Carbon Nanotube Composites

- Lightweighting of aerospace structures confer advantages such as improved performance, payload capacity, maneuverability, efficiency and range. NASA studies show that a 30% reduction in overall launch mass can have game-changing implications for feasible and affordable human missions to Mars.
- One approach to achieving transformative mass savings is through the use of advanced, super-lightweight structural materials such as carbon nanotube (CNT)-based composites.

Research Motivation

- CNT composites are in the very early development phase and do not yet demonstrate the theoretical structural/mass advantages promised by these systems.
- CNT composite research show that significant misalignment between and within CNT bundles, pervasive regions of poor wetting by the matrix polymer, and substantial void volume fraction in the nanostructured composite significantly influence mechanics.
- A gap exists in understanding how nanoscale defects impact load transfer mechanics and failure modes.

Research Objectives

- At mesoscopic dimensions, between the atomic (MD) and the macro- (FEM) scale, a critical gap exists in our ability to model CNT composites.
- We develop hierarchical multiscale simulations to address the nano-, meso-, and macro-scale deformations: separate simulations compute structure-property relations at one length scale in order to pass the “effect” to higher scales.
- The key innovation is in the bridging of the scales with an original mesoscopic distinct element method (mDEM).

MD: Non-Orthogonal Tight Binding Computational Technique

- Models for the energetics of the two crystalline organization modes (hexagonal and ‘dog bone’) are calculated by unit cell CNTs placed under periodic boundary conditions (PBC).
- Structural parameters captured by the lattice vectors a and b of the PBC cell give an approximation of the co-ordination of the unit cells. They quantify the lattice shift and layer spacing across the interface.
- Computed unit cell energies E versus circumference of the CNT show a linear relationship.
- As R increases, E lowering occurs via both inter- and intra-tube vdW energy gains in collapsed CNTs, but only by inter-tube vdW gains in the polygonised CNTs.

MD: Predicted Mechanical Behavior of CNT Bundle Configurations

- Computationally predicted Young’s moduli, Y, versus radius, R, for bundles of hexagonal and “dog bone” collapsed armchair CNTs. The data for the “dog bone” shapes are shown with filled symbols (filled square, circle, rhombus) while the hexagonal bundle configuration are shown with empty symbols (empty square, circle, rhombus).
- Hexagonal CNTs show a strong decrease of Y with R in addition to lowering of Y with wall number. The opposite is the case for “dog bone” collapsed armchair CNTs.
- The effect of radius is more pronounced than the influence of wall number on the mechanical response of the two bundle configurations considered.

Mesoscopic Distinct Element Method (mDEM)

Modeling Framework

- mDEM is build on the framework of the DEM of Civil Engineering.
- mDEM is implemented in existing DEM packages: PFC (Itasca Consulting) and LAMMPS DEM.
- In mDEM, a CNT is coarse grained into a chain of cylindrical distinct elements.
- Each element interacts through contact bonds:
  - Parallel Contacts to capture the mechanics of individual CNTs
  - Van der Waals Contacts - to capture the adhesion between CNTs
  - Viscous Damping Contacts – to capture the friction between CNTs

Essential Features of the mDEM Model

- Capture local bending and twisting of individual CNTs
- Enable smooth intertube sliding: important for self-assembling process

mDEM Simulations: Twisted CNT Ropes

- Twisting a CNT rope offers a way for strengthening it
- mDEM simulations revealed the complexity of the twisting process:
  - CNT ropes developed internal vacancies at twisted states, known as topological defects
  - Further twisting leads to helix transformation
- Mechanical properties are heavily influenced by various factors: porosity, degree of bundling, CNT length, and orientation etc.
- mDEM provides an efficient way to study large system (~1 micron3)
- vdW attraction leads to bundling effect, CNT bending and non-affine deformation
- By filling the pores with nanoparticles, we preserve the entanglement of CNT network and improve load transferability of the network

mDEM Simulations: CNT Networks with Nanoparticle Fillers

- Rings and rackets are stable self-assembled structures often found in nanotubes and proteins (amyloid and kinesin)
- Stability is governed by energy balance between strain and vdW energy
- Packings of collapsed single-, double-, and triple-walled carbon nanotubes (CNTs) into bundles

mDEM Verification: Dynamics of Carbon Nanotube Self-assemblies

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