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Tuning the band gap of semiconducting carbon nanotube by an axial magnetic field

G. Fedorov,[1,a)] P. Barbara,[1] D. Smirnov,[2] D. Jiménez,[3] and S. Roche[4]
[1]*Department of Physics, Georgetown University, Washington, DC 20057, USA*
[2]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA*
[3]*Departament d'Enginyeria Electrònica, Escola d'Enginyeria, Universitat Autònoma de Barcelona, Bellaterra, 08193 Barcelona, Spain*
[4]*CIN2, ICN, CSIC, Campus UAB, Barcelona, E-08193 Bellaterra, Spain and Commissariat a l'Energie Atomique, DSM, SP2M, INAC, Lsim, Grenoble, France*

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We have investigated the magnetic field dependence of transfer characteristics of a device fabricated in a configuration of a field-effect transistor with a conduction channel formed by a semiconducting multiwalled carbon nanotube. Our results unambiguously indicate that an axial magnetic field suppresses the band gap of the nanotube. Quantitative analysis of the data indicates linear dependence of the band gap on magnetic field as well as a linear splitting between the K and K′ subbands of the band structure of the nanotube. © *2010 American Institute of Physics*.
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Since the fabrication of the first field effect transistor[1] (FET) based on a carbon nanotube (CNT) a lot of work has been done to explore the possibilities of integration of CNTs into electronic devices. The ability to tune the band structure of a CNT by an external perturbation may significantly enhance capabilities of such devices and circuits. As early as in 1993, Ajiki and Ando predicted that an axial magnetic field would tune the band structure of a CNT between a metal and a semiconductor one, owing to the modulation of the Aharonov–Bohm (AB) phase of the electronic wave functions.[2,3] When a magnetic flux ϕ threads the nanotube cross section, the electron wave functions accumulate an additional magnetic field dependent phase factor[4–8] (AB-phase), which results in many phenomena.[9–13] One of them is a ϕ_0-periodic modulation of the band gap ($\phi_0=h/e$ is the flux quantum).[14–17] This effect occurs due to peculiar topology of the graphene Fermi surface, and it is unique for CNTs. It was recently shown that a CNT that is metallic in a zero magnetic field is converted into a semiconducting one once an axial magnetic field is applied with the band gap linearly depending on the magnetic field strength.[18,19]

Here we report on the observation of magnetically induced decrease in a band gap of a semiconducting multiwall nanotube (MWNT) under magnetic fields up to 33 T. The effect is manifested as a significant increase in conductance and exponential decay of resistance with magnetic field. According to our estimations, the band gap of the MWNT was decreased from 140 meV at a zero magnetic field down to about 70 meV at 33 T. Such tuning of the band structure of a CNT could be used for optical applications in the mid-infrared and far-infrared range.

As reported in our previous work,[18] we fabricated devices made in the configuration of a standard CNT field-effect transistor (CNFET) with conduction channel formed by an individual CNT. Nanotubes were grown on highly conductive n-doped Si substrates, capped with 310 nm of thermally grown SiO_2 and used as a back gate. CNTs were grown by a chemical vapor deposition method[20] from a CH_4/H_2 mixture using a Fe/Mo catalyst yielding a low density of nanotubes on the substrate. Each nanotube was contacted with 50-nm-thick Pd electrodes patterned using e-beam lithography and deposited by rf-sputtering. Schematic of the resulting device is shown in the Fig. 1(b). Here we report results obtained for a case of a MWNT with a diameter $d=4.9\pm0.5$ nm. The distance between electrodes was 4 μm.

To investigate the effect of magnetic field on transport properties of our devices, we measured the dependence of the device conductance $G=I/V_d$ on the back gate voltage V_g at different values of magnetic field and temperatures $T=150$ and 200 K. The $G(V_g)$ characteristics were recorded at a small dc bias voltage $V_d\sim1$ mV. Figure 1(c) displays $G(V_g)$ curves obtained at a temperature $T=200$ K. The axial

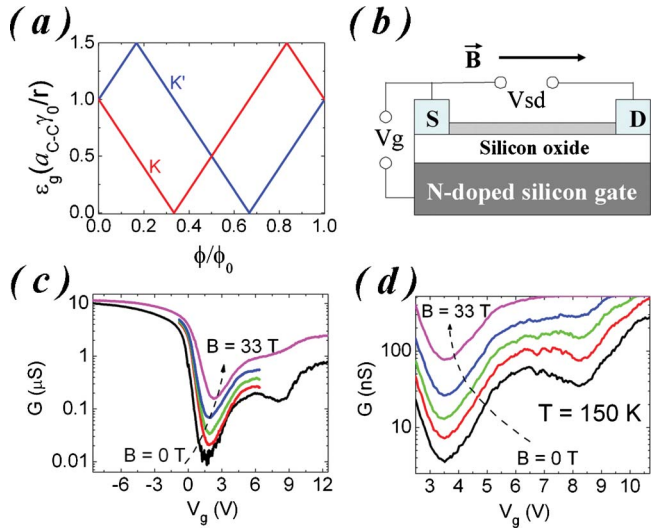

FIG. 1. (Color online) (a) Magnetic field dependence of an energy gap of K and K′ bands of a semiconducting CNT. (b) Schematics of a FET-type device used in this work. [(c) and (d)] Evolution of transfer characteristics ($B=0$; 12; 18; 24; and 33 T) of the studied sample at T=200 K and 150 K, respectively.

a)Author to whom correspondence should be addressed. Present address: Russian Research Centre "Kurchatov Institute," Moscow, Russia. Electronic mail: fedorov@imp.kiae.ru.

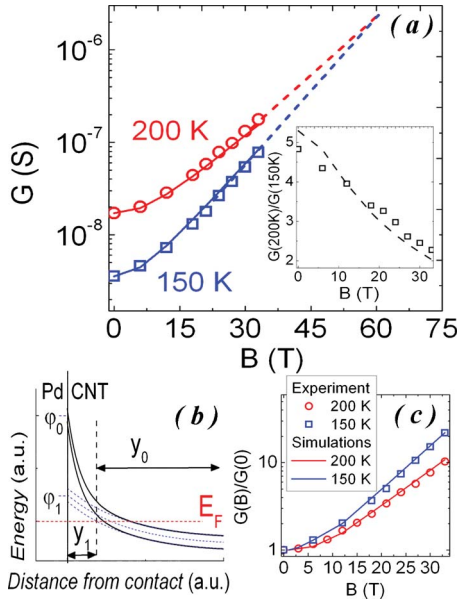

FIG. 2. (Color online) (a) Magnetic field dependence of the device conductance. Conductance G is defined as that at a gate voltage $V_g=V_g^*$. Symbols: experimental points. Solid lines: fits with an expression (5). Extrapolations of the $G(B)$ curves to the point where they intersect are shown with dashed lines. Inset: Ratio of the device conductance at 200 K to that at 150 K as a function of magnetic field. Symbols: experimental points. Dotted line: fit with an expression (6). (b) Band profiles of the CNT (c) Conductance of sample, normalized to its value at zero magnetic field compared to simulations (solid lines); symbols: experimental points.

magnetic field has the strongest effect on $G(V_g)$ at $V_g=V_g^*$(off-state) corresponding to the conductance minima. As seen from Fig. 1(c) the magnetic field has almost no effect for $V_g<-5$ V. This gate voltage range corresponds to "ON"-state of a CNFET when the Fermi level of the system lies deep in the valence band of the CNT forming a conducting channel. As seen in Figs. 1(c) and 1(d) the application of an axial magnetic field result in a significant increase in conductance in the V_g range around V_g^*. We interpret this as an indication of reduction of the CNT band gap.[16,18] Similar effect was observed in other devices with a conduction channel formed by a semiconducting CNT; further we concentrate on the most representative one.

For a further quantitative analysis we concentrate on magnetic field dependence of the device conductance at $V_g=V_g^*$. Figure 2(a) shows the minimum conductance $G_{MIN}=G(V_g^*)$ as a function of magnetic field. Symbols correspond to experimental points.

At high enough fields, $B>10$ T, the conductance of the device increases exponentially at both chosen temperatures. Qualitatively, this observation agrees well with the linear $\varepsilon_g(B)$ dependence and therefore strongly favors the interpretation of our data in terms of an AB effect. We therefore base our analysis of the $G_{MIN}(B)$ curves on an assumption of a thermally activated carrier transport, $G_{MIN}(B)\propto\exp[-\Delta(B)/k_BT]$ (k_B is the Boltzmann constant), with an effective activation energy $\Delta(B)$ being proportional to the CNT band gap and thus scaling linearly with the magnetic strength. In the case of a semiconducting CNT, an axial magnetic field lifts the degeneracy between the states corresponding to the lowest K and K′ bands of the CNT band structure [see Fig. 1(a)] so that the energy gaps of the two bands depend on magnetic field as follows:[3,16,21]

$$\varepsilon_g(B)_{K,K'}=\varepsilon_g(0)\pm\lambda B, \tag{1}$$

where $\lambda=d\varepsilon_g/dB$ is the rate of the energy gap growth in the magnetic field:

$$\lambda=\frac{3\pi\gamma_0 a_{C-C}}{\phi_0}\times r, \tag{2}$$

where $\gamma_0\approx 2.8$ eV is the nearest-neighbor interaction parameter, a_{C-C} is the C–C bond distance, $\phi_0=h/e$ is the flux quantum, r is the nanotube radius, and

$$\varepsilon_g(0)=\frac{a_{C-C}\gamma_0}{r} \tag{3}$$

is the energy gap of a semiconducting CNT under zero magnetic field. While band gap corresponding to one of these branches decreases the other one is increasing as a function of magnetic field.

We first fit magnetic field dependence of the device conductance $G_{MIN}(B)$ considering two bands with and a thermal activation energy Δ proportional to the energy gap, and therefore scales linearly with magnetic field as follows:

$$\Delta(B)_{K,K'}=\Delta(0)\pm\alpha B. \tag{4}$$

Therefore we use the following expression for fitting the $G_{MIN}(B)$ curves:

$$G(B)=\tfrac{1}{2}\times G(0)[\exp(-\alpha B/k_BT)+\exp(\alpha B/k_BT)], \tag{5}$$

where $G(0)$ is the device conductance at zero magnetic field. Varying the value of α as a fitting parameter we obtain the best match between experiment and results obtained with formula (5) [solid lines on the Fig. 2(a)] for the alpha value; $\alpha=1.5$ meV/T.

The value of $\Delta(0)$ is evaluated from fitting the magnetic field dependence of the ratio of the device conductance values at two different temperatures [see the inset of Fig. 2(a)] with the following expression:

$$\frac{G(T_1)}{G(T_2)}=\frac{\exp\{-[\Delta(0)+\alpha B]/k_BT_1\}+\exp\{-[\Delta(0)-\alpha B]/k_BT_1\}}{\exp\{-[\Delta(0)+\alpha B]/k_BT_2\}+\exp\{-[\Delta(0)-\alpha B]/k_BT_2\}}, \tag{6}$$

with $T_1=200$ K and $T_2=150$ K and the value of α obtained from fitting the $G_{MIN}(B)$ curves. The best agreement is obtained for $\Delta(0)\approx 90$ meV.

Now, noting that the ratio $\Delta(0)/\alpha$ should be the same as the ratio $\varepsilon_g(0)/\lambda$ we can use the values of $\Delta(0)$ and α along with the formulae (2) and (3) to estimate the radius of the CNT. We get $r\approx 2.7$ nm that gives $d\approx 5.4$ nm which is within the range defined by the AFM measurements. We thus conclude that the OFF-state conductance of the studied device is defined by the outer shell. This result is reasonable, since the OFF-state conductance of the inner shells should be much smaller than that of the outer one if they are semiconducting (gap is proportional to $1/d$). On the other hand, any noticeable contribution of metallic inner shells would have led to much smaller ON/OFF ratio of studied device.

We also note that in case of a CNT with a diameter of 5.4 nm, the energy gap of the lower branch will vanish for an applied magnetic field of $B_0=60.5$ T [magnetic flux through the nanotube cross-section is equal to 1/3 of the flux quantum, see Fig. 1(a)] Under such a field conductance will be practically temperature independent and should have a value

of $G_{ON}/2$ if only two K and K′ bands contribute into the conductance. As seen from the Fig. 2(a) extended curves $G_{MIN}(B)$ calculated for 200 and 150 K using the formula (5) intersect at $B \approx 61$ T consistently with the estimated value of B_0. Extrapolated conductance value of $G_{MIN}(B_0) \approx 2.5 \times 10^{-6}$ S is about four times smaller than the conductance in the ON-sate ($G_{ON} \approx 10^{-5}$ S). Such a discrepancy may indicate a band gap due to Mott transition[22] or the contribution of the upper lying branches of the CNT band structure that may be noticeable in the ON-state. On the other hand thus obtained estimation of $G_{MIN}(B_0)$ is not very accurate and no definite conclusion can be made at this point. We also not that extrapolated conductance value of $G_{MIN}(B_0) \approx 2.5 \times 10^{-6}$ S is very close to the value of $G_{MIN}(B_0)$ obtained in our previous work for the case of a semimetallic CNT.[18]

Finally, we discuss the relation between the experimentally obtained values of $\Delta(B)$ and predicted values of $\varepsilon_g(B)$ using more thorough simulations based on a realistic band profile. Our results indicate that the ratio $\Delta(B)/\varepsilon_g(B)$ is constant and equal to ~0.7. It has been argued in many works that the effective thermal energy is not equal to any of the barriers created by the bended bands but is rather determined by both these barriers and thermally assisted tunneling through the depleted region.[23,24] Recently we suggested an approach to model transport in one-dimensional semiconducting channel of a FET based on a simplified formula for the shape of the band profile and accounting for tunneling.[18] We consider a CNT energy band diagram with B-dependent Schottky barriers that form at the nanotube/metal interface. The height of the Schottky barrier for electrons equals $\varphi_0 + \varepsilon_g(B)/2$, where φ_0 is approximated as the difference in the work-functions of Pd and CNT ($\varphi_0 \approx 400$ meV). We assume that the band profiles, $E_{C,V}(y)$, have two characteristic length scales along the CNT direction y, as sketched in Fig. 2(b). The length scale of the band bending far away from the electrodes, y_0, is determined by the electrostatic influence of the gate and is of the order of the SiO_2-layer thickness[24,25] $t_{ox}=300$ nm. Close to the electrodes, the midgap energy is shifted from φ_0 down to φ_1 on the short length scale $y_1 \ll y_0$, thus inducing the formation of a thin tunneling barrier for electrons. The existence of such an additional short-scale interface barrier can be attributed to doping-induced effects,[26] as already evidenced experimentally in Ref. 27. Both parameters φ_1 and y_1 depend on the chemical environment and/or the particular geometry of the electrodes.

For a further semiquantitative analysis of the device's magnetoconductance, charge transport through the nanotube is simulated using Landauer–Büttiker formalism, assuming ballistic conduction along the tube axis, whereas the energy band profiles $E_{C,V}(y)$ are described by the following:

$$E_{C,V}(y) = \varphi_1 \pm \frac{\varepsilon_g(B)}{2} + (\varphi_0 - \varphi_1)\exp\left(\frac{-y}{y_1}\right) - [\varphi_1 + e\chi(V_g,B)]\left[1 - \exp\left(\frac{-y}{y_0}\right)\right], \quad (7)$$

where the midgap energy far from the electrodes $e\chi(V_g,B)$ is controlled by the gate voltage[27] with $\varepsilon_g(B)$ dependence obtained by the band structure calculations. To simulate the magnetoconductance curves $G(B)$, the minimum value of conductance as a function of V_g is found at each magnetic field.

As shown in Fig. 2(c), a very good agreement between the experiment and the simulations is obtained with values of $y_0=470$ nm, $y_1=5$ nm, and $\varphi_1=40$ meV.

We thus demonstrate that modification of the band structure has very strong effect on conductance of MWNT-based device. Our results are consistent with the linear dependence of the energy gap on magnetic field within an assumption about proportionality of the thermal activation energy to the band gap of the CNT. Based on our estimations of $\Delta(0)$ and α we find that by changing an axial magnetic field we tune the energy gap of the lower band of the studied CNT from 140 to 70 meV.

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