Mechanics of Nanotubes and Nanotube-Polymer Composites

Deepak Srivastava, NASA Ames Research Center
Chengyu Wei, Stanford University/NASA Ames
Kyeongjae Cho, Stanford University
Madhu Menon, University of Kentucky
Mohamed Osman, Washington State University/Pulham

Onboard computing systems for future autonomous intelligent vehicles
- powerful, compact, low power consumption, radiation hard
- High performance computing (Tera- and Peta-flops)
  - processing ancillary data
  - integrated space vehicle engineering
  - climate modeling
- Revolutionary computing technologies
  - Smart, compact sensors, small volume
- Advanced miniaturization of all systems
  - Microspacecraft
  - 'Thinking' spacecraft
  - Micro-, nano-rovers for planetary exploration

Carbon Nanotube

CNT is a tubular form of carbon with diameter as small as 1 nm.
Length: few nm to microns.

CNT is configurationally equivalent to a two dimensional graphene sheet rolled into a tube.

CNT exhibits extraordinary mechanical properties:
Young's modulus over 1 Tera Pascal, as stiff as diamond, and tensile strength ~ 200 GPa.

CNT can be metallic or semiconducting, depending on chirality.

Outline

- Nanomechanics of nanotubes (C and BN nanotubes)
  - plastic collapse
  - anisotropic strain-release
  - nanostructured skin-effect
- C nanotube reinforced polymer composite
  - increased thermal expansion coefficient
  - increased Young's modulus
  - mechanisms and limits of load transfer

NASA Mission Needs

http://www.ipt.arc.nasa.gov at Ames Research Center

Experimental Nanotechnology at Ames Research Center

CVD Carbon Nanotube SEM Images

http://www.ipt.arc.nasa.gov at Ames Research Center

Nanomechanics of Individual Nanotubes

- High value of Young's Modulus (1.2 - 1.3 TPa for SWNTs)
- Elastic limit up to 10-15% strain

redistribution of strain
sharp buckling leading to bond rupture
SWNT is stiffer than MWNT
- Experiment: buckling and collapse of nanotubes embedded in polymer composites.


BN nanotube based composite with anisotropic plasticity

Nanostructured skin effect!
Simulation: 30% yielding strain from fast strain rate (1/ps) molecular dynamics simulations

Experiments: 6% maximum strain in SWCNT ropes; 12% maximum strain in MWCNTs

Simulation:
- T=0K, Tersoff-Brenner potential: Super-elastic up to 20%
- T=0K, Tight Binding: diamond like defects, collapsed at 12%

Experiment:
- Collapsing of CNT within polymer matrix under compression stress 150GPa (TEM study)

- Previous MD simulations with high strain rate:
  - Elastic up to 30% (Yakobson et al.*)
  - Experimentally feasible strain rate and Temperature

- Transition State Theory
  - Arrhenius formula: \[ t = \frac{1}{n_{\text{site}}} e^{\frac{E_v}{k_B T}} \]
  - Activation energy as a function of strain: \[ E_v = E_v^E \]

- Experimental feasible conditions
  - Length ~ 1/μm; strain rate ~ 1/hour; T = 300K
  - Yield strain: 9 ± 1%
Structural and thermal properties
- Load transfer and mechanical properties

SEM images of epoxy-CNT composite
SEM image of polymer (polyvinylalcohol) ribbon contained CNT fibers & knotted CNT fibers


Polymer-CNT composite

Thermal Characterization of Nanotube and Nanotube/Polymer Composites
- Thermal conductivity of single-wall nanotubes
- Nanotube/polymer composites as high thermal expansion coefficient materials
- Thermal conductivity of nanotube/polymer composite
Thermal peak position has a strong dependence on the radius of the tube and weak dependence on chirality.

Typical peak thermal conductivity is about 2000-3000 W/mK.

High thermal conductivity material with highly directional heat-flow and weak dependence on chirality.

Results:

- Glass transition temperature $T_g$ increased from 150K to 175K.
- Thermal expansion coefficients: $K^{-1}$
  - PE PE-CNT $T<T_g$: $3.5 \times 10^{-4}$, $4.5 \times 10^{-4}$, $18\%$
  - PE PE-CNT $T>T_g$: $8.6 \times 10^{-4}$, $12.0 \times 10^{-4}$, $7.40\%$

Diffusion coefficients of polymer with CNTs embedded

- Diffusion coefficient increased, especially along CNT axis direction, indicating enhancement of thermal conductivity.
- Experiments on ABS/CNT & RTV/CNT show large increase (Rick Berg's group at RICE).

Modulus of Polymer-CNT composites

(Halpin-Tsai's formula)

$E_r = \frac{E_m}{1 - \nu_f \nu_m (1 - \nu_f)}$

$E_c = \frac{E_f}{V_f}$

Dependent on geometry, packing of fiber, aspect ratio of fiber.
- Young's modulus of CNT composites 109% higher than polymer matrix
- Stretching treatments enhance Y by 50%

Young's Modulus

(LD-2, Np=10)
Comments

- Nanomechanics of individual nanotubes explained experimental observations, and revealed novel anisotropic strain release in BN nanotubes.
- Realistic strain-rate, temperature and length dependent deformation of nanotubes under tensile strain is developed.
- Polymer-nanotube composite is a high thermal expansion coefficient and diffusion material above glass transition temperature.
- Young’s modulus increases by up to 30% for low strain values, this can be further increased by stretching-unstretching cycling of composite.
- Multiple-site chemical bonding favors load transfer.