Synopsis:
Molecular Dynamics Modeling and Simulation of Nanotube Reinforced Composites

Molecular dynamics simulation images
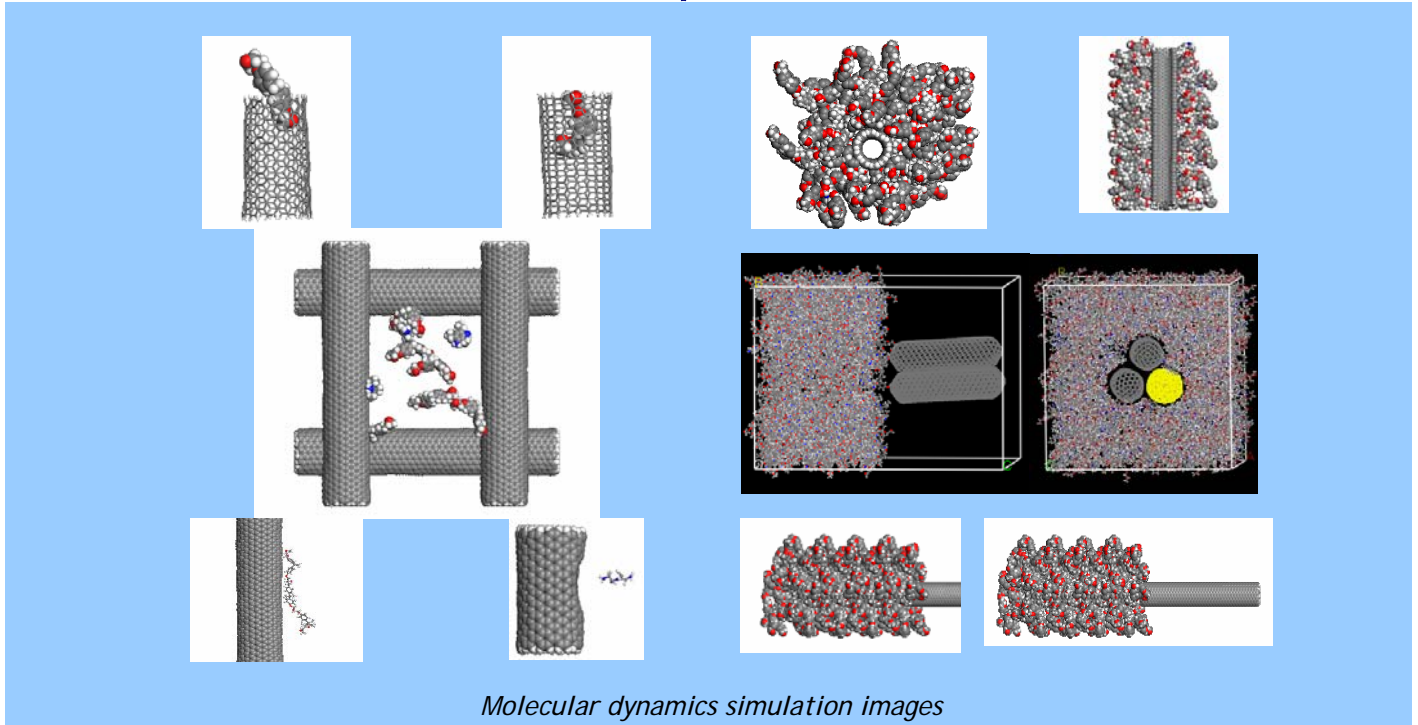
Background

To harness the properties of nanotubes requires special research techniques, considering the nanotube is only about 1,000th the diameter of a human hair. HPMI uses MD modeling-simulation to the nanostructure-processing-property relationships of the nanotube/polymer composites, which is critical for developing the next generation of high-performance composites.

Goals

- Predict mechanical properties of nanotubes embedded in polymeric matrix
- Predict interfacial bonding strength and load transfer in nanocomposites
- Predict nanotube dispersion and resin flow through buckypaper nanotube films

Projects/Research Highlights

- Improved nanotube dispersion and functionalization
- Modeled pullout and pull-through of interface and load transfers
- Validated modeling and simulation through experiments

Benefits to Industry

- Understand nanotube dispersion under different factors
- Accelerate multiscale composite material development
- Optimize performance of nanocomposites

High-Performance Materials Institute HPMI