Elastic Properties of Carbon Nanotube Reinforced Composites

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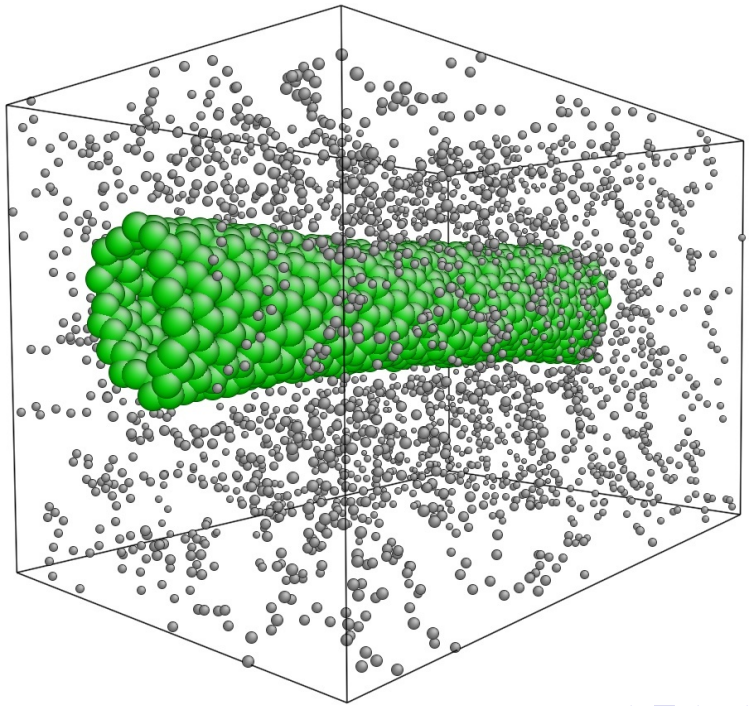
Dec. 11 2008

Simulation Goals

- Simulate a polymer nanocomposite reinforced with single-wall carbon nanotube using LAMMPS.
- Apply strain longitudinally until failure and calculate elastic properties.
- Apply strain transversely until failure and calculate elastic properties.
- Model three different interface strengths between the nanotube and the polymer.

Simulation Volume

- 10 polymer chains, each 260 monomers long.
- One central carbon nanotube containing 930 atoms.
- 63 angstroms long along nanotube axis, 40 angstroms square normal to axis.
- Periodic in all directions.



Restrictions

- Nanotube collapses during simulation, so simulated as a rigid body. Prohibits calculation of longitudinal properties, but can still be used for transverse properties where the nanotube does not directly affect the properties of the composite.
- Harmonic potentials used to model nanotube and polymers, which produces a force directly proportional to atomic spacing. Prevents nanotube and chain from breaking.

Applied Strain

- Uniform tensile strain is applied to the simulation volume normal to the axis of the nanotube.
- Strain is applied by resizing the simulation volume in the direction of the strain and rescaling the coordinates of the atoms to fit the new dimensions. Each iteration increases the length of the volume by 0.05 angstroms.
- After each iteration the system is allowed to equilibrate for 2,000 time steps, then the reported stresses for the next 1,000 time steps are averaged to produce a single value of stress.

Simulation Goals

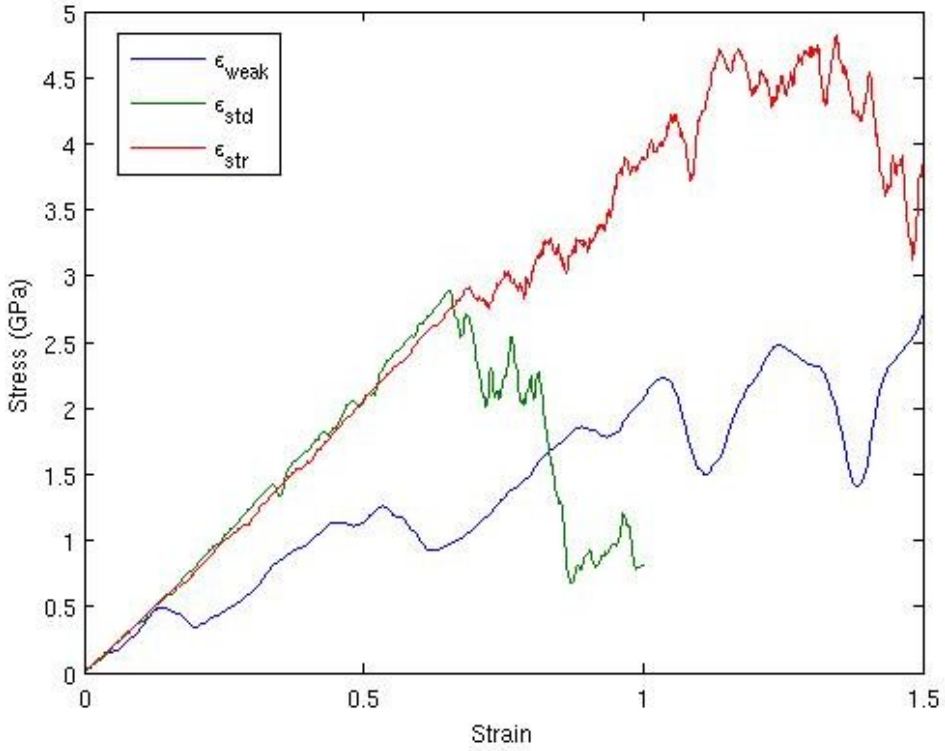
- Simulation is repeated three times with different interface strengths between the nanotube and the polymer.
- Interface strength is based on the standard 12/6 Lennard-Jones potential,

$$E = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad r < r_c \tag{1}$$

  ϵ = depth of potential well, σ = interparticle potential cutoff distance, r = distance between particles.
- Strength is adjusted by using three different values of ϵ
  - $\epsilon_{std} = 0.00286$ eV
  - $\epsilon_{weak} = \frac{1}{4}\epsilon_{std} = 0.000715$ eV
  - $\epsilon_{str} = 4\epsilon_{std} = 0.01144$ eV

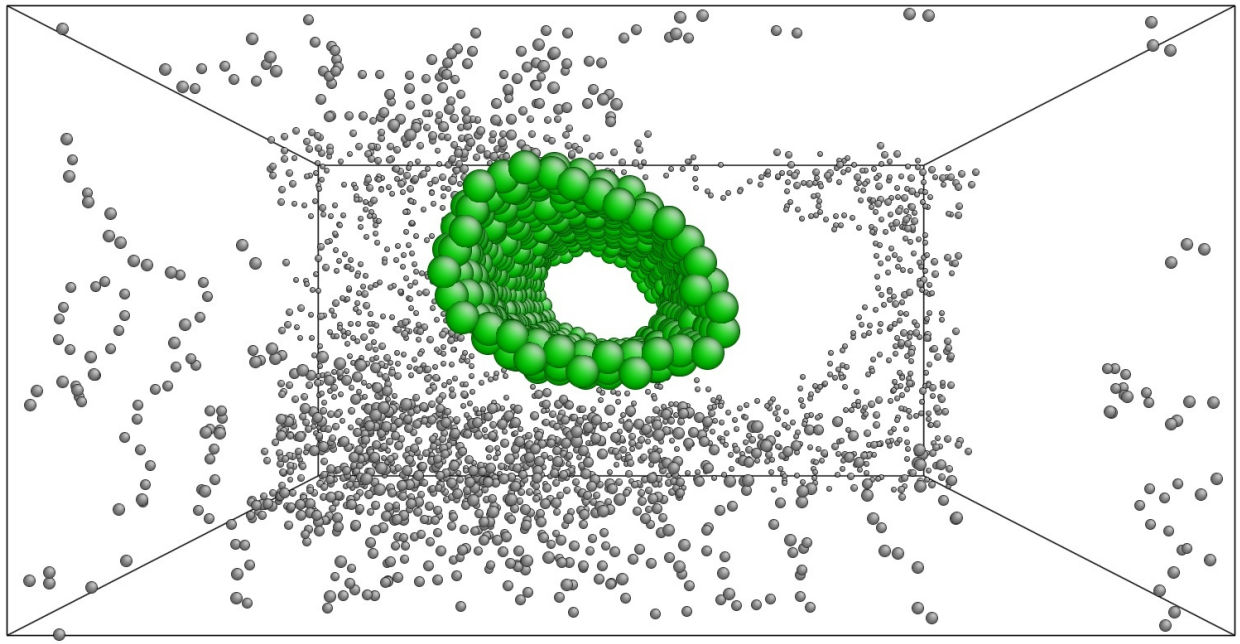
Stress-Strain Curves

- Initially the response is linear-elastic and can be used to calculate Young's modulus according to Hooke's law.
- As the strain increases the polymer begins to fail and the stress-strain curves break down.



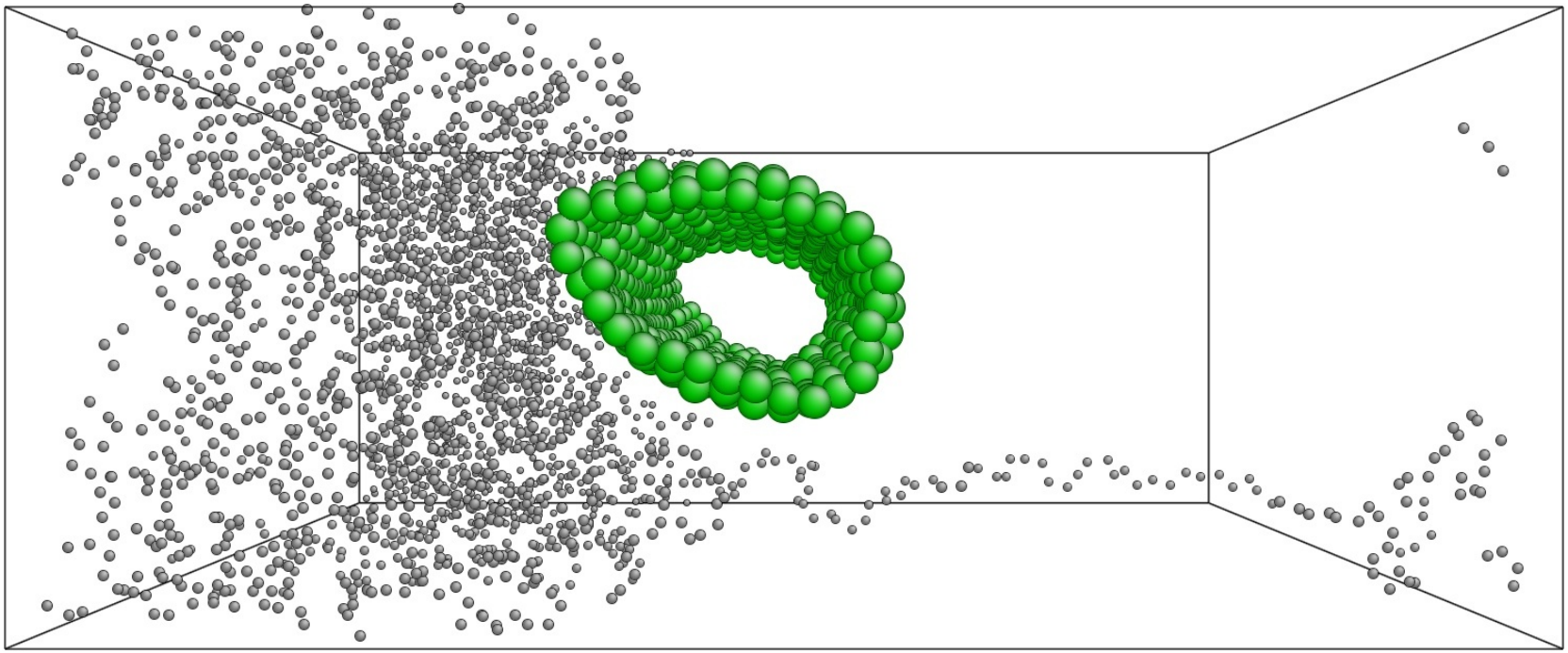
Stress-Strain Curves

- The weakest interfaces experiences several partial failures under relatively low strain as the polymer separates and regroups along the nanotube.



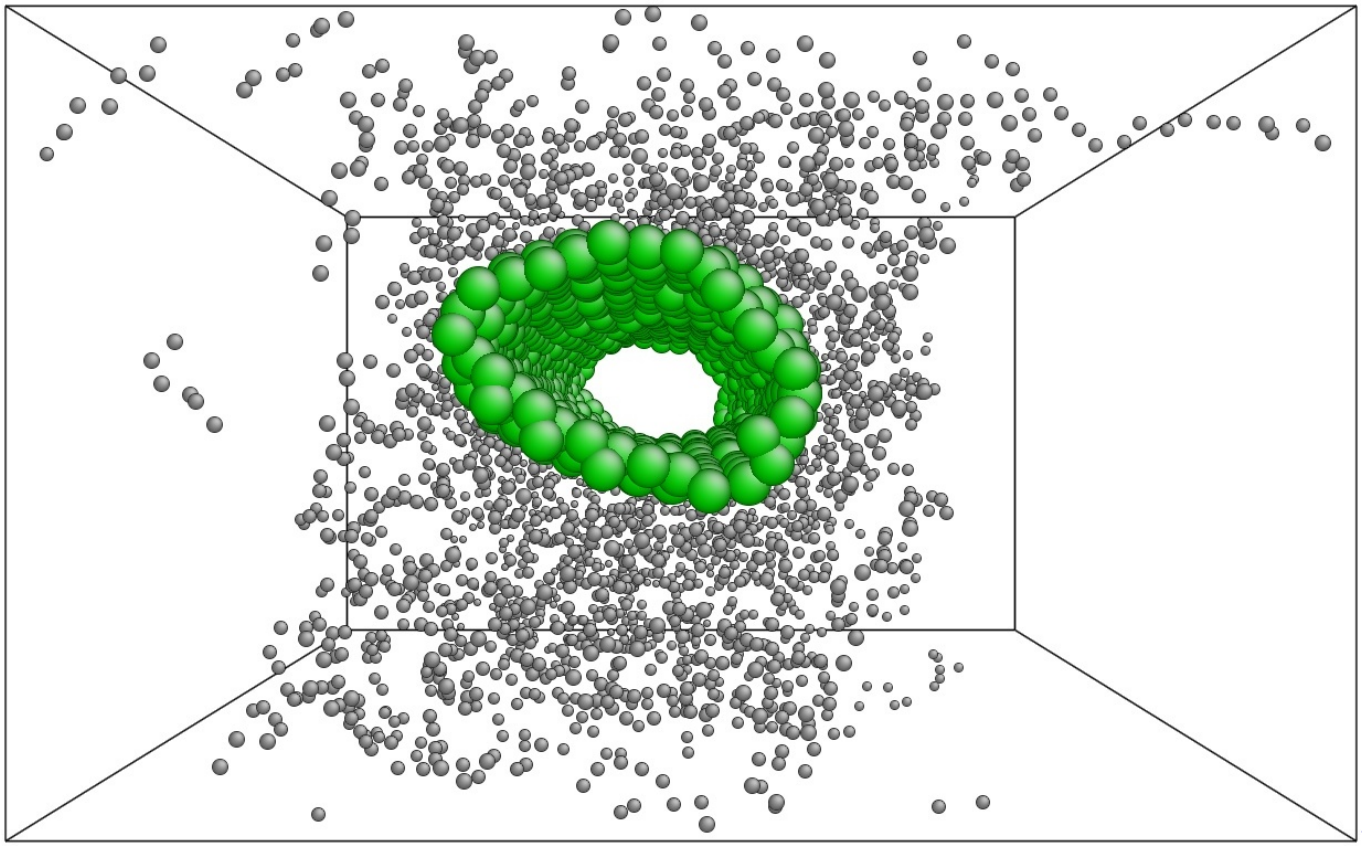
Stress-Strain Curves

- As the strain continues to increase the polymer separates completely from the nanotube and clusters in the gap between.



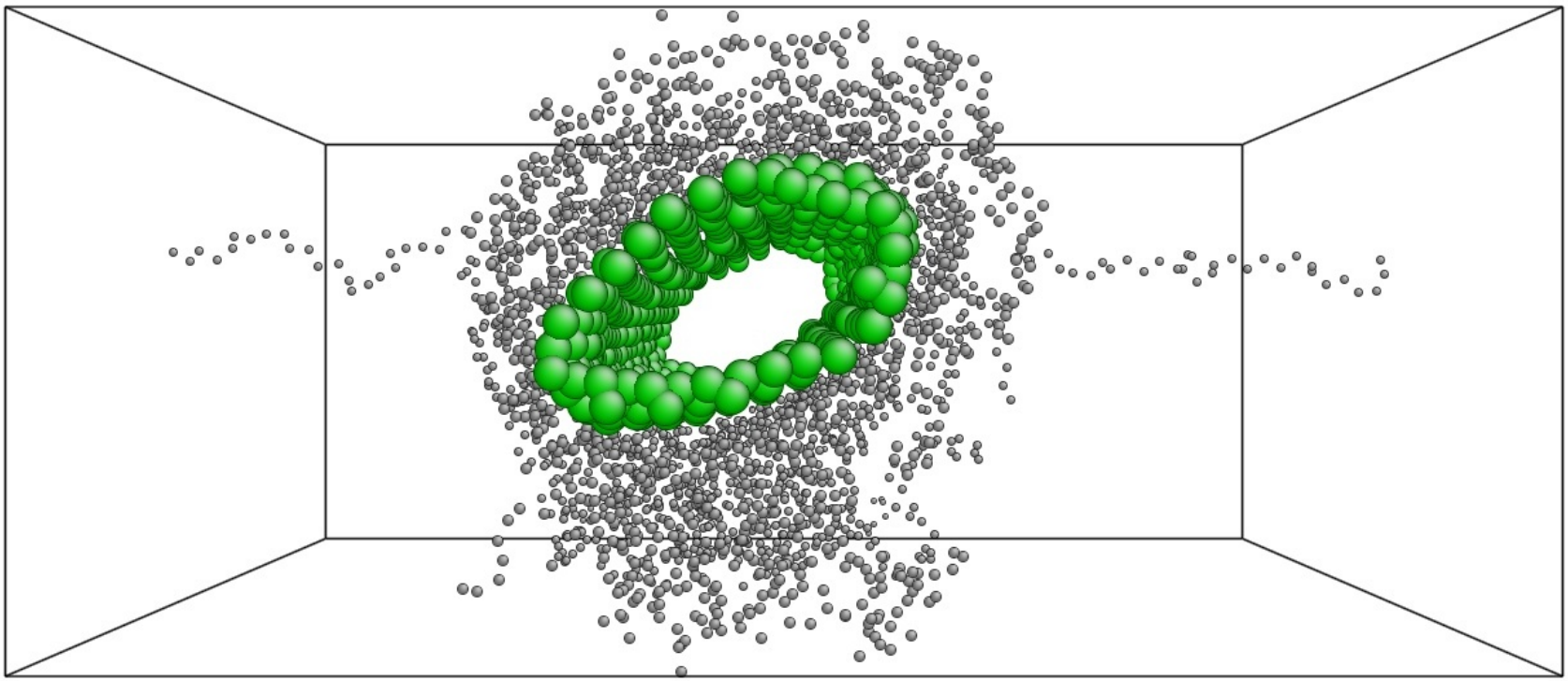
Stress-Strain Curves

- With the standard strength interface the polymer remain evenly distributed along the nanotube, but separate from the polymers in the periodic volumes on either side.



Stress-Strain Curves

- The strong interface is very to the standard interface, except that the polymer chains remain even closer to the nanotube.

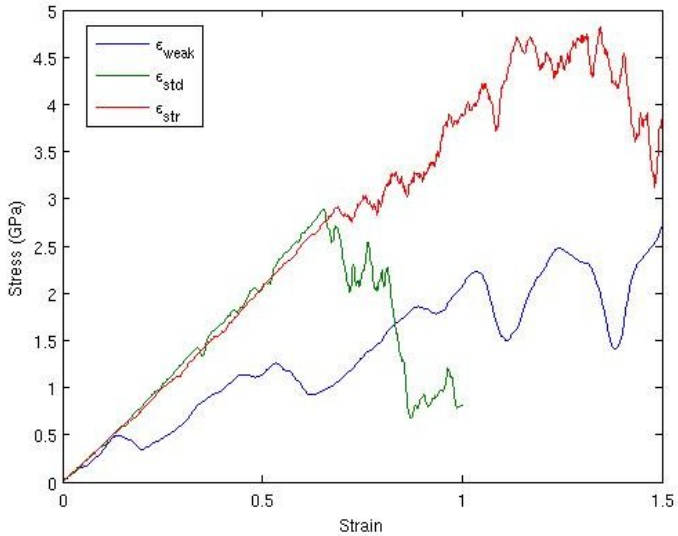


Young's Modulus

- For the system with the weak interface three values of Young's modulus were calculated, corresponding to the initial slope of the stress-strain curve and the slopes after the first two partial failures. Averaging these three values results in an approximate Young's modulus of 3.67 GPa.
- The standard strength interface was calculated using only the linear portion of the graph, giving a Young's modulus of 4.36 GPa.
- The strong interface was calculated the same way as the standard, giving 4.22 GPa.

Ultimate Tensile Strength

- The ultimate tensile strength S_U is for the weak interface is estimated to be 2.5 GPa at a strain of 1.25.
- For the standard interface S_U is nearly 2.9 GPa, occurring at a strain of approximately 0.65.
- For the strong interface S_U is 4.75 GPa and occurs between strains of 1.1 and 1.4



Conclusions

- The stiffest system is the one with the medium strength interface, although the strong interface is only slightly lower. However, the strong interface has a much higher ultimate tensile strength. The weak interface has the lowest Young's modulus and experiences several partial failures as the strain increases.
- Additional time and simulation effort are required to validate some of the presented results, particularly in regards to the weak interface model. Future work should also attempt to overcome the issues requiring the nanotube to be a rigid body, in order to allow calculation of longitudinal properties.