Transport through carbon nanotube wires

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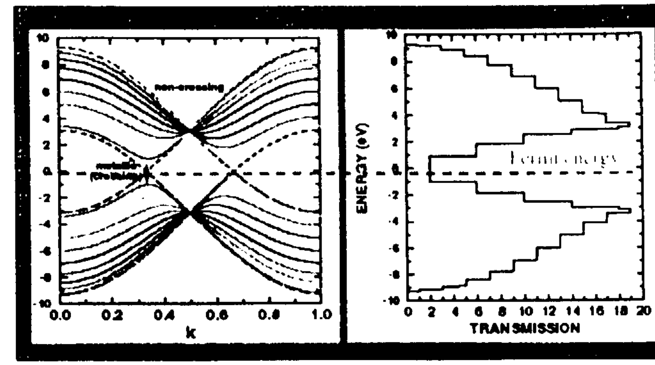
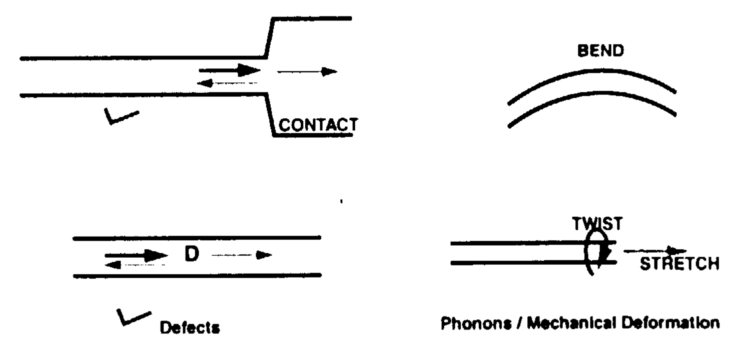
TRANSMISSION vs ENERGY OF (10,10) NANOTUBE



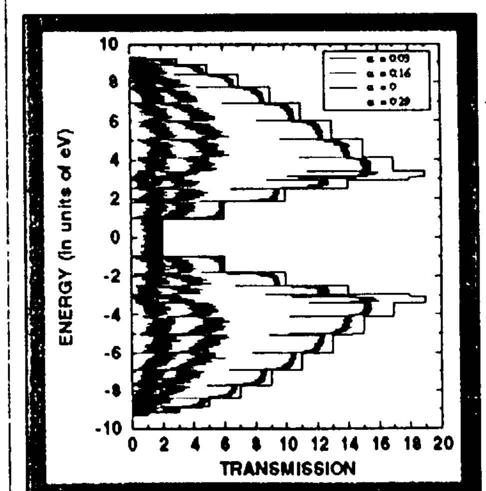
- Close to E=0, Resistance = 6 kΩ; At higher energies, less than 300 Ω
- Experimentally:
  - Max. small bias conductance ~ 12.5 kΩ
  - Max. large bias conductance ~ 4 kΩ

Common reasons for reflection



Bragg reflection: Intrinsic mechanism, which exists even in an ideal situation

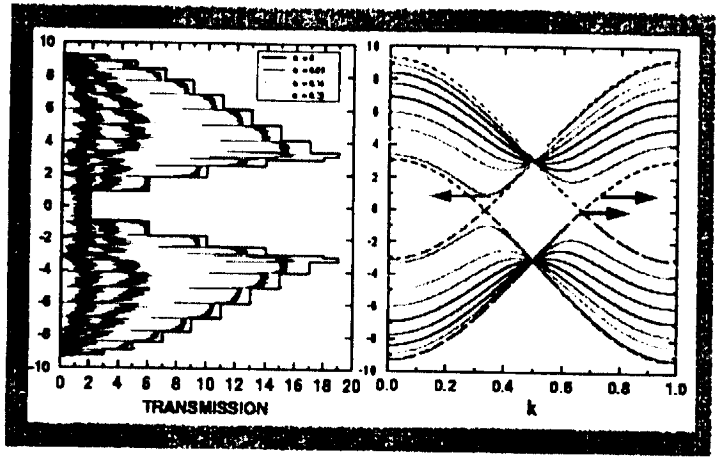
Transmission versus Energy with Defects



Transmission Probability:

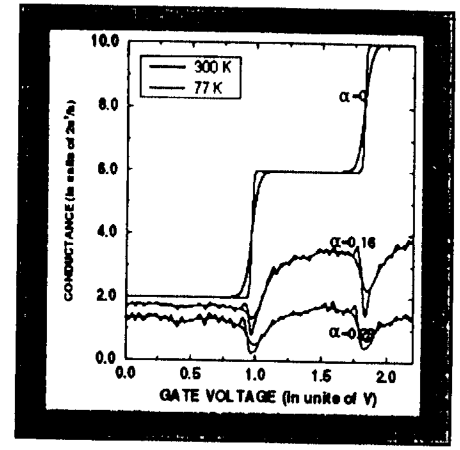
- Decreases with disorder
- Large Dips at some energies
- Very small decrease around E=0 (WIRES?)
- Localization length

Physical explanation of the transmission dips



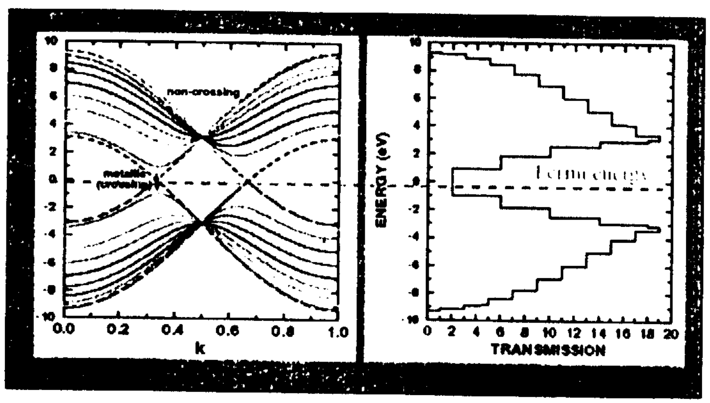
- E=0, Crossing bands: Large velocity (dE/dk)
- Large velocity states (⟶) at higher energies are prone to REFLECTION as they couple to low velocity states (and ⟵)

Conductance vs. Gate Voltage



- DIPS IN THE CONDUCTANCE WHEN THE FERMI ENERGY IS CLOSE TO THE SUB-BAND OPENINGS
- FERMI ENERGY AT THE BAND CENTER: GOOD WIRE

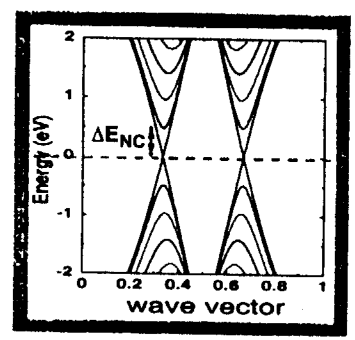
TRANSMISSION vs ENERGY OF (10,10) NANOTUBE



- **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?

At what applied voltage are electrons injected into higher subbands?



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

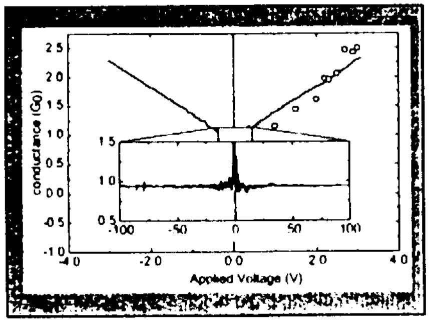
7Å 56Å

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

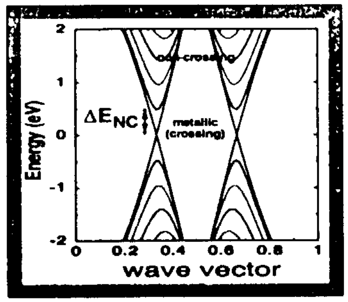
For example, in a (20,20) nanotube electrons are injected into over 20 subbands at an energy of2.5eV.

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

Frank et. al, Science 280 (1998)



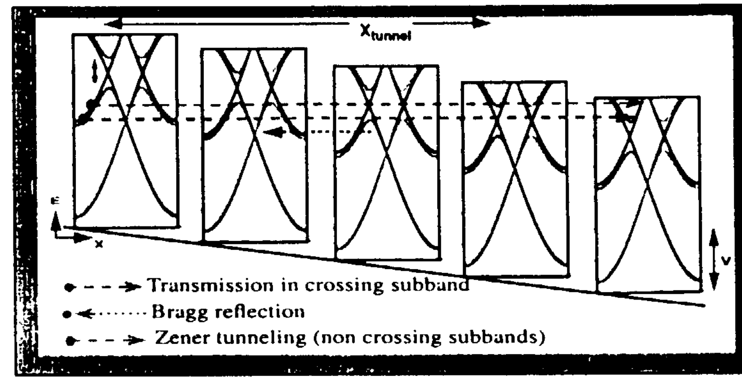
- V < 200mV, G~$2e^2/h$
- V > 200mV, slow increase in G with V.



- 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 picture at an applied bias

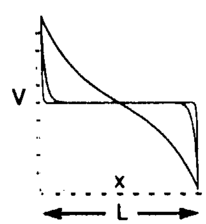


- The strength of the two processes are determined by:
  - Tunneling distance (X_{tunnel}) → Screening length
  - Barrier height, $2\Delta E_{NC}$
  - Scattering and Defects
- ΔE_{NC} α 1/Diameter. So, the importance of Zener tunneling increases with increase in nanotube diameter.

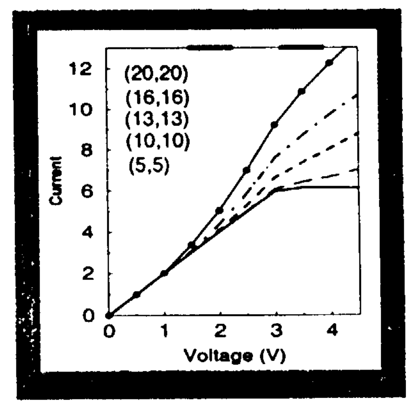
Model

- pi-orbital based tight binding calculation [Phys. Rev. B 58, 4882 (1998)]
- Ideal contacts - reflection less contacts
- Electrostatic potential drop
  - Linear
  - Exponential (Screening length, L_{sc})

$$V(x) = \frac{V_a}{2}\left\{1 + \frac{1+e^{\frac{L}{L_{sc}}}}{e^{-\frac{L}{L_{sc}}} - e^{\frac{L}{L_{sc}}}} e^{-\frac{x}{L_{sc}}} - \frac{1+e^{-\frac{L}{L_{sc}}}}{e^{-\frac{L}{L_{sc}}} - e^{\frac{L}{L_{sc}}}} e^{\frac{x}{L_{sc}}}\right\}$$



- L=2400 Å, L_{sc}=6, 50, 500 Å
- e-e and e-p scattering are not included



- L=10 Å
- $dI/dV \approx 4e^2/h$ for $V_a < 2\Delta E_{NC}$
- Threshold changes with diameter
- Barrier height (ΔE_{NC}) decreases with increase in diameter
- Total Current increases with increase in diameter
- $dI/dV > 0$ for $V_a > 3.1$ V, except for the (5,5) nanotube
- (5,5) nanotube ΔE_{NC}= 1.9eV

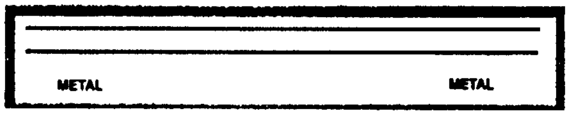
The differential conductance is NOT comparable to the increase in the number of subbands.

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

The main issues here are:

- How does a carbon nanotube couple to simple metals?
- Interplay between chiraliy, diameter and Fermi wave vector.
- Explain the experimentally observed scaling of conductance with contact length.

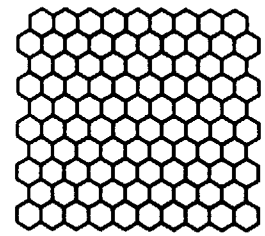
- Experiment: S. J. Tans et. al, Nature 386, 474 (1997)



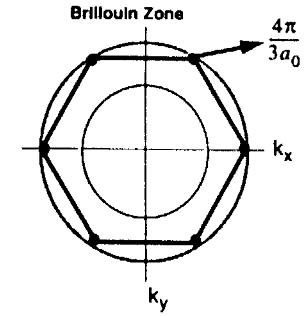
Outline:

- Coupling between a graphene sheet and metal
- What happens when the sheet----->strip (CNT)
- Dependence of coupling on width of strip and disorder

GRAPHENE SHEET IN UNIFORM CONTACT WITH METAL



FEG



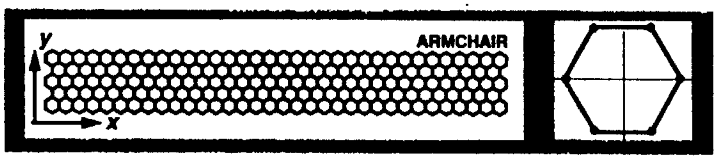
K_{Fermi} $Å^{-1}$	
Cs	0.65
Ag	1.20
Au	1.21
Hg	1.37
Al	1.75
⬡	1.7

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)

NANOTUBE IN UNIFORM CONTACT WITH METAL



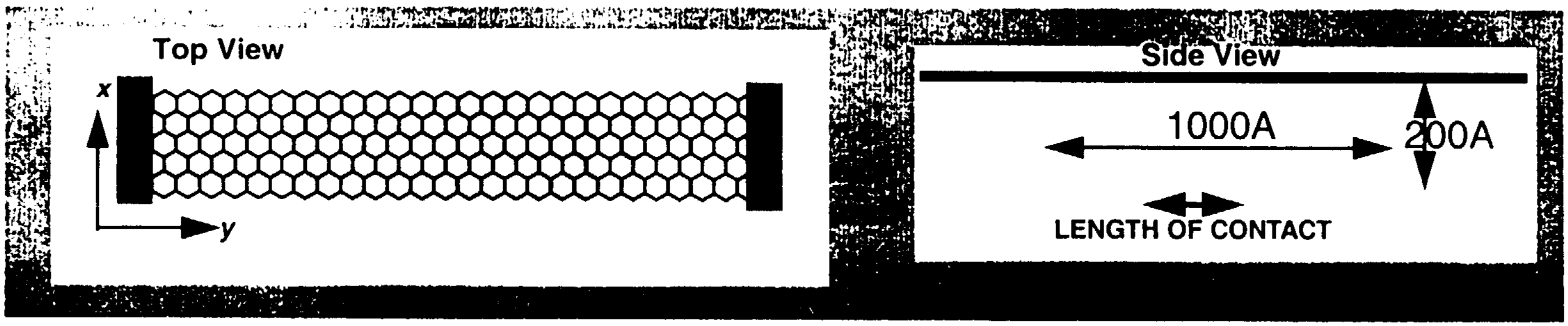
- K_x is conserved
- K_y conservation is relaxed due to finite *width* of *contact area*
- Metal couples better to CNT than to graphite
- Cut-off K_{Fermi} of metal is smaller than $\frac{4\pi}{3a_0}$ =1.7 $Å^{-1}$

$\Psi = e^{imk_x a_0}\phi$ m = integer and ϕ is wave func. of atoms in a 1D unit cell

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	E=0 at $k_x = 0$ No threshold for k_{Fermi}

How do we model the system?

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



- Phys. Rev. B v.58 (1998);
- Compute self energy due to: (i) metal & (ii) semi-infinite CNT leads

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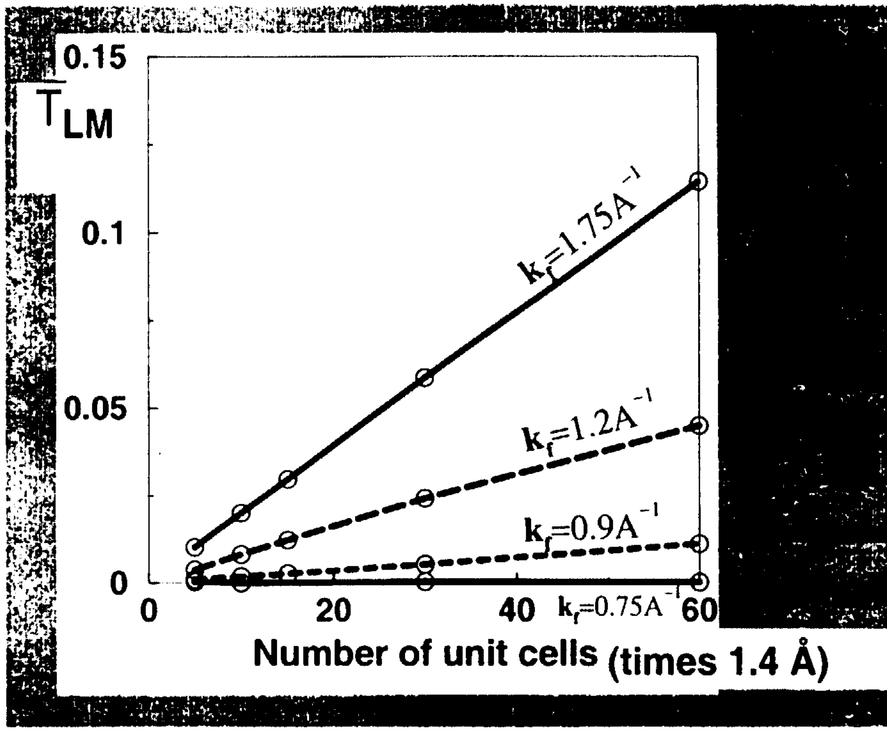

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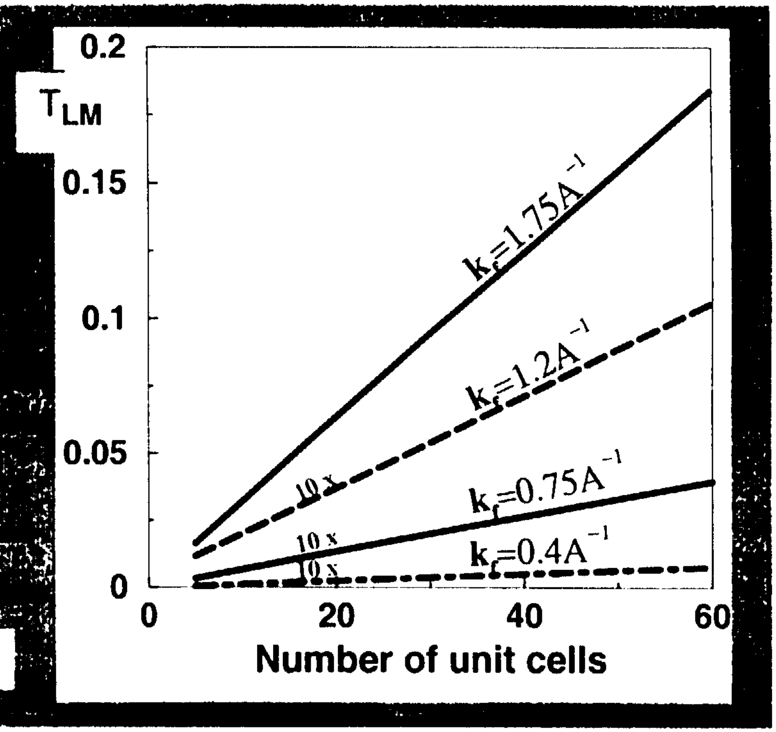

- threshold for k_f is $\frac{2\pi}{3a_0}$ =0.85 Å^{-1} — no threshold for k_f

(see k_f = 0. 75A^{-1} and 0.9A^{-1} curves) — (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)

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