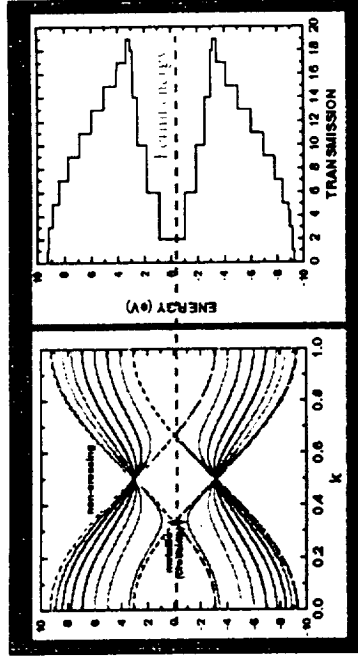


# Transport through carbon nanotube wires

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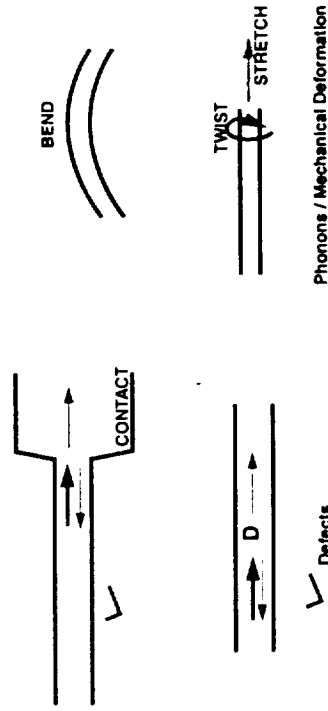
Acknowledgements: T. R. Govindan  
Jie Han  
Supriyo Datta  
Liu Yang  
Natalio Mingo

## TRANSMISSION vs ENERGY OF (10,10) NANOTUBE



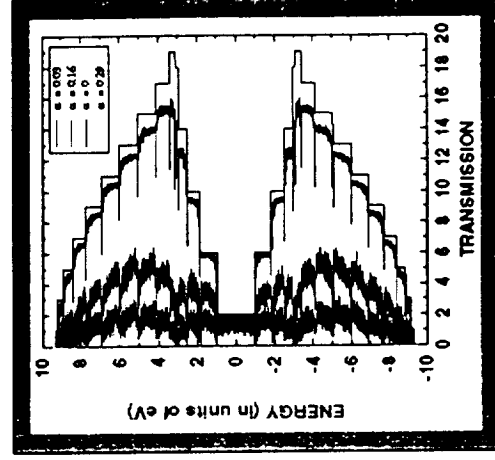
- Close to  $E=0$ , Resistance =  $6 \text{ k}\Omega$ ; At higher energies, less than  $300 \text{ }\Omega$
- Experimentally:
  - Max. small bias conductance  $\sim 12.5 \text{ k}\Omega$
  - Max. large bias conductance  $\sim 4 \text{ k}\Omega$

## Common reasons for reflection



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

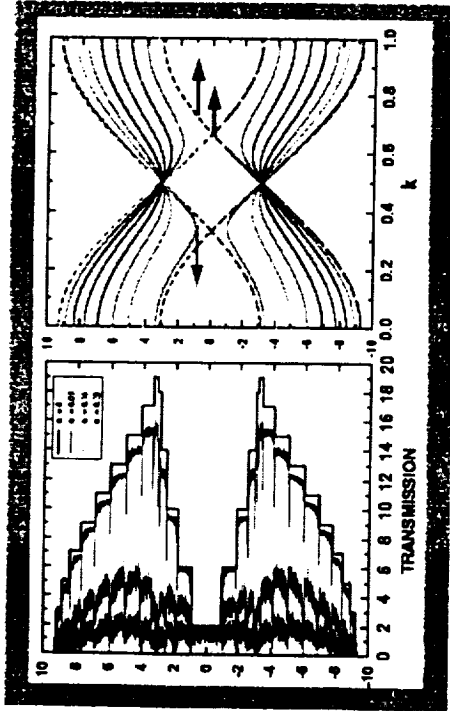
## Transmission versus Energy with Defects



### Transmission Probability:

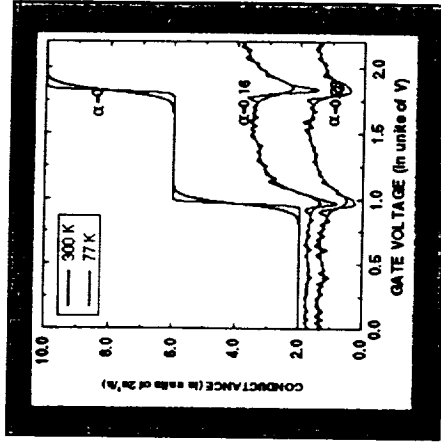
- Decreases with disorder
- Large Dips at some energies
- Very small decrease around  $E=0$  (WIRES?)
- Localization length

## Physical explanation of the transmission dips



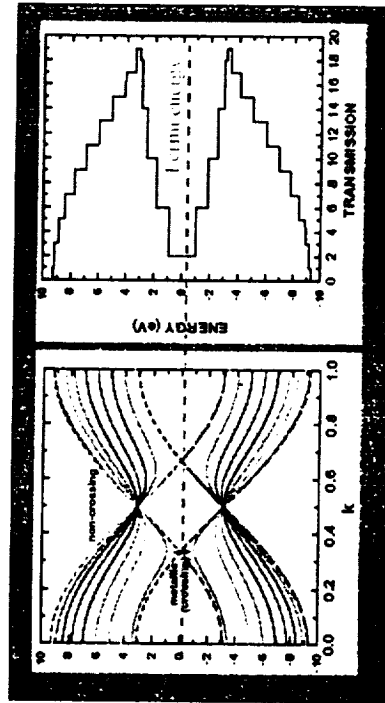
- $E=0$ , Crossing bands: Large velocity ( $dE/dk$ )
- Large velocity states ( $\rightarrow$ ) at higher energies are prone to REFLECTION as they couple to low velocity states ( $\leftarrow$ ) and ( $\leftarrow$ )

## 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

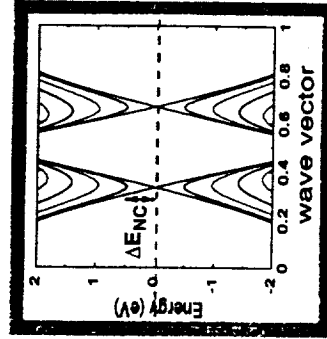
## TRANSMISSION vs ENERGY OF (10, 10) NANOTUBE



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

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?

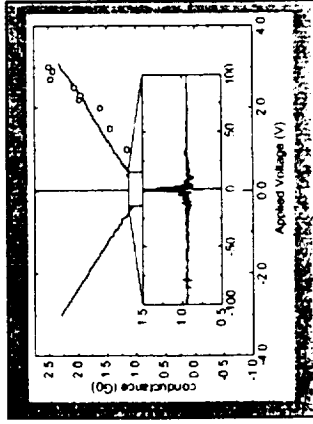


Bias at which electrons are injected into non crossing subbands is  $\Delta E_{NC}$

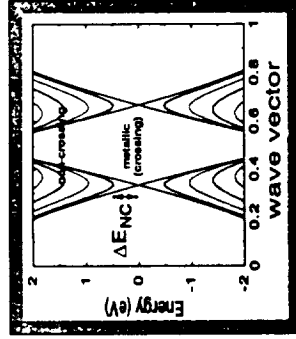
7A		56A	
size	(5,5)	(10,10)	(40,40)
$\Delta E_{NC}$ (eV)	1.9	0.98	0.5
	0.25		

For example, in a (20, 20) nanotube electrons are injected into over 20 subbands at an energy of 2.5 eV.

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



- $V < 200\text{mV}$ ,  $G \sim 2e^2/h$
- $V > 200\text{mV}$ , slow increase in  $G$  with  $V$ .

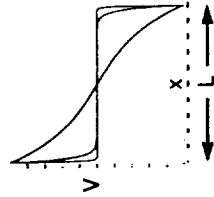


- $E \sim \pm 120\text{meV}$ , non-crossing bands open
- At  $E \sim 2\text{eV}$ , electrons are injected into about 80 subbands
- Yet the conductance is only  $\sim 3.75 e^2/h$

### Model

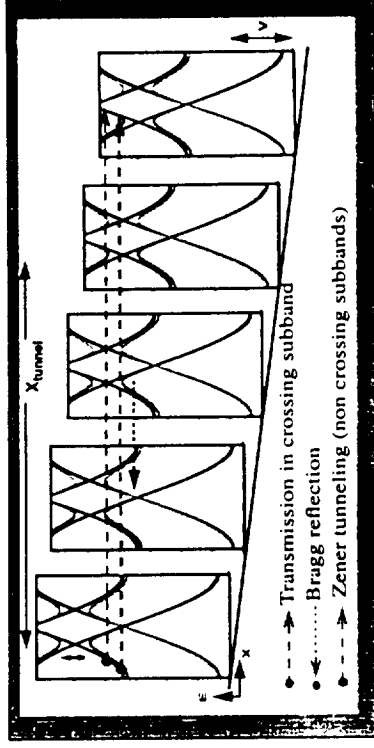
- pi-orbital based tight binding calculation [Phys. Rev. B **58**, 4882 (1998)]
- Ideal contacts - reflection less contacts
- Electrostatic potential drop
  - Linear
  - Exponential (Screening length,  $L_{sc}$ )

$$V(x) = \frac{V_0}{2} \left\{ 1 + \frac{1 + e^{-x/L_{sc}}}{e^{x/L_{sc}} - e^{-x/L_{sc}}} - \frac{1 + e^{-x/L_{sc}}}{e^{x/L_{sc}} - e^{-x/L_{sc}}} e^{x/L_{sc}} \right\}$$

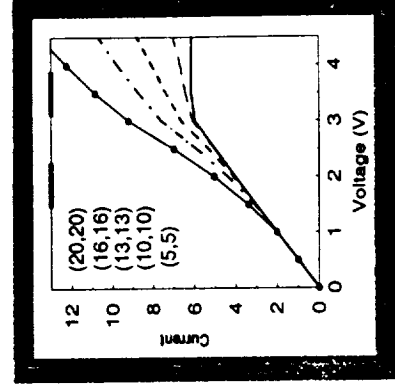


- $L = 2400 \text{ \AA}$ ,  $L_{sc} = 6, 50, 500 \text{ \AA}$
- e-e and e-p scattering are not included

### Semiclassical picture at an applied bias



- The strength of the two processes are determined by:
  - Tunneling distance ( $X_{\text{tunnel}}$ )  $\rightarrow$  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.



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

The differential conductance is NOT comparable to the increase in the number of subbands.  
For a (20,20) nanotube, there are 35 subbands at  $E = \pm 3.5\text{V}$ .

The main issues here are:

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

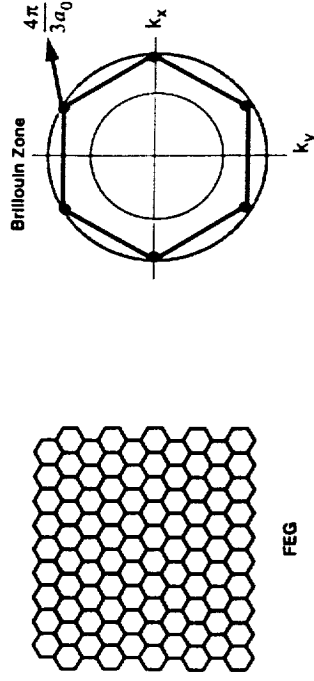
- Experiment: S. J. Tans et. al, Nature 386, 474 (1997)



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



For good coupling: Metal  $k_{\text{Fermi}} > 4\pi/3a_0$  (1.7 Å<sup>-1</sup>)

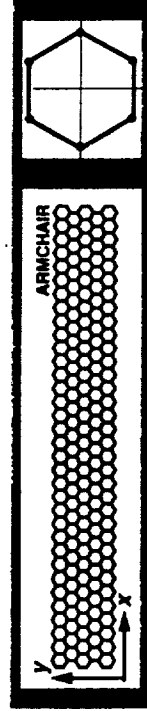
$k_{\text{Fermi}}$ Å <sup>-1</sup>	
Cs	0.65
Ag	1.20
Au	1.21
Hg	1.37
Al	1.75
$\frac{4\pi}{3a_0}$	1.7

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  $k_{\text{Fermi}}$  of metal is smaller than  $\frac{4\pi}{3a_0} = 1.7 \text{ Å}^{-1}$

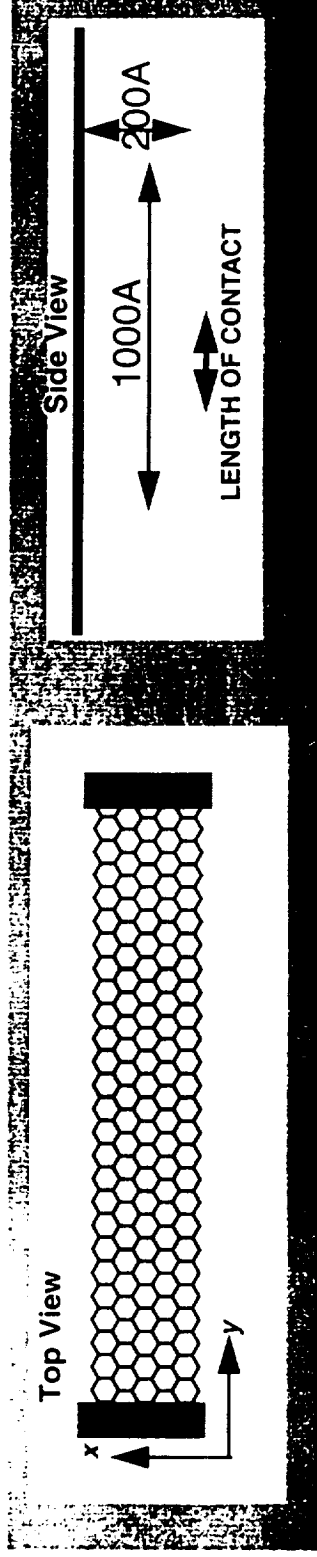
$$\Psi = e^{imk_x a_0} \phi \quad m = \text{integer and } \phi \text{ is wave func. of atoms in a 1D unit cell}$$

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

$$m = 1, 2, 3, 4, \dots$$

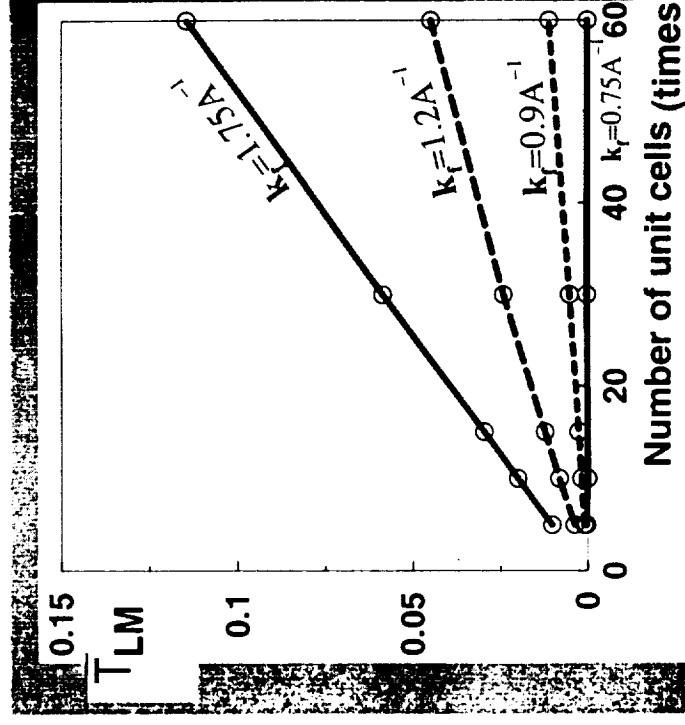
How do we model the system?

- 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

## ARMCHAIR

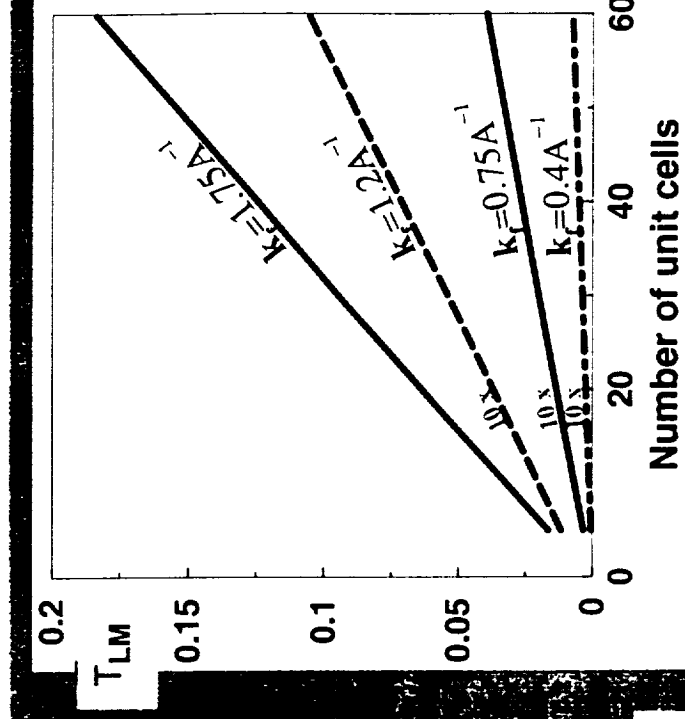


- threshold for  $k_f$  is  $\frac{2\pi}{3a_0} = 0.85 \text{ Å}^{-1}$

(see  $k_f = 0.75 \text{ Å}^{-1}$  and  $0.9 \text{ Å}^{-1}$  curves)

For zigzag tubes,  $T_{LM}$  is small for  $k_f \leq 1.2 \text{ Å}^{-1}$  as a result of the large

## ZIGZAG



- no threshold for  $k_f$

(see  $k_f = 0.4 \text{ Å}^{-1}$  curve)

- 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)