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

Benjamin D. Jensen, Kristopher E. Wise
NASA Langley Research Center

Gregory M. Odegard
Michigan Technological University

13th U.S. National Congress on Computational Mechanics
July 26-30, 2015
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
New ReaxFF$_{C-2013}$ parameterization fitted to:
- Diamond strained in the bulk and <001> direction
- Graphene strained in the bulk and axial directions

In-house analysis of ReaxFF$_{C-2013}$ mechanical properties of diamond, graphene, amorphous carbon, and CNTs:
- Improved Poisson contraction response
- Elastic and fracture properties improved over previous ReaxFF$_{CHO}$ parameterization

**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

Equilibration Step

Potential Energy (kcal/mol)

Temperature (K)

Time (ps)

Potential Energy

Temperature

0 100 200 300 400 500 600

E F G O P O P

−175
−170
−165
−160
−155
0 100 200 300 400 500 600
0 200 400 600 800 1000 1200 1400

0 100 200 300 400 500 600

−175
−170
−165
−160
−155

0 100 200 300 400 500 600

1400
1200
1000
800
600
400
200
0

NASA
Results

Structuring of amorphous carbon at the CNT interface

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

Axial Specific Moduli

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

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

- 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)
MWNT array axial fracture (9% crosslinked)
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

Ultimate Sp. Strength (GPa/(g/cm^3))

Sp. Modulus (GPa/(g/cm^3))

Increasing crosslinking

Axial

Trans.

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
Acknowledgements

NASA Langley Research Center
- Mia Siochi
- LaRC Nano Incubator Team

Michigan Technological University
- Matthew Radue
- S. Gowtham
- Cameron Hadden

Pennsylvania State University
- Adri van Duin (Penn. State)
- Sriram Srinivasan (Penn. State)

SUPERIOR, a high-performance computing cluster at Michigan Technological University, was used in obtaining some of results.
Questions
Supplemental Slides
Results

Individual CNT stress-strain responses within the maximally crosslinked systems

MWNT array

- Exterior CNTs
- Interior CNTs
- Composite

SWNT bundle

- Exterior CNTs
- Interior CNTs
- Composite

• Exterior/functionalized CNTs fracture earlier than interior/unfunctionalized
Results

Axial stress-strain response

Uncrosslinked vs Maximum crosslinking

SWNT array

MWNT array

SWNT bundle

Axial stress-strain response
Results

Transverse specific stress-strain response

![Graph showing stress-strain response over time and strain](image-url)