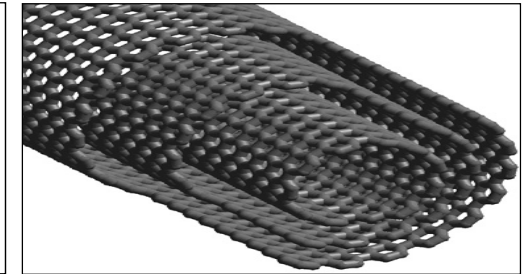
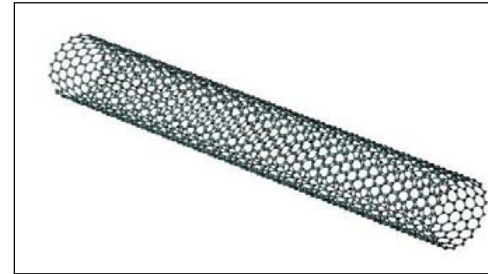


# Multi-physics Simulations of Carbon nanotubes

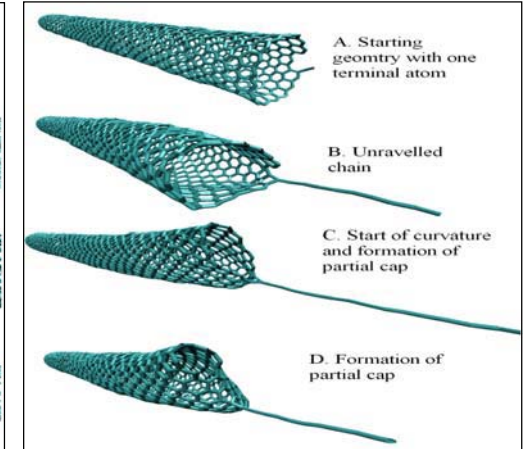
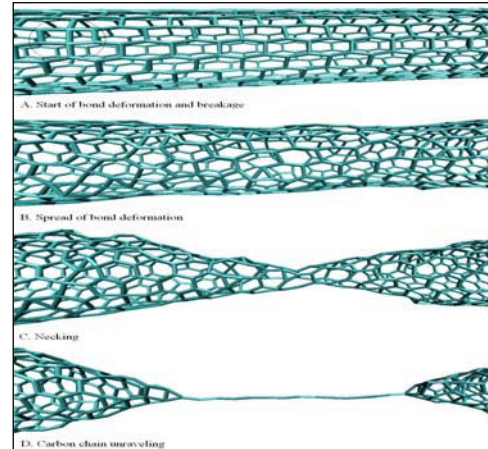
## What are Carbon nanotubes (CNT)?

- They are the tubes formed from folding around a sheet of graphene composed of carbon atoms formed a honey comb shape.
- They can have diameters ranging from 1nm to 60 nm, and lengths ranging from few nanometers to few centimeters.
- They can be single-walled or Multi-walled CNT.



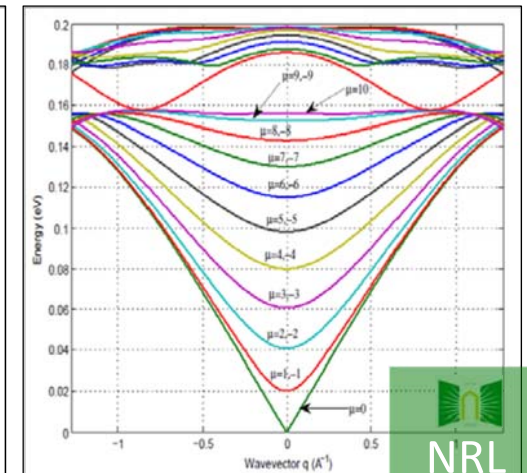
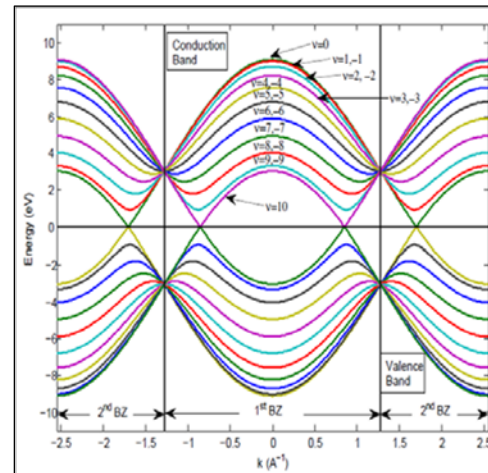
## Mechanical simulations of CNTs

- Due to their extreme small size approaching atomic scale, continuum mechanics (FEM) cannot be used for analysis.
- To understand the mechanics and predict the mechanical properties, accurate Molecular Dynamics (MD) simulations are used with virial stress theory for calculating the stresses till failure.
- The model can be used to analyze SWCNTs and MWCNT.
- MD simulations is used to predict the unraveling of CNTs under electric field during field emission.



## Thermo-electrical simulations of CNTs

- Coupled MD/MC (Monte Carlo) simulations is proposed to model the thermal and electrical properties of SWCNTs.
- A model for accurately including the hot phonon effects will be used for the first time for any material.



## Applications

- Mechanically: CNTs are used in high strength composites for military and high demand applications.
- Thermoelectrically: CNTs is expected to replace copper for ULSI nanoelectronics due to their excellent thermal and electrical properties.