Effects of atomic-scale structure on the fracture properties of amorphous carbon – carbon nanotube composites

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Overview

Motivation

- Carbon nanotubes (CNTs) have high specific stiffness and strength
- Composite design with CNTs will be different than for carbon fibers
- New reactive force field ReaxFF can be applied to model fracture

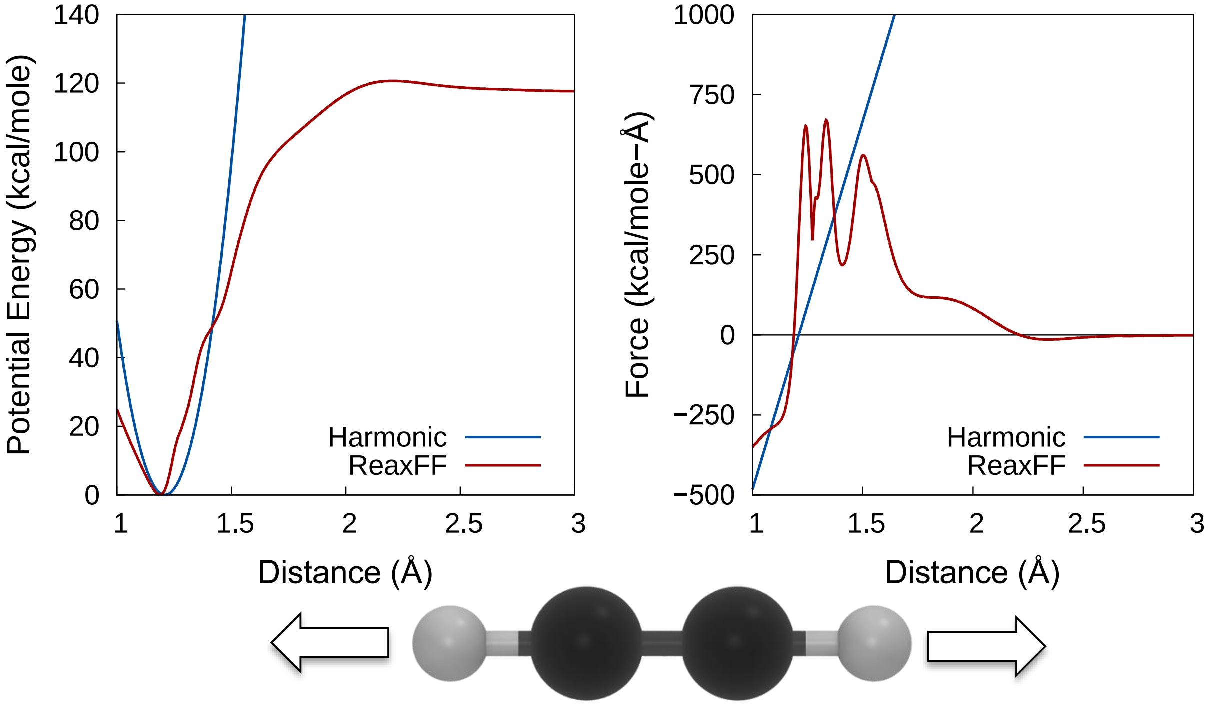
Objectives

1. Estimate maximum CNT composite mechanical properties
2. Compare composite mechanical properties with:
    a. Singlewall vs multiwall CNTs
    b. Dispersed vs bundled CNT arrangements
    c. CNT-matrix crosslinking

Bond breaking with ReaxFF

Molecular dynamics using ReaxFF:

- Allows bond breaking and formation to be modeled
- Multibody interactions via bond order function



Modeling Fracture with ReaxFF

New ReaxFF$_{C\text{-}2013}$ parameterization fitted to:

- Diamond strained in the bulk and <001> direction
- Graphene strained in the bulk and axial directions

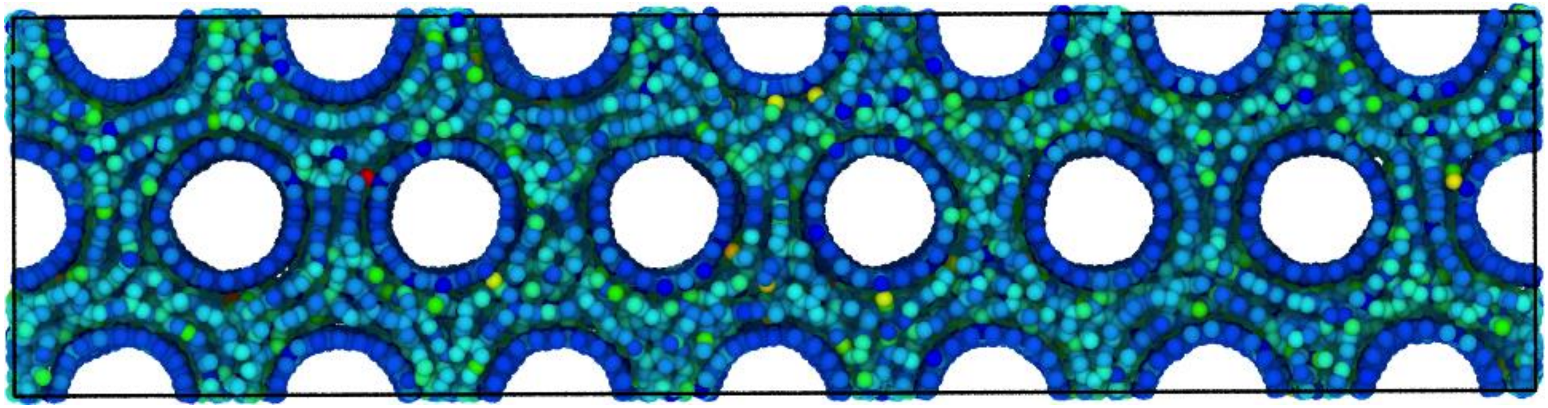
In-house analysis of ReaxFF$_{C\text{-}2013}$[*] mechanical properties of diamond, graphene, amorphous carbon, and CNTs:[**]

- Improved Poisson contraction response
- Elastic and fracture properties improved over previous ReaxFF$_{CHO}$ parameterization

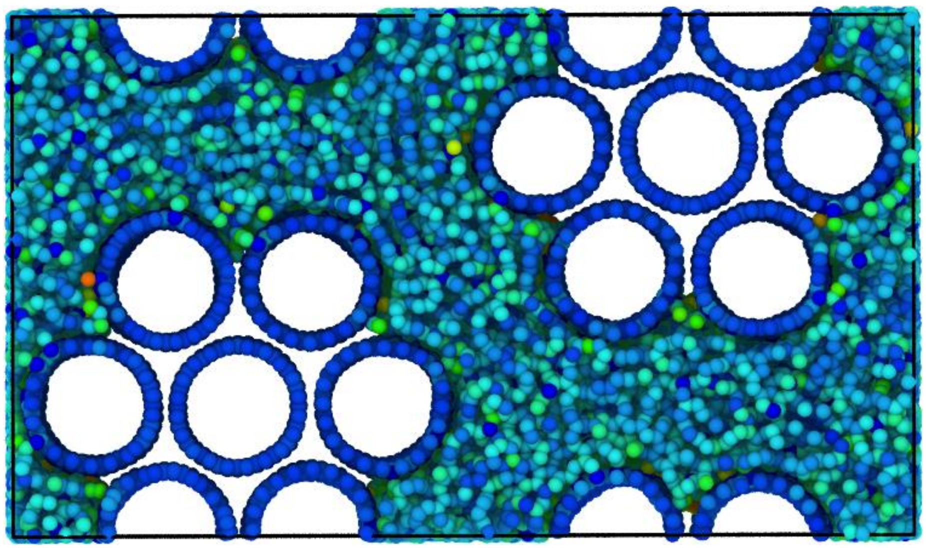
*Goverapet Srinivasan, S.; van Duin, A. C. T.; Ganesh, P., *J. Phys. Chem. A* 2015, 119 (4), 571-580.

**Jensen, B.D.; Wise, K.; Odegard, G.M., *Submitted to J. Phys. Chem A*

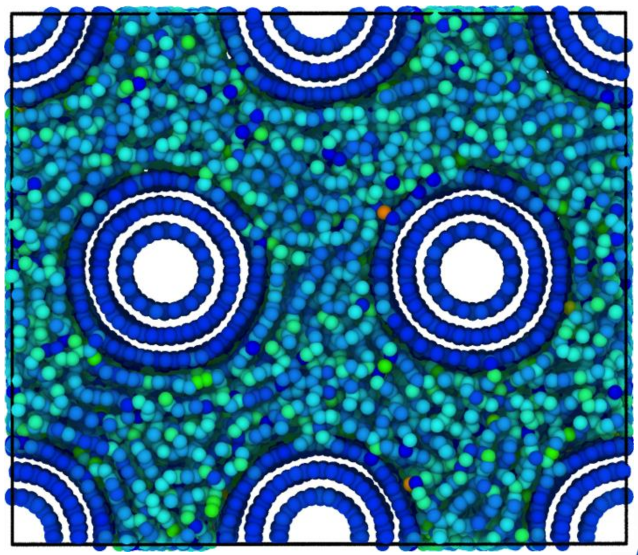
Simulation Setup



SWNT Array



SWNT Bundle



MWNT Array

Simulation Setup

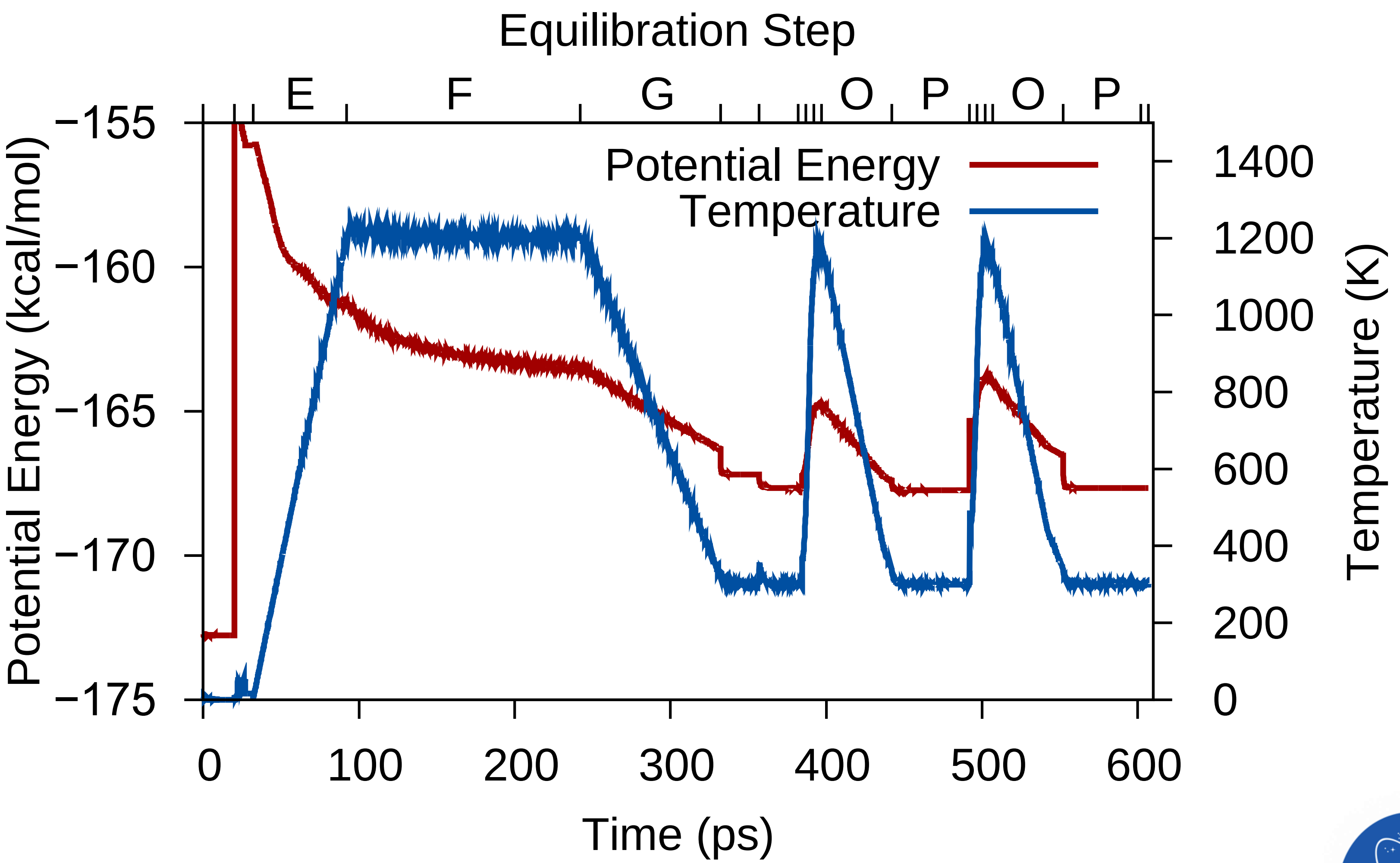
1. Continuous/straight CNTs

2. Amorphous carbon (AC) matrix:
   – Relative simplicity
   – High mechanical properties

3. Three CNT arrangements:
   – SWNT array, MWNT array, SWNT bundle

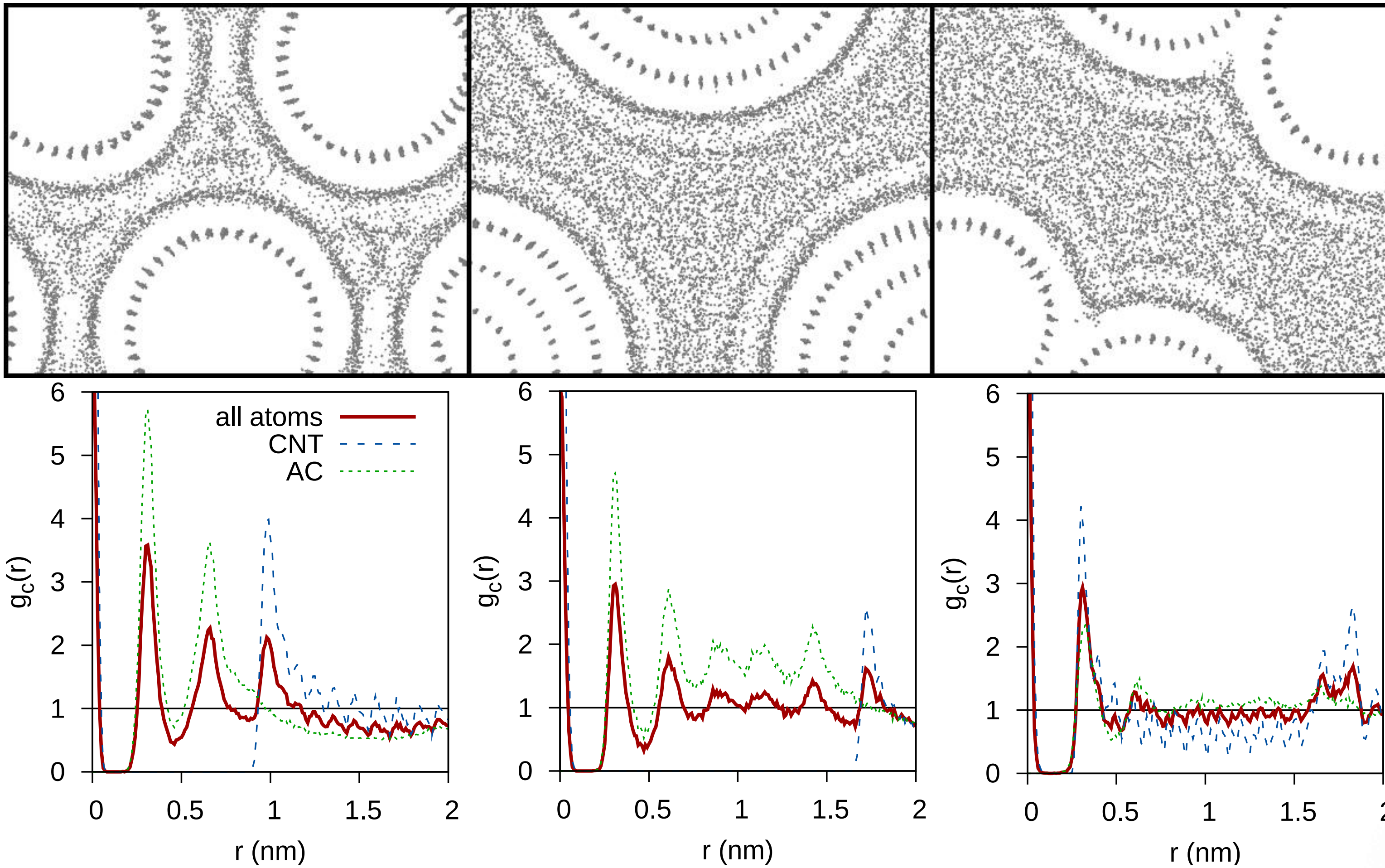
4. Five crosslinking fractions for each system:
   – 0%, 5%, 10%, 15%, 20%

Equilibration Procedure



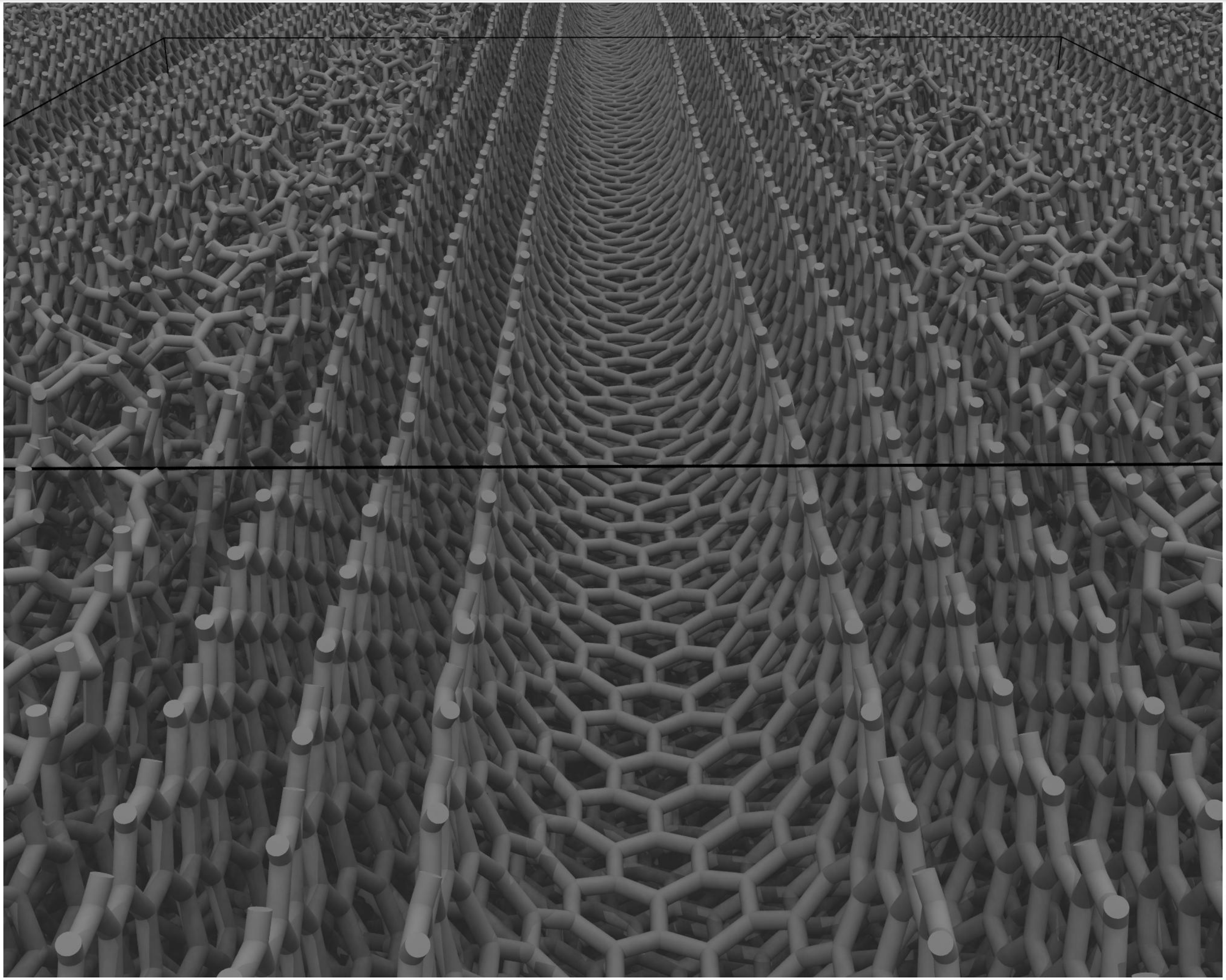
Results

Structuring of amorphous carbon at the CNT interface

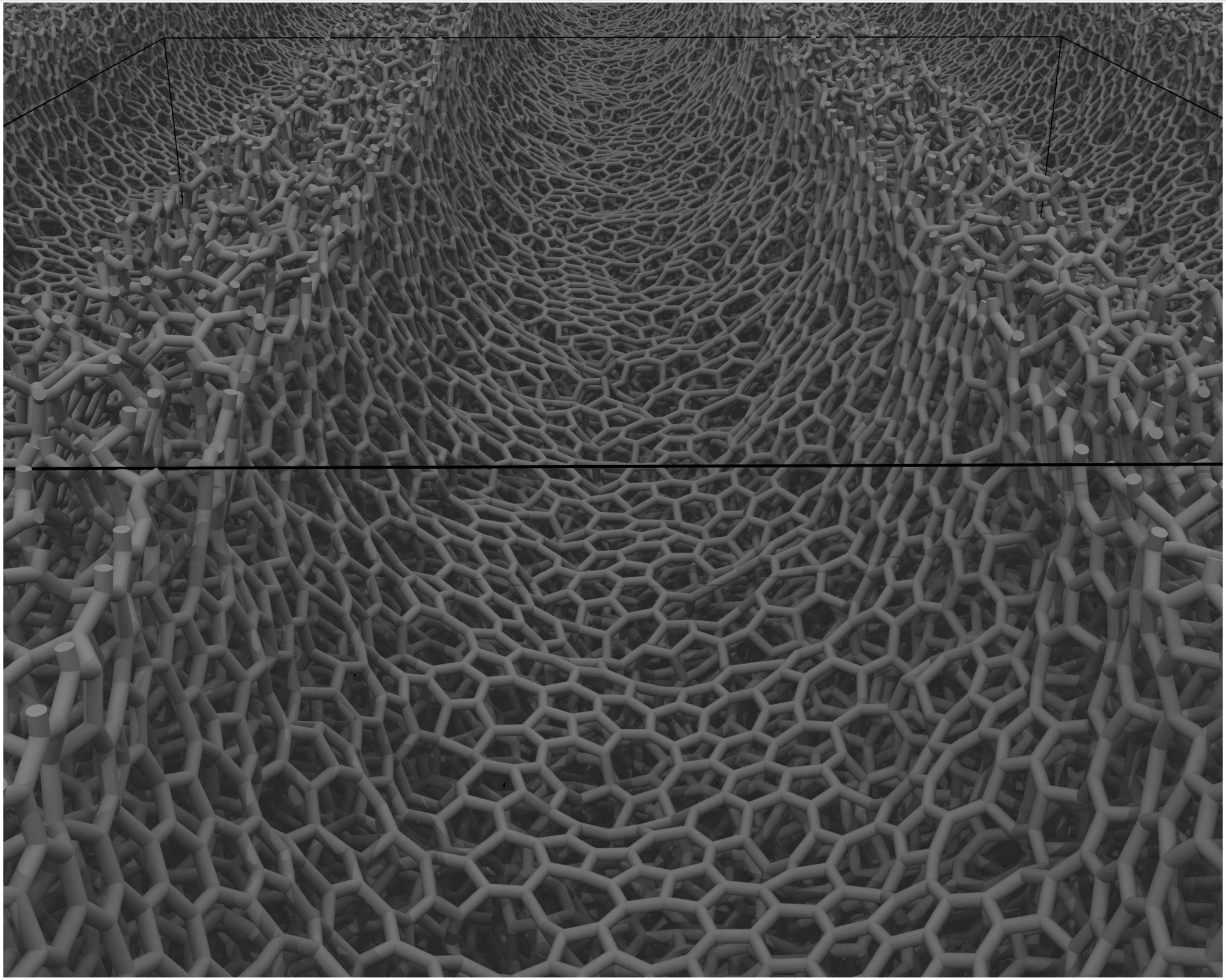


Nanotube-centered cylindrical distribution functions, zeroed at the exterior nanotube wall

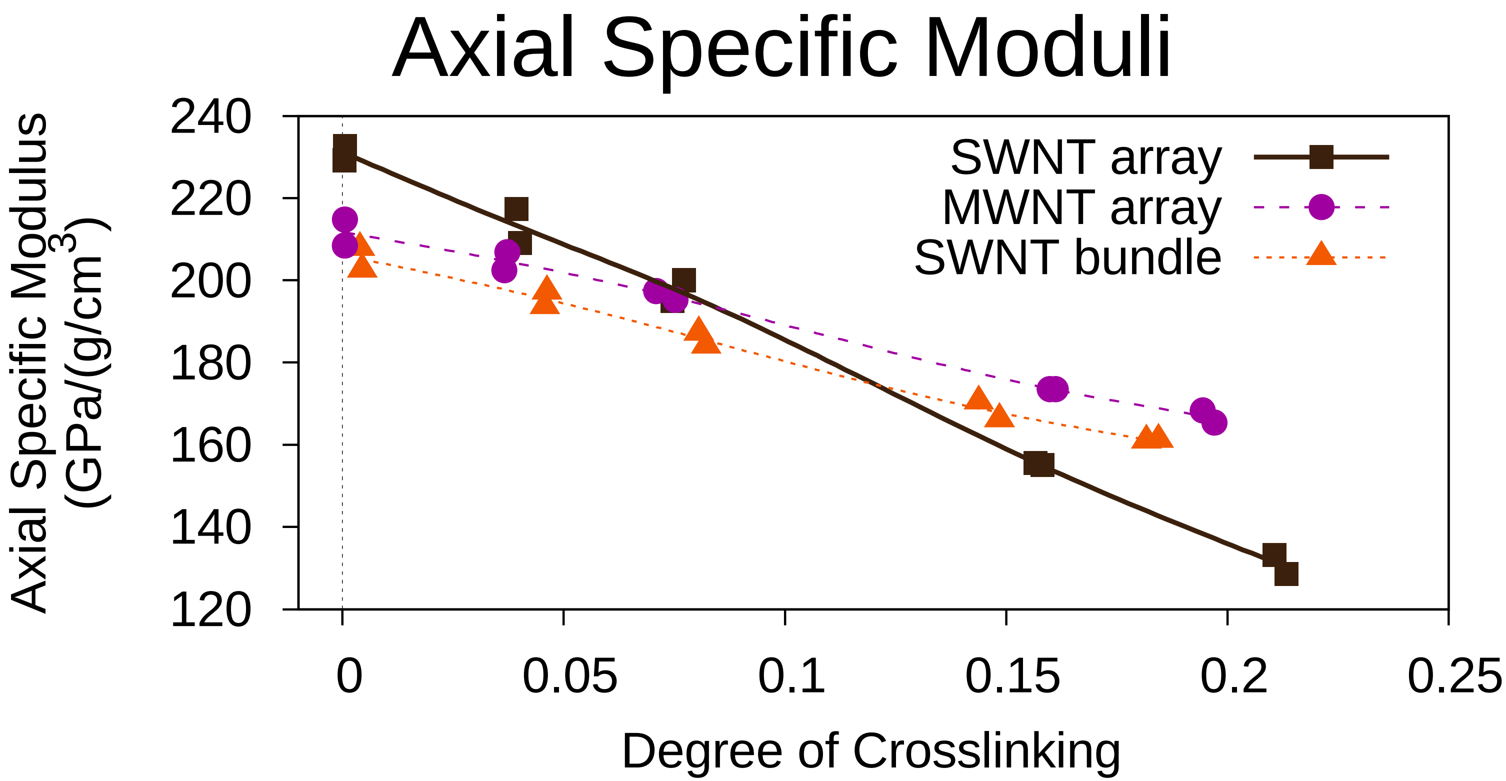
Results



Results

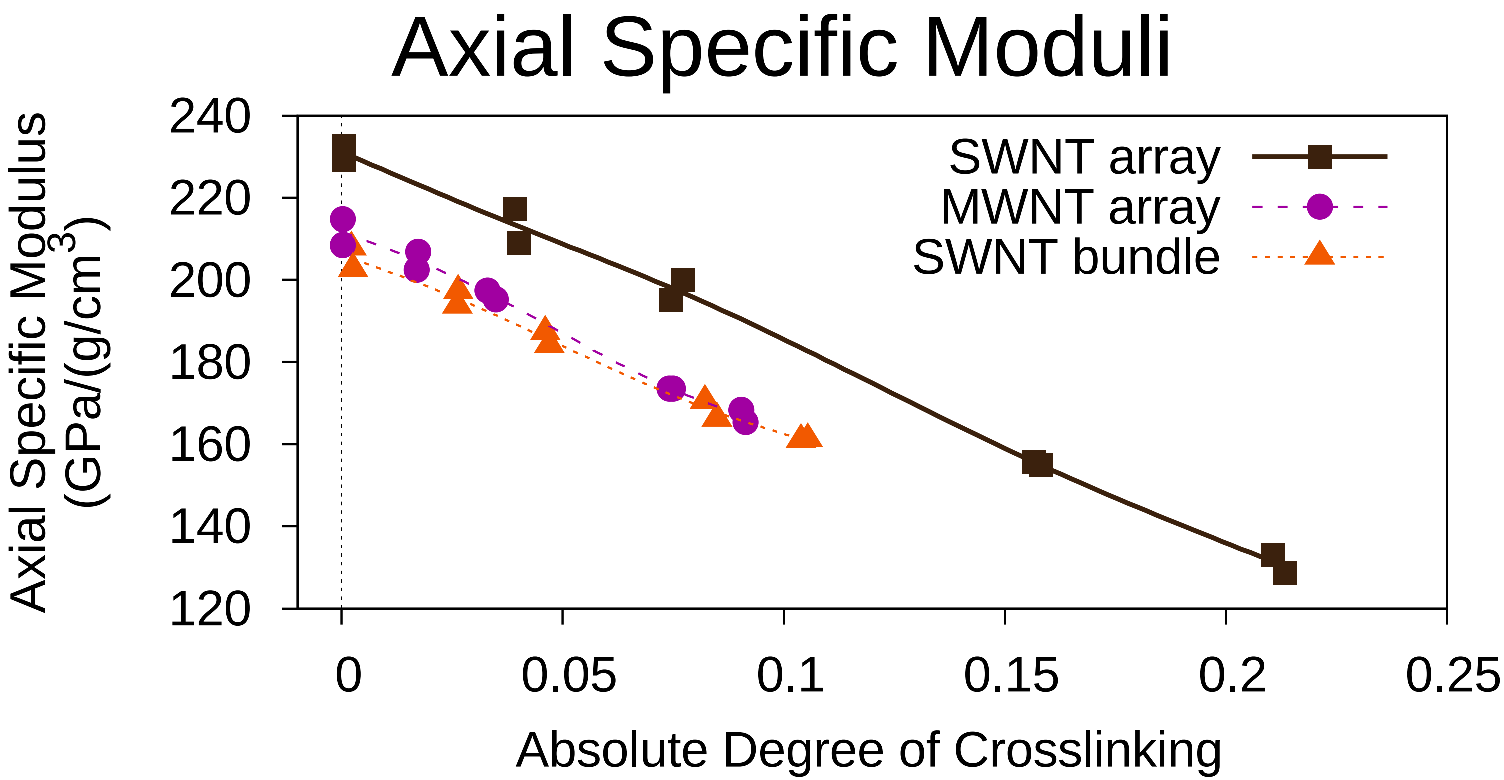


Results



- Templating of the matrix substantially increases the axial modulus
- Dispersion of crosslink sites does not strongly influence axial modulus

Results



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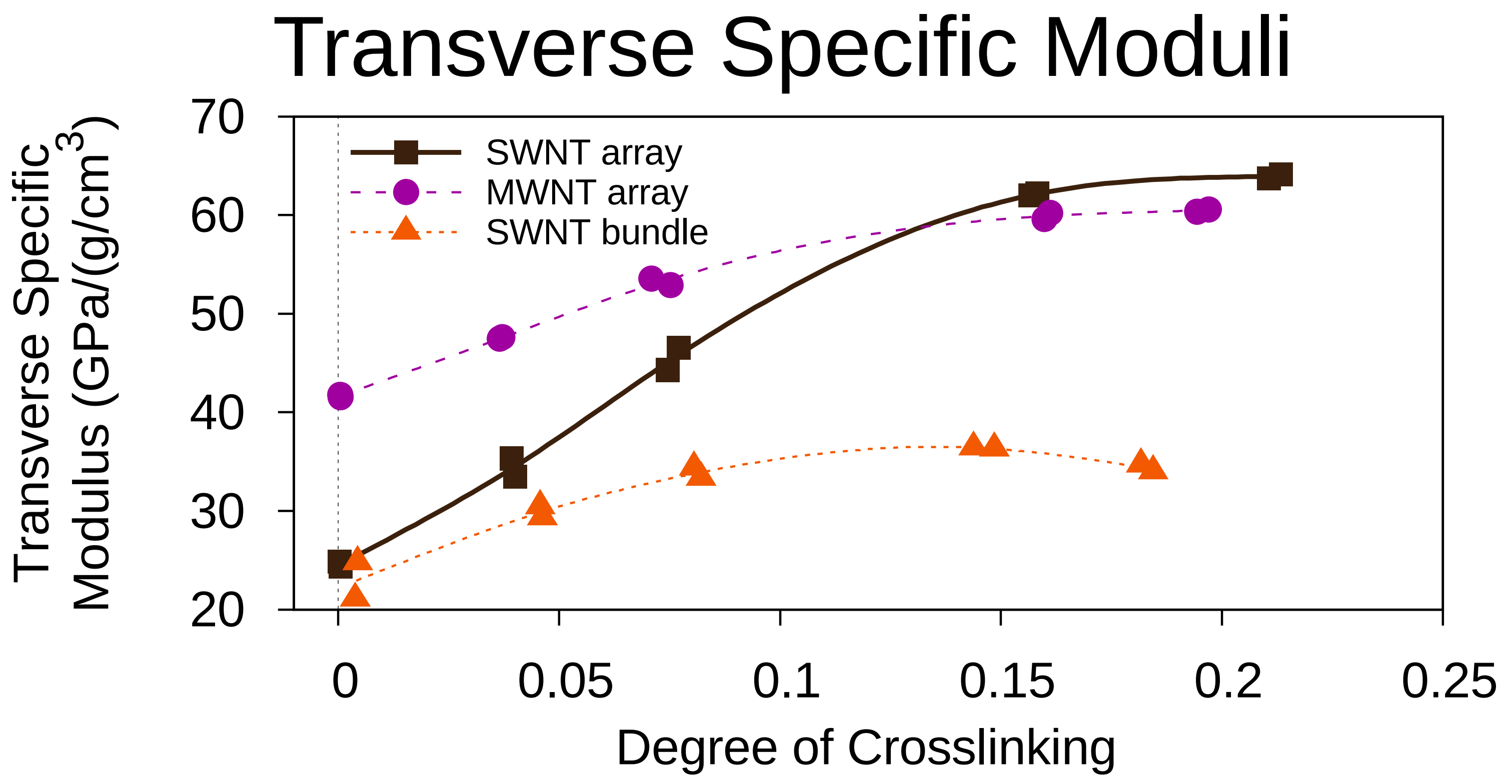
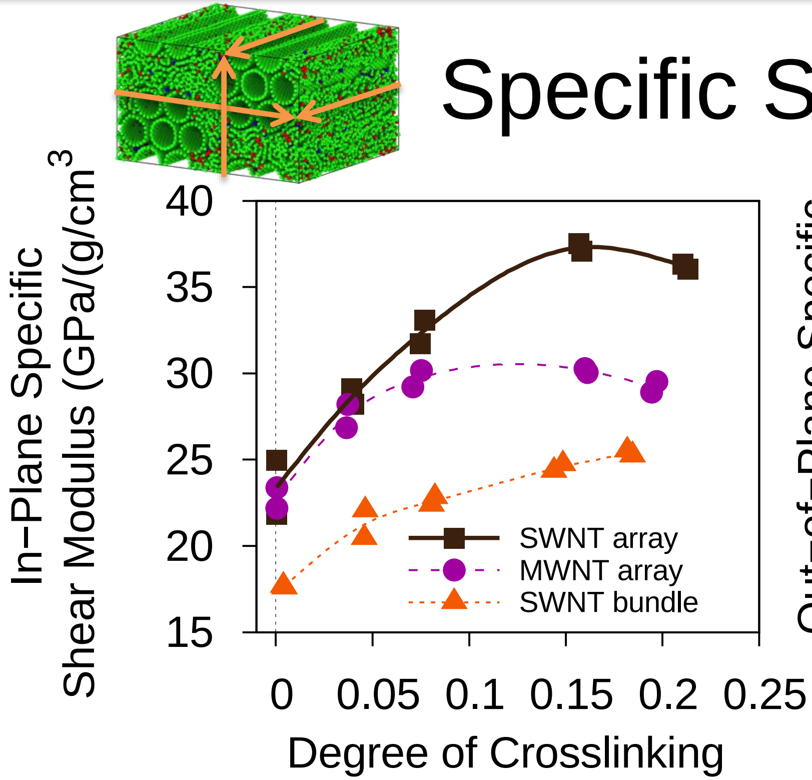
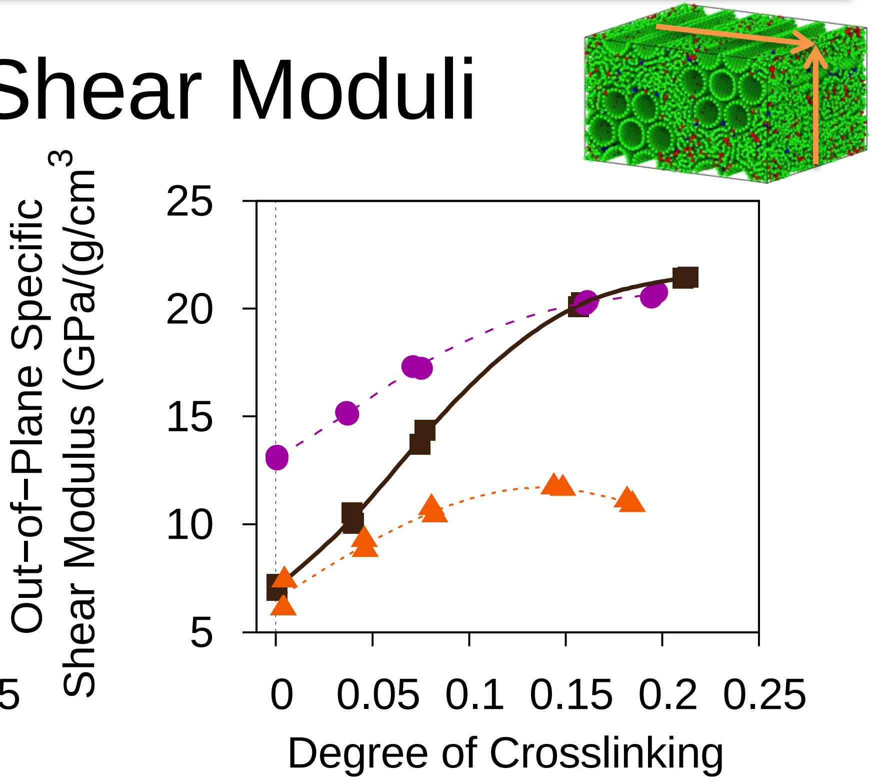


- Multiwalled CNT resists CNT flattening, increasing the transverse modulus
- Lack of crosslinks within the bundle limits effectiveness of crosslinking for transverse stiffness

Results

Specific Shear Moduli

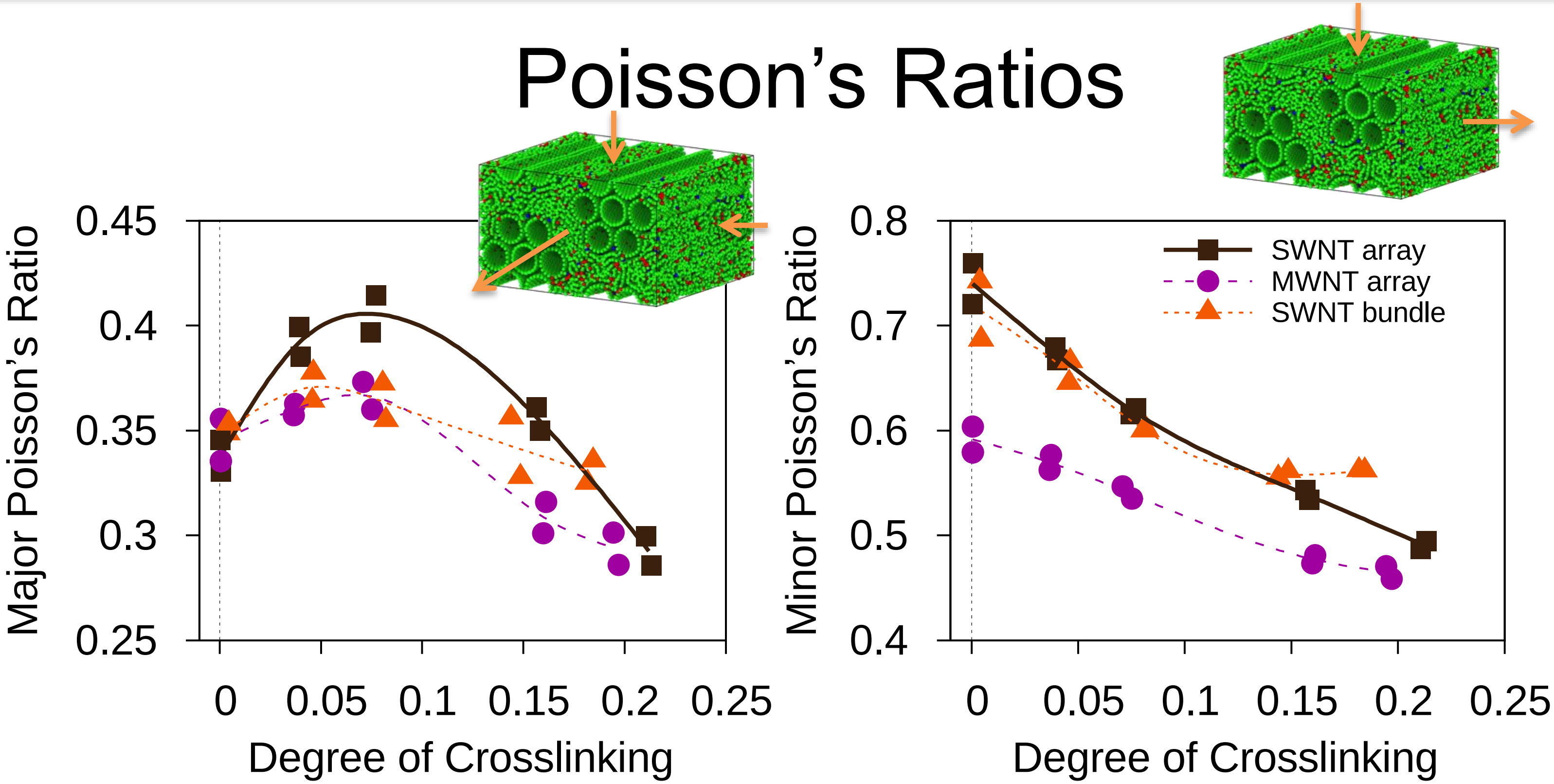




- SWNT bundle system has lowest specific shear moduli in both directions
- Inner MWNT walls reinforce circular shape resulting in higher out-of-plane specific shear modulus

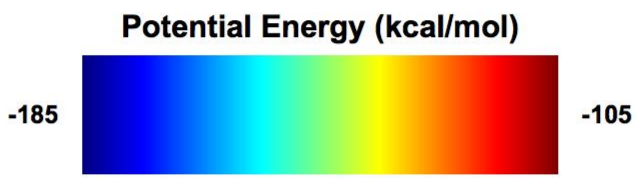
Results

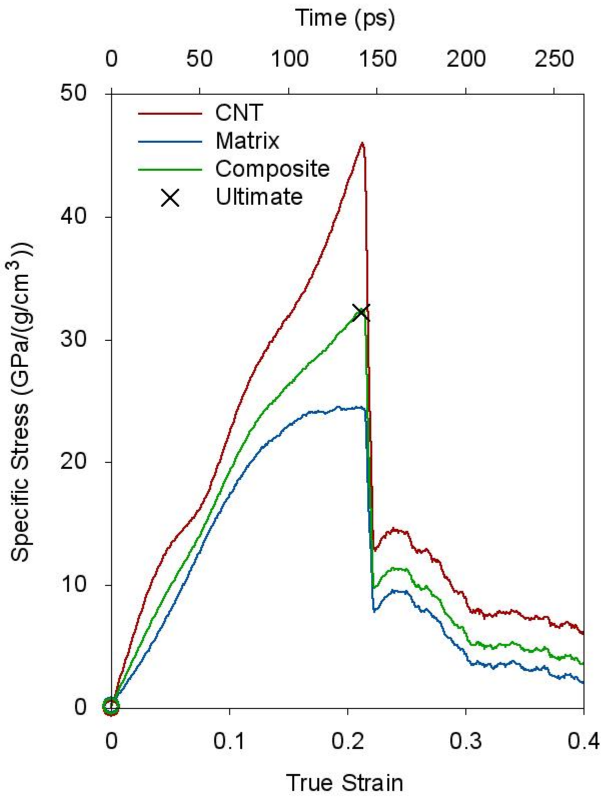
Poisson's Ratios

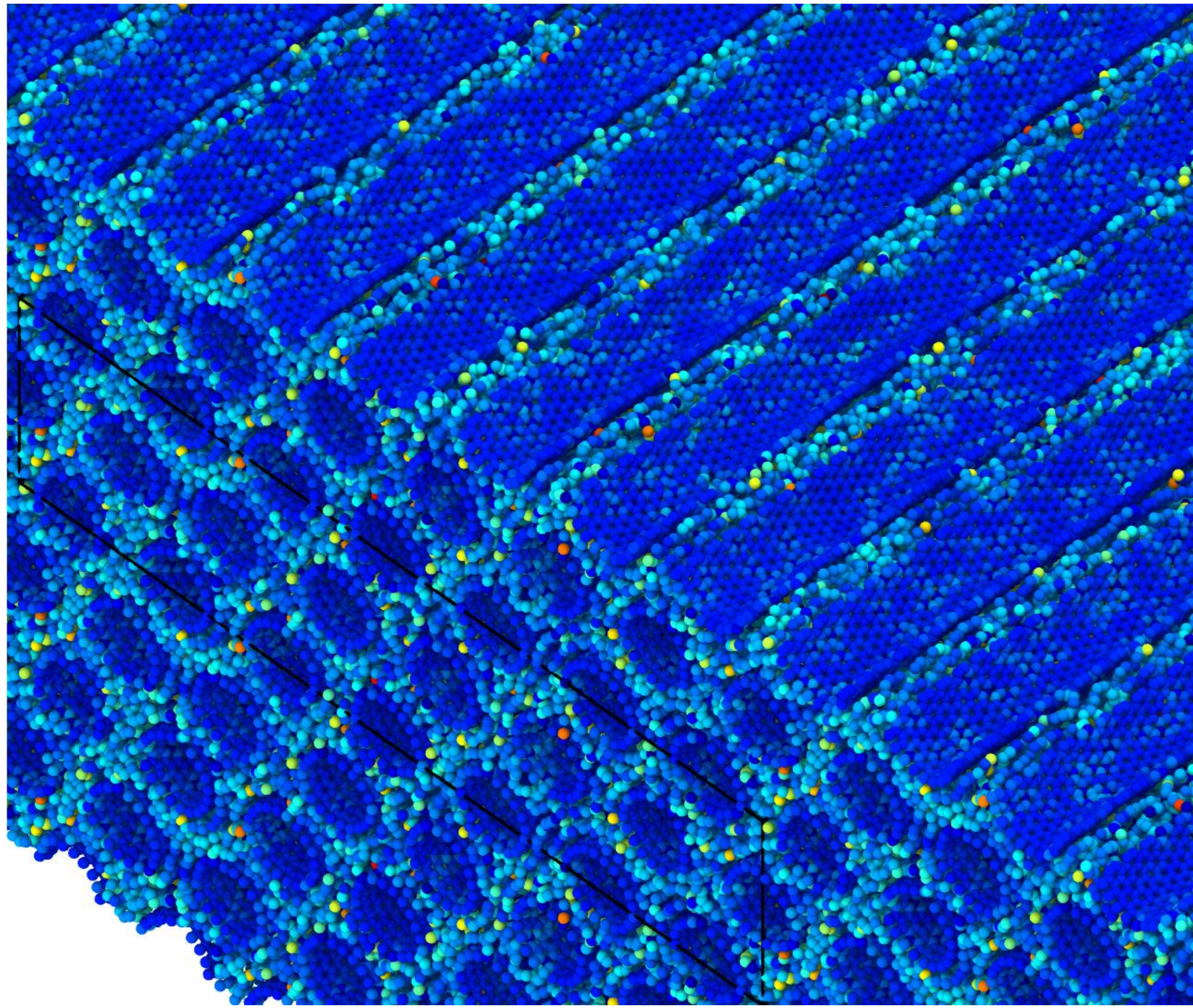


- Major Poisson's ratio largest around 7% crosslinking
- MWNT array resists deformation of the circular cross-section resulting in lower minor ratios

SWNT array axial fracture (9% crosslinked)







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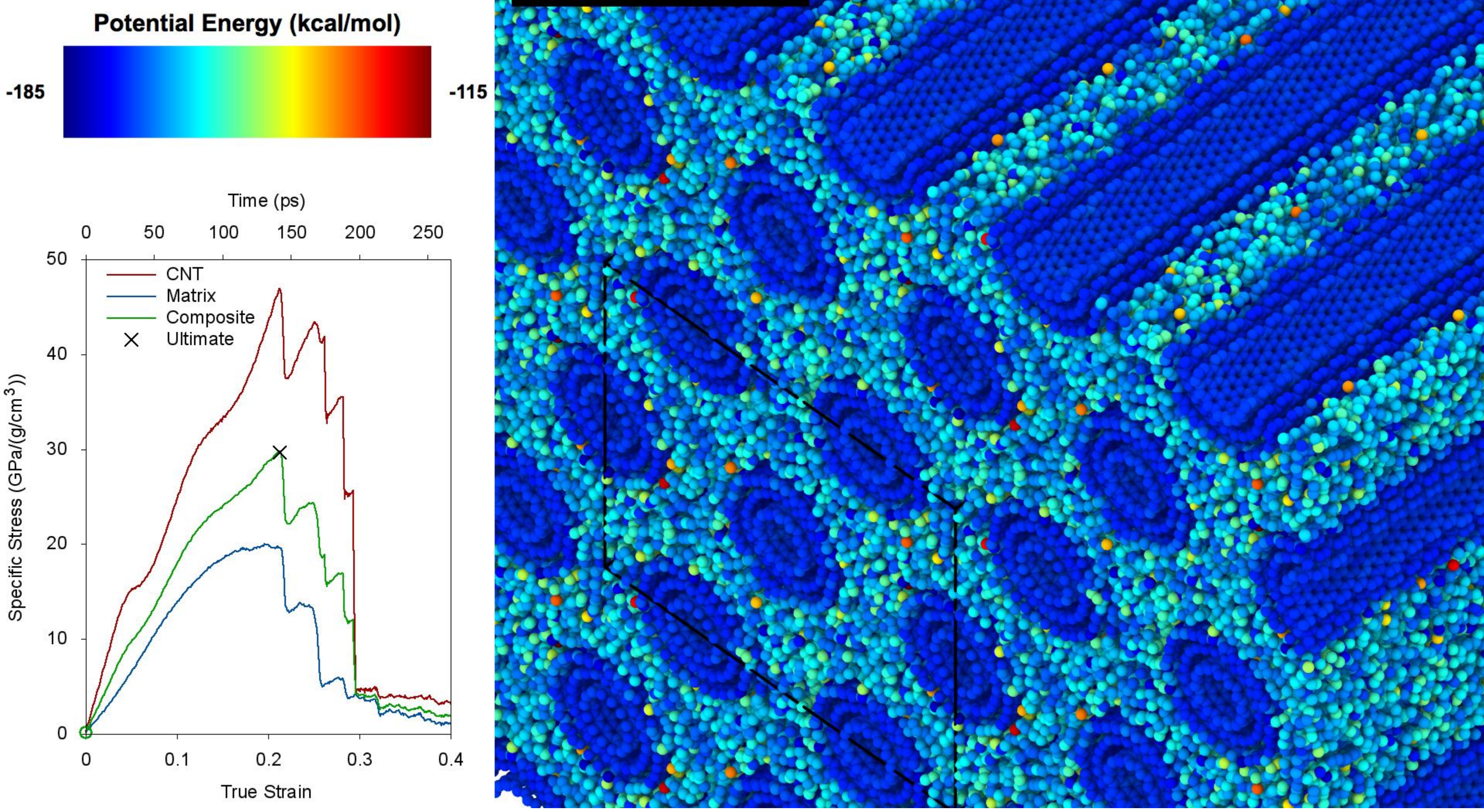
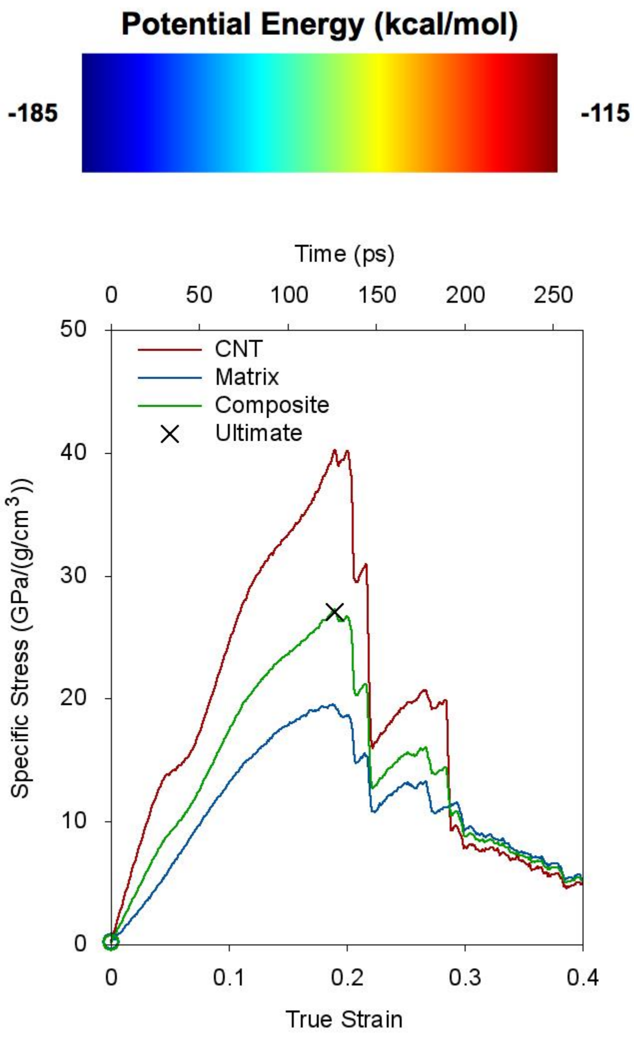
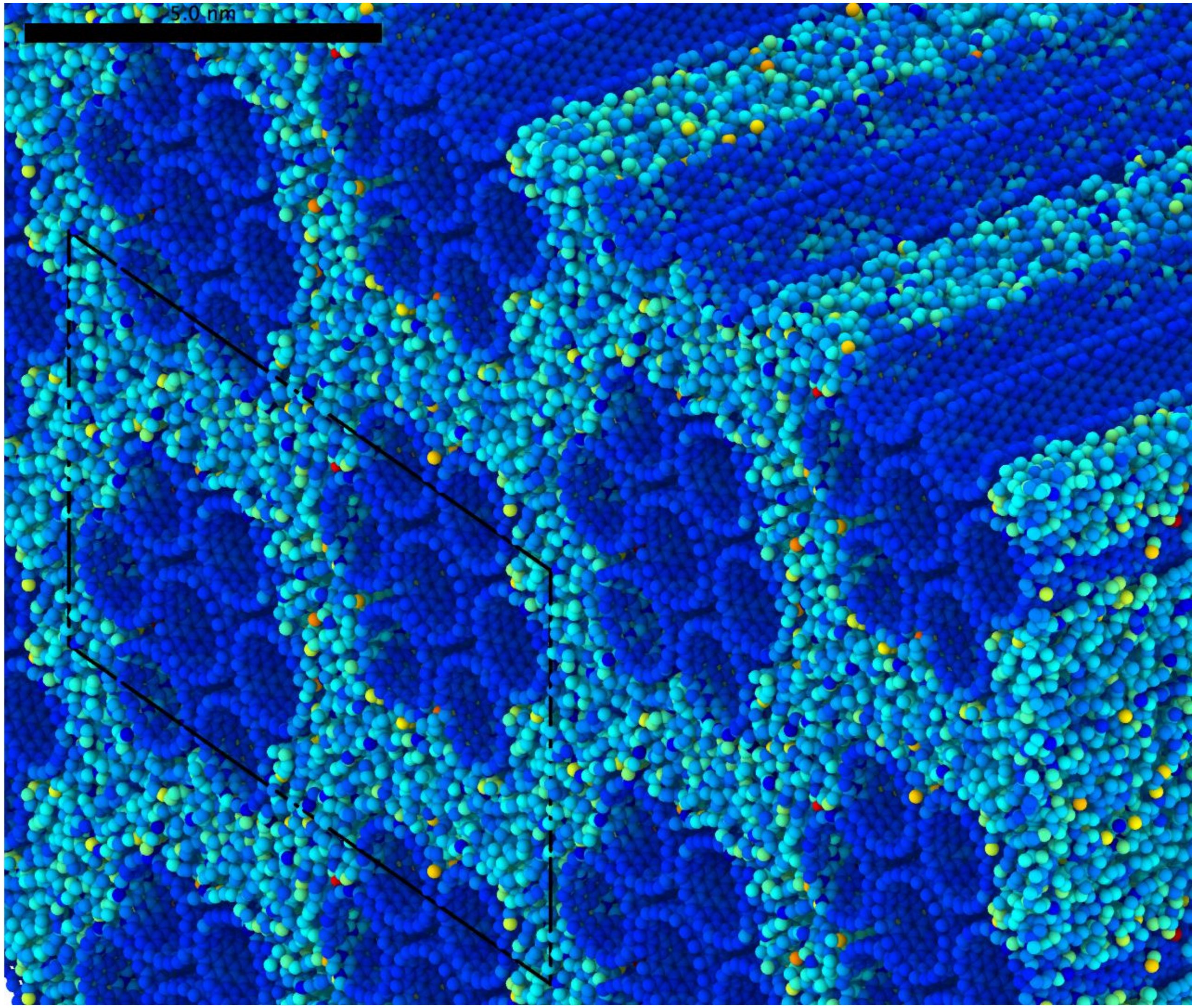


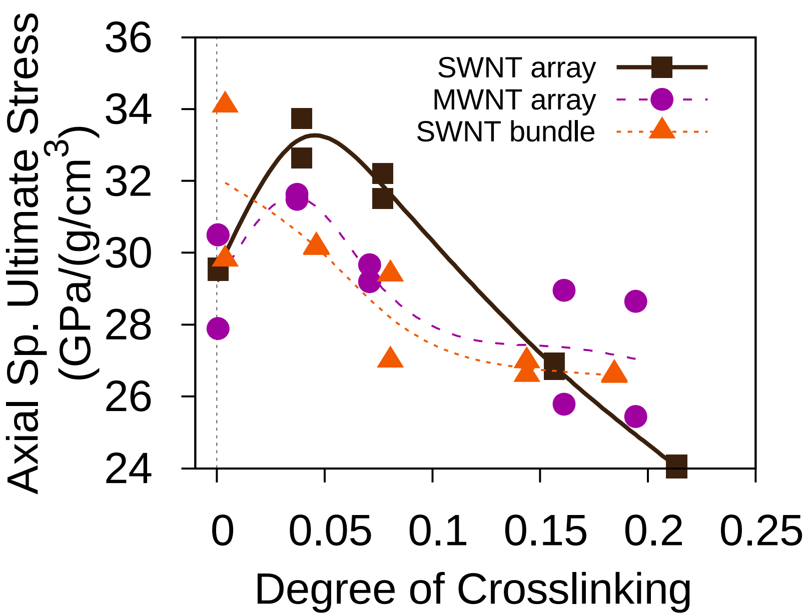
SWNT bundle axial fracture (9% crosslinked)

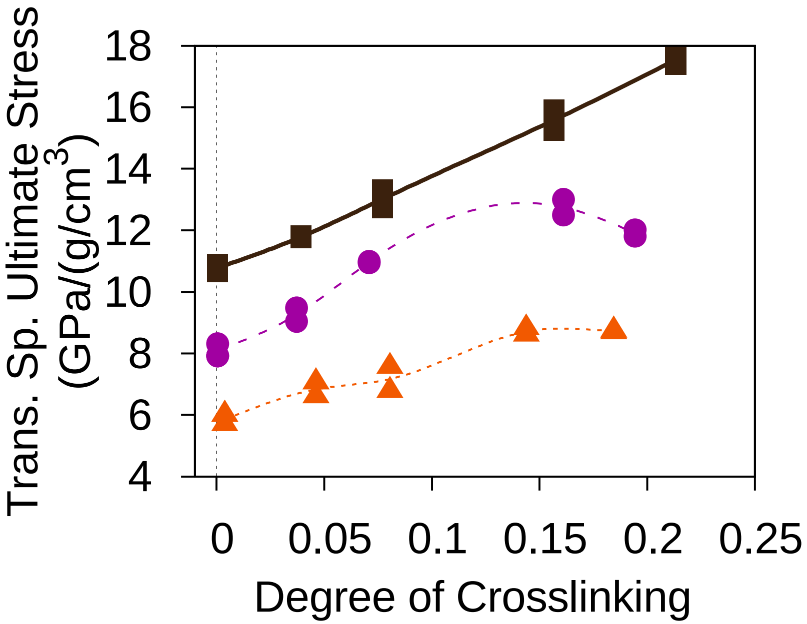




Results

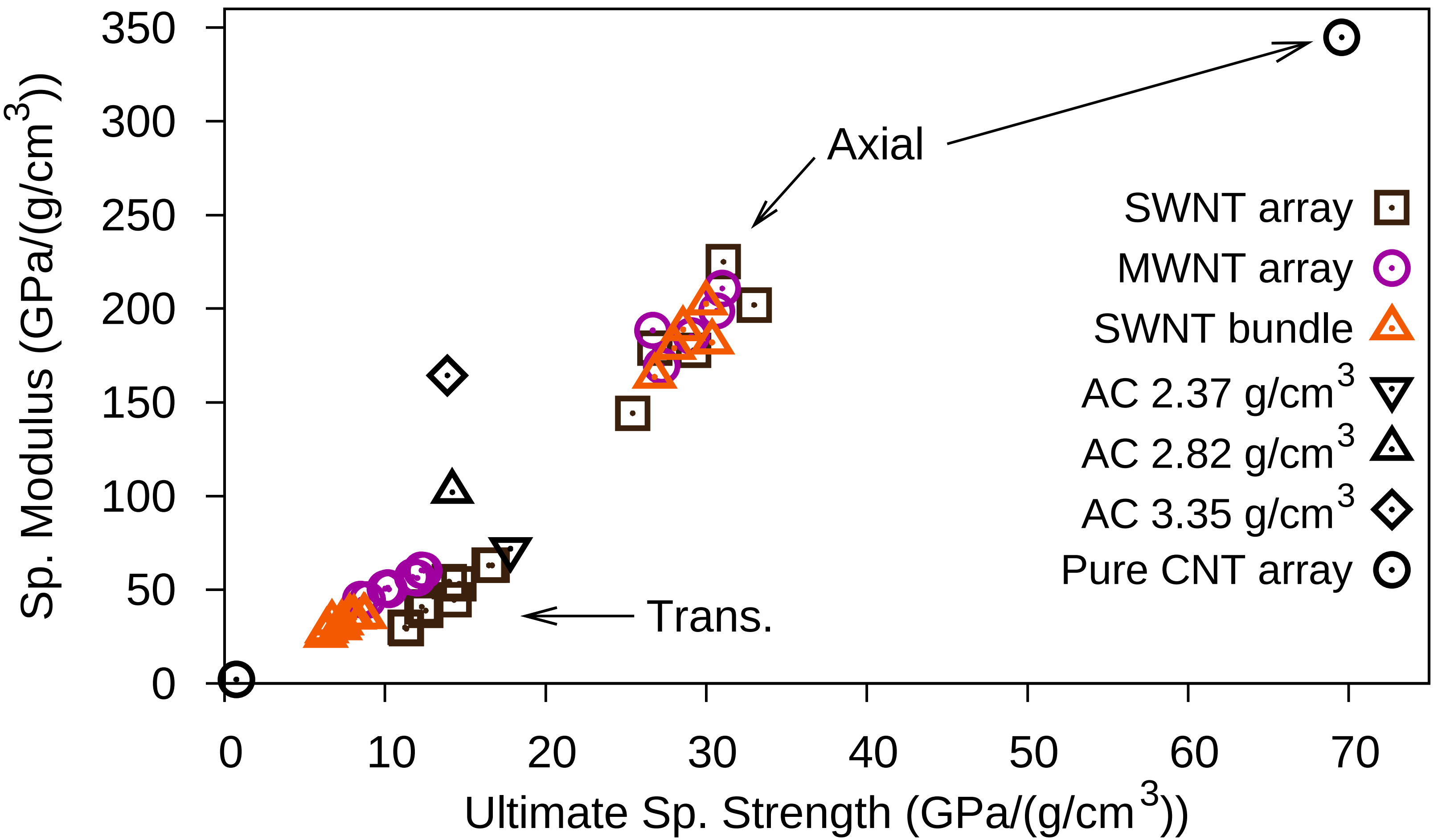
Specific Ultimate Stress





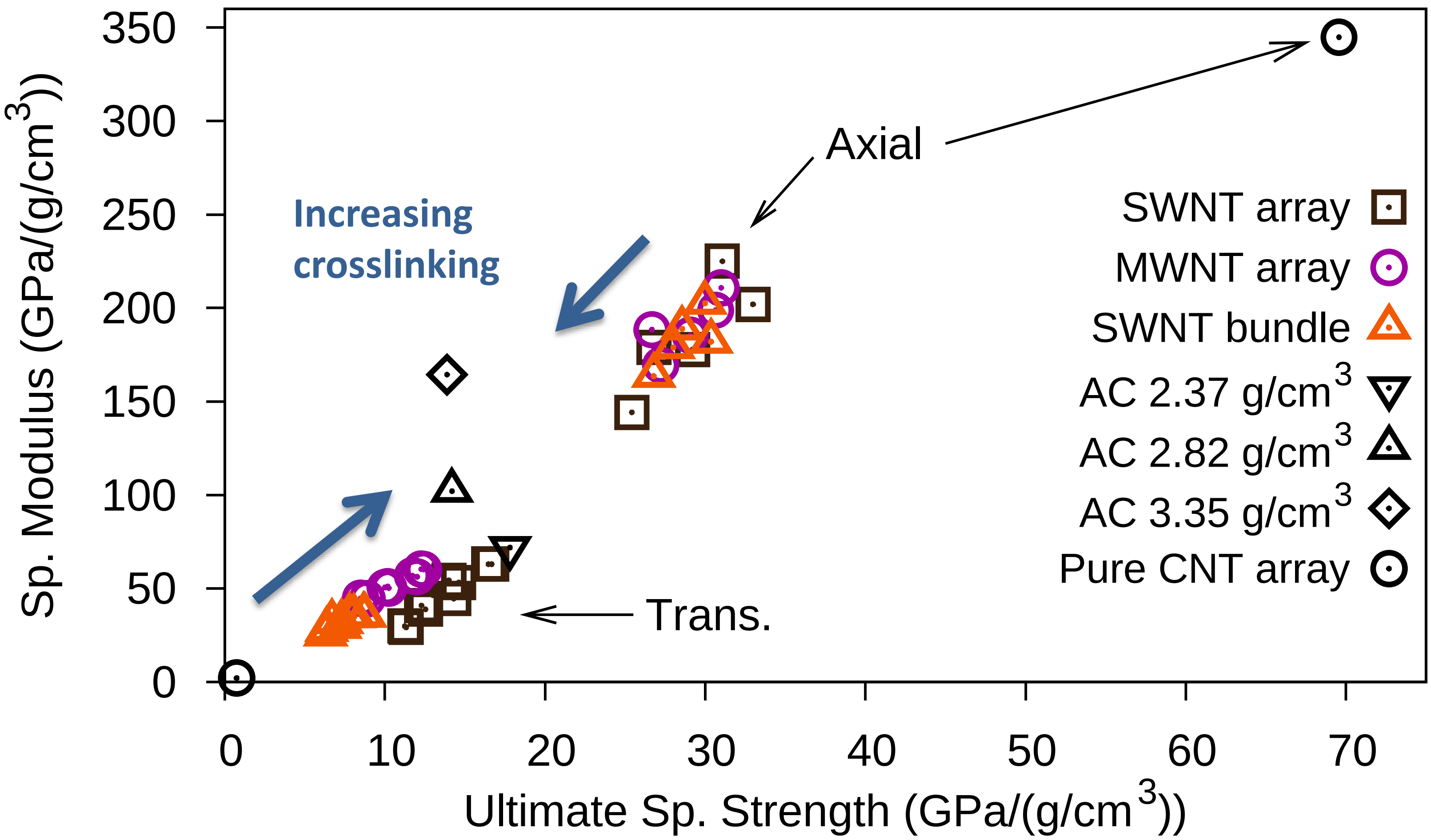
- Axial specific strength maximized around 4% crosslinking
- Transverse strength continually improved through crosslinking

Conclusions



Multiple data points for each system reflect impact of crosslinks to matrix

Summary



Multiple data points for each system reflect impact of crosslinks to matrix

Summary

SWNT vs MWNT

- Interface templating has a substantial impact on the matrix properties, and SWNTs maximize the surface area per CNT mass
- Inner MWNT walls reinforce the circular cross section

Arrays vs bundle

- Very weak bonding within bundle reduces the properties that require transferring load through the bundle

Crosslinking

- Crosslinks decrease axial specific modulus, increase transverse modulus
- Axial specific ultimate strength is maximized around 4% crosslinking
- Transverse specific ultimate strength is continually increased with crosslinking
- Crosslinking may inhibit void nucleation at the CNT/matrix interface

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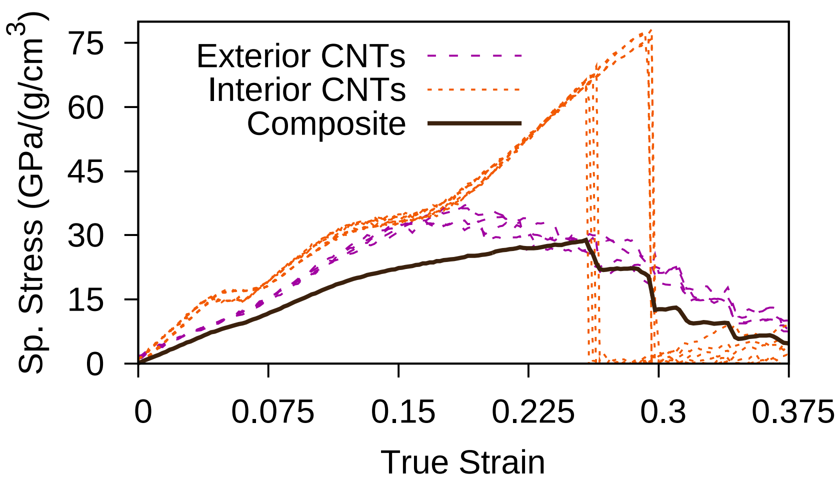
Questions

Supplemental Slides

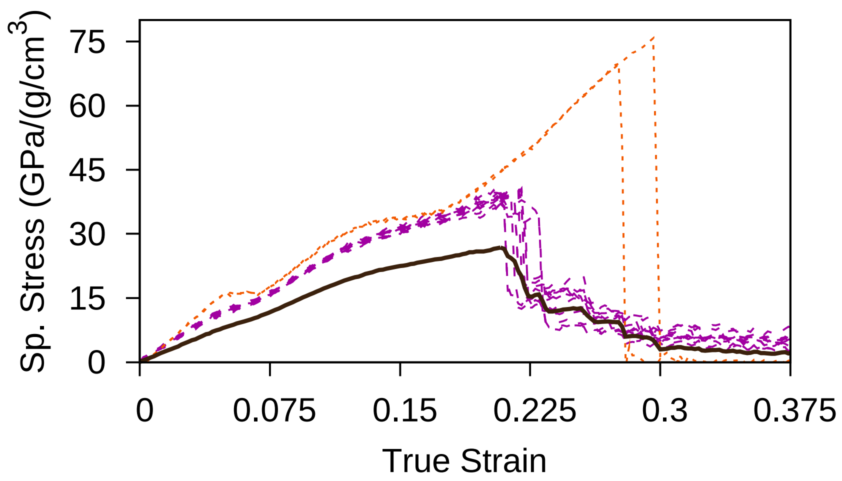
Results

Individual CNT stress-strain responses within the maximally crosslinked systems

MWNT array



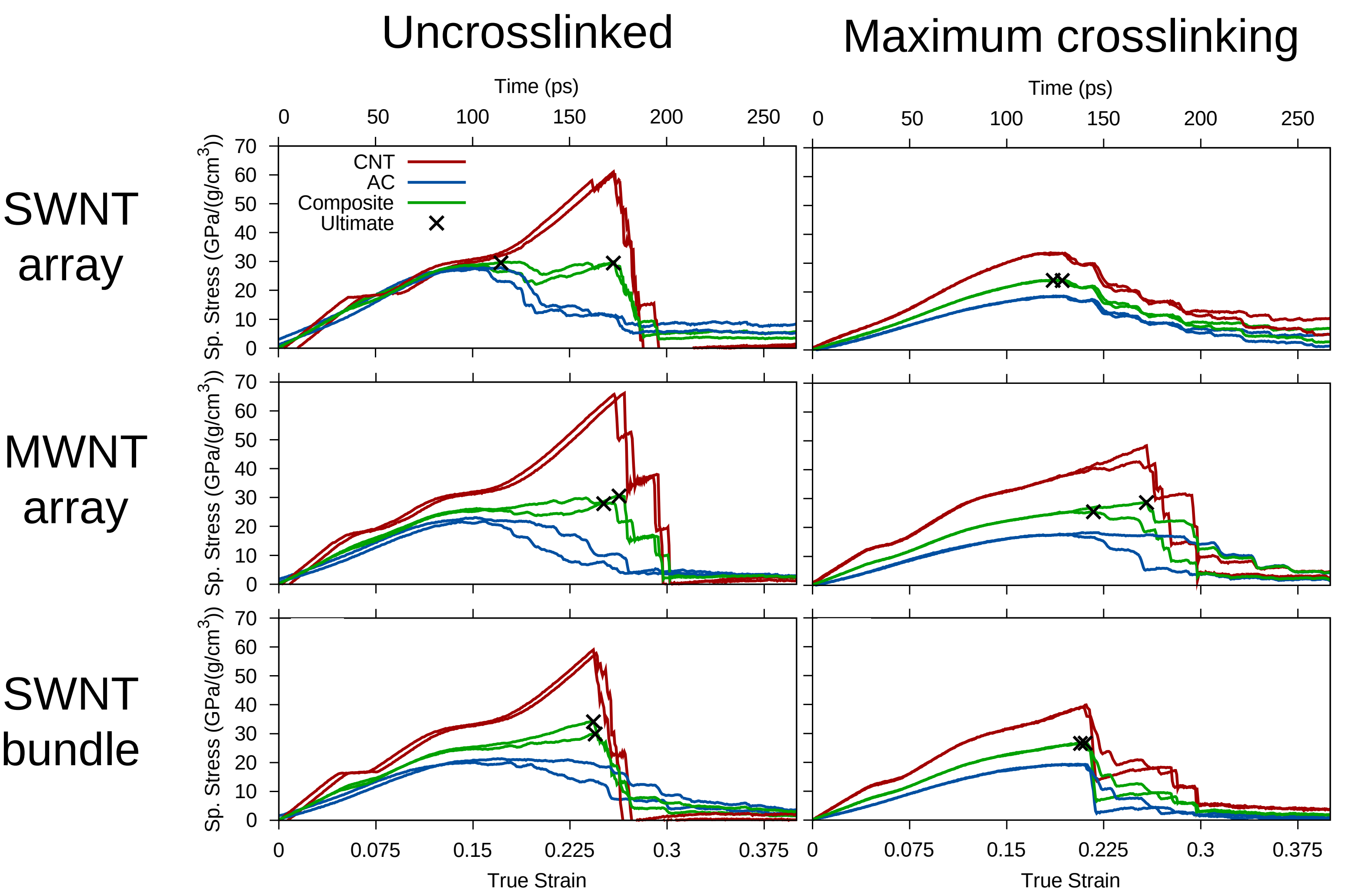
SWNT bundle



- Exterior/functionalized CNTs fracture earlier than interior/unfunctionalized

Results

Axial stress-strain response



Results

Transverse specific stress-strain response