Conductance of AFM deformed Carbon Nanotubes

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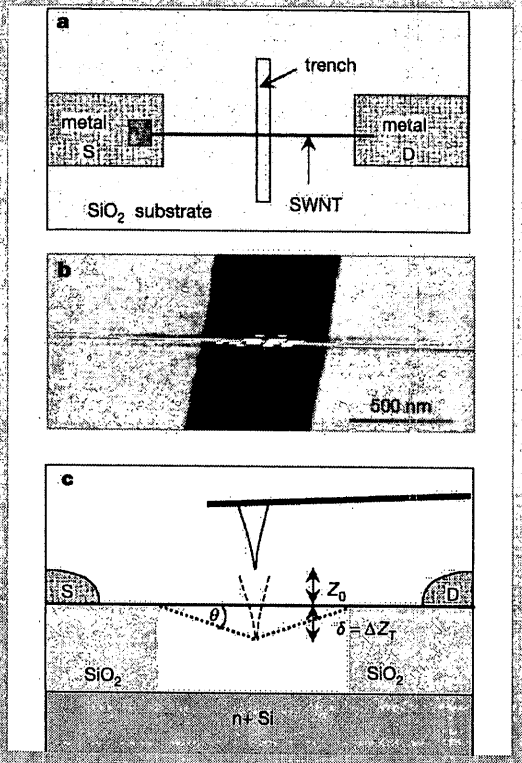
Tombler et. al, Nature 405, 769 (2000)



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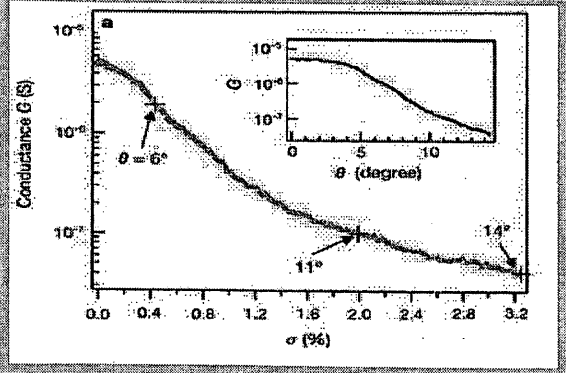
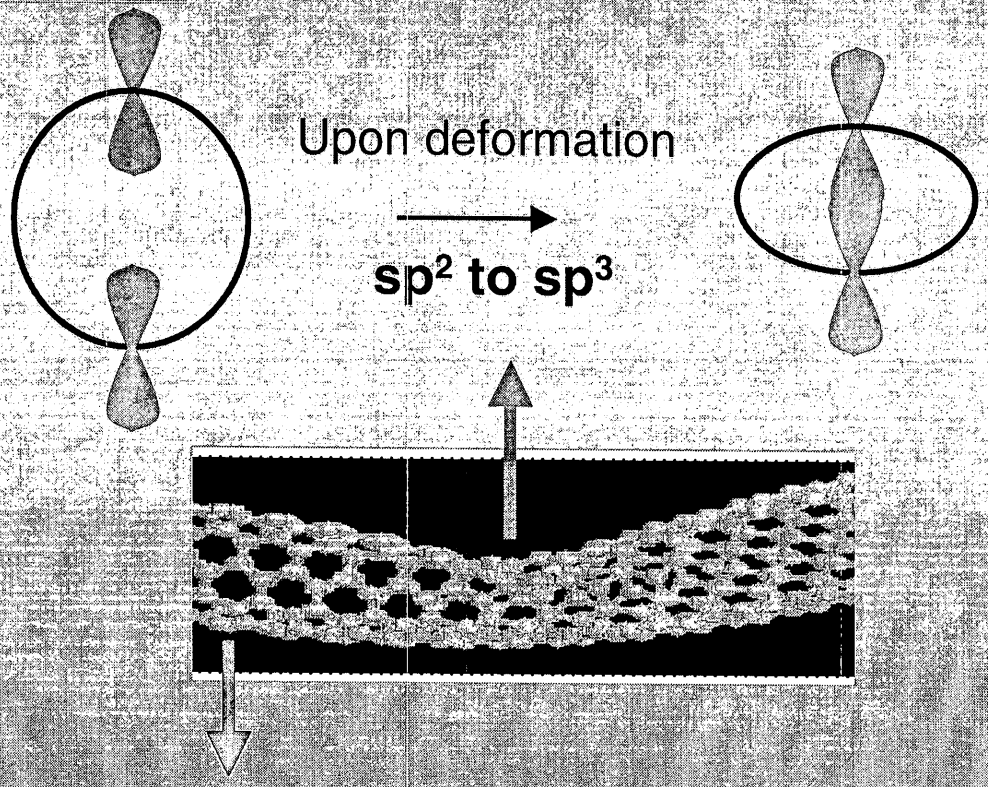




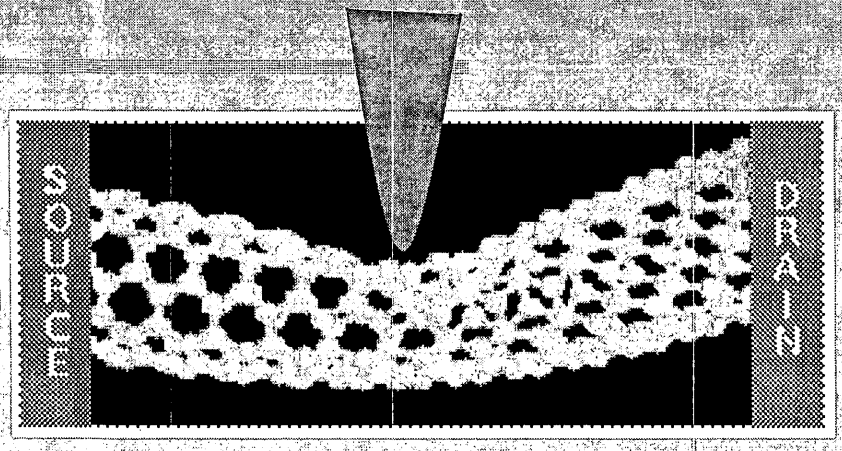
Stretching of bonds

Opens bandgap in most nanotubes
[Phys. Rev. B, vol. 60 (1999)]

What is the conductance decrease due to?

Approach

1) AFM Deformation



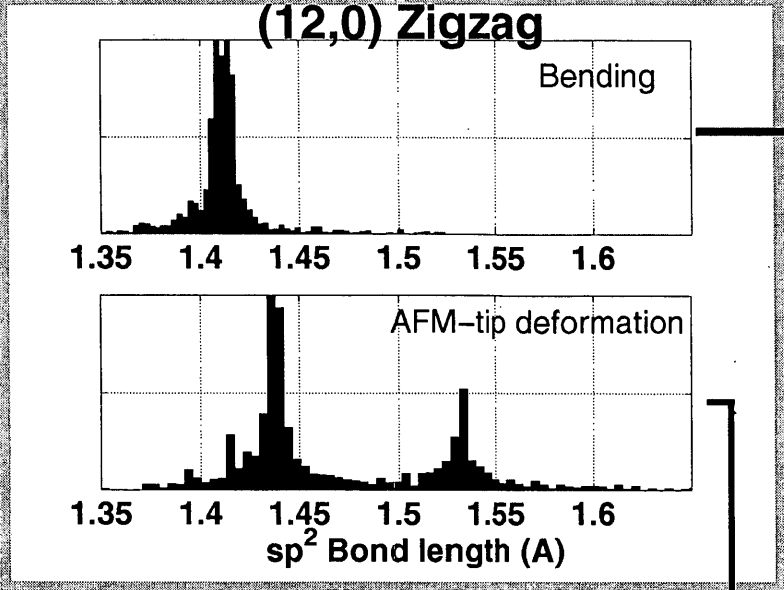
2) Bending

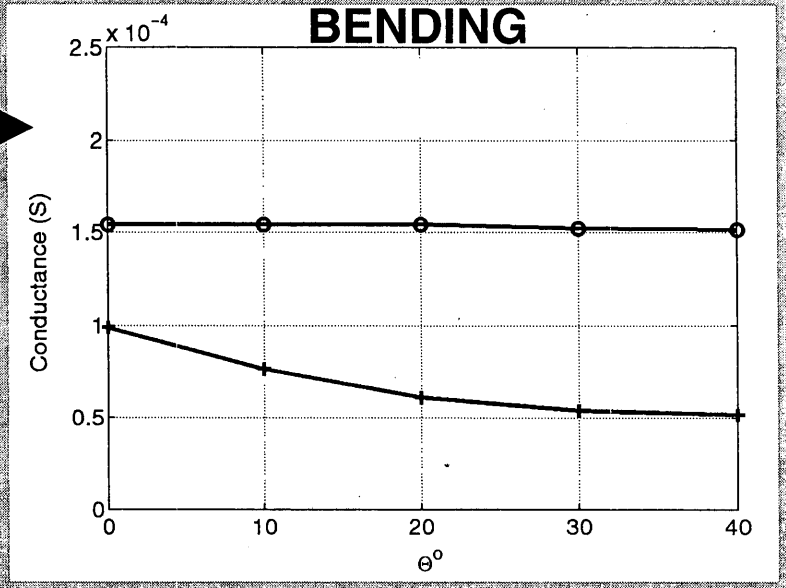
Relaxed structure using molecular dynamics

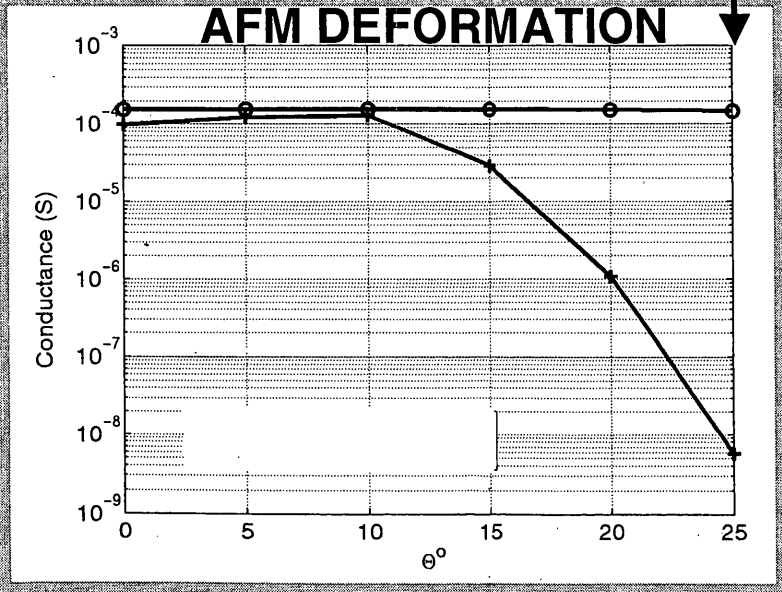
Central 150 atoms were relaxed using DFT and the remaining 2000+ atoms were relaxed using a universal force field

Density of states and conductance were computed using four orbital tight-binding method with various parametrizations

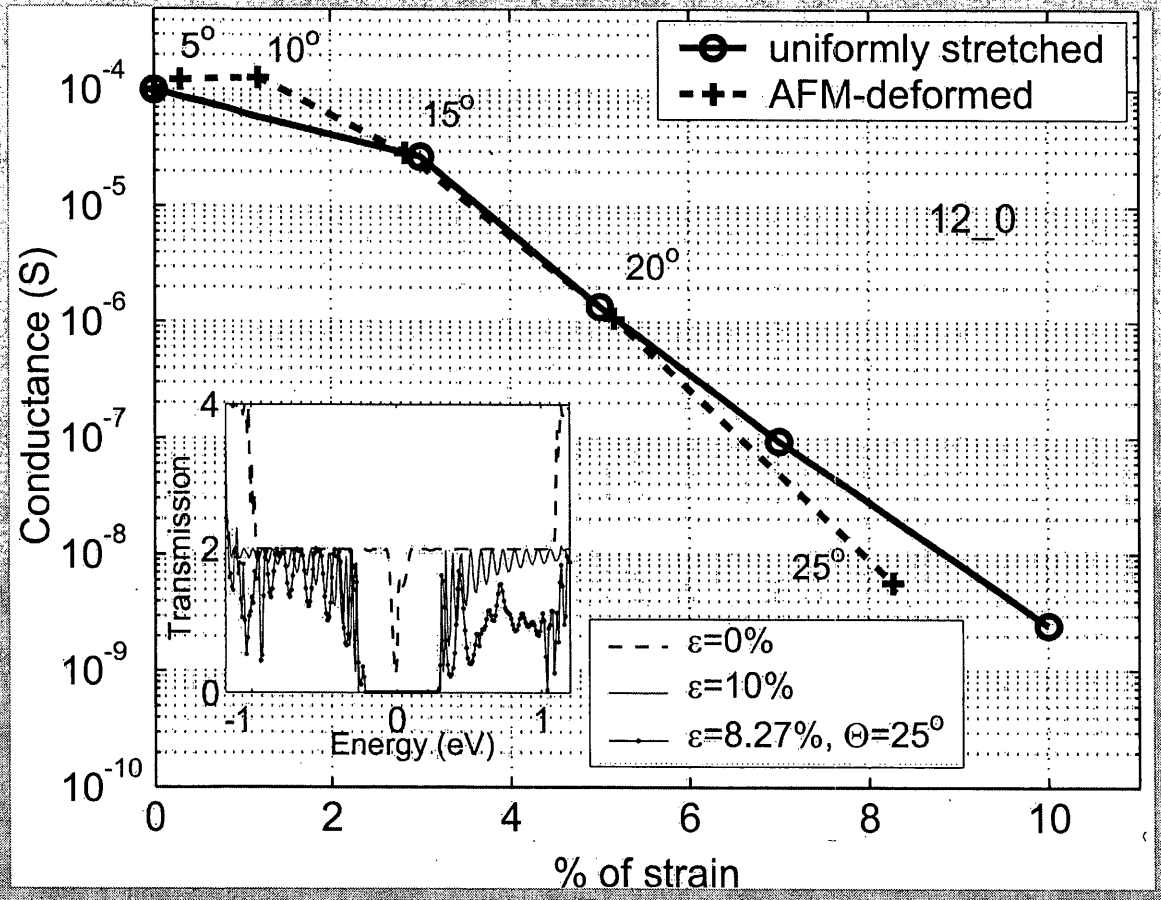
Bond Length Distribution & Conductance



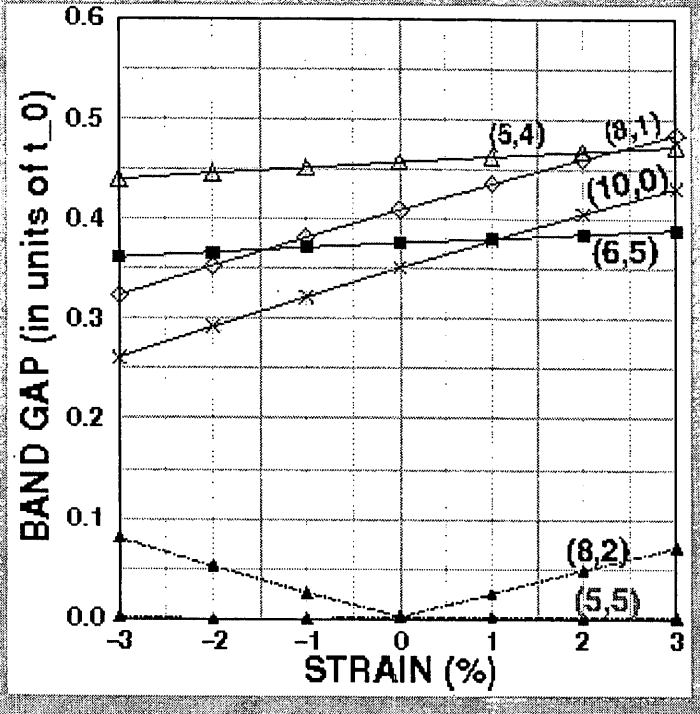


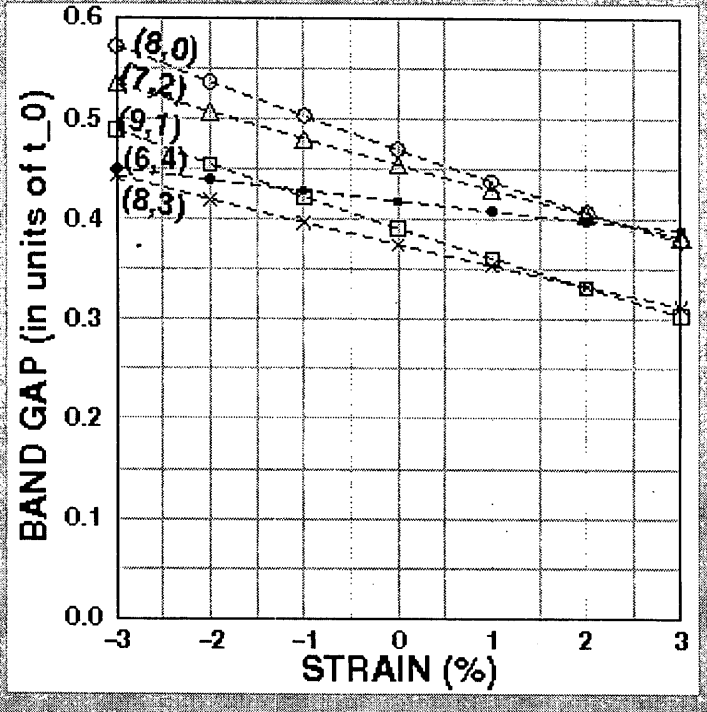


AFM Deformed versus Stretched



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.