



- Meso-scale modeling DEM

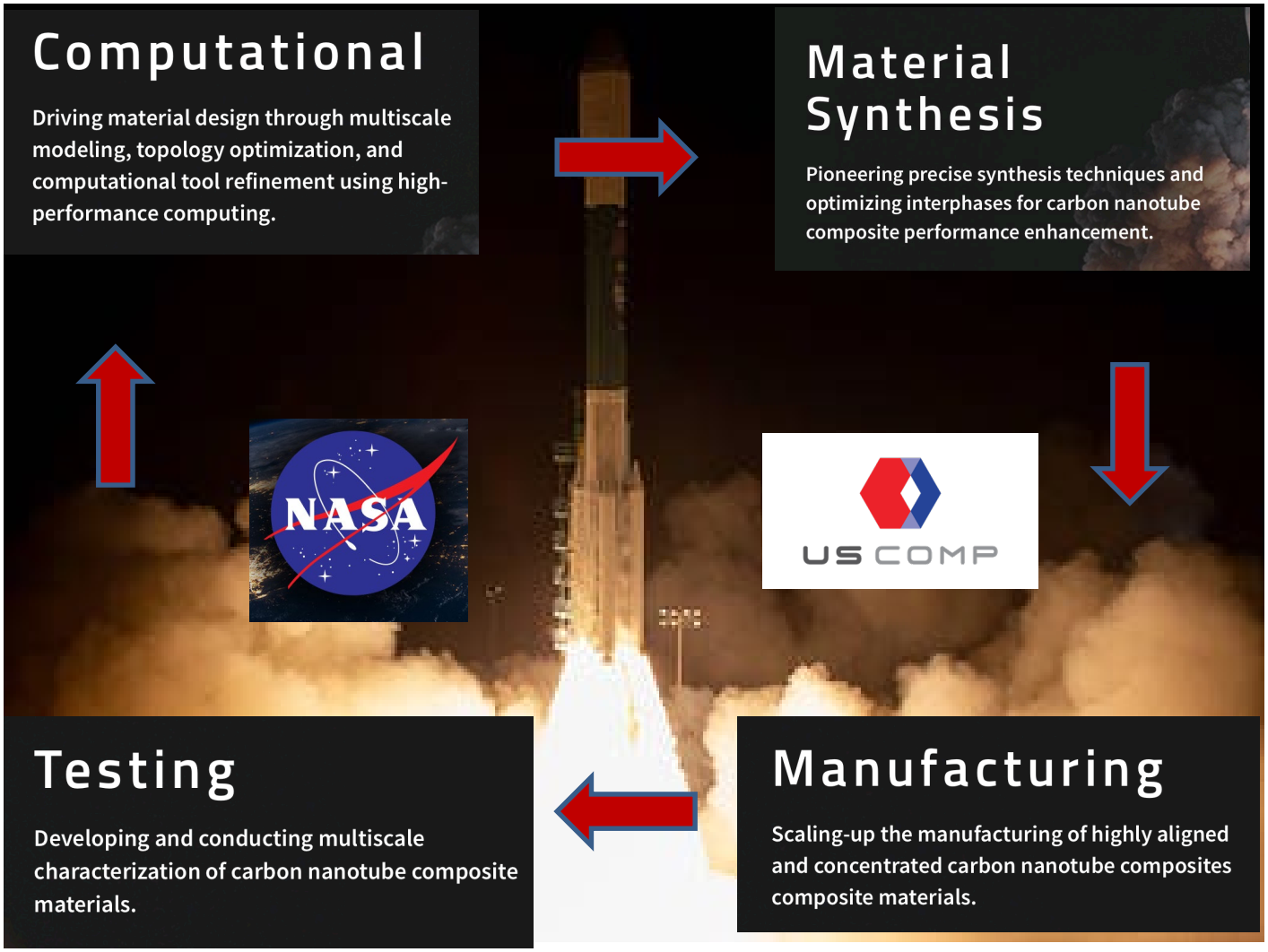


- Continuum modeling

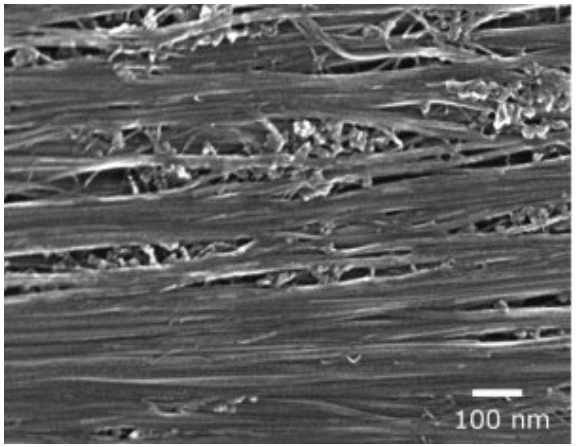


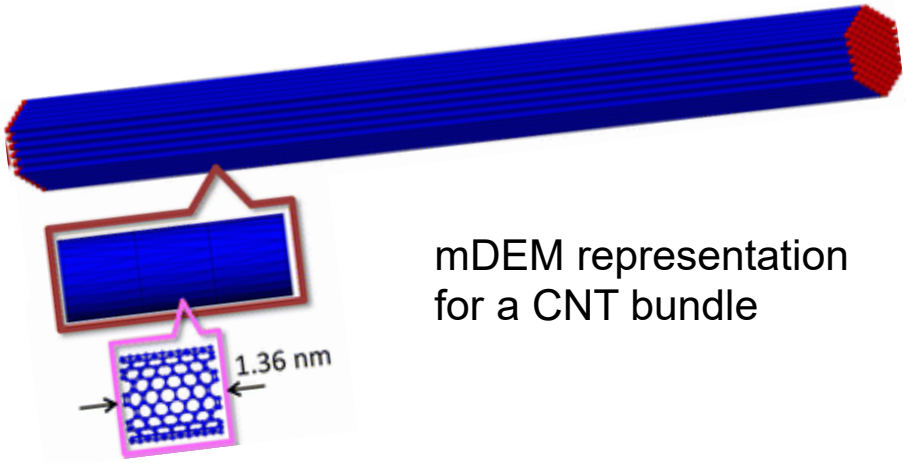
Institute for Ultra-Strong Composites by Computational Design (US-COMP) - a NASA Space Technology Research Institute awarded in 2017

"Manhattan Project"



- We utilize the concepts of **mesoscopic distinct elements** interacting via **mesoscopic contacts** to develop a technology for bridging atomistic and macro-scale computations.





mDEM representation for a CNT bundle

HR-SEM image of a CNT yarn surface.

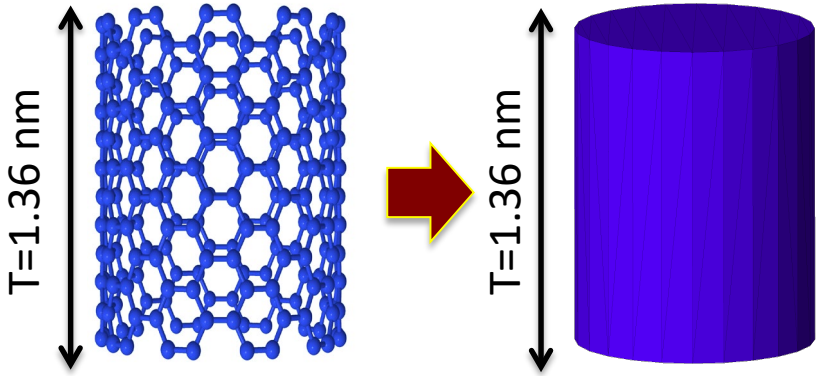
Kim, Jae-Woo, et al. Composites Part A: 84 (2016): 256-265.

- Simulate the meso-scale mechanics, and the strain to failure of purified and hybrid (nanoparticle/polymer) carbon nanotube (CNT) sheets and yarns.

- The technical compatibility with the classical distinct element method (DEM), a solid mechanics method, allows for the embedding of these concepts into existing codes, PFC3D, and thus for the creation of easy-to-use simulation environment.

The Technical Approach
The Mesoscopic Distinct Element Method (mDEM)

I. "Ultra" coarse-graining: a large number of atoms represented by a mesoscopic distinct element



(10,10) CNT -- 220 atoms

Rigid tube element

M -- Mass

I -- Inertia

II. For each mesoscopic distinct element we solve:

$$\mathbf{F} = m\ddot{\mathbf{x}},$$
$$\mathbf{M} = I\dot{\boldsymbol{\omega}},$$

+ local damping (both force and moment)

Example Algorithm:

$$\mathbf{x}(t+\Delta t) = \mathbf{x}(t) + \mathbf{v}(t+0.5\Delta t)\Delta t.$$

$$\mathbf{v}(t+0.5\Delta t) = \mathbf{v}(t-0.5\Delta t) + \frac{\mathbf{F}(t)}{m}\Delta t,$$

$$\boldsymbol{\omega}(t+0.5\Delta t) = \boldsymbol{\omega}(t-0.5\Delta t) + \frac{\mathbf{M}(t)}{I}\Delta t.$$

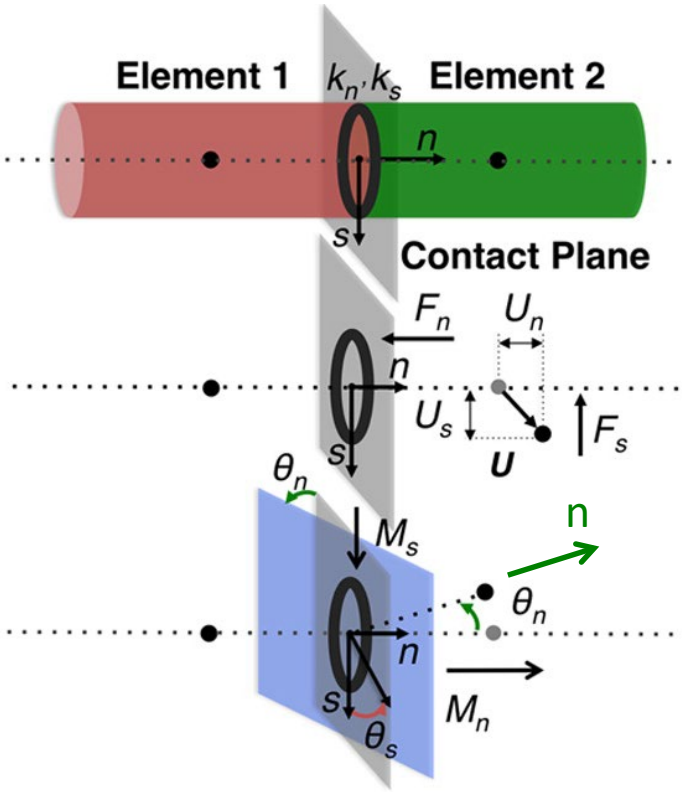
Published in: I. Ostanin; R. Ballarini; D. Potyondy; Traian Dumitrică; J. Mech. Phys. Solids 2013, 61, 762–782. doi:10.1016/j.jmps.2012.10.016

The Mesoscopic Distinct Element Method

Two Main Contact Models: **1) Parallel-Bond Contact (Strain energy storing)**

Adjacent distinct elements on a CNT connected by a parallel-bond contact.

Restoring forces F_n and F_s and moments M_n and M_s in response to the normal and shear relative displacements u_n and u_s and rotations θ_n and θ_s, respectively.



$$F_n = -k_n A\, u_n$$

$$F_s = -k_s A\, u_s$$

$$M_n = -k_s J\, \theta_s$$

$$M_s = -k_n I\, \theta_n$$

How to find k_n and k_s?

$$k_n = E/T$$

$$k_s = G/T$$

Table 1. Parameters for the mDEM Model of a (10,10) CNT Used in our Simulations[22]

A (nm^2)	I (nm^4)	J (nm^4)	k_n (eV/nm^4)	k_s (eV/nm^4)
1.427	0.348	0.696	4740	2110

Published in: Yuezhou Wang; Igor Ostanin; Cristian Gaidău; Traian Dumitrică; *Langmuir* 2015, 31, 12323-12327.
DOI: 10.1021/acs.langmuir.5b03208

The Mesoscopic Distinct Element Method

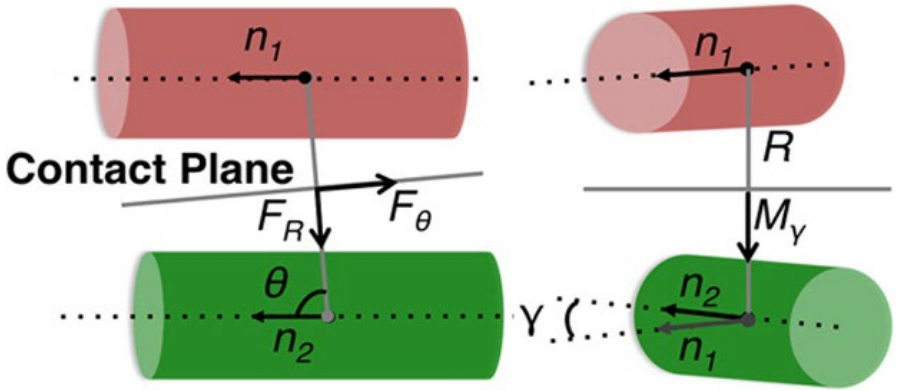
Two Main Contact Models: **2) van Der Waals potential (vdW cohesive energy storing)**

$$U=U(R,\theta,\gamma)$$

Parallel distinct elements on two CNTs connected by a vdW contact.

Restoring forces in response to changes in center-to-center distance R and alignment angle θ. (Right)

Restoring moment at a nonzero crossing angle γ. n_1 and n_2 indicate the axes of the elements.



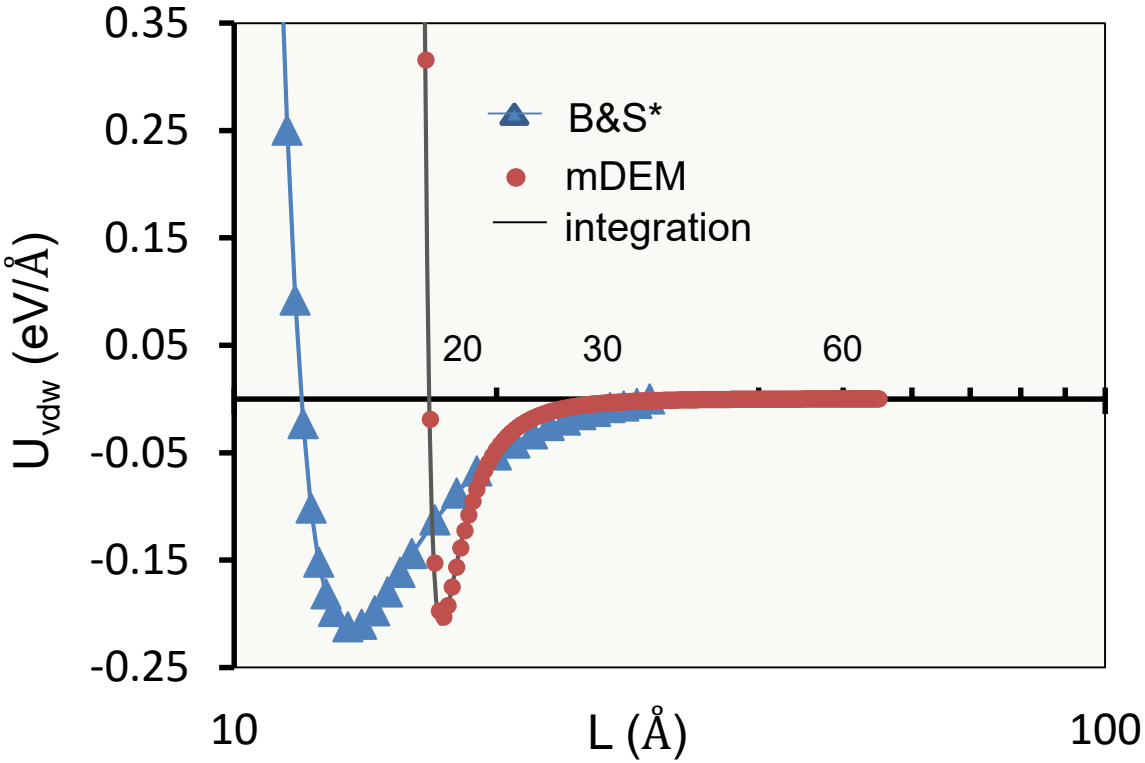
$$F_R = -\partial U/\partial R,\ RF_\theta = -\partial U/\partial\theta, \text{ and } M_\gamma = -\partial U/\partial\gamma.$$

How to find U?

It should match the integrated Lennard-Jones atomistic potential between two CNTs

Published in: Yuezhou Wang; Igor Ostanin; Cristian Gaidău; Traian Dumitrică; *Langmuir* 2015, 31, 12323-12327.
DOI: 10.1021/acs.langmuir.5b03208

The Challenge of “Ultra” Coarse-graining

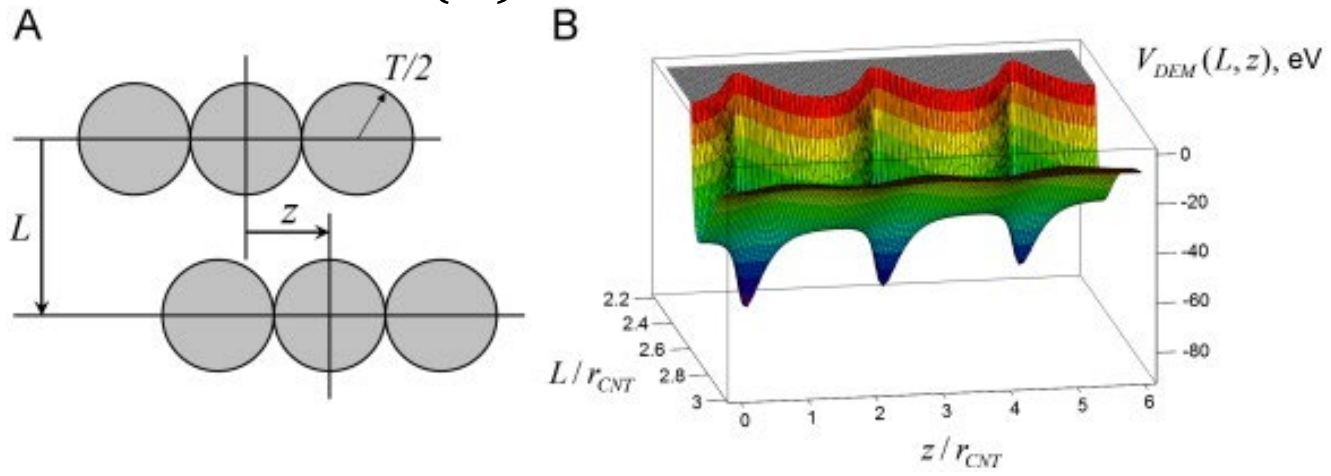


Van der Waals Interaction between 2 parallel (10,10) CNTs

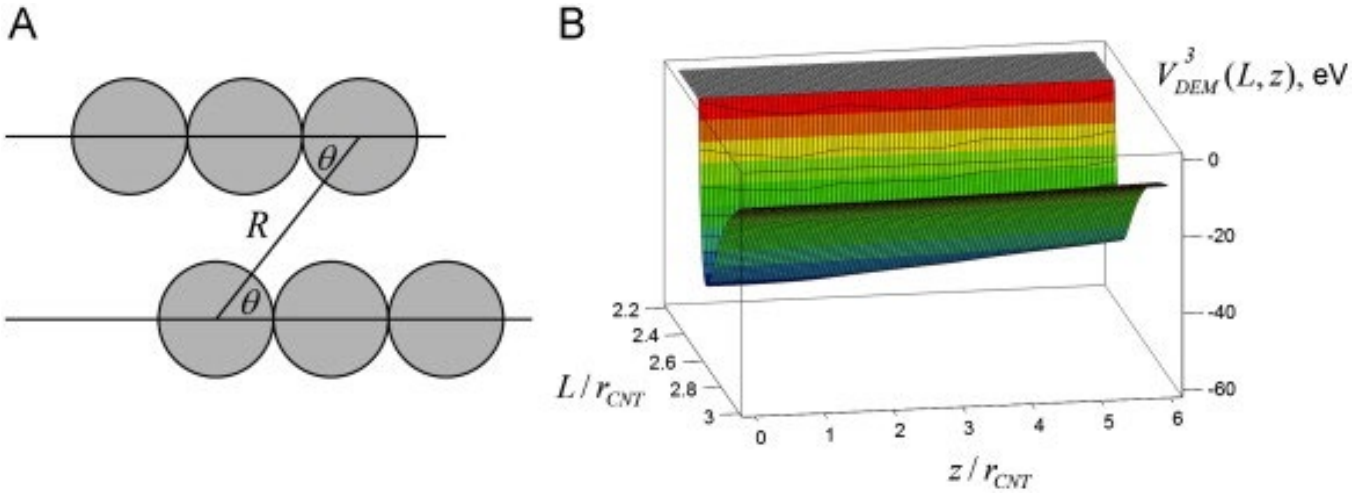
*B&S potential from A Sengab, RC Picu - Composites Science and Technology, 2018

The Challenge of "Ultra" Coarse-graining

Isotropic vdW Contact (B&S): $U=U(R)$



Anisotropic vdW Contact: $U=U(R,\theta,\gamma)= V(R,\theta)\Gamma(R,\gamma)f_c(R)$

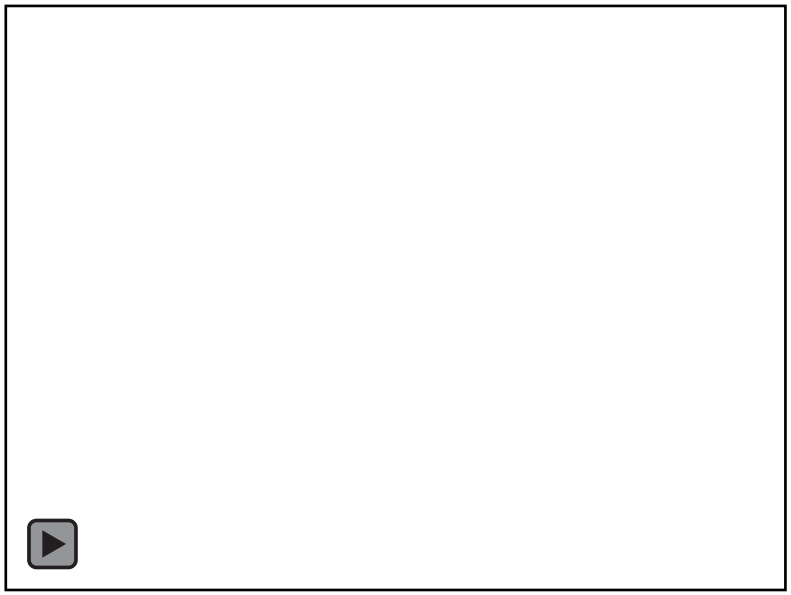


For the detailed *U* expression see: I. Ostanin; R. Ballarini; D. Potyondy; Traian Dumitrică; J. Mech. Phys. Solids 2013, 61, 762–782. doi:10.1016/j.jmps.2012.10.016

The Mesoscopic Distinct Element Method

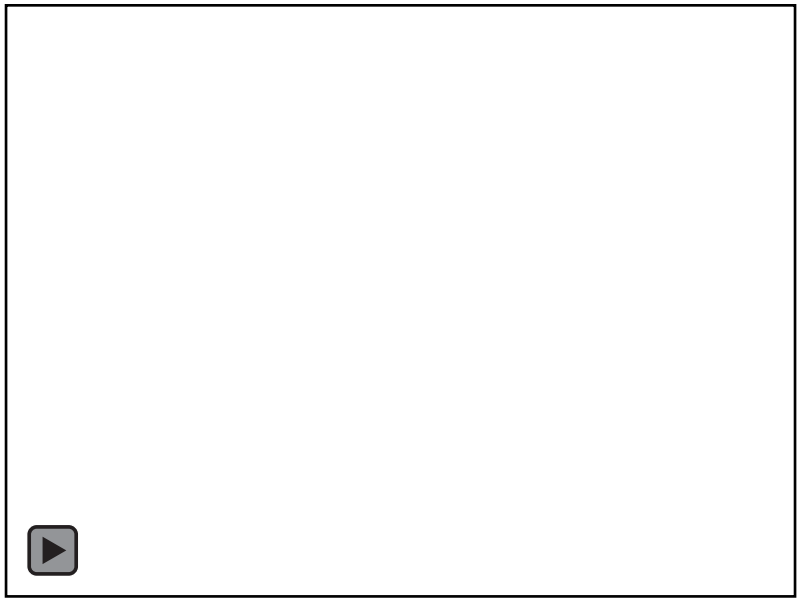
- **vdW Interactions "at work"**

Time Evolution of Two Misaligned Carbon Nanotubes - each 40.7 nm in length



Relaxation time ~800 ps

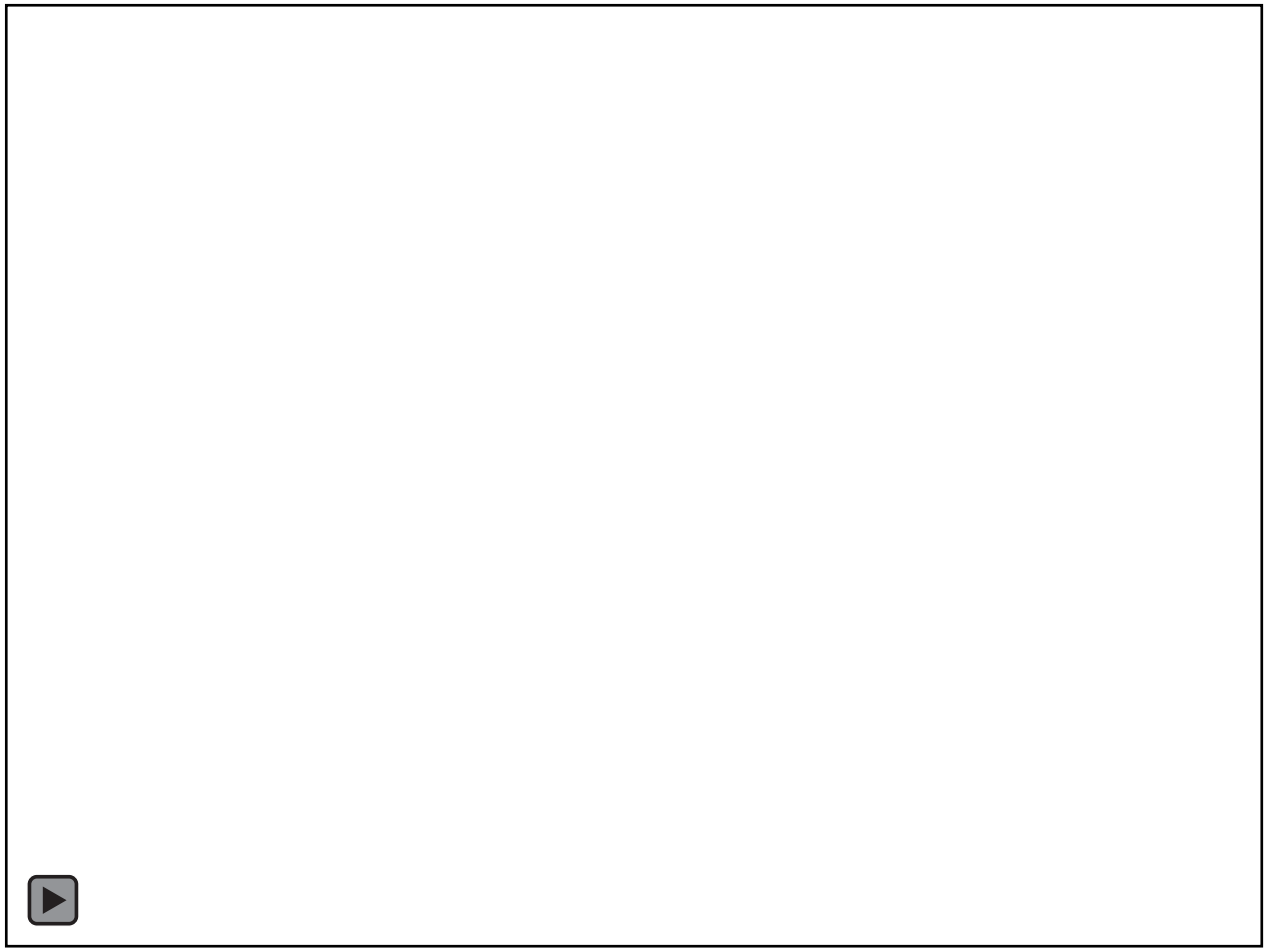
Time Evolution of Two Crossed Carbon Nanotubes - each 40.7 nm in length



Relaxation time 100 ps

The Mesoscopic Distinct Element Method

- **vdW + parallel contact bonds "at work"**



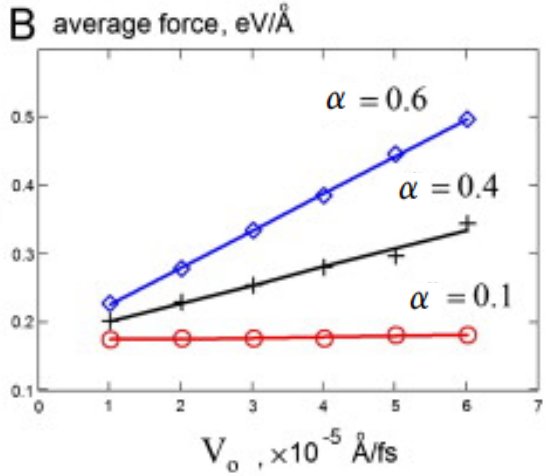
T. Anderson, E. Akatyeva, I. Nikiforov, D. Potyondy, R. Ballarini, and T. Dumitrică, ASME Journal of Nanotechnology in Engineering and Medicine **1**, 041009 (2010).

The Mesoscopic Distinct Element Method

+ damping: **a) local damping -** artificial dissipative damping for both force and moment equations

$$\boldsymbol{F}_{\alpha} = -\alpha \cdot \boldsymbol{F} \cdot sign(\boldsymbol{v}) \text{ and } \boldsymbol{M}_{\alpha} = -\alpha \cdot \boldsymbol{M} \cdot sign(\boldsymbol{\omega})$$

displacement controlled set-up



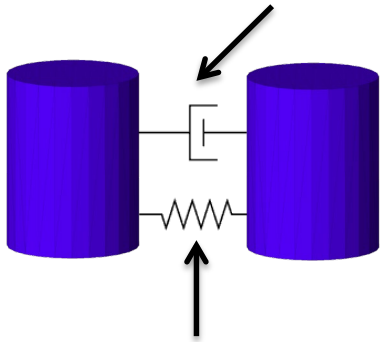
α =0.4 the resulting viscous friction coefficient is very small:

local damping constant

$4.3 \times 10^{-5}\ \mu N\,s/m$

$10\ \mu N\,s/m$ - the "realistic" value

b) viscous damping - to capture the complex energy losses during CNT sliding



$$\boldsymbol{F}_{\boldsymbol{d}} = \gamma \cdot \boldsymbol{v}_{\boldsymbol{r}}.$$

Force developed by the "dashpot" proportional to the relative velocity of the two elements in vdW contact

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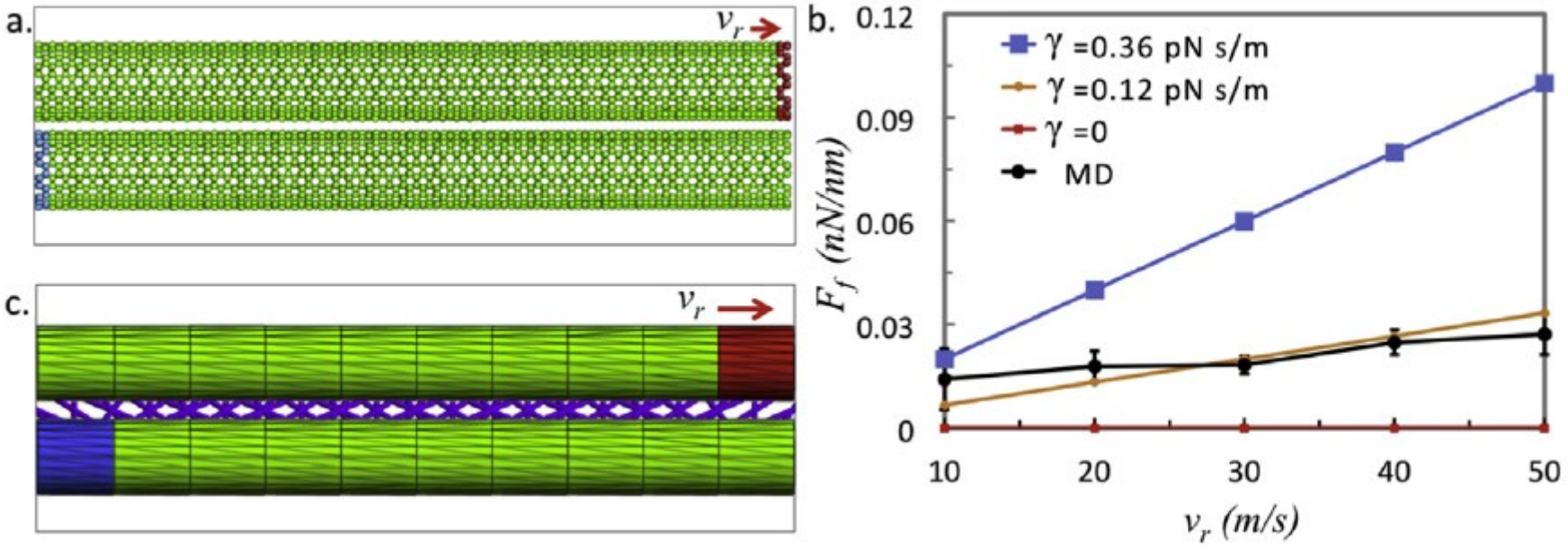
For the detailes see: I. Ostanin; R. Ballarini; D. Potyondy; Traian Dumitrică; J. Mech. Phys. Solids 2013, 61, 762–782. doi:10.1016/j.jmps.2012.10.016 and J. Appl. Mech. 81 061004 2014.

The Mesoscopic Distinct Element Method

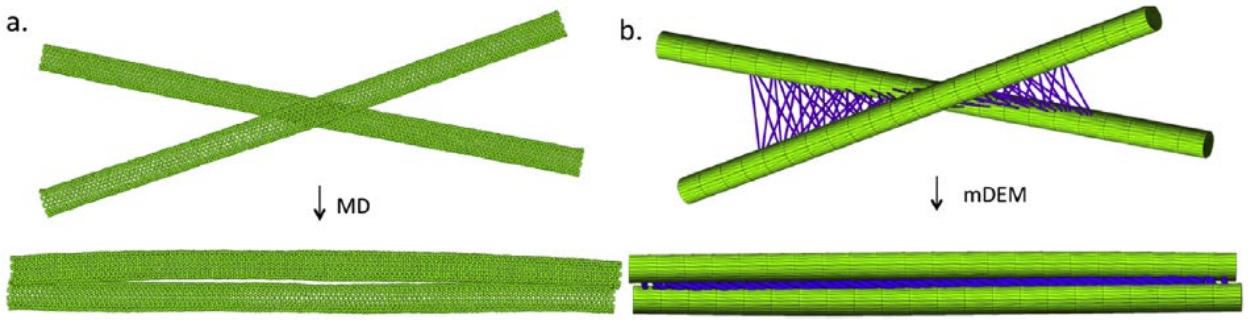
Bridging across length scales to capture dissipation effects



(a) MD setup used to compute dynamical friction between two aligned cylindrical (10,10) CNTs. The desired sliding velocity is imposed to the one unit cell "ring" and one distinct element (red) belonging to the upper CNT. One unit cell "ring" and one distinct element (blue) belonging to the lower CNT is at rest. (b) F_f (per unit length) vs. v_r. MD data (black circles) shows smooth sliding. (c) mDEM setup used to calibrate mesoscale friction. The purple lines indicate the vdW contacts between distinct elements located on the two CNTs.

The Mesoscopic Distinct Element Method

Bridging across length scales to capture dissipation effects



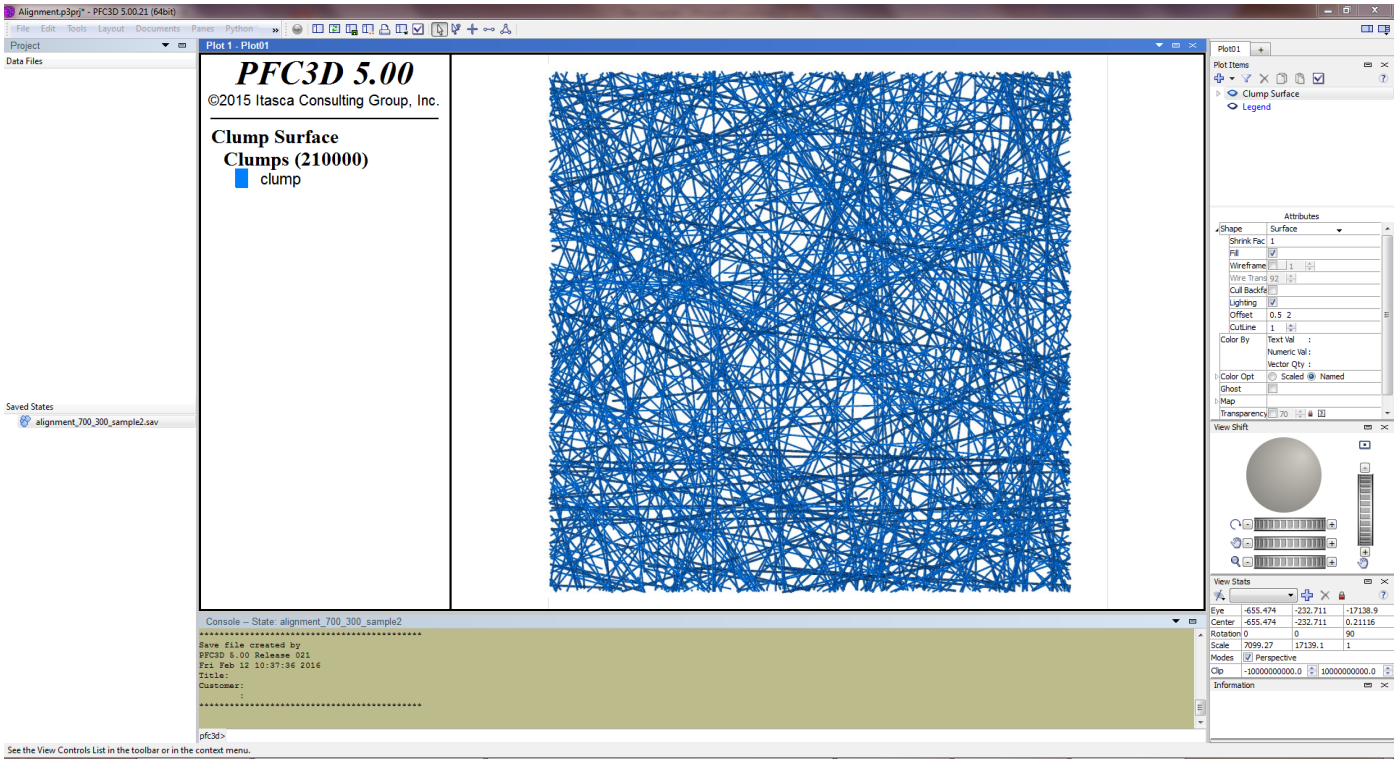
(a) MD setup used to compute the relaxation time of two crossed (10,10) CNTs each 30 nm in length. (b) mDEM setup used to calibrate the crossing relaxation at the mesoscale. The purple lines indicate the vdW contacts between distinct elements.

Table 1
Computed zipping relaxation time of two crossed (10,10) CNTs each 30 nm in length. In the mDEM simulation results of the last two columns, we selected $\alpha = 0.4$.

Crossing Angle	Zipping time (ps)		
	MD	mDEM $\gamma = 0.12$ (pN s/m)	mDEM $\gamma = 0$
30°	50	55	40
45°	140	144	118
60°	220	216	180

Y. Wang et al. Mesoscopic friction and network morphology control the mechanics and processing of carbon nanotube yarns. Carbon 139 (2018) 94-104.

mDEM Simulations of CNT Networks



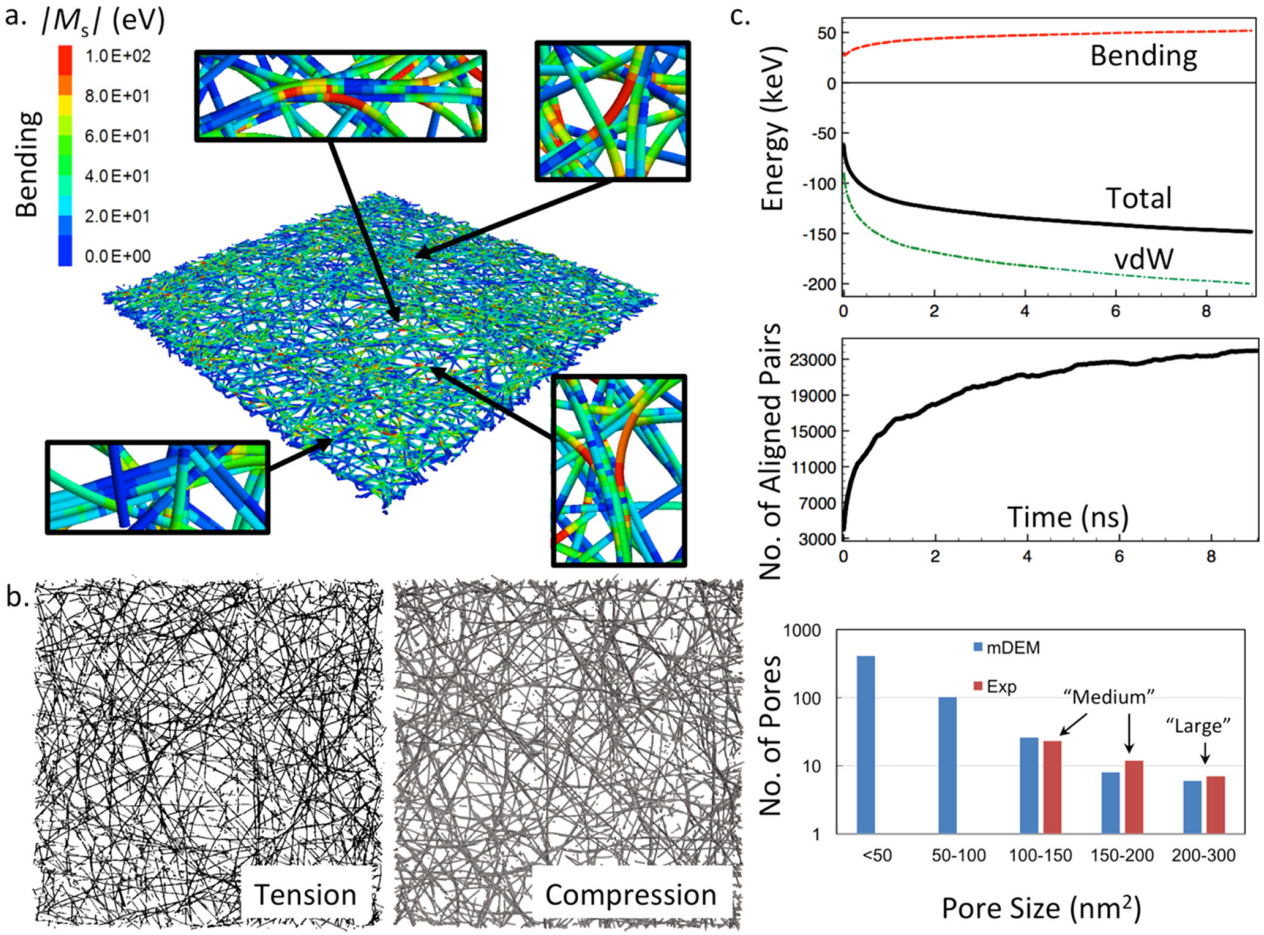
The PFC3D Modeling Interface showing a CNT thin film with dimension: 1000 nm *1000 nm* 11 nm

- Number of CNTs: 350
- Length of individual CNT: 475 nm (350 elements)
- Number of distinct element: 122,500

6 x

Processor: Core™ i7-6700K Quad-Core 4.2 GHz 64 GB DDR4
Graphics Card: GeForce® GTX 970 SuperClocked ACX 2.0 1165-1317MHz, 4GB GDDR5 7010MHz
Liquid Cooling: CPU Liquid Cooling Kit, Single Loop, 360mm Single Radiator

mDEM Simulations of CNT Network Relaxation



(a) mDEM-simulated SWCNT network, measuring 500 nm × 500 nm × 11 nm in size, after relaxation. The color reflects the magnitude of the bending moments stored by the parallel contact bonds. The callouts detail the entangled structure of SWCNT bundles and bent SWCNTs. (b) Force chains (tension and compression) and pore size distribution in the relaxed SWCNT network. (c) Energy and number of aligned pairs during the network relaxation process.

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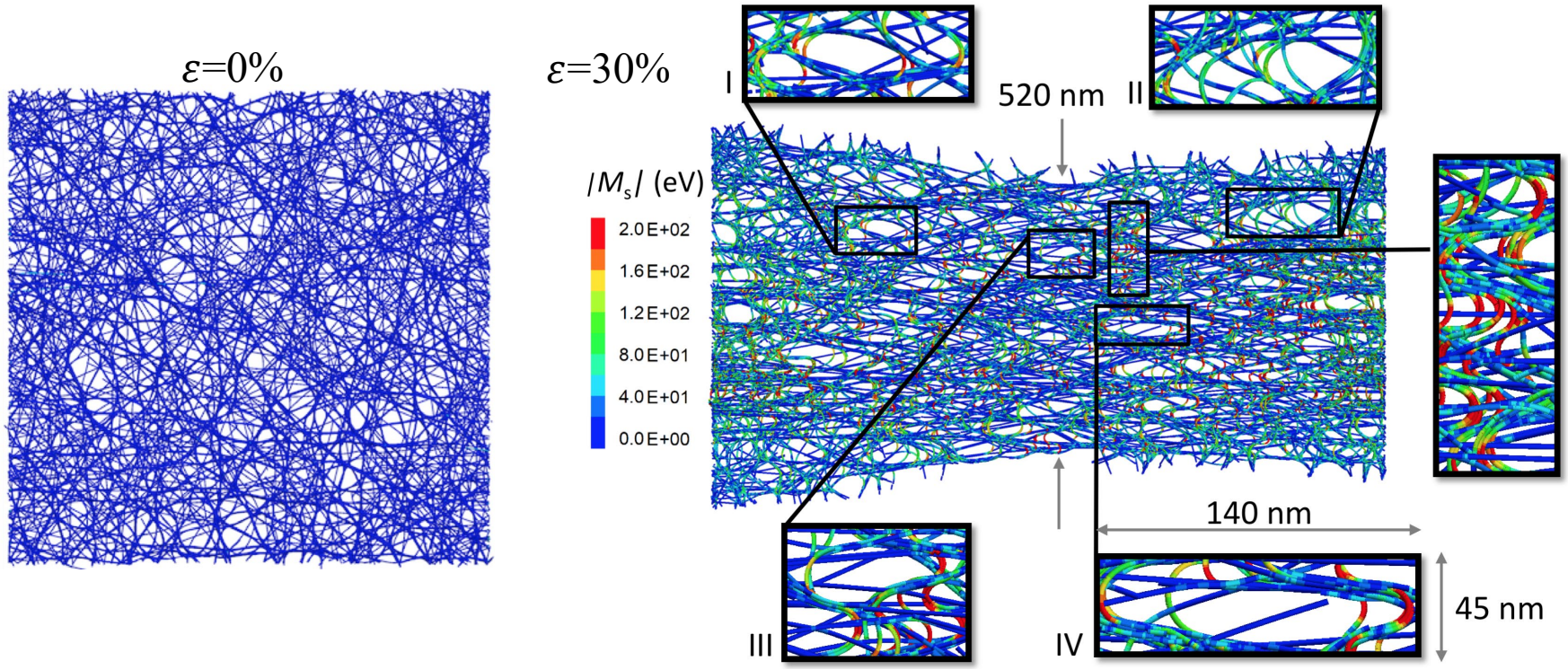
DOI: 10.1021/acsami.7b01434

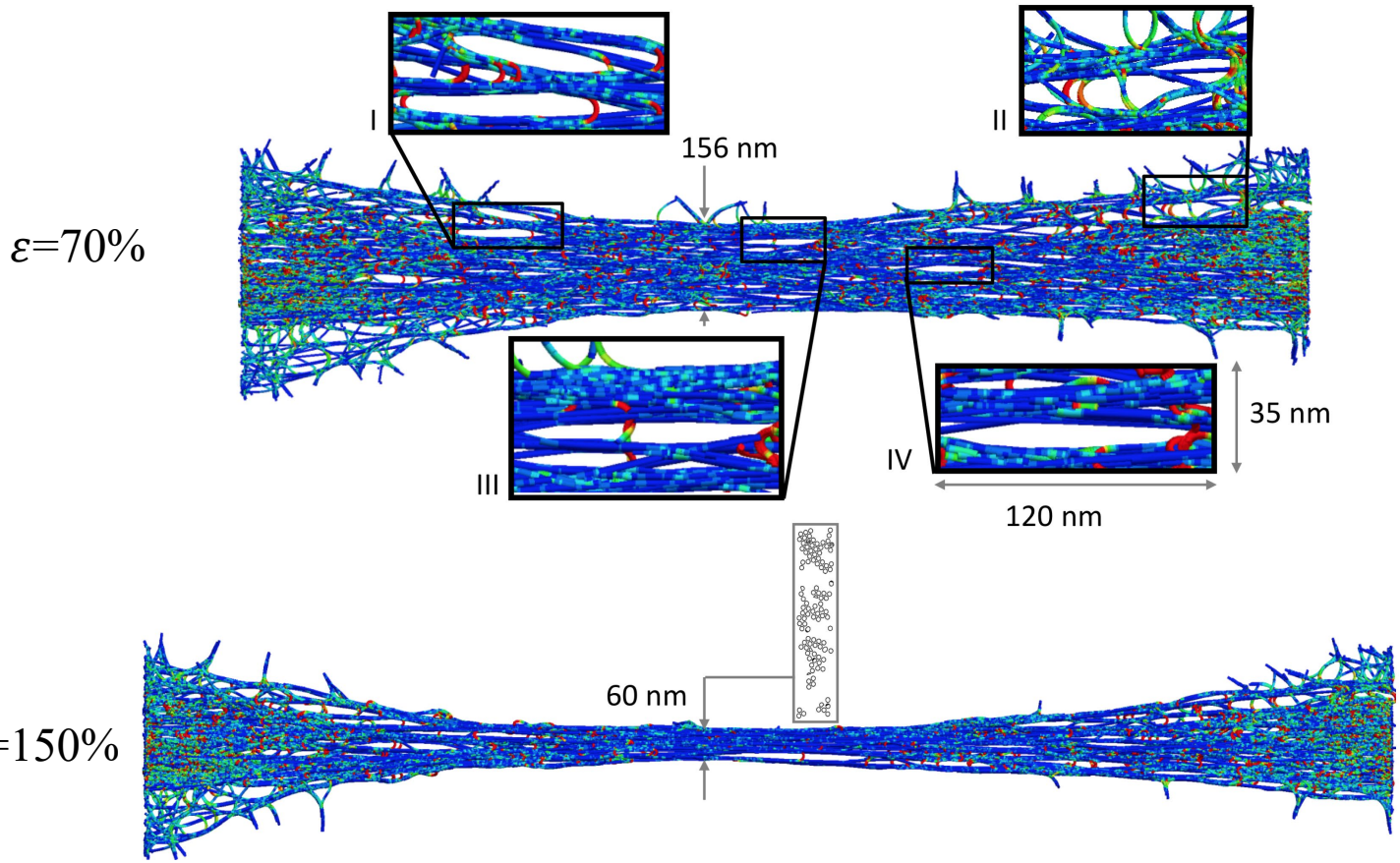
mDEM Simulations of CNT Networks In Tension



The 1000 nm x 1000 nm x 11 nm CNT network under axial strain. Color gives the magnitude of the bending moments stored by the parallel bonds. The callouts detail the structure around selected pores. The length of each CNT is 950 nm. Here γ=0.12 pN s/m (phononic friction).

Y. Wang et al. Mesoscopic friction and network morphology control the mechanics and processing of carbon nanotube yarns. Carbon 139 (2018) 94-104.

mDEM Simulations of CNT Networks In Tension Leading to Yarn Formation



The 1000 nm x 1000 nm x 11 nm CNT network under axial strain. Color gives the magnitude of the bending moments stored by the parallel bonds. The callouts detail the structure around selected pores. The length of each CNT is 950 nm. Here γ=0.12 pN s/m (phononic friction).

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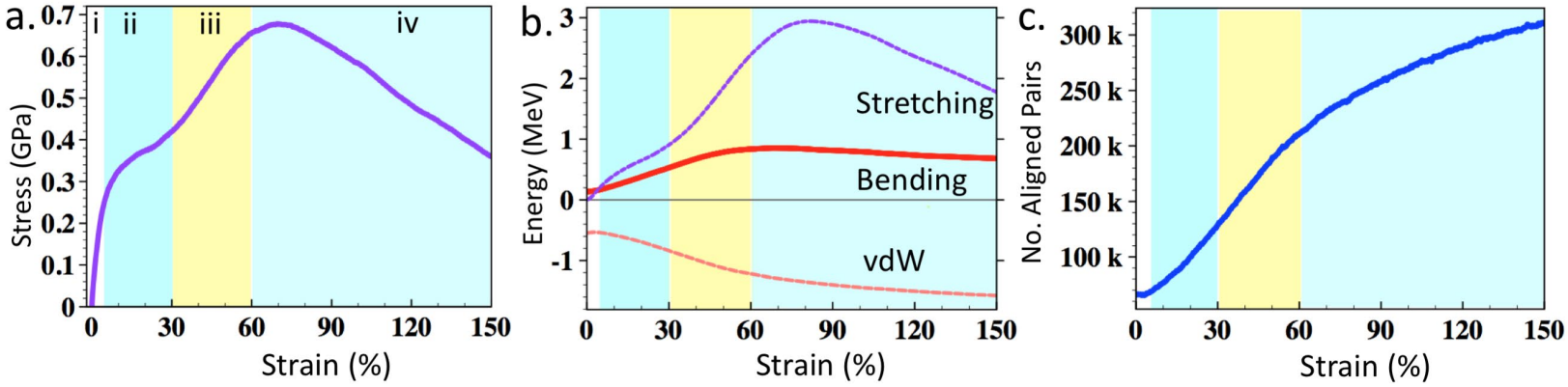
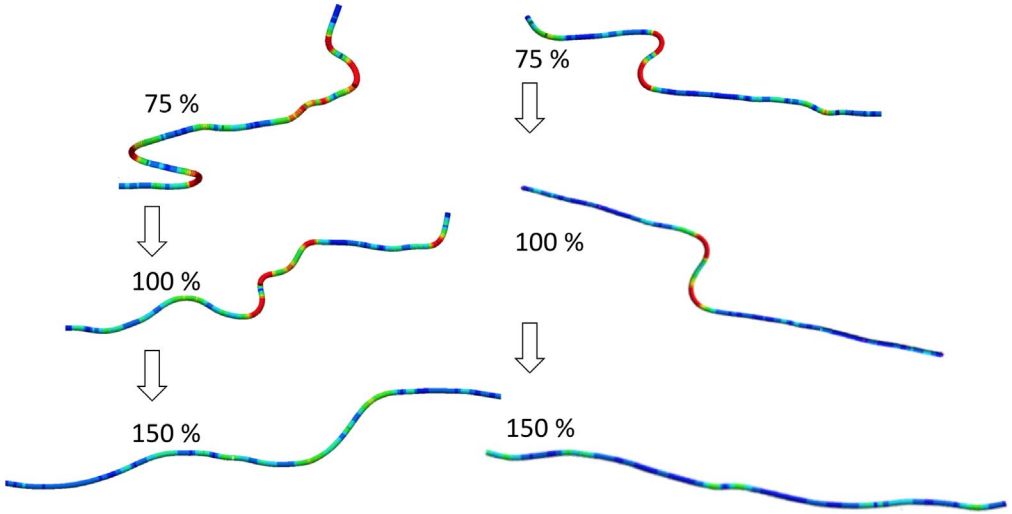
mDEM Simulations of CNT Networks In Tension



(a) Engineering stress, (b) energy, and (c) number of aligned distinct element pairs, vs. strain.



Two CNTs during horizontal network stretching, showing the removal of waviness

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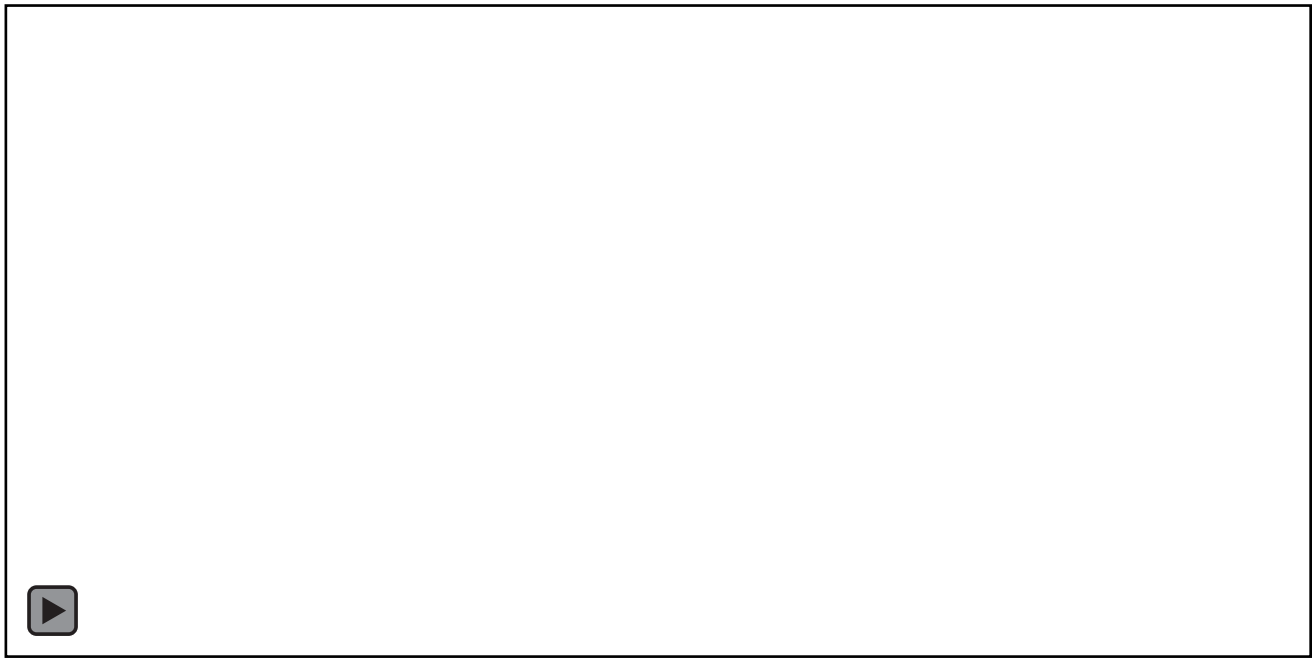
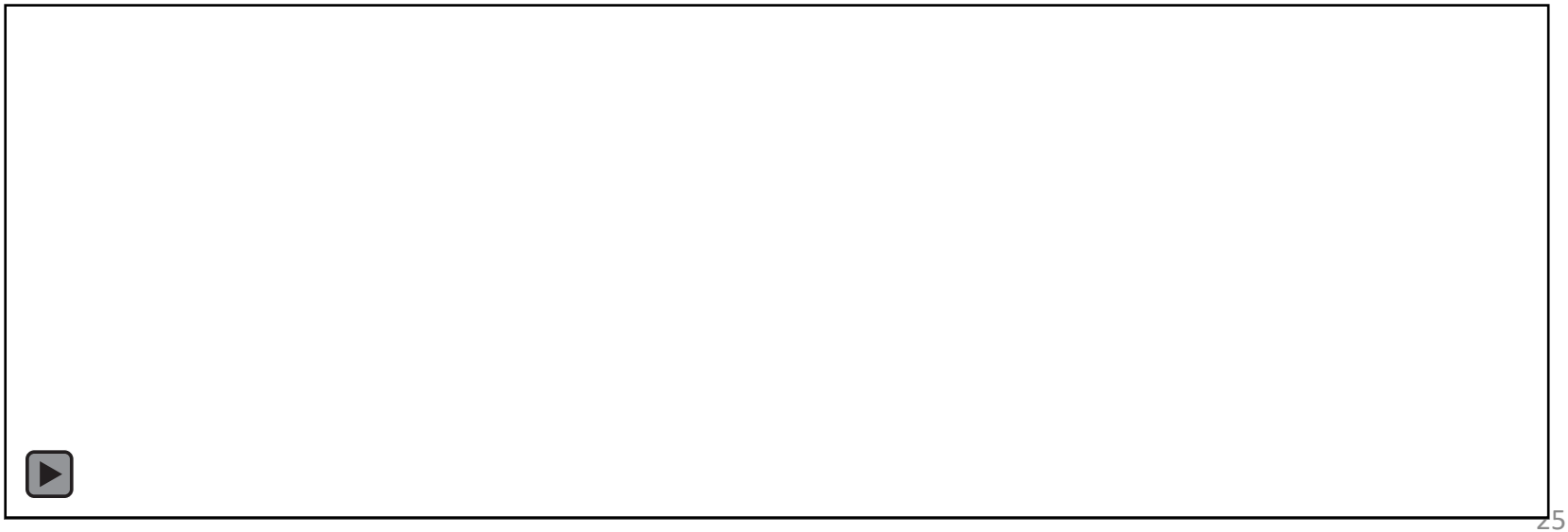
mDEM Simulations of CNT Networks In Tension

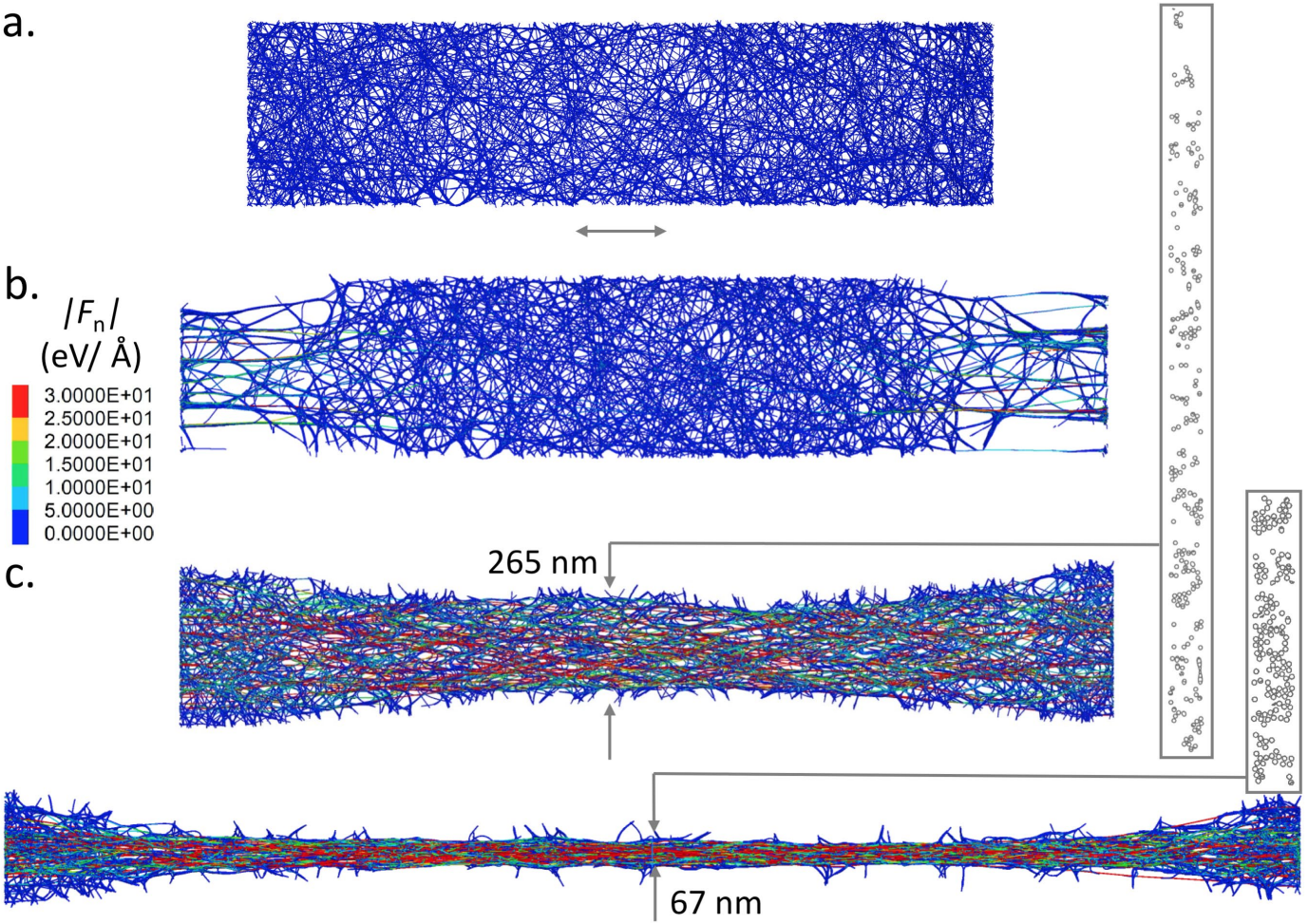


No Friction

With Friction

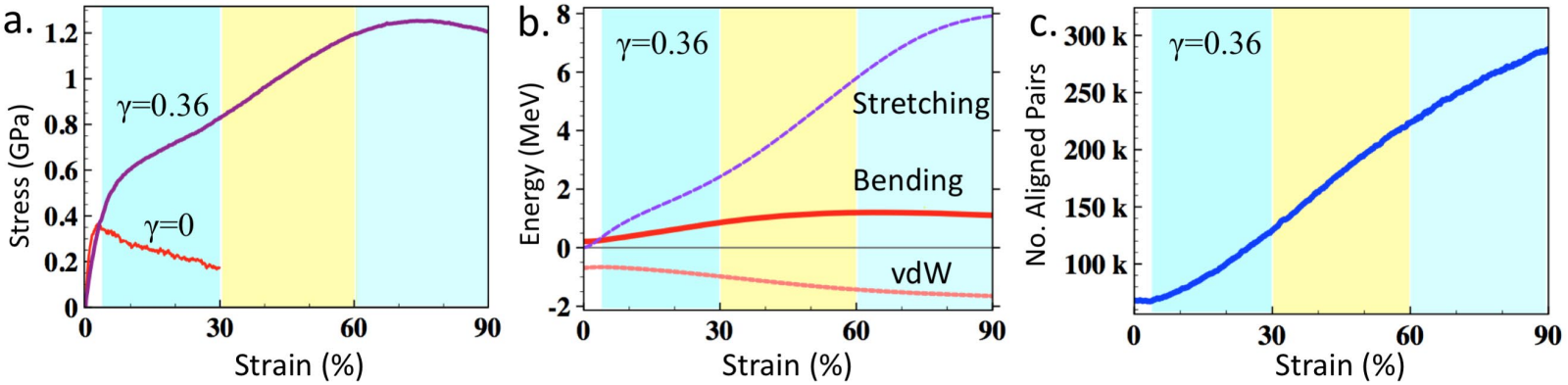


mDEM Simulations of CNT Networks In Tension

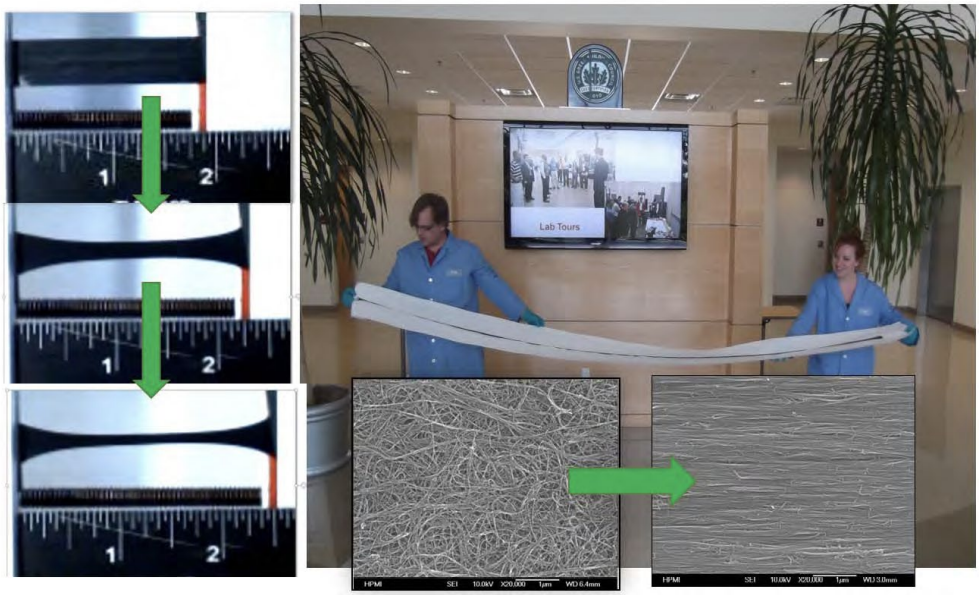


(a) mDEM relaxed CNT ribbon, measuring 2000 nm x 500 nm x 11 nm in size. (b) The ε =30 % ribbon. The double arrow indicates the ε direction. Friction was not accounted for (i.e., γ=0). (c) ε =30 % (top) and ε =90% (bottom) ribbon. Here, γ=0.36 pN s/m. Color reflects the magnitude of the normal force stored by the parallel bonds. The callouts detail the yarn packing.

mDEM Simulations of CNT Networks In Tension



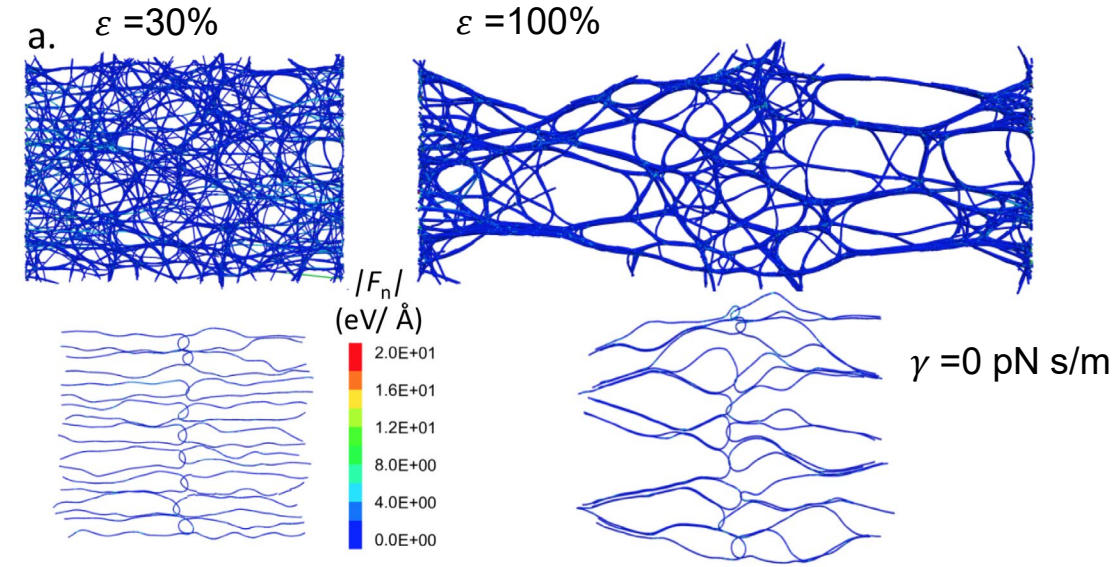
(a) Engineering stress, (b) energy, and (c) number of aligned distinct element pairs, vs. ε. The shadings mark the four contiguous regimes (i-iv) occurring during the stretching of the preequilibrated CNT ribbon. The units for γ are pN s/m.

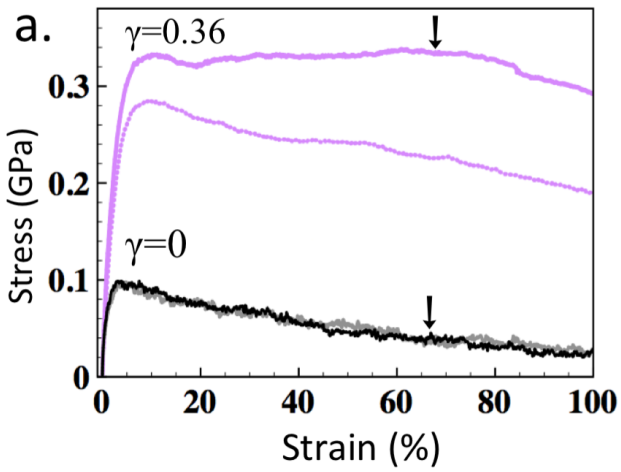


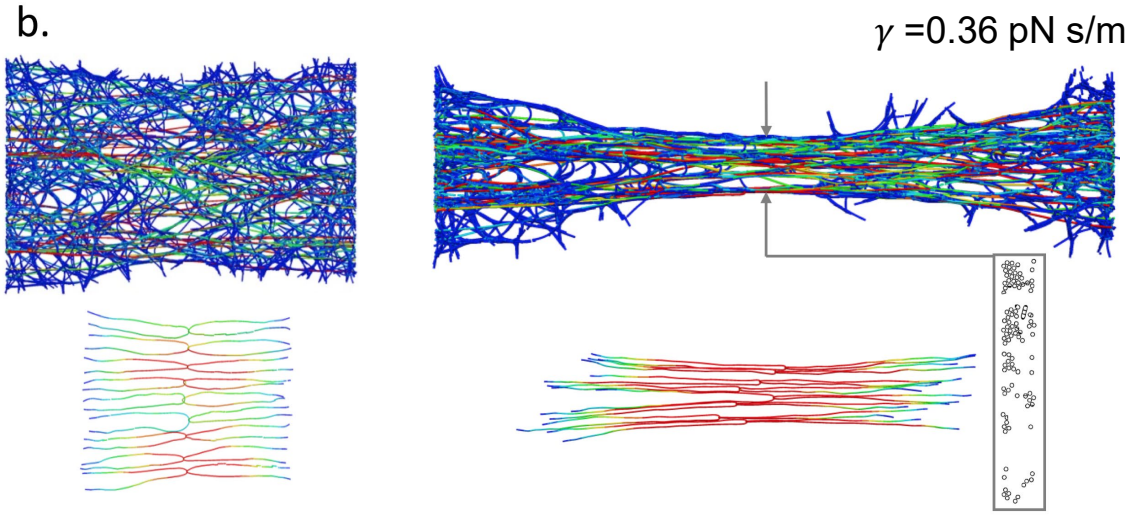
Mechanical stretching process to produce a highly aligned CNT tape. Florida State.

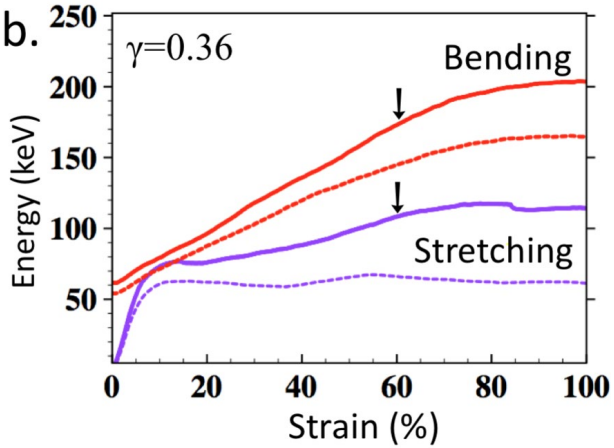
mDEM Simulations of CNT Networks In Tension

Role of Entanglement and Mesoscopic Friction





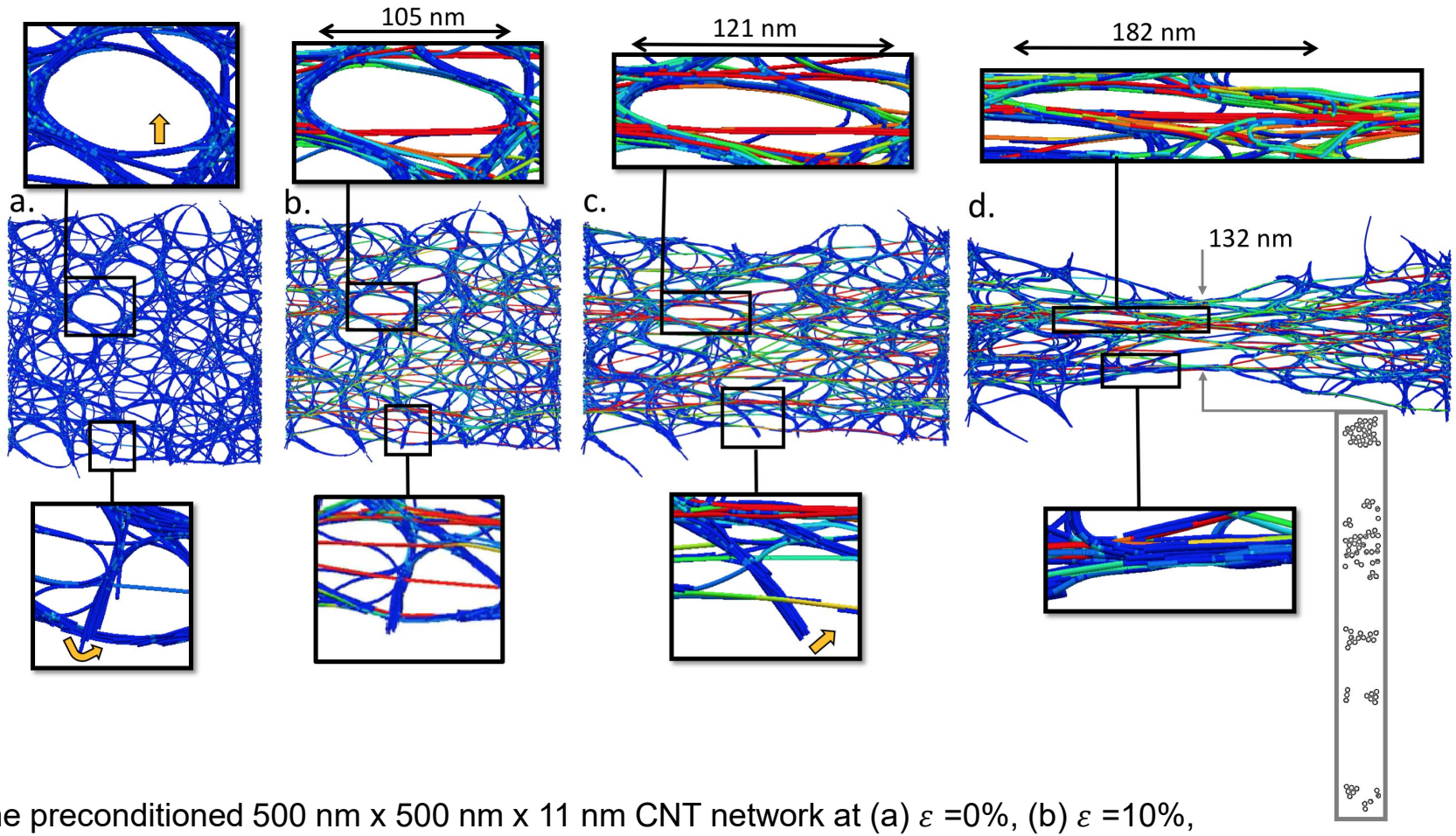




The 500 nm x 500 nm x 11 nm CNT network with added hooked rackets.

mDEM Simulations of CNT Networks In Tension

Role of the Network Morphology



The preconditioned 500 nm x 500 nm x 11 nm CNT network at (a) ε =0%, (b) ε =10%, (c) ε =30%, and (d) ε =75%. Color gives the magnitude of the normal force stored by the parallel bonds. The upper callouts detail un-zipping (yellow arrow) followed by zipping. The lower callouts exemplify zipping of bundles (yellow arrows). The yarn packing at ε =75% is also shown.

Conclusions

- **The Distinct Element Method might be the missing method for bridging the atomistic and large scale mechanics of nanofibrous systems**
- **PFC3D code parallelization would aid enormously**
- **Demonstrated the applicability of the method to simulation the stretching of a carbon nanotube network**
- **DEM simulations of the network under stretching reveled the important role of mesoscale friction in obtaining the experimental trends**
- **Ongoing work: CNT bundles with polymeric friction**