Molecular Dynamics Simulations of Carbon Nanotube Composite Fracture using ReaxFF

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Overview

Motivation

– Carbon nanotubes (CNTs) have high specific stiffness and strength
– CNT yarns can now be manufactured by the kilometer
– Composite design with CNTs will be different than for carbon fibers
– New reactive force field ReaxFF can be applied to model fracture

Objectives

– Compare mechanical properties of composites made with:
  • Continuous and discontinuous CNT bundles
  • CNT-matrix covalent bonding (crosslinking)
ReaxFF reactive force field
– Allows bond breaking and formation to be modeled
– New ReaxFF\textsubscript{C-2013} parameters\(^*\) developed to improve carbon accuracy

Analysis of ReaxFF\textsubscript{C-2013} performance for diamond, graphene, amorphous carbon, and CNTs shows\(^**\)
– Improved Poisson contraction response
– Improved elastic and fracture properties compared to ReaxFF\textsubscript{CHO}\(^***\)

**Simulation Setup**

**Discontinuous**

- 5 nm CNT diameter
- 34% CNT by mass
- 50% CNT by volume
- 2.2-2.4 g/cm³ matrix density
- CNT lengths
  - 22 nm – discontinuous
  - 10 nm – continuous
- Atoms
  - 155k – discontinuous
  - 72k – continuous

**Continuous**
Simulation Setup

CNT-matrix crosslinks

- Crosslinking fractions (per CNT atom)
  - Approx.: <1%, 4%, 7%, 14%, 19%
  - 2 independent systems near each fraction
- Matrix atom bonding
  - Primarily 3 coordinate
  - Some 2 coordinate
- CNT atom bonding
  - Primarily 4 coordinate
  - Some 3 coordinate

matrix interface

- 2 coordinate
- 3 coordinate
- 4 coordinate

outer CNT
center CNT
bulk matrix
Results – Matrix Interface Structuring

<1% crosslinking, discontinuous

<1% crosslinking, continuous
Results – Matrix Interface Structuring

<1% crosslinking, discontinuous

<1% crosslinking, continuous

<1% crosslinking discontinuous - CNTs and matrix

discontinuous CNTs
continuous CNTs
 discontinuous matrix
continuous matrix

matrix interface

discontinuous matrix with varying crosslinking

<1%
5%
8%
15%
18%
g_c(r)

radius (nm)
Results – Axial Specific Modulus

Axial specific modulus
- Optimal crosslinking - discontinuous: 4-7%, continuous: 0%
Results – Axial Specific Modulus

Axial specific modulus
- Optimal crosslinking - discontinuous: 4-7%, continuous: 0%
- Matrix interface is up to 82% stiffer than bulk matrix
Axial specific modulus

- Optimal crosslinking - discontinuous: 4-7%, continuous: 0%
- Matrix interface is up to 82% stiffer than bulk matrix
Results – Discontinuous Fracture

(7% crosslinked)
Results – Discontinuous Fracture

(20% crosslinked)
Axial specific ultimate stress
- Optimal crosslinking - discontinuous: $\geq 14\%$, continuous: 0\%
Results – Axial Specific Ultimate Stress

- Optimal crosslinking - discontinuous: ≥14%, continuous: 0%
- Matrix interface is up to 50% stronger than bulk matrix
Results – Axial Specific Ultimate Stress

- Optimal crosslinking - discontinuous: \( \geq 14\% \), continuous: 0%
- Matrix interface is up to 50% stronger than bulk matrix
Results – Comparison to Experiment

exp. measured single CNT*

exp. CNT yarn composite**

Experimental knockdown


Results – Comparison to Experiment


Results – Comparison to Experiment


Results – Comparison to Experiment

Summary

- Mechanically significant structuring of the matrix at the nanotube interface
- Continuous composite crosslinking was mechanically detrimental
- Discontinuous composite crosslinking between 4%-7% maximized modulus, above 14% maximized ultimate stress
- Observed void at the ends of the discontinuous tubes
- Simulation results were compared to experimental nanotube yarn composites and experimental single tube measurements
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NASA Pleiades Supercomputer

LAMMPS – Free open source molecular dynamics by Sandia National Labs
Questions