Random Telegraph Signal in Carbon Nanotube Device



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Feb 28, 2008



Introduction

- 1. Structure of Single-walled Carbon Nanotube (SWCNT)
- 2. Electronic properties of SWCNT
- 3. Sample preparation: Catalytic synthesis of SWCNT, Fabrication.
- 4. Electronic transport: carbon nanotube field effect transistor (CNT-FET), ideal IV curves.
- 5. RTS basics, Other groups' data, our data
- 6. Future work
- 7. Group and Collaboration



Motivation:

- 1. Interaction between single molecular defects and 1D conduction channel in nano scale
- 2. Potential sensing technology in nano scale





•Graphene sheet rolled up into a hollow cylinder

- •Graphene is rolled along Chiral vector into cylinder
- •Chiral Vector $\mathbf{C} = n\mathbf{a}_1 + m\mathbf{a}_2$
- Chirality indices (n, m) uniquely define a tube





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Dresselhaus et al., P

•Diameter
$$d = \frac{|C|}{\pi} = \frac{a_0}{\pi} \sqrt{(n^2 + nm + m^2)}$$

- •Metallic if |n-m| = 3q , q=1,2,3...
- •Semiconducting if $|n-m| = 3q \pm 1$



$$a_0 = 1.42 \times \sqrt{3} = 2.46 \overset{o}{A}$$



•Bonding in graphene

Tight Binding Description of graphene
Dispersion of graphene
Zone-folding Approximation
1D electronic density of states

- Many CNT properties derived from Graphene
- Origin of conductivity in Graphene
- Zone folding approximation: graphene to CNT





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Origin of conductivity in Graphene

- 4 outer most shell electrons

- energies are so close together, new orbtials formed by mixing orbitals

World of Carbon, invsee.asu.edu/nmodules/Carbonmod/bonding.html



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Sp₂ hybridization

•Sp₂ orbitals are trigonal planar

•2p_z orbital is not hybridized



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Sigma bond:

- overlapping between sp_2 orbitals
- responsible for hexagonal network
- no energy band close to Fermi level, doesn't contribute to conductivity





•Bonding in graphene

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Pi bond:

- overlapping between 2p_z orbitals in side way manner
- responsible for electrical conduction





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- Dispersion obtained by tight binding approximation

$$E^{\pm}(\mathbf{k}) = \frac{\varepsilon_{2p} \mp \gamma_0 \sqrt{f(\mathbf{k})}}{1 \mp s_0 \sqrt{f(\mathbf{k})}}.$$

3 empirical parameters:

$$\varepsilon_{2p} \sim -0.28 eV$$

 $\gamma_0 \sim -2.97 eV$

 $s_0 \sim 0.073 eV$



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Bonding in graphene
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Upper band: anti-pi bond, conduction band

-Lower band: pi valence band

-Meet at K point, metallic behavior in Graphene



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Dispersion of a (4,2) Chiral tube**

- $\vec{k_z}$ continuous along the tube
- $\overrightarrow{k_{\perp q}}$ Quantized along Circumference:
- Only certain k vector is allowed along Circumference
- $\overrightarrow{k_{\perp q}} \cdot \overrightarrow{C} = 2\pi q$,q=integer
- one line in Brillouin zone for each q
- allowed k-vectors on these lines.

**R. Saito, et. al, *Physical Properties of Carbon Nanotubes*, Imperial College Press,1998.



Bonding in graphene
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Dispersion of a (4,2) Chiral tube**

-Only K point has energy band crossing Fermi level

- Metallic if K point $(\frac{1}{3}\vec{k_1} \frac{1}{3}\vec{k_2})$ is allowed:
 - $\vec{K} \cdot \vec{C} = (\frac{1}{3}\vec{k_1} \frac{1}{3}\vec{k_2}) \cdot (n\vec{a_1} + m\vec{a_2}) = \frac{2\pi}{3}(n-m) = 2\pi q$

=>
$$n-m=3q$$
 where $\vec{a_1} \cdot \vec{b_1} = \vec{a_2} \cdot \vec{b_2} = 2\pi$

- (4,2) is a semi-conducting tube

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Dispersion of a (4,2) Chiral tube**

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Different between CNT and graphene:

- Highly peaked DOS in 1D system









E/E0 2







E/E0 2



•Catalytic synthesis of SWCNT •Field effect transistor

CVD tubes:

-Mostly single-walled, 1-3nm

-tens of micron in length

-long, straight, in designated area

-cannot control chirality

-random orientation







•Catalytic synthesis of SWCNT •Field effect transistor

Growth Mechanism

- Present of catalyst metal (Fe, Mb, Al)
- -**Mutual dissolution of carbon and metal at ~1000°C
- Decompose and Defuse
- Root growth: favor single walled CNT
- Tip growth: favor multi-walled CNT





Kong. J., Soh. H.T., Cassell. A.M., Quate. C.J., Nature, **395**, **878.(1998)** Qian D,Dickey E.C.,Andrews R,Jacques D ,Center for applied energy research, Univ. of Kentucky



•Catalytic synthesis of SWCNT •Field effect transistor

Growth process:

- 1. Furnace
- 2. Catalysts (Fe, Mb, Al)
- 3. Methane as carbon feedstock

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Kong. J., Soh. H.T., Cassell. A.M., Quate. C.J., Nature, **395, 878.(1998)**



•Catalytic synthesis of SWCNT •Field effect transistor

Device preparation:

-CNT growth on catalysts site

-Fabricate markers

-Identify the location by markers







•Catalytic synthesis of SWCNT •Field effect transistor

Device preparation:

-contact electrodes by photolithography by picking the right electrodes



Signal A = InLens

Photo No. = 809

Date :19 Aug 2007

Time :16:19:34



EHT = 0.83 kV

WD = 3 mm

2 µm

•Catalytic synthesis of SWCNT •Field effect transistor

Device structure:

-CNT Field effect transistor

-control the electric field at the CNT by back-gate

-channel insulated with the back gate





•Catalytic synthesis of SWCNT •Field effect transistor

Device preparation:

-successful device image





•Basic transport theory

Transport of Ideal CNT
Metallic versus semi-conducting
Schottky barrier transistor
Coulomb Blockade

Conduction channel modulated by gate $\rm V_{G}$





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•Basic transport theory

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Coulomb Blockade



Level between source and drain is needed for conduction

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Basic transport theory
 Transport of Ideal CNT
 Metallic versus semi-conducting

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Metallic



•Basic transport theory •Transport of Ideal CNT •Metallic versus semi-conducting

•Schottky barrier transistor •Coulomb Blockade





Basic transport theory
Transport of Ideal CNT
Metallic versus semi-conducting
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•Basic theory

•Other group's data •Our data

• RTS origin

- Charge trap defects inside SiO_2 or SiO_2/CNT interface

- defect filled: local electric field affect conductivity
- trapped defect center => coulomb scattering center
- charge trapping and detrapping of the defect change the current level



Modeling electrostatic and quantum detection of molecules S. Vasudevan1, K. Walczak1, N. Kapur2, M. Neurock2, A.W. Ghosh1, in press S. Heinze, J. Tersoff, R Martel, V. Derycke, J. Appenzeller, Ph. Avouris Phys Rev Let.. 89, 106801 (2002)



•Basic theory •Other group's data •Our data

- RTS origin
 - defects level \mathcal{E}_T
 - control defect level by $\rm V_{G}$
 - emptied when above both fermi levels
 - filled if below both fermi levels
 - finite probability filled or empited



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Basic theory
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 - filled if below both Fermi levels
 - finite probability filled or emptied if between Fermi levels



Modeling electrostatic and quantum detection of molecules S. Vasudevan1, K. Walczak1, N. Kapur2, M. Neurock2, A.W. Ghosh1, in press F. Liu, K. L. Wang, C. Li, and C. Zhou, IEEE Transaction on



•Basic theory •Other group's data •Our data

- RTS origin
 - capture time au_c and emission time au_e
 - detailed balance equation

$$\frac{\tau_c}{\tau_e} = 2 \exp[\frac{\varepsilon_T - \varepsilon_F - \kappa e V_G}{k_B T}]$$

- switching frequently between discrete level if

$$\mathcal{T}_c \sim \mathcal{T}_e \quad \text{so,} \quad \mathcal{E}_T \approx \mathcal{E}_F - \kappa e V_G$$



F. Liu, K. L. Wang, C. Li, and C. Zhou, IEEE Transaction on Nanotechnology, 5, 411 (2006)



Basic theory
Other group's data
Our data

• RTS origin





F. Liu, K. L. Wang, C. Li, and C. Zhou, IEEE Transaction on Nanotechnology, **5**, 411 (2006)





F. Liu, K. L. Wang, C. Li, and C. Zhou, IEEE Transaction on Nanotechnology, 5, 411 (2006)



•Basic theory •Other group's data •Our data

- Well defined in Room temperature
- discrete current jumping in both sides
- Unexpected RTS "windows"





•Basic theory •Other group's data •Our data

- See discrete jumping in both side of RTS windows
- τ_c and τ_e changing with V_G







•Basic theory •Other group's data •Our data

• Agreed with principle of detailed balance

$$\frac{\tau_c}{\tau_e} = 2 \exp[\frac{\varepsilon_T - \varepsilon_F - \kappa e V_G}{k_B T}]$$

$$\log \frac{\tau_c}{\tau_e} lpha V_G$$



•Basic theory •Other group's data •Our data

- Hysteresis effect due of water molecules on oxides surface
- Annealing in H₂ removed RTS
- Hysteresis effect enhanced after annealing
- No confident explanation on the data yet





6. Future works

- Explain our data, further characterization
- Decorate molecular defect on CNT FET, O₂, N₂
- Identify corresponding RTS signature



7. Group, Collaborations:

Advisor: Prof. Keith Williams Graduate student: Brian Burke, Jack Chan. Undergraduate student: Kenneth Evans, Andrew Spisak. Collaborator:

Prof. Avik Ghosh, Kamil Walczak, Smitha Vasudevan. (theoretical) NSF award for Novel Transistor Research at the Nanoscale

Prof. Joe Campbell Group (experimental).

Future collaborator: CNMS in ORNL.

End







Bonding in grapheneTight Binding Description of graphene

•Dispersion of graphene •Zone-folding Approximation

•1D electronic density of states



• Ready to get
$$E(k)$$
 and $\begin{pmatrix} C_A \\ C_B \end{pmatrix}$

$$\frac{H_{AA}(\mathbf{k}) - E(\mathbf{k})S_{AA}(\mathbf{k})}{H_{AB}^{*}(\mathbf{k}) - E(\mathbf{k})S_{AB}^{*}(\mathbf{k})} = 0,$$

$$E(\mathbf{k})^{\pm} = \frac{-(-2E_0 + E_1) \pm \sqrt{(-2E_0 + E_1)^2 - 4E_2E_3}}{2E_3},$$

with

$$E_{0} = H_{AA}S_{AA}, \quad E_{1} = S_{AB}H_{AB}^{*} + H_{AB}S_{AB}^{*}$$
$$E_{2} = H_{AA}^{2} - H_{AB}H_{AB}^{*} \quad E_{3} = S_{AA}^{2} - S_{AB}S_{AB}^{*}.$$

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$$\begin{split} H_{AA} &= \frac{1}{N} \sum_{\mathbf{R}_{A}} \sum_{\mathbf{R}_{A'}} e^{i\mathbf{k}(\mathbf{R}_{A'} - \mathbf{R}_{A})} \langle \varphi_{A}(\mathbf{r} - \mathbf{R}_{A}) | H | \varphi_{A}(\mathbf{r} - \mathbf{R}_{A'}) \rangle \\ &= \frac{1}{N} \sum_{\mathbf{R}_{A}} \langle \varphi_{A}(\mathbf{r} - \mathbf{R}_{A}) | H | \varphi_{A}(\mathbf{r} - \mathbf{R}_{A}) \rangle \!=\! \varepsilon_{2p}, \end{split}$$

$$H_{AB} = \frac{1}{N} \sum_{R_A} \sum_{R_B} e^{ik(R_B - R_A)} \langle \varphi_A(r - R_A) | H | \varphi_B(r - R_B) \rangle$$
$$= \gamma_0(e^{ikR_{11}} + e^{ikR_{12}} + e^{ikR_{13}})$$

with

$$\gamma_0 = \langle \varphi_A(\mathbf{r} - \mathbf{R}_A) | H | \varphi_B(\mathbf{r} - \mathbf{R}_A - \mathbf{R}_{1i}) \rangle \quad (i = 1, 2, 3),$$

$$S_{AB} = s_0(e^{ikR_{11}} + e^{ikR_{12}} + e^{ikR_{13}})$$

with

$$s_0 = \langle \varphi_A(\mathbf{r} - \mathbf{R}_A) | \varphi_B(\mathbf{r} - \mathbf{R}_A - \mathbf{R}_{1i}) \rangle \quad (i = 1, 2, 3),$$

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a) Rolled up of a graphene sheet, graphene is a layer of graphite.

- b) Chirality vector: **C**=n**a**₁+m**a**₂, graphene is rolled along **C** into cylinder.
- c) Chirality indices (n, m) determines electronic band structure.
- d) diameter: C/pi=.....
- e) Metallic if n-m=3q, semiconducting otherwise.
- f) talk about Brillouin zone?
- g) Physical properties:

Electrically conductive

High current carrying capacity

Can be functionalized (doped).

High Length/Diameter aspect ratio

Extra ordinary mechanical properties, eg. Young Modulus>1T Pascal.







•Basic transport theory •Transport of Ideal CNT •Schottky barrier (SB) transistor •Coulomb Blockade

• SB

- formed between metal and semi-cond



- IV_G changes with dopant level:
 - Whole curve shifted
 - Shape doesn't change
- SB device IV_G :
 - change with work function, i.e. metal
 - formed between semi-cond and metal
 - minimum current range almost unchang $\boldsymbol{\varepsilon}$
 - curve change shape



S. Heinze, J. Tersoff, R Martel, V. Derycke, J. Appenzeller, Ph. Avouris Phys Rev Let., **89**, **106801 (2002)**



•Basic transport theory •Transport of Ideal CNT •Schottky barrier (SB) transistor •Coulomb Blockade

• SB

- formed between metal and semi-cond
- matching fermi level by electron flowing
- build in voltage developed



S. Heinze, J. Tersoff, R Martel, V. Derycke, J. Appenzeller, Ph. Avouris

55

Phys Rev Let., 89, 106801 (2002)

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Keith Williams' Nanophysics Group – University of Virginia



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Ingredients:

- Schrodinger's equation $H\psi(k) = E\psi(k)$
- Normalized $2p_z$ orbitals of C atom $\varphi(r)$
- 2 atoms in graphene unit cell
- Bloch function of graphene sublattice

$$\Phi_{A} = \frac{1}{\sqrt{N}} \sum_{R_{A}} e^{ik \cdot R_{A}} \varphi(r - R_{A})$$
$$\Phi_{B} = \frac{1}{\sqrt{N}} \sum_{R_{B}} e^{ik \cdot R_{B}} \varphi(r - R_{B})$$

- Eigenfunctions $\psi(k) = C_A \Phi_A(k) + C_B \Phi_B(k)$
- Approximation:

-Only nearest neighbor

-Overlapping integral So is non-zero

• Ready to get
$$E(k)$$
 and $\begin{pmatrix} C \\ C \end{pmatrix}$

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$$E^{\pm}(\mathbf{k}) = \frac{\varepsilon_{2p} \mp \gamma_0 \sqrt{f(\mathbf{k})}}{1 \mp s_0 \sqrt{f(\mathbf{k})}}.$$

where

$$\begin{split} f(k) &= 3 + u(k) \\ &= 3 + 2 \cos k \cdot a_1 + 2 \cos k \cdot a_2 + 2 \cos k \cdot (a_1 - a_2) \\ &= 3 + 2 \cos 2 \pi a k_1 + 2 \cos 2 \pi a k_2 + 2 \cos 2 \pi a (k_1 - k_2), \\ \gamma_0 &= \left\langle \varphi_A(r - R_A) \left| H \right| \varphi_B(r - R_A - R_{1i}) \right\rangle \quad (i = 1, 2, 3), \\ s_0 &= \left\langle \varphi_A(r - R_A) \right| \varphi_B(r - R_A - R_{1i}) \right\rangle \quad (i = 1, 2, 3), \\ H_{AA} &= \frac{1}{N} \sum_{R_A} \sum_{R_{A'}} e^{ik(R_{A'} - R_A)} \langle \varphi_A(r - R_A) | H | \varphi_A(r - R_{A'}) \rangle \\ &= \frac{1}{N} \sum_{R_A} \left\langle \varphi_A(r - R_A) | H | \varphi_A(r - R_A) \rangle = \varepsilon_{2p}, \end{split}$$

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