A HYBRID CONTINUUM/TIGHT-BINDING ANALYSIS TO STUDY THE EFFECT OF MECHANICAL DEFORMATION ON THE ELECTRICAL PROPERTY OF CARBON NANOTUBES

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Carbon nanotubes show great promise for nano-electronic applications due to their superb electrical properties. Recent experiments, however, show that the electrical conductance of carbon nanotubes may change by two orders of magnitude upon mechanical deformation. This makes carbon nanotubes suitable for NEMS, but may also constitute a potential problem for the reliability of carbon nanotube-based electronics.

We have developed a continuum theory based on the interatomic potential for carbon. This continuum analysis provides the atomic positions of the deformed carbon nanotube. The k-space tight-binding calculations then give the band gap, which is an indication whether the deformed carbon nanotubes has the metal-like or semiconductor-like electrical properties.