Nonlinear Properties of Carbon Nanotubes in a Strong Electric Field

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Abstract

A theoretical model and computations of the I-V characteristics of both doped and undoped long carbon nanotubes in a strong axial dc-fields at room temperatures have been presented. Negative differential conductivity has been predicted. It has been shown that $|dI/dV|$ for metal carbon nanotubes in the region of the negative differential conductivity significantly exceeds corresponding values for semiconducting ones. The predicted effect makes possible the design of wave-generating nanotube-based diods for submillimeter and infrared ranges.

1. Introduction

Since the discovery by Iijima of carbon nanotubes (CNs), a great deal of interest has been focused on these quasi-one-dimensional monomolecular structures because of their unique physical properties (mechanical, electrical, optical, etc.) and the rapid experimental progress in the controlled preparation. Processes of electron transport in strong external fields when nonlinear effects are constitutive are of a great interest for potential applications in nanoelectronics and for experimental diagnostic of CN themselves.

The current-voltage (I-V) characteristics for tunnelling electrons in individual single-wall CNs at law temperatures were measured in Refs.[1, 2]. At such temperatures $k_B T \ll \mathcal{E}_c, \Delta\mathcal{E}$ and conduction occurs through well separated discrete electron states; here k_B is the Boltzmann constant, T is the temperature, $\mathcal{E}_c$ is charging energy, $\Delta\mathcal{E} = \pi\hbar v_F/L$ is the energy level spacing with v_F as the Fermi speed and L as the CN length. At the above condition the current is produced by the electrons tunneling through CN in the presence of the Coulomb blockade induced by the long-ranged (unscreened) Coulomb interaction.

Current instability in CNs is of great interest. The instability appears due to the negative differential conductivity (NDC) in I-V curves of CNs. Nonlinear coherent transport through doped nanotube junctions was considered in Ref.[3]. It was also shown the possibility of NDC for tunelling electrons. In Ref.[4] a theoretical phenomenological analysis of the I-V characteristics of undoped CNs at room temperatures, when $k_B T > \mathcal{E}_c, \Delta\mathcal{E}$. The current was produced by free charge carriers (quasiparticles) which are π-electrons moving in the field of the crystalline lattice. The nonlinearity of the I-V characteristic appears due to the nonlinear properties of the quasiparticle gas . The *negative differential conductivity* region with $dI/dV < 0$ in CNs aws predicted in a certain range of the field strength.

2. Theory

This report extends Ref.[4] for the case of doped CNs. Let us consider an doped single-wall zigzag CN (m,0) exposed to a homogeneous axial dc-field E_z, $E_z = V/L$, where V is the voltage between the CN ends. We shall apply the semi-classical approximation considering the motion of π-electrons as a classical motion of free quasi-particles with dispersion law extracted from the quantum theory in the tight-binding approximation [5].

The motion of quasi-particles in an external axial electric dc-field is described by the Boltzmann kinetic equation

$$eE_z \frac{\partial f(\mathbf{p})}{\partial p_z} = -\frac{1}{\tau}[f(\mathbf{p}) - F(\mathbf{p})], \tag{1}$$

where e is the electron charge, $F(\mathbf{p})$ is the equilibrium Fermi distribution function and τ is the relaxation time. The relaxation term of the equation (1) describes the electron-phonon scattering [6, 7], electron-electron collisions etc.

Utilizing the method originally developed in the theory of quantum semiconductor superlattices [8] we can construct an exact solution of kinetic equation (1) without assuming the electric field to be weak. First, note that the distribution function $f(\mathbf{p})$ is periodic in p_z with period $2\pi/a$, $a = 3b/2\hbar$, $b = 1,42$Å. Then, taking into account the transverse quantization, the distribution function can be presented by:

$$f(\mathbf{p}) = \Delta p_\phi \sum_{s=1}^{m} \delta(p_\phi - s\Delta p_\phi) \sum_{r\neq 0} f_{rs} e^{iarp_z}, \tag{2}$$

where f_{rs} are coefficients to be found, $\delta(x)$ is the Dirac delta-function, $\Delta p_\phi = \pi\sqrt{3}/am$. The equilibrium distribution function $F(\mathbf{p})$ can be expanded in the analogous series with the coefficients as follows

$$F_{rs} = \frac{a}{4\pi} \int_0^{2\pi/a} \left[\frac{e^{-iarp_z}}{1 + \exp\{(\mathcal{E}_s(p_z) - \mu)/k_B T\}} - \frac{e^{-iarp_z}}{1 + \exp\{(-\mathcal{E}_s(p_z) - \mu)/k_B T\}} \right] dp_z. \tag{3}$$

In this equation first term descirebes the contribution of conduction band and the second one of valence band. Here μ is a chemical potential of CN. It describes doping (μ=0 for undoped CNs [4]). μ can be varied within wide range of values. Accordingly to [3] $\mu \sim 0.3$ eV for dopping by Au substrate, -0.5 eV $< \mu <$ 0.5 eV for doping by typical alcali and halogen atoms. For the KC_8 doped CNs $\mu \sim 2.0$ eV [9]. Substitution of both expansions into Eq. (1) gives $f_{rs} = F_{rs}/(1 + i\tau r\Omega)$, where $\Omega = aeE_z$ is the Stark frequency.

The surface current density is defined by

$$j_z(E_z) = -\frac{8e\gamma_0}{\sqrt{3}\hbar bm} \sum_{r=1}^{\infty} \frac{r^2\Omega\tau}{1 + (r\Omega\tau)^2} \sum_{s=1}^{m} F_{rs}\mathcal{E}_{rs}. \tag{4}$$

Here $\gamma_0 \sim 3.0$eV is the overlapping integral. This equation states the basis for the evaluation of I-V characteristics. As it has been stated above, the quasi-particles motion is described classically. Thus, both interband transitions and quantum-mechanical corrections to the intraband motion are left out of account in this model. This imposes the limitation on the external electric field strength: $|E_z| < \gamma_0/2eR$.

The Coulomb electron-electron interaction has been also left out of account in our approach. The role of this mechanism as applied to CNs was considered in a number of papers, see [10] for example. It has been established that the short-range electron-electron interaction, typical for CN arrays ('ropes'), have only a weak effects at high temperatures.

3. Numerical Results

The I-V characteristics obtained via numerical calculation of Eq.(4) are presented in Fig.1 and Fig. 2 for metal ($m = 3q$, q is an integer) and Fig. 3 and Fig. 4 for semiconducting ($m \neq 3q$) zigzag CNs.

The figures show the linear dependence of j_z on E_z at weak strengths of the external field both for doped and undoped CNs; it corresponds to the region of ohmic conductivity. As E_z increases, the value $\partial j_z/\partial E_z$ growth smaller and at $E_z = E_z^{(max)}$ the current density reaches the maximum value j_z^{max}. Further increase of E_z results in the decrease of j_z. Thus, predicted in [4] the region with the negative differential conductivity ($\partial j_z/\partial E_z < 0$), in the I-V characteristics of undoped CNs can be also observed in the case of doped CNs.

Fig.1 and Fig. 3 demonstrate that $E_z^{(max)}$ depends on neither number m nor the conductivity type (metal or semiconductor), whereas, j_z^{max} shows the different dependencies on m for undoped metal and semiconducting CNs. For metal CNs, j_z^{max} decreases with m while it increases for semiconducting ones. As $m \to \infty$, j_z^{max} for metal and semiconducting CNs tends to the same limit from opposite sides. Generally, at large m, the I-V characteristics of different CNs are coming close and in the limit case $m \to \infty$ they reduce to I-V characteristic of the plane graphite monolayer. It should be noted that the metal CNs exhibit much lager NDC as compared to semiconducting ones. Fig. 2 shows that the doping of metal CNs makes J_z^{max} some times larger. Doping of semiconducting CNs with small m does not lead to noticeable changes but as m increses, current through doped doped semiconducting CNs increases and values of current density become one order with ones for conducting undoped CNs (Fig. 4).

4. Conclusion

In Summary, we have predicted the NDC effect in both doped and undoped CNs, which is expected to be observable in sufficiently long CNs at room temperatures. I-V curves are expected to be effectevely controlled due to doping.

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