Conductance of AFM deformed Carbon Nanotubes

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Upon deformation

$\text{sp}^2 \rightarrow \text{sp}^3$

Stretching of bonds

Opens bandgap in most nanotubes


What is the conductance decrease due to?
Approach

1) AFM Deformation

2) Bending

Relaxed structure using molecular dynamics

Central 150 atoms were relaxed using DFT and the remaining 2000+ atoms were relaxed using a universal force field

Density of states and conductance were computed using four orbital tight-binding method with various parametrizations
Bond Length Distribution & Conductance

(12,0) Zigzag

Bending

AFM-tip deformation

AFM DEFORMATION

Conductance (S)

Conductance (S)

BENDING

Conductance (S)

\( \theta^o \)
AFM Deformed versus Stretched

Graph showing the conductance (S) as a function of % of strain for different energies (eV). The graph compares uniformly stretched and AFM-deformed samples.

- **Uniformly Stretched**
- **AFM-deformed**

Inset graph shows transmission as a function of energy for different strains:
- ε=0%
- ε=10%
- ε=8.27%, Θ=25°
What happens to other chiralities?

- Metallic zigzag nanotubes develop largest bandgap with tensile strain.
- All other chiralities develop bandgap that varies with chirality.
- Experiments on a sample of metallic tubes will show varying decrease in conductance.
- Some semiconducting tubes will show an increase in conductance upon crushing with an AFM tip.