Carbon Nanotube Diode Design

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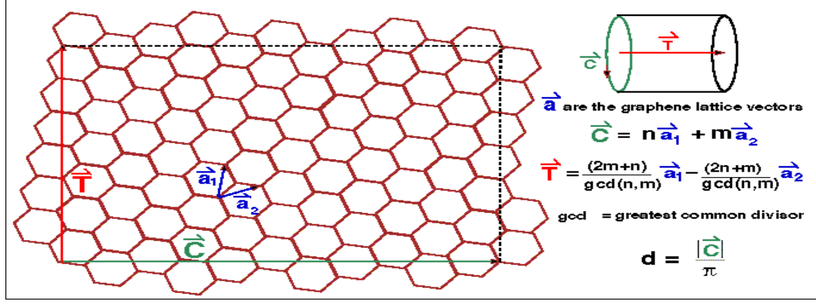
Motivation:

Recently techniques for the production of junctions between different carbon nanotubes (CNT) have been developed. The experimental observation that these contacts exhibit nonlinear IV characteristics leads to their potential application as molecular nanoscale device components.

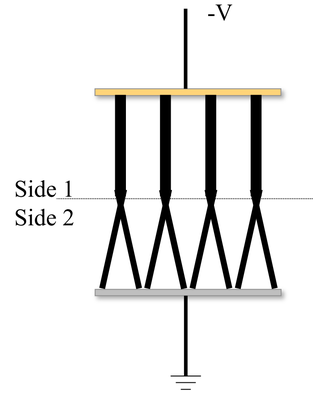
Objective:

Develop tube-diameter dependent models for the effective mass, doping, band offset, and dielectric constant of a CNT and then, using standard heterojunction physics, relate the physical properties of a y-junction array of CNTs (diameters) to its electrical properties (IV).

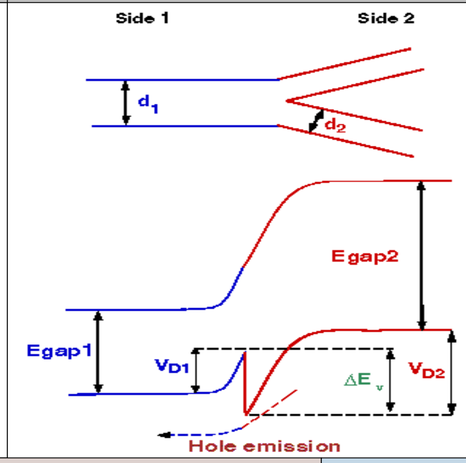
Unit cell



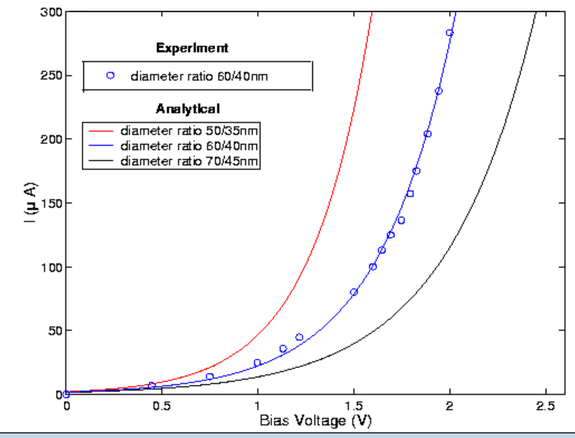
CNT Y-junction array



Band edge of junction



IV plot for a y-junction array



- **Electron orbital hybridization gives acceptor density:**

$$N_A \propto N(a_{cc}/d)^{\beta} \quad (N,\beta) \text{ constants}$$

- **Average bond energy method gives band offset:**

$$\Delta E_v = \gamma a_{cc}\left(1/d_2 - 1/d_1\right)$$

- **Linear response approximation gives dielectric constant :**

$$\varepsilon \propto \left(dN_A/m^*\right) \text{ X (CNT number in array)}$$

- **Treating semiconducting CNT y-junction as a thermionic emitter of holes, obtain the forward bias current:**

$$I_{d_1d_2}(V) = I_o(d_1,d_2)\exp\left(\frac{eV+\gamma a_{cc}\left(1/d_2-1/d_1\right)}{k_bT\left(1+8(d_1/d_2)^{2(\beta-2)}\right)}\right)$$

$$I_o = \alpha\left(\frac{a_{cc}}{d_2}\right)^{(\beta-3/2)}\left(\frac{d_2}{2^{(1/2-\beta)}d_1}\right)^{\left[(\beta-1/2)/\left(1+8(d_1/d_2)^{\beta(\beta-2)}\right)\right]}$$

$$\alpha \approx \left(eN_2a_{cc}^{\,2}\sqrt{\pi k_bT}/10\right)$$

- **Comparison with experiments of:**

[C. Papadopoulos et al., Phy. Rev. Lett. **85,** 3476 (2001).]

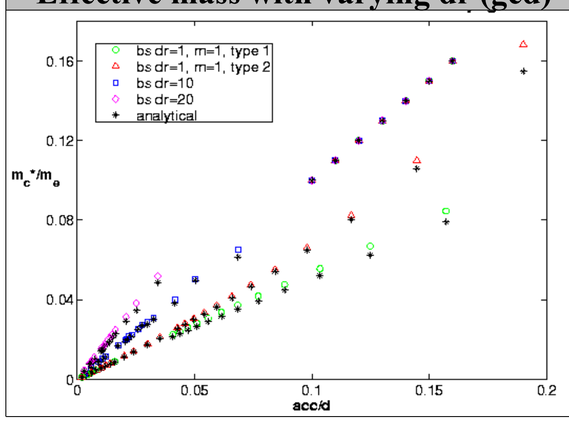
$$\beta = 2.74 \qquad N_2 \cong 3X10^{28}\,cm^{-3}$$

Effective mass averaged over indices (n,m)

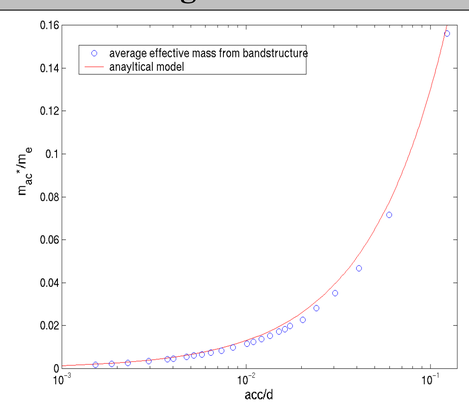
$$m^* = 1.3m(a_{cc}/d)$$

m_e :Electron mass a_{cc}:C bond length d :diameter

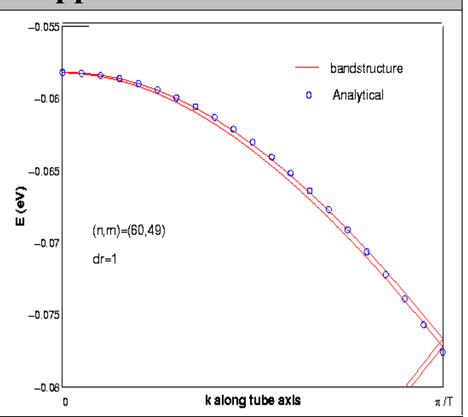
Effective mass with varying dr (gcd)



Average effective mass



Upper valence bands of CNT



Conclusion:

- **Theory for CNT diameter dependence of effective mass, doping, band offset, and dielectric constant useful in predicting electric properties of rectifying junctions.**
- **Comparison with limited data available gives a donor level of about one in every 60 Carbon atoms in the CNT.**