Presentation/Publication Information: APS Meeting, March 11-16, 2001, Seattle, WA

Acknowledgments:

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Abstract:

(Transparencies enclosed)

[K40.042] Coupling of armchair and zigzag tubes to a free electron metal

M. P. Anantram (NASA Ames Research Center, Moffett Field, CA 94035-1000)

The effect of nanotube chirality is of prime importance in determining its electronic properties. We address the issue of how chirality affects the coupling of a nanotube to metal contacts. We model coupling of armchair and zigzag nanotubes to metal contacts, in both the side- and end-contacted geometries. In the side-contacted geometry, the coupling of armchair and metallic-zigzag nanotubes to a free electron metal are significantly different. Namely, it is possible to drive a larger current through a metallic-zigzag nanotube. The predicted difference holds good when both (a) the entire circumference and (b) only a finite sector of the nanotube makes contact to the metal electrode. It might be possible to observe the predicted difference between armchair and zigzag nanotubes using gold contacts.

Which nanowire couples better electrically to a metal contact: Armchair or Zigzag NT?

M. P. Anantram

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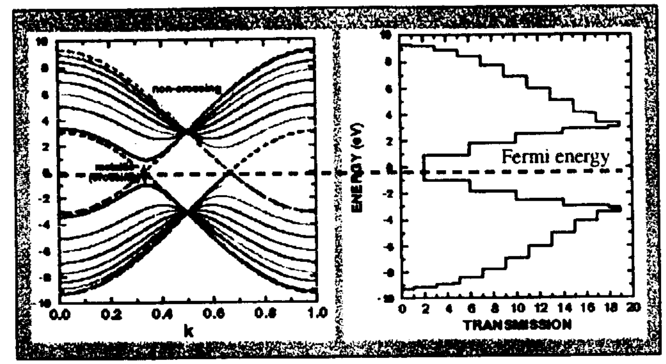
Transmission vs Energy of a (10,10) Nanotube



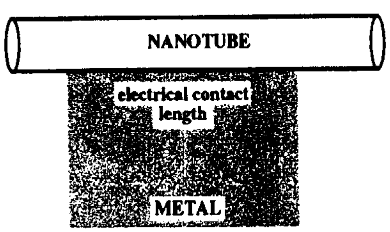
- Close to E=0: Total Transmission (T) = 2, Resistance = 6.5 kΩ

Electronic properties of nanotubes are closely related to chirality:

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

Question:

Is there a preferable nanotube chirality to maximize current flow?



Parameters that influence current flow:

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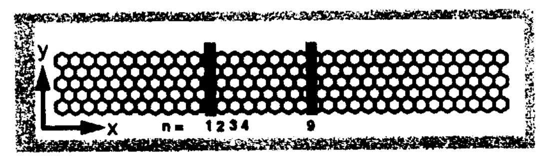
- Metal Fermi wave vector

Scattering rate



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

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

$$\alpha \ | < e^{ink_x L} \mid e^{ink_x^m L} > < \phi \mid V_{m\text{-}nt} \mid \phi_m > |^2$$

$$\alpha \quad \delta(k_x - k_x^m) \quad | < \phi \mid V_{m\text{-}nt} \mid \phi_m > |^2$$

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

- K_x is conserved
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How do we model the system?

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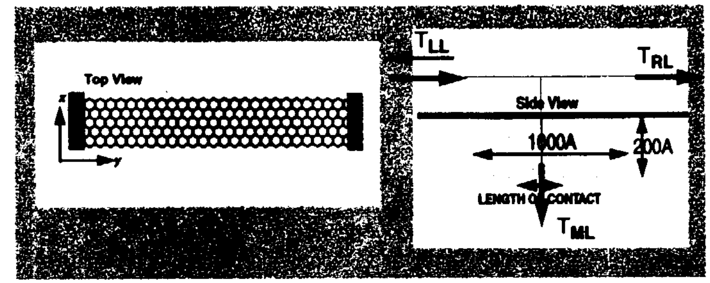
- Metal is modeled as a free electron gas (k_F)



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

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

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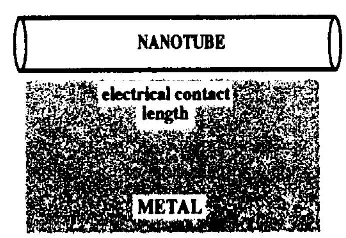

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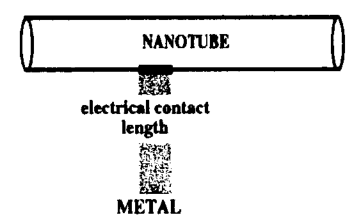

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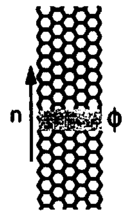

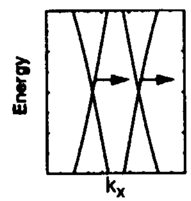

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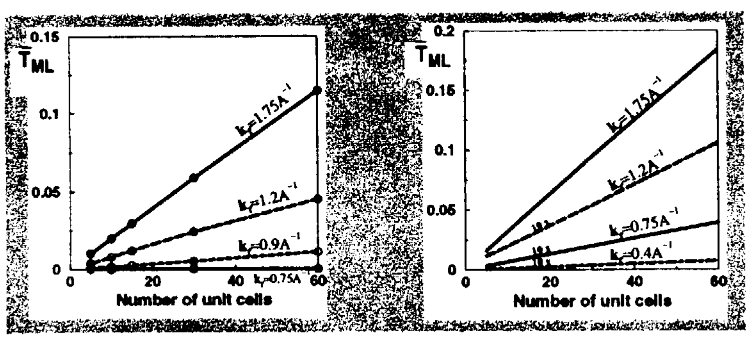

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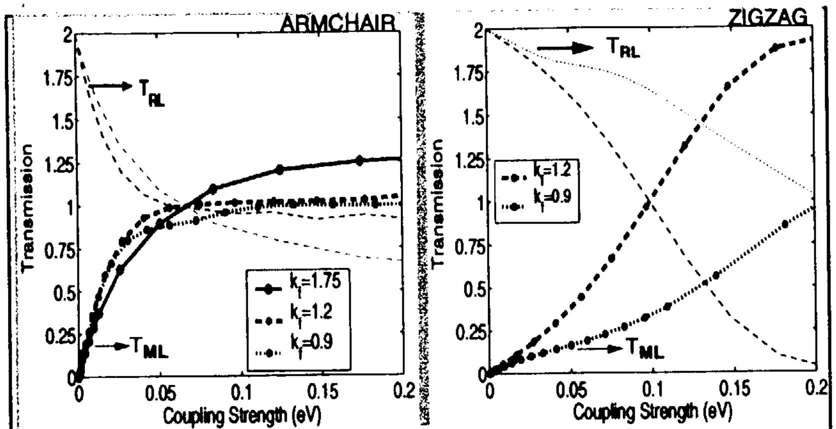

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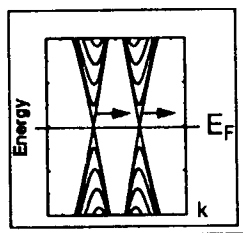

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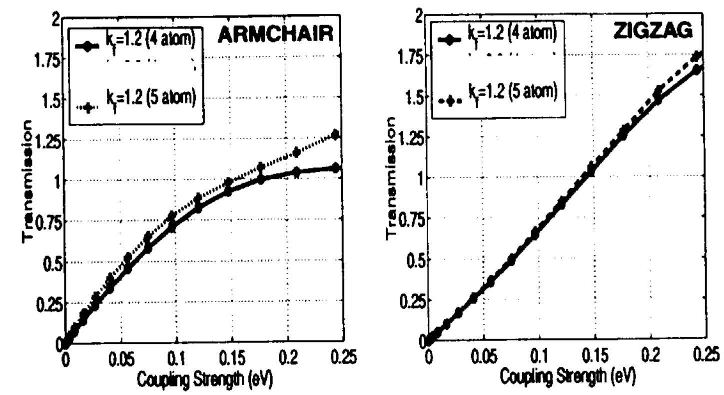
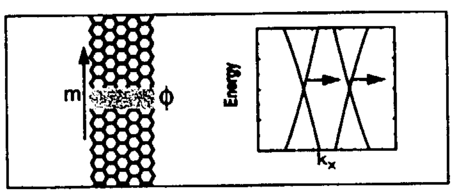
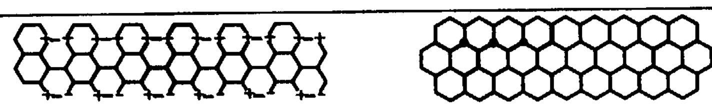


Nodes on the cylinder - Shape of NT wave function

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





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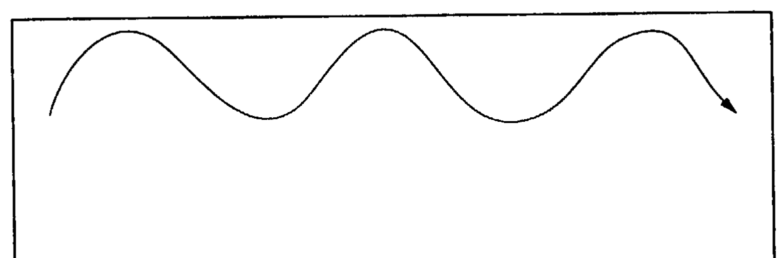

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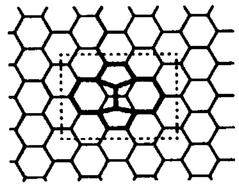

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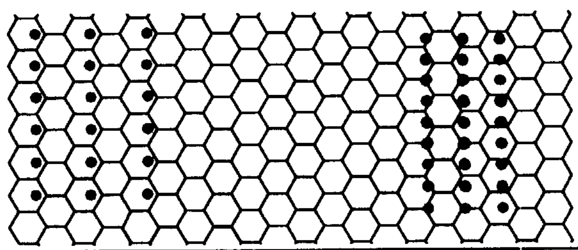

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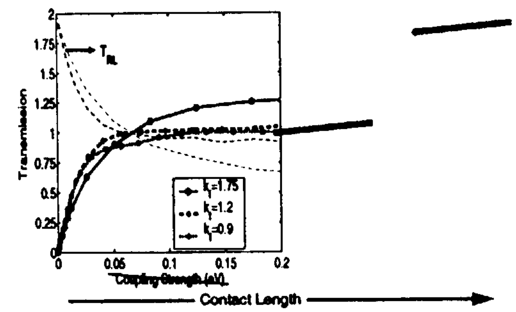

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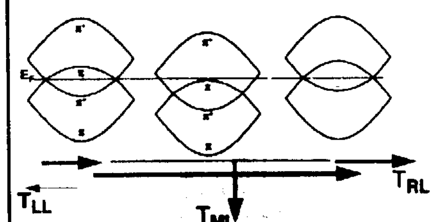

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This is different from the present case, where,

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Conclusions

- Requirement for axial wave vector conservation causes non trivial difference in coupling of zigzag and armchair tubes.

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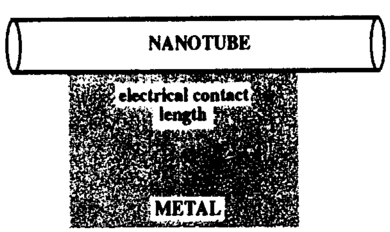

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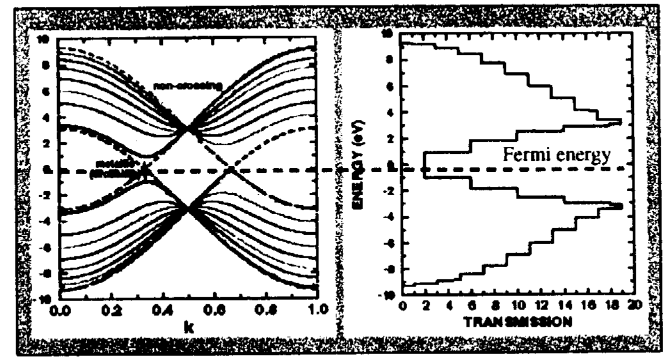

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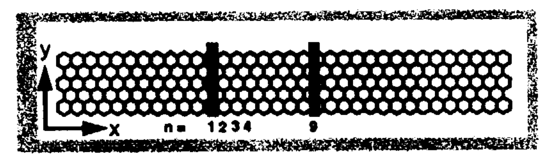

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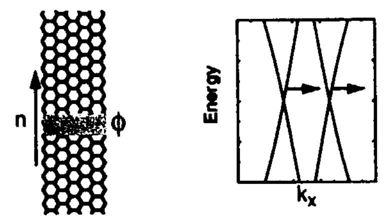

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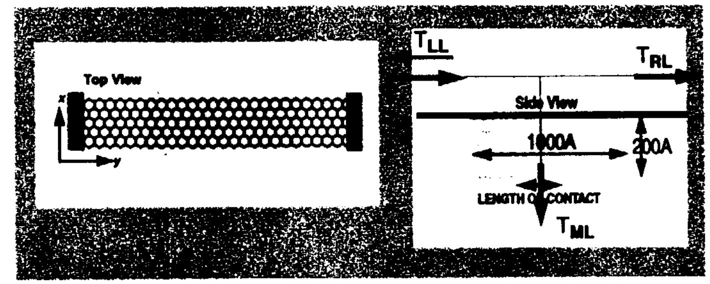

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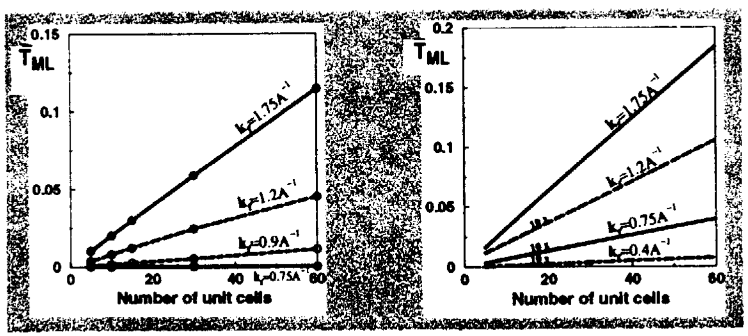

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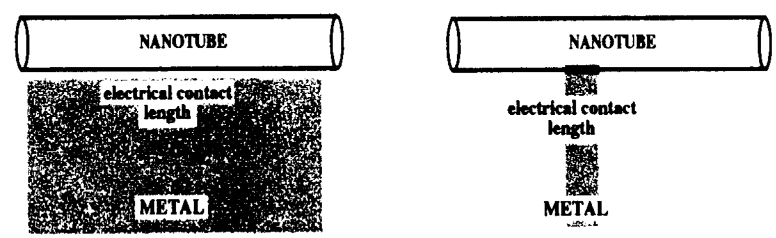

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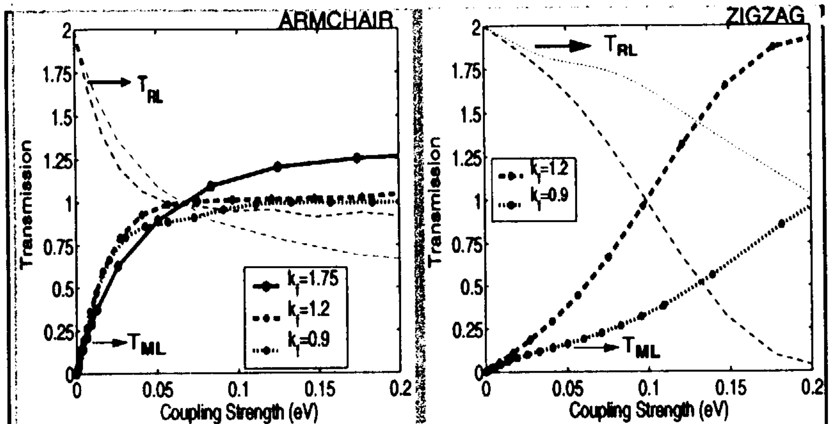

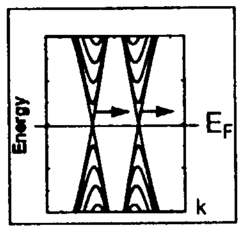

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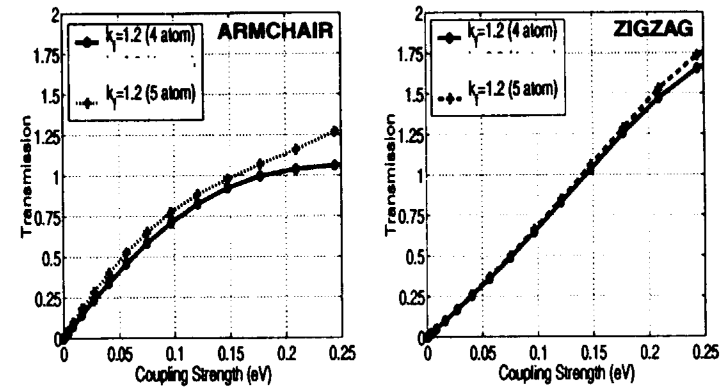

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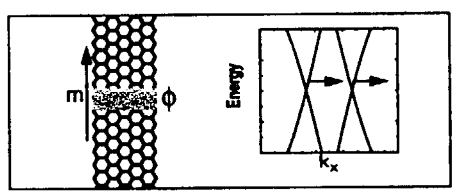

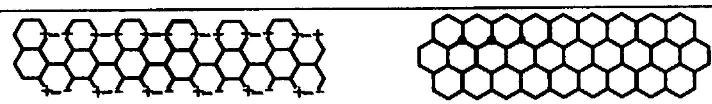

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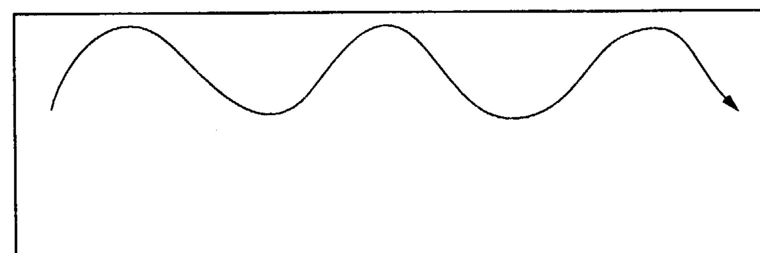

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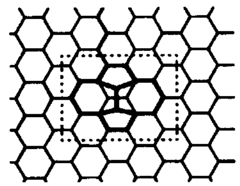

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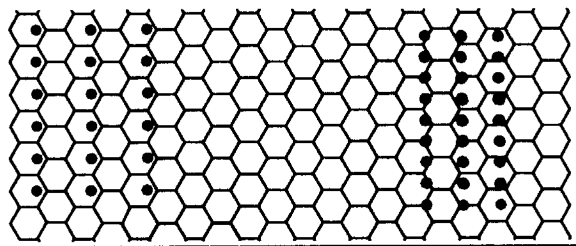

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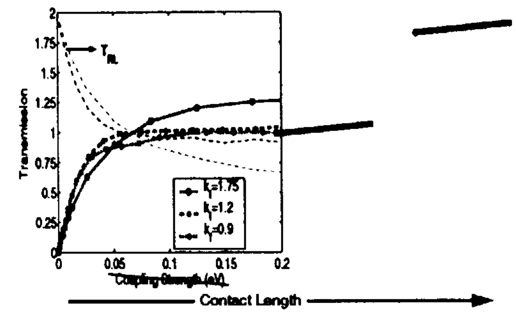

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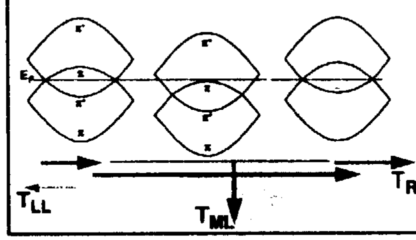

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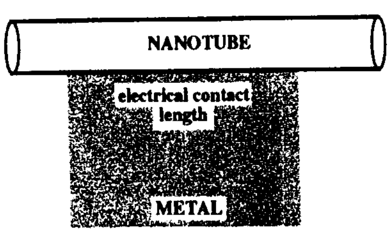

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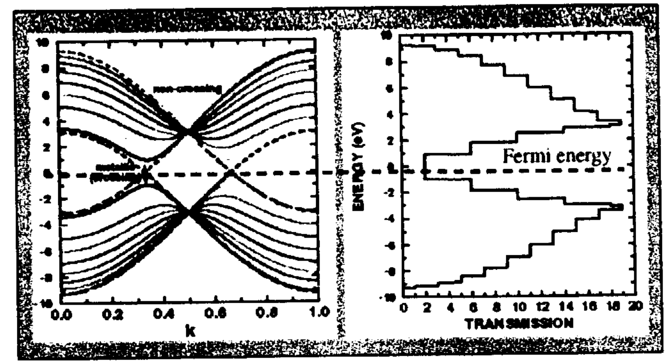

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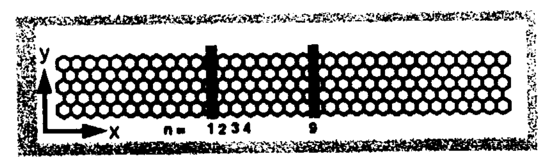

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$$\alpha \ | < e^{ink_x L} \, | \, e^{ink_x^m L} > < \phi \, | \, V_{m\text{-}nt} \, | \, \phi_m > |^2$$

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

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

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