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ELECTROPHYSICAL PROPERTIES OF CNT. THE AUGMENTED CYLINDRICAL WAVE METHOD

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Current-voltage characteristics of tunnel contact between semiconducting (and conducting) carbon nanotubes (CNT) of various diameters and system of periodically located quantum dots (and also in contact to metal) was obtained using density of states (DOS) investigation. DOS has been calculated by means of the method of attached cylindrical waves. At certain parameters for quantum dots, the current-voltage characteristics observed testify to the presence of negative differential conductivity.

Keywords: carbon nanotubes, density of the states, current-voltage characteristics.

1. Introduction

In the last few years, the interest of many researchers has been focused on the properties of carbon nanotubes [1]. It is known from classical works that the "Arm-chair" type of nanotube, in Huckel's approximation, are conductors at any temperature [2]. However, using the linear augmented cylindrical wave (LACW) method allows a gap in the band structure of this type of nanotube. This makes it possible to use them in different applications. The simplest method to experimentally verify the change in the state density is to study the tunneling current [3, 4], for example, of the contact with quantum dots. In these papers, the density of states were calculated by the method of Green's functions [5], however, not every system has a density of states for electrons can be determined analytically. For such a system, the more versatile method is based on ab initio calculations .

Theoretically, investigation was done by tight-binding calculations only, but it is known from the band structure theory of solids that the linear combination of atomic orbitals (LCAO) basis is adequate to achieve good results for the valence band, but not for the conduction band. The reason for this is that this basis does not include the delocalized conducting plane-wave type functions. As to the π electron band structure models, they are adequate for calculating the energy curves located in a Fermi level region only. Therefore, we have calculated the complete band structures of metallic armchair (n, n) CNTs with $4 < n < 100$ and zigzag semiconducting $(0, n)$ CNTs with $10 < n < 49$ indivisible by 3 in terms of a LACW method. The LACW method is just a reformulation of the linear augmented plane wave (LAPW) theory for cylindrical multiatomic systems. Its basis functions have both localized and delocalized components. Finally, the main argument for using cylindrical waves is to account for the cylindrical geometry of the nanotubes in an explicit form that offers obvious advantages [6].

2. Basic equations

2.1. Cylindrical muffin-tin potential

Similar to the LAPW technique used in the band structure theory of solids, we apply the muffin-tin (MT) and local density functional approximations for electronic potentials of tubules. However, the potential of a nanotube differs drastically from that of bulk material. Indeed, infinite motion of an electron is possible in any direction in a crystal, but it is obviously limited in the case of nanotubes by their size and cylindrical shape. Therefore, in terms of the LACW method, the atoms of nanotube are considered to be enclosed between two impenetrable cylinder-shaped potential barriers Ω_a and Ω_b, because there are two vacuum regions Ω_v on the outside and on the inside of the tubule. The radii a and b of these barriers are chosen so that the region confined by barriers accommodates a significant portion of the electron density of the tubule. Based on our previous calculations of the CNTs, we take $a = R_{NT}+2.3$ a.u., $b = R_{NT}+2.3$ a.u., where, R_{NT} is radius of the tubule. Finally, the electronic potential is spherically symmetrical in the regions of MT-spheres of atoms α and constant in the interspherical region. Inside these spheres, we calculate the electron potential by means of the local density approximation with Slater exchange. As usually, the radii of the MT spheres were chosen so that the atomic spheres touch, but do not overlap. Outside the MT spheres up to the impenetrable potential barriers Ω_a and Ω_b, the potential is approximated by a constant value taken to be the energy zero point [6,7].

2.2. Solution of the Schrdinger equation

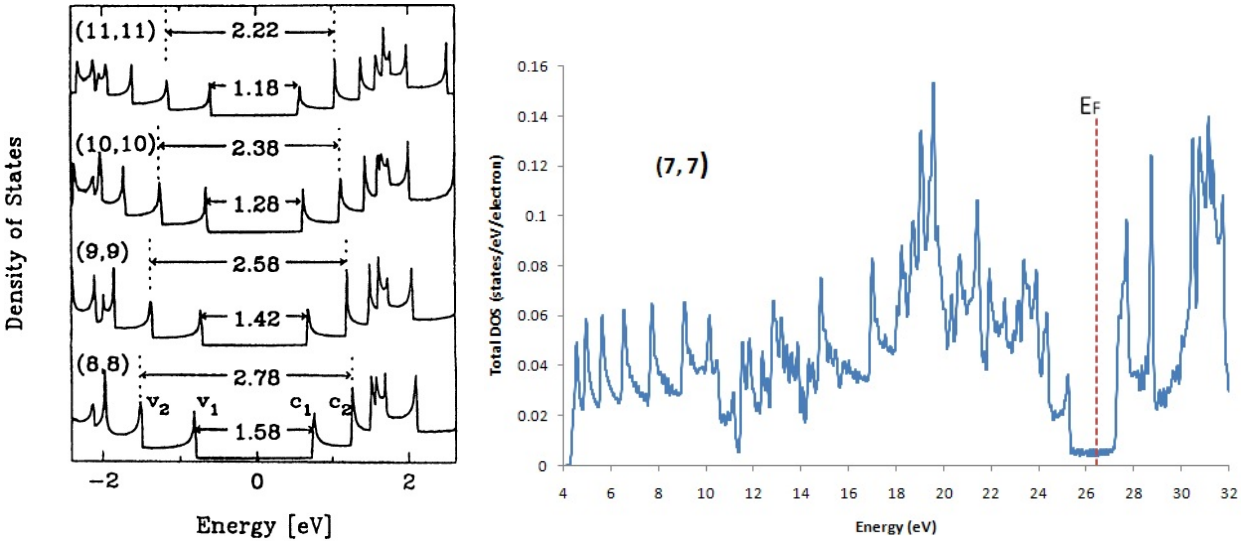
The basis functions called LACWs are solutions of the Schrodinger equation for the interspherical and MT regions of tubule sewn together so that the resulting LACWs are continuous and differentiable anywhere in the system. In the interspherical region, the LACWs are the solutions of the Schrdinger equation for free electron movement in the infinitely long potential well between two impenetrable cylindrical potential barriers. Here, the solutions are the superpositions of the cylindrical Bessel functions of the first and second kinds. In any MT sphere, the solutions are expanded in terms of the spherical harmonic functions and the eigenfunctions of the radial Schrdinger equation. To obtain the basis wave functions, the solutions of Schrdinger equation in these two regions are matched on the surfaces of the MT spheres so that both the basis functions and their normal derivatives are continuous across these surfaces. The eigenfunctions of electrons in the tubule are the linear superpositions of these basis LACWs. The coefficients of the expansions of any eigenfunction in terms of these basis functions and the electron dispersion curves are defined by the variational method.

In this work, we apply the symmetry-adapted version of the LACW method developed previously. In this version, one takes into account that every single-walled CNT can be generated by first mapping only two nearest-neighbor C atoms onto a surface of a cylinder and then using the rotational and helical symmetry operators to determine the remainder of the tubule. With account of these symmetries, the cells contain only two carbon atoms, and the *ab initio* LACW theory becomes applicable to any tubule independent of the number of atoms in a translational unit cell. In the LACW studies, we use only this structural information as input parameters.

The dispersive relation for quantum wells is similar to the band structure of superlattice [8]:

$$E_{QD} = \varepsilon_0 - \Delta\cos(p),$$

where ε_0 is electron energy in quantum well, Δ is tunnel integral, defining by overlap of electron wave functions of nearest wells.



a) b)

FIG. 1. Density of states for CNT arm-chair type: a) Huckel's approximation; b) LACW method

The density of states for arm-chair CNTs, calculated under the π-electron approximation [2], was shown in Fig. 1a. The LACW method allows in the calculation consideration of more deep-seated σ-orbital electrons at very high temperatures ($\sim$ 25–27 eV) to get a gap in the energy spectrum (see Fig. 1b). This fact allowed the calculation of the electrical properties of conductive nanotubes in contact with the quantum dots.

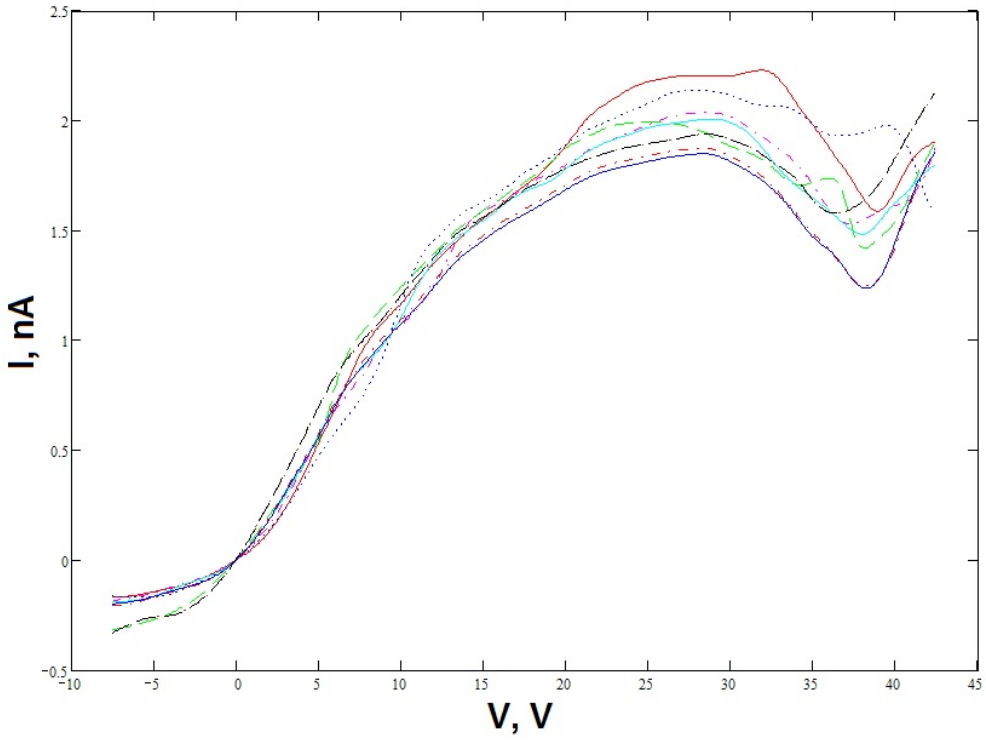


FIG. 2. Current-voltage characterictics for CNT type "zig-zag" of various diameter ((10, 0) – (50, 0)) in contact with quantum dots system

3. Tunnel characteristics

In order to study tunneling effects, we will set Hamiltonian of our model in a form:

$$H = \sum_p \varepsilon_p^A a_p^+ a_p + \sum_q \varepsilon_q^B b_q^+ b_q + \sum_{pq} T_{pq}(a_p^+ b_q + b_q^+ a_q), \tag{1}$$

where a_p^+, a_p - production (annihilation) operators of electrons with a momentum p in carbon nanotubes; ε_p^A - electron energy spectrum of nanotubes (1); T_{pq} - matrix element of the operator of tunneling between conditions p and q; b_q^+, b_q - creation (annihilation) operators of electrons with an momentum q in matter, resulted in contact with carbon nanotubes; ε_p^B - electron energy spectrum of quantum dots. Note, that in (1) p and q are multi-indices. Also, if we consider the external electric field $\vec{E}$ which we will investigate using the gauge: $\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t}$, it is possible to take it into account by means of replacement the corresponding momentum components: $p \to p - eA/c$.

Defining a tunnel current as [5]:

$$J = ie \sum_{pq} \left(a_p^+ b_q - b_q^+ a_p\right), \tag{2}$$

and carrying out calibration transformation [5]:

$$a_p \to S^{-1} a_p S,$$
$$S = \exp\left(ieVt \sum_p a_p^+ a_p\right),$$

where V applied, for definiteness, to CNT voltage, - electron charge, it is possible to reduce formally a problem about calculation characteristic current-voltage to calculation of the response of the operator: $J_t = ie \sum_{pq} \left(a_p^+ b_q e^{ieVt} - b_q^+ a_q e^{-ieVt}\right)$ on external action [5]:

$$H_t = \sum_{pq} T_{pq} \left(a_p^+ b_q e^{ieVt} + b_q^+ a_q e^{-ieVt}\right).$$

Within the framework of Kubo theory, the answer is set by the formula:

$$\begin{gathered} J = 4\pi e \left|T\right|^2 \int\limits_{-\infty}^{\infty} d\varepsilon \nu_A\left(\varepsilon + eV\right) \nu_B\left(\varepsilon\right) \left(n_f(\varepsilon) - n_f(\varepsilon + eV)\right), \\ \nu_A\left(\varepsilon\right) = \sum_p \delta\left(\varepsilon - \varepsilon_p^A\right), \quad \nu_B\left(\varepsilon\right) = \sum_q \delta\left(\varepsilon - \varepsilon_q^B\right), \end{gathered} \tag{3}$$

where $\delta(x)$ - Dirac delta-function, $\nu_{A(B)}\left(\varepsilon\right)$ - tunnel density of states; $n_f\left(\varepsilon\right)$ - equilibrium number of fermions with energy ε. We used the approach of "rough" contact: $T_{pq} = T$ (a nanotube is perpendicular to the quantum dot surface). After integrals calculation entering in (3) it is easy to obtain current-voltage characteristic of the contact presented in Fig. 2–3.

The existence of a descending section of the current-voltage characteristic of the tunneling conductance between the nanotubes and the quantum dots system can be clearly seen in Fig. 2. This indicates the presence of negative differential conduction. The descending section is observed at the same parameters of quantum dots: $\varepsilon_0 = 22$ eV - energy of electrons a quantum

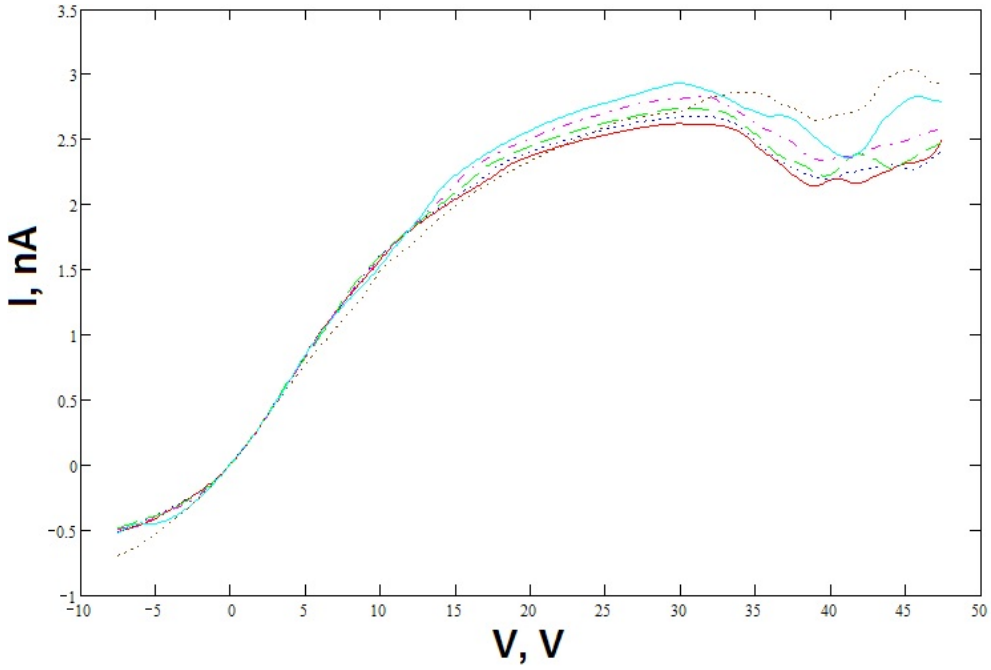


FIG. 3. Current-voltage characteristics for CNT type "arm-chair" of various diameter ((4,4) – (9,9)) in contact with quantum dots system

hole, and $\Delta = 3$ eV - the tunnel integral defined by overlapping of wave electronic functions of the next holes. The size of the resistance obtained in such a system was $R \approx -24$ kOhm.

Similarly, the current-voltage characteristics for semiconducting CNT of various diameters ((10,0)–(50,0)) in contact with systems of quantum dots are represented in Fig. 2. For semiconducting CNT in contact with a quantum dots system, the descending section in the current-voltage, characteristic of tunnel conductivity, was also observed. The resistance obtained for such a system was $R \approx -18$ kOhm (should be -18 kOhm) for the same parameters of the quantum dots system.

It should be noted that the descending section in CVC for system CNT-QD is absent in the case of pi-approximation for CNT DOS.

The obtained dependencies can have the important practical applications for studying noncontact and the design of tunneling diodes based on carbon nanotubes.

4. The conclusion

In summary we will formulate the basic conclusions from the made work.

(1) Current-voltage characteristics of contacts CNT - a superlattice of quantum dots are obtained.
(2) The descending section with negative differential conduction is observed for certain characteristics of quantum dots. This effect can be used to create various frequency amplifiers.

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