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TUNNELING CURRENT IN CARBON NANOTUBES WITH DEEP IMPURITIES

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In this paper we study the tunneling contact of carbon nanotubes with deep impurities and metal. The tunneling current in contact nanotube-metal was investigated. The dependence of current-voltage characteristic of such contact on the band gap of the impurity was analyzed. An area with negative differential conductivity was observed.

Keywords: Carbon nanotube, deep impurity, band gap, negative differential conductivity.

1. Introduction

In this paper the tunneling current flowing in contact of carbon nanotubes (CNTs) with deep impurities and metal. A deep impurity is one which creates a deep energy level [1]. It should be noted that research related to the study of such impurities, as well as their influence on the electronic structure and thus the properties of semiconductors is very popular now [2,3]. Such attention to this problem is primarily caused by the trends of modern opto-, micro- and microwave electronics, and, specifically, more stringent requirements for the quality of semiconductor materials having content of impurities which give rise to deep levels in the band gap. The presence of these impurities impart both positive and negative characteristics. Therefore, to minimize undesirable effects, it is important to study the nature of deep impurities to make the most effective use of positive effects on the functional characteristics of these devices.

At the same time, the attention of researchers is attracted to tunneling, as devices based on the tunneling effect have become a part of the basic elements of modern electronics and are thus of great practical application.

2. Statement of the problem and basic equations

The matrix form of the Hamiltonian of the problem is:

$$H = \begin{bmatrix} 0 & f & \alpha_1 & \beta_1 & \gamma_1 & \Delta_1 \\ f^* & 0 & \alpha_2 & \beta_2 & \gamma_2 & \Delta_2 \\ \alpha_1^* & \alpha_2^* & t_1 & 0 & 0 & 0 \\ \beta_1^* & \beta_2^* & 0 & t_2 & 0 & 0 \\ \gamma_1^* & \gamma_2^* & 0 & 0 & t_3 & 0 \\ \Delta_1^* & \Delta_2^* & 0 & 0 & 0 & t_4 \end{bmatrix} \tag{1}$$

where $|f|$ determines the energy spectrum of the CNT; t_i - the value of the energy level of deep impurities, α, β, γ, Δ - hopping integral between the sublattices and impurity levels.

Hamiltonian (1) can be rewritten by using the structure of the block matrices [4]:

$$H = \begin{bmatrix} 0 & f & \alpha_1 & \beta_1 & \gamma_1 & \Delta_1 \\ f^* & 0 & \alpha_2 & \beta_2 & \gamma_2 & \Delta_2 \\ \alpha_1^* & \alpha_2^* & t_1 & 0 & 0 & 0 \\ \beta_1^* & \beta_2^* & 0 & t_2 & 0 & 0 \\ \gamma_1^* & \gamma_2^* & 0 & 0 & t_3 & 0 \\ \Delta_1^* & \Delta_2^* & 0 & 0 & 0 & t_4 \end{bmatrix} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}.$$

Considering the electronic system in the long-wave approximation, we can write the effective Hamiltonian of the problem [4]:

$$H_{\text{eff}} = H_{11} - H_{12}H_{22}^{-1}H_{21}. \tag{2}$$

We solve the eigenvalue problem and find:

$$\begin{gathered} \lambda_{1,2}^2 = \frac{R + Q \pm \sqrt{(R-Q)^2 - 4\left(\varepsilon D^* + \varepsilon^* D - |\varepsilon|^2 - |D|^2\right)}}{2}, \\ R = -\left(\frac{|\alpha_1|^2}{t_1} + \frac{|\beta_1|^2}{t_2} + \frac{|\gamma_1|^2}{t_3} + \frac{|\Delta_1|^2}{t_4}\right), \\ Q = -\left(\frac{|\alpha_2|^2}{t_1} + \frac{|\beta_2|^2}{t_2} + \frac{|\gamma_2|^2}{t_3} + \frac{|\Delta 2|^2}{t_4}\right), \\ D = \left(\frac{\alpha_1\alpha_2^*}{t_1} + \frac{\beta_1\beta_2^*}{t_2} + \frac{\gamma_1\gamma_2^*}{t_3} + \frac{\Delta_1\Delta_2^*}{t_4}\right). \end{gathered} \tag{3}$$

Parameters R, Q reflect the probability of a jump from the first (second) CNT sublattice to the impurity, while D reflects the probability of a jump from one CNT‘s sublattice to another.

We note that the dispersion relation, which describes the properties of CNTs, is [5]:

$$\varepsilon\,(p,s) = |f| = \pm\gamma\sqrt{1 + 4\cos(ap_x)\cos\left(\frac{\pi s}{m}\right) + 4\cos^2\left(\frac{\pi s}{m}\right)}, \tag{4}$$

where $s = 1, 2, \ldots, m$, the nanotube is of the type $(m, 0)$, $\gamma \approx 2.7$ eV, $a = 3b/2\hbar$, $b = 0.142$ nm is the distance between the adjacent carbon atoms.

Typical band structure of carbon nanotube with deep impurities is presented in Fig. 1.

In the framework of the Kubo theory, the expression for the current density of the contact is the following [6]:

$$\begin{gathered} J = 4\pi e\,|T|^2 \int\limits_{-\infty}^{+\infty} dE\nu_A(E+eV)\nu_B(E)(n_f(E) - n_f(E+eV)), \\ \nu_A(E) = \sum_p \delta(E - E_p^A); \quad \nu_B(E) = \sum_q \delta(E - E_q^B), \end{gathered} \tag{5}$$

where $\delta(x)$ is the Dirac delta function, $\nu_{A(B)}(E)$ is the tunneling density of states, $n_f(E)$ is the equilibrium number of fermions with energy E. Here and below, we use the approach of "rough" contact T (tunneling matrix element between the two states): (in fact, we impose restrictions on the geometry of the contact that is, in what follows we consider the case where the nanotube is perpendicular to the surface of the contact material).

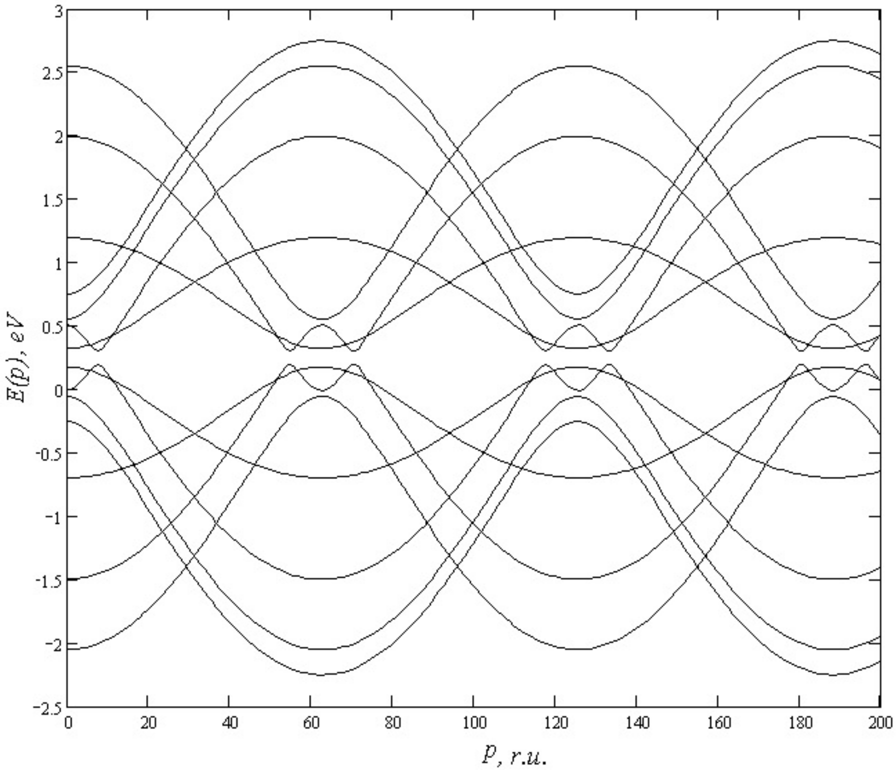

FIG. 1. The band structure of CNT (7,0) with the deep impurities

The metal dispersion law of free electrons in the effective-mass m is:

$$E_q^B = \frac{p^2}{2m}. \tag{6}$$

3. Results

Equation (5) was solved numerically. The current-voltage characteristic (CVC) of the contact is presented in Fig. 2.

A significant influence of the parameters on the behavior of the current-voltage curve can be seen. It should be noted that when R increases, both the current and the area with negative differential conductivity decrease. Also, it should be noted that we have an area with negative differential conductivity (NDC).

The current-voltage characteristic of the contact in the case of different values of D is shown in Fig. 3.

The effect of parameter D appears to weaken of the current, which can be attributed to a stronger bond between the electrons and the impurity levels.

Therefore, we can conclude that the influence of impurities on the tunneling characteristics of CNT-metal contact was investigated. The effect of hopping integrals, and the width of the band gap of deep impurities on the dependence of the tunneling current and the voltage between the contact were also observed. By careful selection of the impurity parameters (D, R, Q), we can control the CVC and the value of the area with NDC. This effect can be used in many practical applications (for example in tunneling diodes).

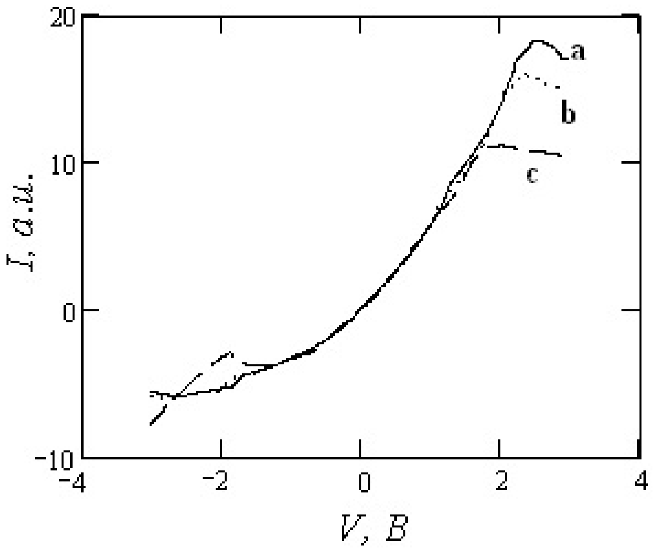

FIG. 2. The current-voltage characteristics of metal-doped CNTs ($Q = 0.03$ eV, $D = 0.05$ eV - fixed): a) $R = 0.02$ eV; b) $R = 0.04$ eV; c) $R = 0.1$ eV

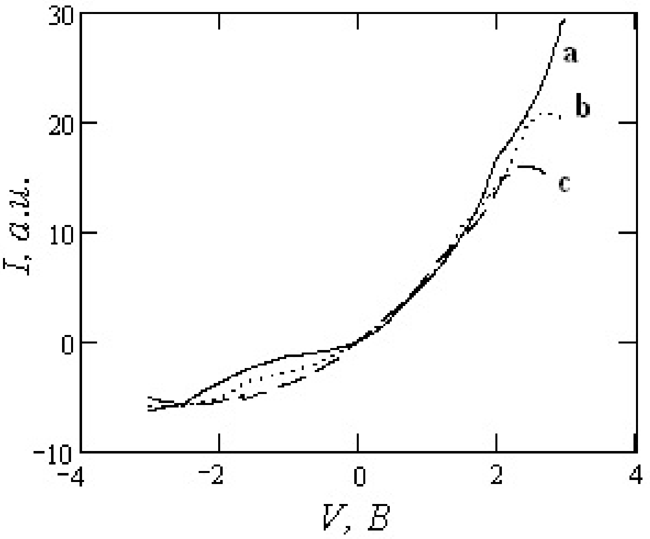

FIG. 3. The current-voltage characteristics of metal-doped CNTs ($R = 0.02$ eV, $Q = 0.03$ eV - fixed): a) $D = 0.01$ eV; b) $D = 0.04$ eV; c) $D = 0.06$ eV

References

[1] A.A. Gvelisiani, E.A. Shelonin. *Behavior and properties of dopped impurities in semiconductors*. IPC MITHT M.V. Lomosov, Moscow: 2004. 80 p.

[2] V.N. Mantsevich, N.S. Maslova. Spatial effects of Fano resonance in local tunneling conductivity in vicinity of impurity on semiconductor surface. *Pis'ma v ZheTF*, **91**, P. 150–153 (2010).

[3] V.N. Mantsevich, N.S. Maslova. The influence of localized states charging of formula nor shown tunneling current noise spectrum. *Solid state communications*, **150**, P. 2072–2075 (2010).

[4] A. Cortijo, F. Guinea, M.A.H. Vozmediano. Geometrical and topological aspects of grapheme and related materials. `arXiv.org 1112.2054v1`, (2011).

[5] P. Harris. *Carbon nanotubes and related structures. New materials of XXI century.* Technosphera, Moscow: 2003. 336 p.

[6] L.S. Levitov,.V. Shitov. *Green's functions. Tasks with solutions*. Fizmatlit, Moscow: 2003. 392 p.