Abstract:

Modeling Ballistic Current Flow in Carbon Nanotube Wires

M. P. Anantram

Experiments have shown carbon nanotubes (CNT) to be almost perfect conductors at small applied biases [1]. The features of the CNT band structure, large velocity of the crossing subbands and the small number of modes that an electron close to the band center / Fermi energy can scatter into, are the reasons for the near perfect small bias conductance. We show that the CNT band structure does not help at large applied biases - electrons injected into the non crossing subbands can either be Bragg reflected or undergo Zener-type tunneling. This limits the current carrying capacity of CNT [2]. We point out that the current carrying capacity of semiconductor quantum wires in the ballistic limit is different, owing to its band structure.

The second aspect addressed is the relationship of nanotube chirality in determining the physics of metal-nanotube coupling [3]. We show that a metallic-zigzag nanotube couples better than an armchair nanotube to a metal contact. This arises because in the case of armchair nanotubes, while the pi band couples well, the pi* band does not couple well, to the metal. In the case of zigzag nanotube both crossing modes couple reasonably well to the metal. Many factors such as the role of curvature, strain and defects will play a role in determining the suitability of nanotubes as nanowires. From the limited view point of metal-nanotube coupling, we feel that metallic-zigzag nanotubes are preferable to armchair nanotubes.

Modeling Ballistic Current Flow in Carbon Nanotube Wires

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Topics Studied

Nanotube = carbon nanotube

Defects

BEND

TWIST
STRETCH

Phonons / Mechanical Deformation

* Bragg reflec.: Intrinsic mechanism, which exists even in an ideal situation
* = This Poster

Frank et. al, Science 280 (1998)

- \( V_{\text{APPLIED}} < 200 \text{mV}, G = 2e^2/h \)
- \( V_{\text{APPLIED}} > 200 \text{mV}, \) slow increase

- \( E < 120 \text{meV}, \) non-crossing bands open
- At \( E = 2eV \), electrons are injected into about 80 subbands
- Yet the conductance is only \( 3.75 e^2/h \)

Current-carrying capacity of carbon nanotubes

- Close to \( E = 0 \), only two sub-bands, \( \text{Conductance} = \frac{4e^2}{h} \) \( (6 \text{ kJ}) \)
- At higher energies, \( \text{Conductance} = \frac{(20 - 30)e^2}{h} \) \( (< 1 \text{kJ}) \)

Can subbands at the higher energies be accessed to drive large currents (small resistance) through these molecular wires?
**Semiclassical viewpoint**

- The strength of the two processes are determined by:
  - Tunneling distance ($X_{tunnel}$) → Screening length
  - Barrier height, $2\Delta E_{NC}$
  - Scattering and Defects
- $\Delta E_{NC} \propto 1/\text{Diameter}$. So, the importance of Zener tunneling increases with increase in nanotube diameter.

Bragg reflection severely limits the current carrying capacity

The crossing metallic-type bands conduct current.
Current carrying capacity of non-crossing subbands is limited.

Large diameter nanotubes: non-crossing bands will partially conduct due to Zener-type tunneling.
Conductances significantly larger (ten times) than $4e^2/h$ would be difficult.

**Coupling of carbon nanotubes to metallic contacts**

Electronic properties of nanotubes are closely related to chirality:
- Metal versus Semiconductor
- Bandgap change with deformation / strain

Questions:
Is there a preferable nanotube chirality to maximize current flow?
Role of wave vector conservation?
Explain experimentally observed scaling of conductance with contact length

**Parameters that influence current flow:**
- Strength of coupling to metal
- Length of metal-nanotube contact
- Defects
- Metal Fermi wave vector
**GRAFHE NE SHEET IN UNIFORM CONTACT WITH METAL**

![Graphene Sheet Image]

For good coupling: Metal $k_{\text{Fermi}} > 4\pi/3a_0$ (1.7 Å)

<table>
<thead>
<tr>
<th>Metal</th>
<th>$k_{\text{Fermi}}$ Å⁻¹</th>
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<tbody>
<tr>
<td>Cs</td>
<td>0.65</td>
</tr>
<tr>
<td>Ag</td>
<td>1.20</td>
</tr>
<tr>
<td>Au</td>
<td>1.37</td>
</tr>
<tr>
<td>Hg</td>
<td>1.75</td>
</tr>
</tbody>
</table>

K-vector along plane is not conserved for most metals

→ Poor coupling


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**Scattering rate**

$$\Psi = e^{i\hbar k_x L} \phi \quad n = \text{integer and } \phi \text{ is wave func. of atoms in a 1D unit cell}$$

Scattering rate from metal to nanotube (Born approx.):

$$1/\tau \propto | < \Psi_{nt} | V_{m-nt} | \Phi_m | |^2$$

$$\delta(k_x - k_x^m)$$

$| < \phi | V_{m-nt} | \phi_m | |^2$

- $k_x$ is conserved
- $k_y$ conservation is relaxed due to finite width of contact area

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**How do we model the system?**

- $\pi$ electron tight binding model
- Metal is modeled as a free electron gas ($k_F$)

<table>
<thead>
<tr>
<th>ARMCHAIR</th>
<th>ZIGZAG</th>
</tr>
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</table>
| E=0 at $k_x = 2\pi/3a_0 = 0.85$ Å⁻¹ | E=0 at $k_x = 0$
| Metal with $k_{\text{Fermi}} < 0.85$ Å⁻¹ couples weakly; threshold $k_{\text{Fermi}}$ | No threshold for $k_{\text{Fermi}}$

Below threshold $k_{\text{Fermi}}$, $T$ does not scale with increase in contact length.

- $T_{RL} + T_{ML} + T_{LL} = 2$

- Compute self energy due to: (i) metal & (ii) semi-infinite CNT leads
LARGE DIAMETER TUBES

- Use $k_{\text{Metal}}$ larger than $4\pi/3a_0$

ARMCHAIR

- Threshold for $k_f$ is $2\pi/3a_0 = 0.85 \, \text{Å}^{-1}$
- For zigzag tubes, $T_{\text{LM}}$ is small for $k_f \leq 1.2 \, \text{Å}^{-1}$ as a result of the large angular momentum, i.e. armchair tubes couple better than zigzag tubes.

ZIGZAG

- No threshold for $k_f$
- (see $k_f = 0.4 \, \text{Å}^{-1}$ curve)

ARMCHAIR

- Technologically, the second option (right) is better
- We consider a contact length of 30 unit cells (72 Å for armchair and 125 Å for zigzag nanotubes), and vary the coupling strength.

ZIGZAG

- Armchair: Transmission is pinned at values close to unity for metal $k_f$ of 0.9 and 1.2 Å$^{-1}$
- Zigzag: Transmission increases to two (maximum possible value)
- At small coupling strengths, transmission increases more rapidly in the armchair case
Nodes on the cylinder - Shape of NT wave function

\[ \Psi = e^{ik_x a_0 \phi} \]

Scattering rate from Metal to Nanotube \( \propto \langle \phi_{\text{nanotube}} | H_{\text{coupling}} | \phi_{\text{metal}} \rangle \)

- Side-contacted: zigzag nanotube are more desirable (curvature)
- Larger metal Fermi wave vector helps.

Conclusions

- \( \text{d}I/\text{d}V \text{ versus } V \) does not increase in a manner commensurate with the increase in number of subbands.

- The increase in \( \text{d}I/\text{d}V \) with bias is much smaller than the increase in the number of subbands - a consequence of bragg reflection

- Requirement for axial wave vector conservation:
  \( \text{ARMCHAIR} \)
  cut-off \( K_{\text{Fermi}} = 2 \alpha / 3 a_0 \approx 0.85 \text{Å}^{-1} \)
  cut-off \( K_{\text{Fermi}} = 0 \)

- Our calculations show an increase in transmission with length of contact, as seen in experiments.

- It is desirable for molecular electronics applications to have a small contact area, yet large coupling. In this case, the circumferential dependence of the nanotube wave function dictates:
  - Transmission in armchair tubes saturates around unity
  - Transmission in zigzag tubes saturates at two

At what applied voltage are electrons injected into higher subbands?

Bias at which electrons are injected into non crossing subbands is \( \Delta E_{\text{MC}} \)

<table>
<thead>
<tr>
<th>ΔE_{\text{MC}} (eV)</th>
<th>(5,5)</th>
<th>(10,10)</th>
<th>(20,20)</th>
<th>(40,40)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7Å</td>
<td>1.9</td>
<td>0.98</td>
<td>0.5</td>
<td>0.25</td>
</tr>
<tr>
<td>56Å</td>
<td></td>
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For example, in a (20,20) nanotube electrons are injected into over 20 subbands at an energy of 2.5 eV.

The maximum conductance if the Fermi energy is at 2.5 eV is \( 40e^2/\hbar \).