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ABSTRACT OR SUPPORTING INFORMATION

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Abstract:

Modeling Ballistic Current Flow in Carbon Nanotube Wires

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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.

[1] S. Frank, P. Poncharal, Z. L. Wang and W. A. de Heer, Conductance quantization in multi-walled carbon nanotube, Science, vol. 280, p. 1744 (1998); P. G. Collins, M. Hersam, M. Arnold, R. Martel, and Ph. Avouris, Current Saturation and Electrical Breakdown in Multiwalled Carbon Nanotubes Phys. Rev. Lett., v. 86, p. 3128 (2001)
[2] M. P. Anantram, Current Carrying Capacity of Carbon Nanotubes Phys. Rev. B, vol. 62, p. R4837, (2000)
[3] M. P. Anantram, Which nanowire couples better to metals: Armchair or zigzag carbon nanotubes? Appl. Phys. Lett., v. 78, p..2055, (2001)

Modeling Ballistic Current Flow in Carbon Nanotube Wires

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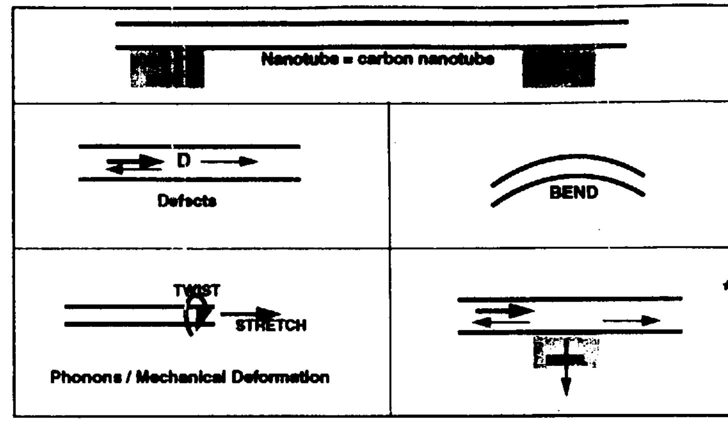
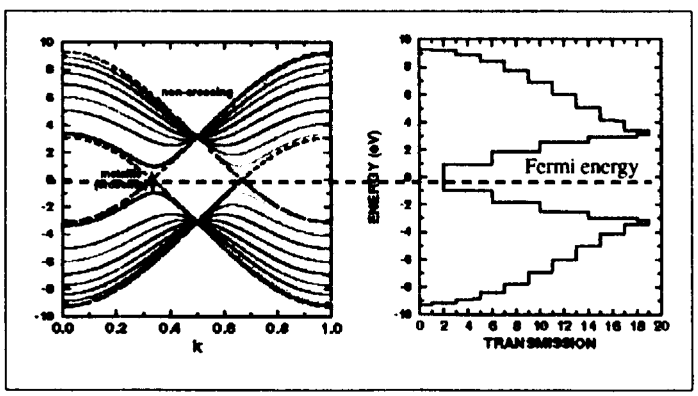
Topics Studied



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

* = This Poster

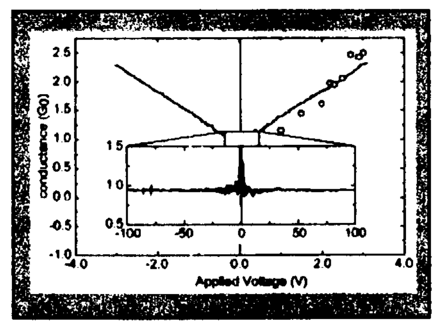
Current-carrying capacity of carbon nanotubes



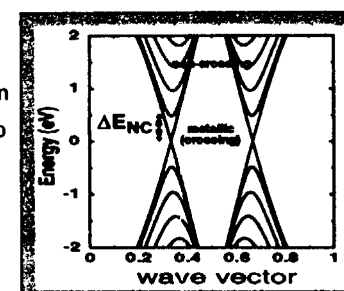
- **Close to E=0, only two sub-bands,** $Conductance = \frac{4e^2}{h}$ **(6 kΩ)**
- **At higher energies,** $Conductance = \frac{(20-30)e^2}{h}$ **(< 1kΩ)**

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

Frank et. al, Science 280 (1998)



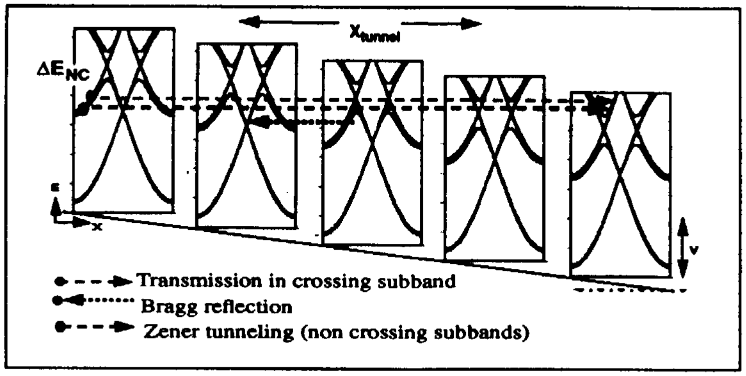
- $V_{APPLIED}$ < 200mV, G~$2e^2/h$
- $V_{APPLIED}$ > 200mV, slow increase



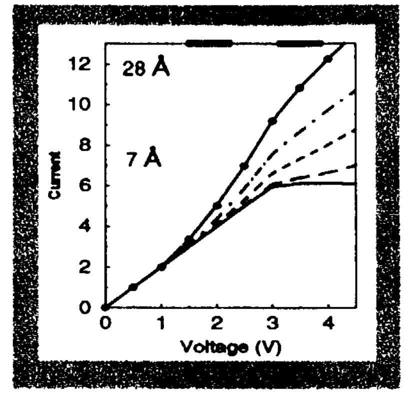
- E~ ±120meV, non-crossing bands open
- At E~2eV, electrons are injected into about 80 subbands

- Yet the conductance is only ~ 3.75 e^2/h

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
- ΔE_{NC} α 1/Diameter. So, the importance of Zener tunneling increases with increase in nanotube diameter.



- L=10 Å
- $dI/dV \sim 4e^2/h$ for $V_a < 2\Delta E_{NC}$
- Threshold changes with diameter
- What happens with increase in nanotube diameter?
- Barrier height (ΔE_{NC}) decreases with increase in diameter
- Total Current increases with increase in diameter

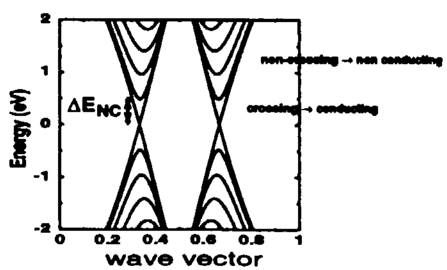
The differential conductance is NOT comparable to the increase in the number of subbands.

For a (20,20) nanotube, there are 35 subbands at E = ± 3.5V.

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:

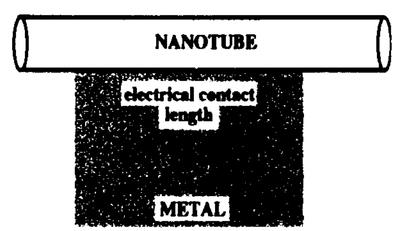
- Metal versus Semiconductor
- Bandgap change with deformation / strain.

Questions:

Is there a preferable nanotube chirality to maximize current flow?

Role of wave vector conservation?

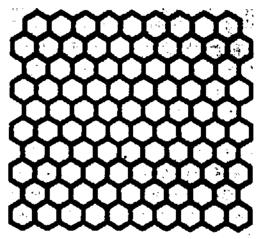
Explain experimentally observed scaling of conductance with contact length



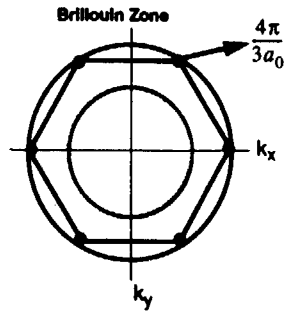
Parameters that influence current flow:

- Strength of coupling to metal
- Length of metal-nanotube contact
- Defects
- Metal Fermi wave vector

GRAPHENE SHEET IN UNIFORM CONTACT WITH METAL



FEG



K_{Fermi} Å^{-1}	
Cs	0.65
Ag	1.20
Au	1.21
Hg	1.37
	1.75
⬡	1.7

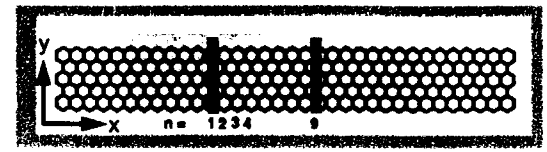
For good coupling: Metal $K_{Fermi} > 4\pi/3a_0$ (1.7Å)

K-vector along plane is not conserved for most metals
⇒ Poor coupling.

Ashcroft & Mermin, Solid State Physics

J. Tersoff, Appl. Phys. Lett, v. 74, p. 2122 (1999)

Scattering rate



$\Psi = e^{ink_xL}\phi$ n = integer and ϕ is wave func. of atoms in a 1D unit cell

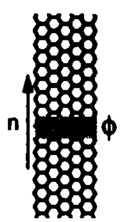
Scattering rate from metal to nanotube (Born approx.):

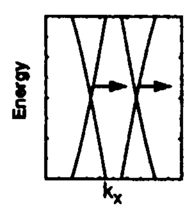
$$1/\tau \propto |< \Psi_{nt} | V_{m-nt} | \Phi_m >|^2$$

$$\delta(k_x - k_x^m) \qquad |< \phi | V_{m-nt} | \phi_m >|^2$$

- K_x is conserved
- K_y conservation is relaxed due to finite *width* of *contact area*

$$1/\tau \propto \quad \delta(k_x - k_x^m) \quad |< \phi | V_{m-nt} | \phi_m >|^2$$



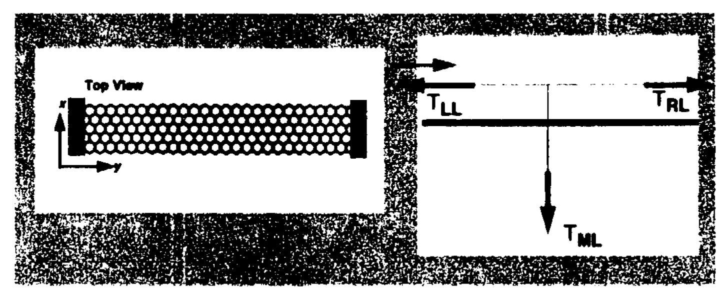


ARMCHAIR	ZIGZAG
E=0 at $k_x = 2\pi/3a_0 = 0.85$ Å^{-1} Metal with $k_{Fermi} < 0.85$ Å^{-1} couples weakly; threshold k_{Fermi}	E=0 at $k_x = 0$ No threshold for k_{Fermi}

Below threshold k_{Fermi} - T does not scale with increase in contact length.

How do we model the system?

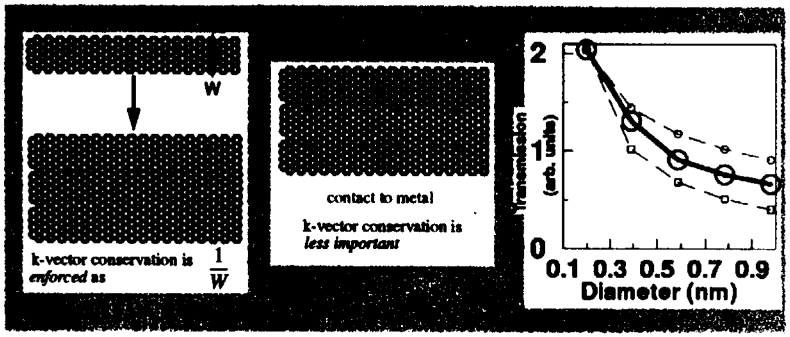
- π electron tight binding model
- Metal is modeled as a free electron gas (k_F)



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

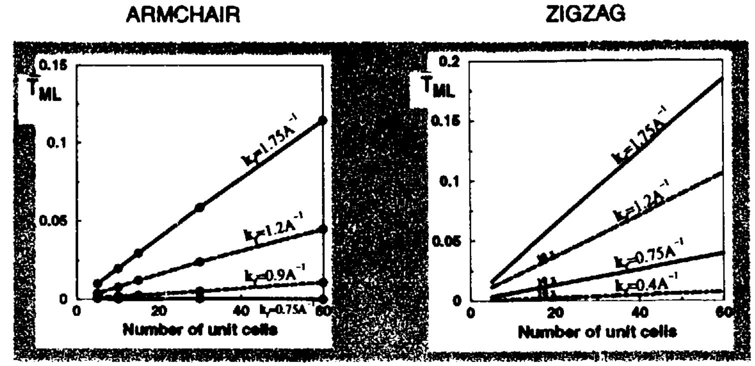
- Phys. Rev. B, v.58, p. 4882 (1998) and v. 61, p. 14219 (2000)
- Compute self energy due to: (i) metal & (ii) semi-infinite CNT leads

LARGE DIAMETER TUBES



- Increase Transmission: Small phase coherence length in metal / disorder in metal-CNT coupling [Frank et.al, Science, v.280 (1998)]

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

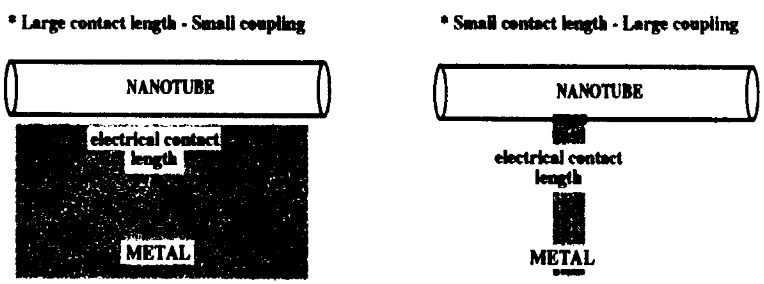


- threshold for k_f is $\frac{2\pi}{3a_0}$ =0.85 Å^{-1} (see k_f = 0. 75A^{-1} and 0.9A^{-1} curves)

no threshold for k_f (see k_f = 0.4Å^{-1} curve)

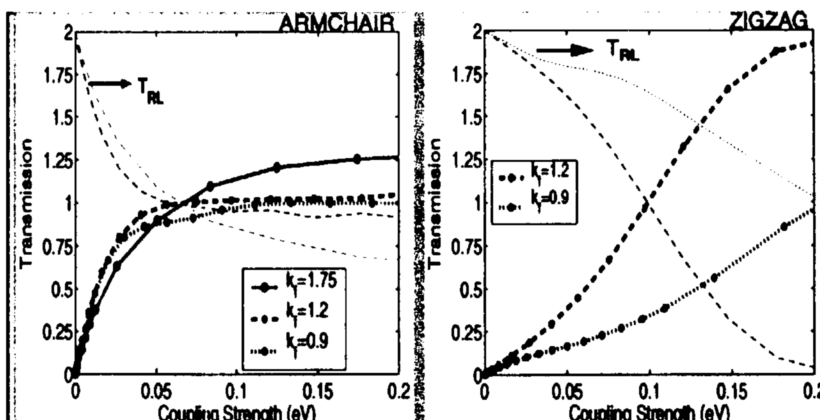
- For zigzag tubes, T_{LM} is small for $k_f \leq 1.2$ Å^{-1} as a result of the large angular momentum. i.e. armchair tubes couple better than zigzag tubes
- Transmission *increases* with contact length as seen in experiment by Tans et. al., Nature, vol. 386, 474 (1997)

- T is small compared to the maximum possible value of 2.
- Experimentally two possible scenarios are possible to increase T:

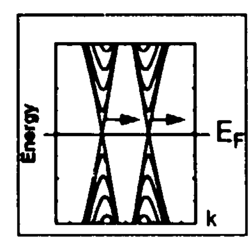


- Technologically, the second option (right) is better

- We consider a contact length of *30 unit cells* (72 Å for armchair and 125 Å for zigzag nanotubes), and vary the coupling strength.

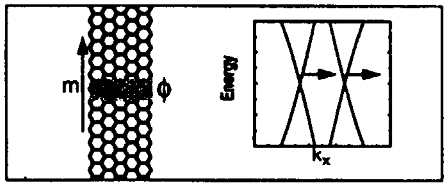


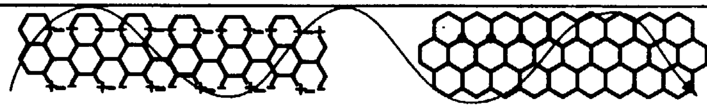
- Armchair:Transmission is pinned at values close to unity for metal k_f of 0.9 and 1.2 Å^{-1}
- Zigzag: Transmission increases to two (maximum possible value)
- At small coupling strengths, transmission increases more rapidly in the armchair case



Nodes on the cylinder - Shape of NT wave function

$$\Psi = e^{imk_x a_0}\phi$$





k_x 0.85 Å^{-1} $\qquad \phi(\bullet)+\phi(\bullet)+\phi(\bullet)=0 \qquad 0\ k_x$

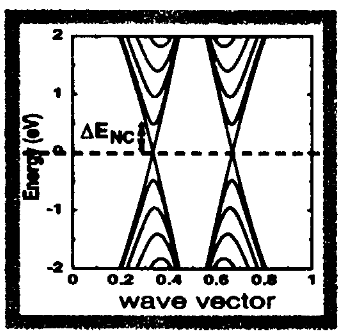
metal k_f=0.90 Å^{-1} → distance between nodes 6 Å
Gold k_f=1.20 Å^{-1} → distance between nodes 3.4 Å
Aluminum k_f=1.75 Å^{-1} → distance between nodes 2 Å

Scattering rate from Metal to Nanotube α $\langle \phi_{nanotube} | H_{coupling} | \psi_{metal} \rangle$

$\langle + - | H_{coupling} | \psi_{metal} \rangle \sim 0$. Hence, Transmission is pinned close to unity.

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

At what applied voltage are electrons injected into higher subbands?



Bias at which electrons are injected into non crossing subbands is ΔE_{NC}

7Å $\qquad$ 56Å

size	(5,5)	(10,10)	(20,20)	(40,40)
ΔE_{NC} (eV)	1.9	0.98	0.5	0.25

For example, in a (20,20) nanotube electrons are injected into over 20 subbands at an energy of2.5eV.

The maximum conductance if the Fermi energy is at 2.5 eV is ~ $40e^2/h$

Conclusions

- dI/dV versus V does not increase in a manner commensurate with the increase in number of subbands.

- The increase in dI/dV with bias is much smaller than the increase in the number of subbands - *a consequence of bragg reflection*
- Requirement for axial wave vector conservation:

ARMCHAIR: cut-off $K_{Fermi} = 2\pi/3a_0 = 0.85$Å^{-1}

ZIGZAG: cut-off $K_{Fermi} = 0$

- 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