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Effects of Different Junction Parameters on Junction Conductances of Crossed Metallic Carbon Nanotubes

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ABSTRACT We have studied the effect of different junction parameters on the junction conductances made of two crossed metallic carbon nanotubes. We have found that because of the intrinsic asymmetries of the junction, forward and backward tunneling between one tube and the other are unequal. Passing a current in one tube leaded to the development of non zero voltage across the other one, a zero field Hall like conductance for the junction was found. We have found that this zero field Hall conductance relates to the contact conductance of the junction. The result also shows that the electronic properties of the junction sensitively depend on the degree of matching between the tube lattices. This matching is controlled by the crossing angel, which resulted in an intertube conductance that varied by an order of magnitude for different angles. We have derived a tunneling matrix element that coupled the low energy electronic states on the two tubes. The magnitude of the coupling was determined by the intertube separation of the crossing angle. We have found that the intrinsic symmetries of the junction created a discrepancy between the forward and backward hopping between the tubes. Using Landauer-Buttiker formalism, we have calculated the different conductances of the four terminal junctions. We have found that the contact conductance scaled inversely with the zero field Hall conductance of the junction. We have also found that the two crucial parameters in determining the conductance are the tube chiralities and the crossing angle. The obtained results were found in good agreement with previously obtained results.

KEYWORDS Junction parameters, Junction conductance, metallic carbon nanotube, Intrinsic, asymmetry, tunneling, chiralities.

1. INTRODUCTION

Charlier et al. [1] studied the bulk behavior of carbon nanotube systems, the electronic properties of different carbon nanotube geometries and on the multiwall tubes [2-6]. These studies presented the intertube transport and its dependence on the chiralities of the tubes and the geometrical details. Wu et al. presented that the films of carbon nanotubes can be used as transparent conducting electrodes [7].

Fuhrer et al. [8] and Youneya [9] studied experimentally the junctions of crossed carbon nanotubes. In this work they explored the different electrical properties of different combinations of crossed metallic and semiconducting tubes. Metal insulator junctions showed a contact conductance of the order of the 0.02 $\left(4e^2/h\right)$, despite the small junction area. This was attributed to the elastic deformation of the tube arising from the

interaction with substrate, resulting in one intertube distance smaller than the 3.4 Å. This increased the coupling at the contact region and provided a natural explanation of relatively high measured conductance. Crossed nanotube junctions have been theoretically studied for high symmetry cases only [10-12], where it was found that maximal contact conductance occurred when the tube lattices are commensurate.

Hong Liu et al. [13] studied and extended Su-Schrieffer-Heeger model multiband semiconductor Bloch equations were formulated in momentum space and applied to the analysis of the linear optical response of semiconducting carbon nanotubes. This formalism included the coupling of electron-hole pair excitations between different valence and conduction bands, originating from the electron-hole coulomb attraction. The influence of these couplings, which are referred to as nondiagonal interband coulomb interaction on the linear excitonic absorption spectra were studied for light fields polarized parallel to the tube direction. The results showed that the intervally non diagonal interband coulomb interaction leaded to a significant increase of the band gap and a decrease of the exciton binding energy depends on the symmetry of the carbon nanotube. For incident fields polarized along the tube's axis, the linear absorption coefficient [14-16] and excitonic resonances [17-20] have been studied both experimentally and theoretically. Two groups proposed that the first and second excitonic transition of single carbon nanotubes have been measured through photoconductivity [21-23]. Also cross polarized optical transitions which varied with the carbon nanotube chirality have been studied by several groups [24-26].

Hongxia et al. [27] presented armchair single wall carbon nanotubes and studied theoretically and predicted to be metallic in the simple zone folding scheme and protected from the curvature effects. They found to be small gap semiconductors, experimentally. They showed that the carbon nanotubes without corrugation are not metastable. The size of corrugation increased rapidly with nanotubes curvature and vanished for flat graphene.

Singh and Aparajita [28] studied the origin of the electron energy relaxation in clean single channel quantum wires and quantum dots, according for the scattering process that involved three particle collisions. Thermal transport of single channel quantum wires, where a lower value of the thermal conductance that predicted by Weidemann-Franz law as observed at the plateau of the electrical conductance. Momentum resolved tunneling spectroscopy provided direct evidence for the electronic thermalization in one dimensional system. They found that interaction effects are responsible for the observed features. They found that the thermal conductance was reduced by interactions.

Kumar et al. [29] studied electronic and transport properties of carbon nanotubes using tight binding models. The depolarization effect shifted the excitation energy to higher energy side and suppressed intensity of the absorption peaks. As a result excitation energy became closer to that associated with that of the second gap for parallel polarization. The intensity of the absorption peaks was weakly dependent on the coulomb interaction and the tube diameter through the cut off energy.

2. METHOD

We have introduced tunneling model and derived tunneling matrix element coupling low energy tube states. We have derived a equation for the junction conductance in terms of the microscopic conductance of the junction in a Landauer - Buttiker framework and presented some numerical results showing the dependence of the junction conductance on various junction parameters. We have presented the low energy coupling between two crossed tubes within tight binding formalism. Nanotubes have been assumed to be long and free of defects. Matching between the two lattices have been quantified by a registry angle-ϕ given by

$$\phi = \theta_1 + \theta_2 + \beta$$

Where β the crossing is angle, θ_1 and θ_2 are the chiral angles. The un-coupled tubes are described by a nearest neighbour tight binding Hamiltonian

$$\mathrm{H}_0 = -\sum_{a=1,2}\sum_{\langle i,j\rangle} t_\pi c_{ai}^\dagger c_{aj}$$

Where the index a labels the carbon nanotubes and $\langle i, j\rangle$ is a sum over nearest neighbour atoms on each carbon nanotube. The eigen states of H_0 are plane waves localized on each carbon nanotube. The interaction

Hamiltonian H_T is built in such a way that an electron can hop from any atom on one carbon nanotube to any atom on the other

$$H_T = \sum_{ij} t_{ij}$$

Where t_{ij} depends on the positions and relative orientation of the π orbitals on atoms *i* and *j* and varies exponentially with the distance between the two hopping sites.

$$t_{ij} = t_0 e^{-d_{ij}/a_0}$$

Where 't_0' is a free parameter to be determined and $a_0 = 0.529$ Å is the range of the π - orbitals. The intersite distance d_{ij} is given by

$$\begin{aligned} d_{ij}^2 = & \left(b + 2R - R\cos\frac{y_1}{R} - R\cos\frac{y_2}{R} \right)^2 \\ & + \left(z_2 \sin\beta + R\sin\frac{y_1}{R} - R\sin\frac{y_2}{R}\cos\beta \right)^2 \\ & + \left(z_2\cos\beta - z_1 - R\sin\frac{y_2}{R}\sin\beta \right)^2 \end{aligned}$$

Where $z_a(y_a)$ is the distance along the length waist of carbon nanotube a and b is the intertube separation at the point of closest contact. The carbon nanotubes are assumed to be of approximately equal radii, which are denoted by R. We have assumed that hopping between the carbon nanotubes is dominated by y_a, Z_a, b, R.

The total Hamiltonian of the system

$$H = H_0 + H_T .$$

Expressed in a plane wave basis by the transformation

$$c_{ai} = \frac{1}{\sqrt{N}} \sum_{k_a} e^{ik_a \cdot r_{ai}} c_{a\eta(i)k_a}$$

Where r_{ai} is the position vector of site *i* on tube *a*, η specifies the A or B subsites, N is the number of graphene unit cells in the tube and $k_a = (k_{ay}, k_{ax})$. In this basis

$$H_0 = -t_\pi \sum_{a=1,2} \sum_{k_a} \gamma k_a c_a^\dagger A k_a c_a B k_a + H.c.$$

where $\gamma k_a = \sum_{j=1}^{3} e^{ik_a \cdot d_{aj}}$

d_{aj} are the three nearest neighbour vectors connecting the two sublattices of the tube a. The Brillouin zones of the graphene sheets forming the two crossed tubes have been taken into account. The wrapping of graphene sheet corresponds to slicing the two dimensional zone in a direction parallel to the tube axis. This yields a series of one dimensional band and in the case of a metallic tube, two bands cross at the Fermi energy. At low energy on the neighborhood of the Fermi points, corners of the Brillouin zone, where

$k = \alpha K_p + q,\ \ q = (0, q), \alpha = \pm 1$ and $p = -1, 0, 1$. Denote the three equivalent Fermi points. In this limit the tube Hamiltonian is diagonalized by the transformation

$$U = e^{-i\left(\frac{1}{2}\right)\alpha\theta\sigma^z e^{-i\left(\frac{\pi}{4}\right)\alpha\sigma^y}}$$

where $\sigma^{y,z}$ are the Pauli matrices and we get two eigen modes ψ_{Lq}. In this $\frac{R}{L}$ basis H_0 becomes

$$H_0 = \sum_{a=1,2}\sum_{q_a} v_F q_a \left(\psi^{\dagger}_{aRq_a}\psi_{aRq_a} - \psi^{\dagger}_{aLq_a}\psi_{aLq_a}\right)$$

Where $v_F = \frac{3t_c d}{2}$ and d is the nearest neighbour distance. The tunneling Hamiltonian H_T can be expressed in the propagating states basis procedure. The coupling between propagating modes on the tubes depends on the geometry of the junction. The Fermi energy of the system has an effect on the coupling as the momentum difference between propagating states on the two tubes changes as the Fermi energy is changed. This developed theory is a low energy one and is applied where the localization of the tube band structure is valid. An upper limit of the energy range where this model is applicable is determined by the diameters of the tubes forming the junction.

3. RESULTS AND DISCUSSION

Figure (1) shows the angular dependence of contact conductance G_c for three junctions. The Fermi energy $E_0 = O$ is at K point and the carbon nanotube lattices are oriented with an orientation. For junction one we see that there are three main peaks in the conductance, which are related to maxima in the transmission probabilities between the two tubes at these crossing angles. The tubes are of different chirality there exist certain crossing angles at which lattice commensuration occurred, in such case the transmission probabilities are largest leading to a conductance maximum. The crossing angles where such peaks are $\beta^+ = 36^\circ, 96^\circ$ and 156° for junction one (I) as shown in Figure (1). The crossing angles that maximized the lattice mismatch resulted in a contact conductance that is roughly an order of magnitude lower. Junction two (II) shows qualitatively similar behaviour as shown in Figure 1 by dashed dot. For this junction lattice matching occurred at $\beta^+ = 22^\circ, 82^\circ$ and 142°. For junction three (III), $\beta^+ = 40^\circ, 100^\circ$ and 160°. For this junction the conductance increased as $\beta^+ \to 0^\circ, 180^\circ$ as the system became periodic and tunneling matrix element taken as $\delta -$function form. The transmission probability and hence the conductance, increased with the area of overlap between the two lattices. This area is minimum at perpendicular crossing, which made the conductance peak closer to $\beta = 0^\circ, 180^\circ$ relatively larger than those near $\beta = 90^\circ$. The slight deviation of the conductance peaks from the lattice commensuration angles that has been shown in Figure (1) is due to the finiteness of the tube radii. For radius of ~1.5nm the curvature causes a deviation of a couple of degrees. This deviation decreased with increasing tube radii. This deviation is smallest at perpendicular crossing as the curvature effects are minimal. Figure (2) shows that as the radii increased the deviation from the angles β^+ became negligible small. We have found that the peaks occurring at angles β^- get increasingly small as the radii of the tube increased. These are the angles at which there is a finite mismatch in only one of the two dimensional momentum components, which caused these peaks to be suppressed as the tube radii are increased. The dependence of the conductance on the relative orientation of the tube lattices are shown in Figure (3). The Figure 3 shows the angular dependence of the conductance of junction I for two orientations. A first observation is that the relative orientation has a negligible effect on the position of the conductance peaks. The varying the cross angle of a certain junction we have found that change the Fermi level be easily achievable through electrostatic doping. The Fermi level dependence of the contact conductance have been shown in Figure (4). In Figure (4) we have found that the angular dependence of the contact conductance for junction one (I) for different energies we have found that changing the Fermi level has a negligible effect on the position of the conductance peak, it does affect the magnitude of the conductance. Tuning the Fermi level away from the K points changed the momentum mismatch between the initial and final states involved in the tunneling, there by changing the transmission probability and the conductance. A sign

change of η reflected the fact that the Fermi level affects the forward and backward conductances differently. The unique point in parameter space that has $\eta = 0$ is a point of high symmetry in the sense that the many asymmetries of the junction counteract to give equal forward and backward transmission probabilities. The obtained results were compared with previously obtained results of theoretical and experimental works and were found in good agreement.

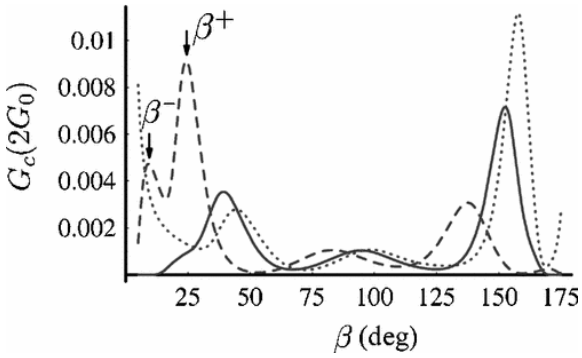

Figure 1: Dependence of G_c on the crossing angle β for three junctions, I (17,2) - (10,10) (solid), II (17,2)-(15,6) (dashed), and III (13,7) - (13,7) (dotted), for $E_0 = 0$. Different peaks in each plot mark the angles where three is high registry between the two tube lattices. The two arrows mark the angles β^- and β^+ for junction II.

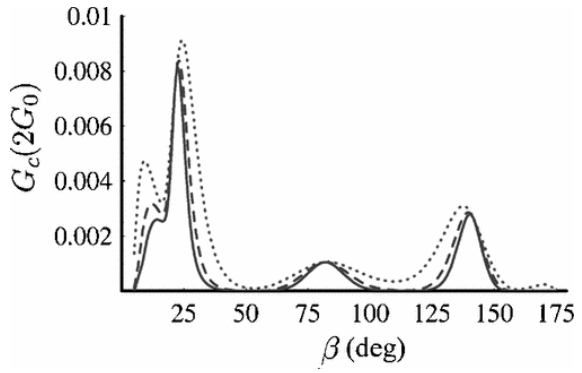

Figure 2: Dependence of G_c on the crossing angle β for 3 junctions. The radii of the tubes in the 3 junctions are *R* (solid), 2R (dashed), and 3R (dotted), and R~1.5 nm. The Carbon nanotubes are assumed to have an HH-orientation contact, and the Fermi energy $E_0 = 0$.

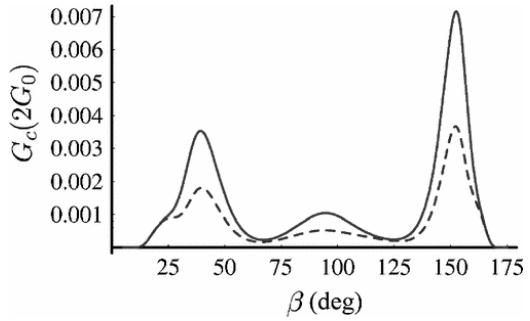

Figure 3: Dependence of G_c on the crossing angle β for junction I (17, 2) - (10, 10) with HH (solid) and AH (dashed) orientations at $E_0 = 0eV$.

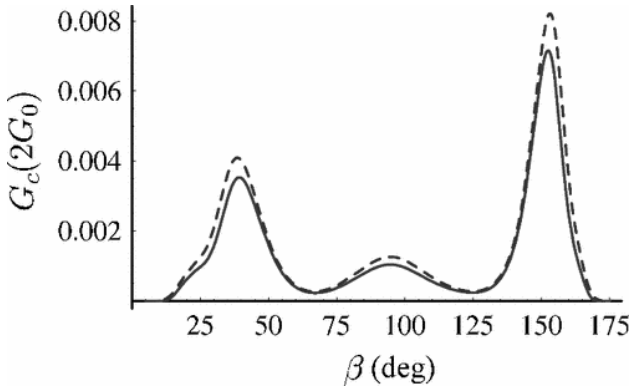

Figure 4: Dependence of G_c junction I (17, 2) - (10,10) on the crossing angle β for different energies, $E_0 = 0\text{eV}$ (solid) and $E_0 = -0.2\text{eV}$ (dashed).

4. CONCLUSION

We have studied the effects of the different junction parameters on the junction conductance. We have derived a tight binding tunneling matrix element that coupled low energy states on the two tubes which allowed calculating the contact conductance of the junction. We have found that the intrinsic asymmetries of the junction caused the forward and backward hopping probabilities from one tube to another tube were different. The matrix element depended on the chiral angles, the cross angle and the Fermi level of the junction. Passing a current in one tube leaded to the development of a non zero voltage across the other one and produced a zero field Hall conductance of the junction. The obtained results have important implications on the study of carbon nanotube network. We have found that the contact conductance scaled inversely with zero field Hall conductance of the junction. We have also found that the crossing angle has the dominant role that determined magnitude of the conductance. The results also shown the electronic properties of the junction sensitively depend on the degree of matching between the tube lattices. For a given junction this matching is controlled by the crossing angle which resulted in an intertube conductance that varied by an order of magnitude for different angles. Deformations slightly increased the contact are between the two tubes and also caused the on tube conductance to be slightly lower than the assumed value due to possible back scattering. These two effects have been found for large diameter tubes where faceting at the contact region is more pronounced. The obtained results were found in good agreement with previously obtained results.

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