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Features of the Electrical Characteristics of an Octagraphene Nanotube

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In the framework of the density functional theory (in the local density approximation) and the method of nonequilibrium Green functions (DFT + NEGF), electron transport in graphene and octagraphene nanotubes with approximately the same geometric dimensions (with diameters of 7.08 Å and 7.15 Å and lengths of 41.2 Å and 39.92 Å, respectively) was studied. The transmission spectra, the density of states, current-voltage *dI*/*dV* characteristics of graphene and octagraphene nanotubes are calculated. It is shown that, by the nature of the current-voltage characteristic, a graphene nanotube has semiconductor properties, and an octagraphene nanotube has metallic properties. It was revealed that the *dI*/*dV* spectrum shows an equidistant series of differential conductivity of Coulomb origin. It is shown that, at resonance voltage, the features of differential conductivity in the form of a maximum in a graphene nanotube are accompanied by a minimum in an octagraphene nanotube. It was found that the amplitudes of the differential conductivity in the form of an equidistant series of graphene nanotubes decrease exponentially, while those of octagraphene nanotubes increase exponentially. The results can be useful for calculating new promising electronic switching nanodevices.

Keywords: Carbon nanotube, Octagraphene nanotube, Electron transport, Transmission spectrum, Density of states, Current-voltage characteristic, Differential conductivity.

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1. INTRODUCTION

After the discovery of graphene [1], other graphene-like quasi-two-dimensional nanostructures were found and predicted [2-5]. One of such nanostructures predicted on the basis of first-principle calculations is octagraphene, which consists of alternating octahedra and squares [6, 7]. The atomic binding energy calculated using the generalized gradient approximation (GGA) in octagraphene is 7.39 eV/atom, while in graphene it is 7.92 eV/atom [6], i.e. from a thermodynamic point of view, octagraphene is less stable and metastable with respect to graphene [8]. By electronic properties, octagraphene is a semimetal with a nonzero density of states at the Fermi level: its valence band overlaps with the conduction band.

Note that in [9], two more types of octagraphene (OPG-L and OPG-Z) were theoretically discovered, where the "square" elements were replaced by "pentagons", and it turns out that one of them, OPG-L, is a metal, and the other, OPG-Z, is a gapless semimetal.

When the octagraphene layer is folded, carbon nanotubes (CNT) of a new type are obtained, which in the future can serve to create elements of nanoelectronics.

In this work, in the framework of DFT + NEGF, we calculated the main electrical characteristics of graphene (GNT) and octagraphene (OGNT) nanotubes with approximately equal geometric parameters (diameters 7.08 Å and 7.15 Å, lengths 41.2 Å and 39.92 Å, respectively) obtained by folding nanoribbon of graphene and octagraphene.

2. SIMULATION MODEL AND METHODS

The geometry of the studied GNT and OGNT is shown in Fig. 1. A GNT consists of 504 atoms and has three regions with a total size of ~ 58.255 Å: the central region, left and right regions of the electrodes. Electrodes were obtained by expanding the central region along the *C*-axis by ~ 8.525 Å. The distance between the electrodes is ~ 41.205 Å, where the central region of the nanosystem of 360 atoms is located. Similarly, an OGNT is formed of 540 atoms and has a length of ~ 60.4 Å. OGNT electrodes were also obtained by expanding the central region along the *C*-axis by ~ 10.24 Å, and 360 carbon atoms were placed in the central region.

Computer simulation of the electron transport characteristics of the GNT and OGNT was carried out within the framework of the density functional theory (DFT) using the non-equilibrium Green's function (NEGF) method in the local density approximation (LDA) [10].

Simulation of characteristics implemented in the program Atomistix ToolKit with Virtual NanoLab [11]. (The basic equations of this method are described in detail in our previous works [12, 13]).

The current-voltage characteristic (CVC) of the nanostructure is calculated on the basis of the well-known Landauer equation, which indicates the fundamental relationship of the electric current with the transmission spectrum:

$$I(V_L,\ V_R,\ T_L,\ T_R) = \frac{2e}{h}\int_{-\infty}^{+\infty} T(\varepsilon)\left[f\left(\frac{\varepsilon-\mu_R}{k_B T_R}\right)-f\left(\frac{\varepsilon-\mu_L}{k_B T_L}\right)\right]d\varepsilon\,, \quad (1)$$

where e is the electronic charge, h is the Planck constant, ε is the energy, $T(\varepsilon)$ is the transmission function (spectrum), $f(\varepsilon)$ is the Fermi function of quasiparticle energy distribution, k_B is the Boltzmann constant, T_L,

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T_R are the current temperatures of the left and right electrodes, respectively, μ_R, μ_L are the electrochemical potentials of the left and right electrodes, respectively.

The geometry of CNT was optimized by the parametrization of functional GGA PBE (Perdew-Burke-Ernzerh) [14]. The structure of the nanotubes was optimized until the maximum residual force on all atoms was less than 0.02 eV/Å.

3. RESULTS AND DISCUSSION

The results of the calculation of the local density of states (LDOS) of CNT are presented in Fig. 2. As can be seen, the minima of GNT LDOS appear between carbon atoms and are repeated every $(n-1)\cdot 0.05l$ Å, and the LDOS maxima occur in the region where C atoms are located and is repeated every $((n-1)\cdot 0.05 + 0.025)\cdot l$ Å (n is the natural number, l is the length of the CNT).

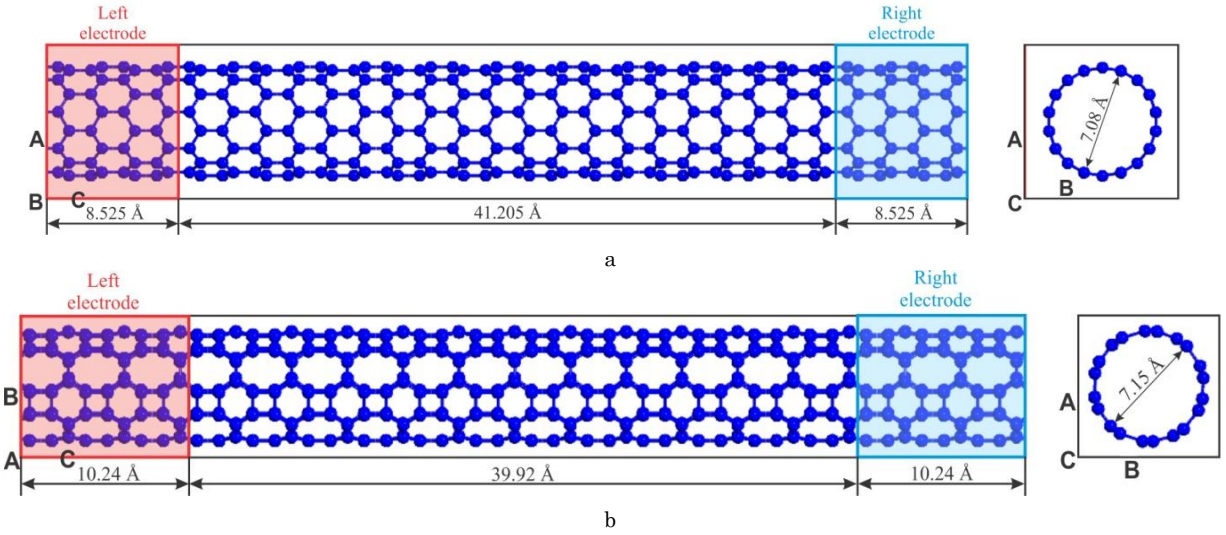

Fig. 1 – The geometry of carbon nanotubes: a) GNT; b) OGNT

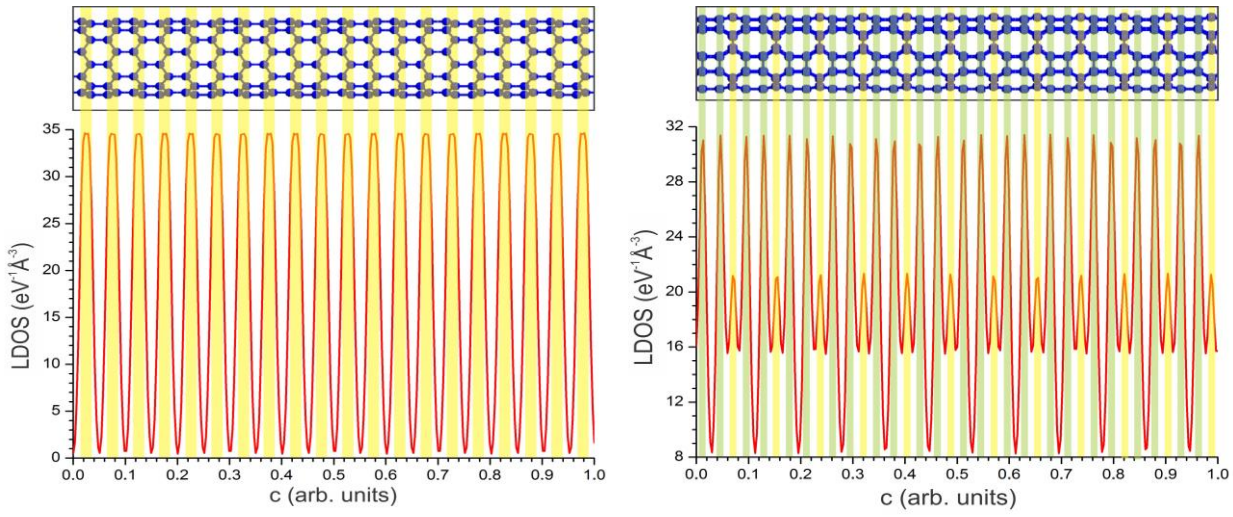

Fig. 2 – LDOS of CNT: a) GNT; b) OGNT (yellow indicates LDOS features associated with hexagonal elements; green indicates LDOS features associated with square elements)

LDOS of OGNT has three characteristic maxima: two large peaks are associated with the square OGNT elements and the third peak is associated with the hexagonal element. Large peaks of LDOS appear every $((n-1)\cdot 0.013 + 0.083)\cdot l$ Å and $((n-1)\cdot 0.046 + 0.083)\cdot l$ Å. The third small peak of LDOS is repeated every $((n-1)\cdot 0.07 + 0.083)\cdot l$ Å.

The transmission spectra of the considered CNT at zero bias voltage are presented in Fig. 3. The transmission spectrum of GNT near the Fermi energy ($\varepsilon_F = 0$) takes a minimum value of ~ 1 arb. units, and of OGNT – takes a maximum value of ~ 8 arb. units. Note that the transmission spectrum of OGNT is uniform. The uniformity of the transmission spectrum of the OGNT is responsible for the quasilinear evolution of CVC. The GNT spectrum decreases with negative energy (– 3÷0 eV) and increases with positive energy (0÷2 eV).

Features of the transmission spectrum are also observed in the device density of states (DDOS) (Fig. 4), since these values $T(\varepsilon) = D(\varepsilon - U)2\pi\gamma_1\gamma_2/\gamma$ are directly proportional (where U is the self-consistent potential, γ is the Luttinger parameter) [15]. As seen, DOS of CNT is very different, high levels of GNT states occur at negative energies of – 5.8 eV, – 5 eV, – 4.6 eV, – 4 eV and of

OGNT states – at energies – 4.8 eV, – 3 eV, – 1.6 eV. At the Fermi level ($\varepsilon_F = 0$), OGNT have a nonzero density (~ 22 eV^{-1}). In the energy range – 1.45 ÷ 0.68 eV, the DDOS and OGNT transmission spectra are almost two times larger than the similar GNT characteristics (Fig. 4).

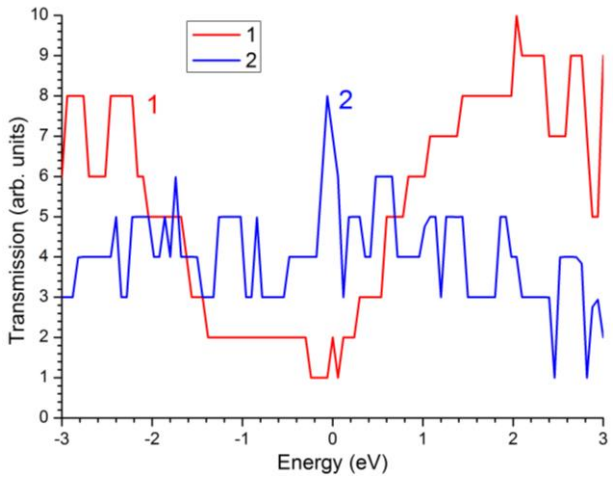

Fig. 3 – Transmission spectra of CNT at $V_{bias} = 0$: 1 – GNT; 2 – OGNT

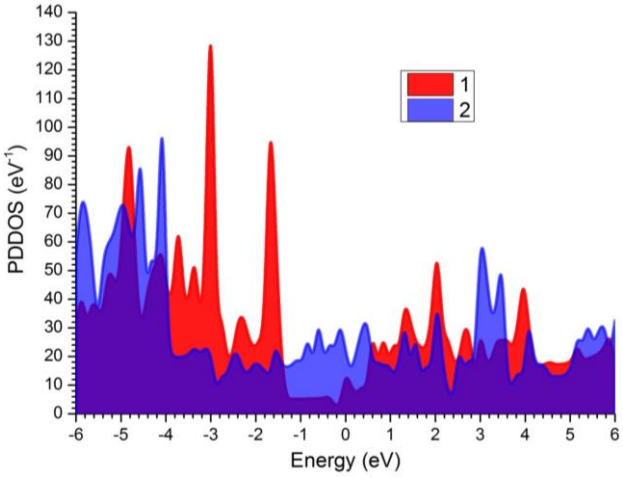

Fig. 4 – The DOS of CNT: 1 – GNT; 2 – OGNT

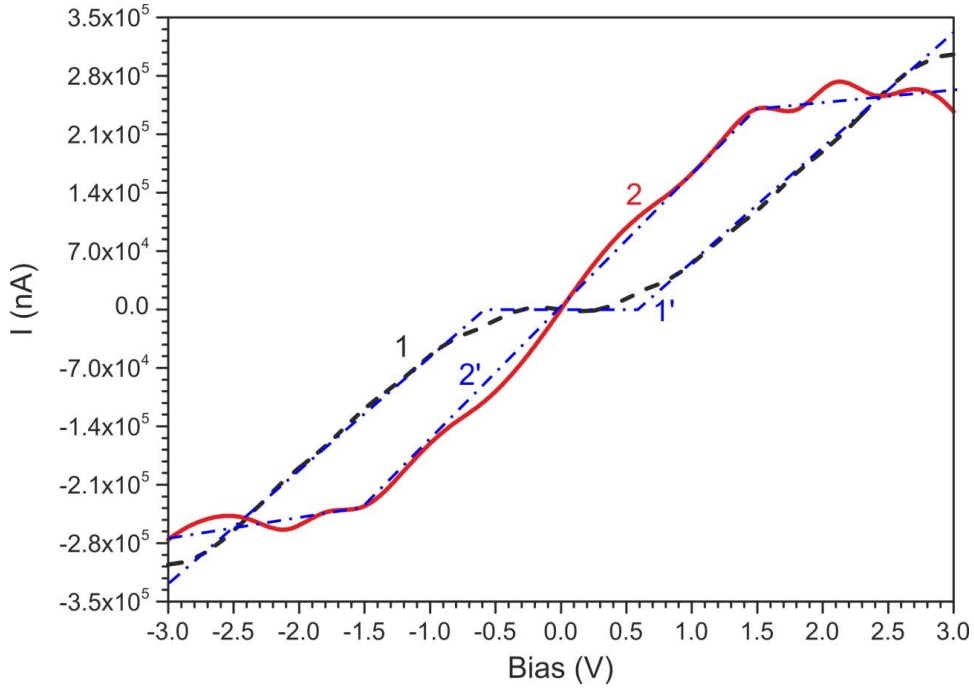

Fig. 5 – CVC of CNT: 1 – GNT (dashed line); 2 – OGNT (solid line); 1', 2' – piecewise linear approximations of characteristics 1 and 2

The results of computer simulation of the CVC and differential conductivity in the framework of DFT + + NEGF are shown in Fig. 5 and Fig. 6. In the voltage range – 0.3 ÷ 0.3 V, a small current ~ 0 ÷ 2.15 μA flows through the GNT. We believe that this is due to the Coulomb blockade of quasiparticles. Outside this interval, a quasilinear increase in current is observed. In the intervals – 3 ÷ – 1.5 V and 1.5 ÷ 3 V, the transport current flowing through the OGNT grows slowly with small oscillations, a sharp increase in current according to the quasilinear law occurs in the voltage range – 1.5÷1.5 V. Moreover, the Coulomb blockade of quasiparticles is not observed. Such switching of the current in the SWCNT from one "state" to another can be used to create nanotriggers, given the low level of $V_0 \approx -2.4\ 10^5$ nA and the high level of $V_1 \approx 2.4\ 10^5$ nA.

Differential conductivity has a peak structure resembling a series of equally spaced differential conductivities of ultrafine nanoparticles in the form of alternating peaks (maxima) and dips (minima) (Fig. 6) [16]. In Fig. 6, for convenience, these features of the dI/dV spectrum are highlighted and numbered.

The series of equally spaced differential conductivities of GNT in the form of peaks occur at a voltage of ± 2.3 V, ± 1.68 V, ± 1.08 V, ± 0.5 V, and of OGNT – at a voltage of ± 1.92 V, ± 1.2 V, 2.6 V. Typically, these features of differential conductivities are observed with periods ΔV from 0.1 V to 5.0 V [16]. In our case, the val-

ue of ΔV varies from ~ 0.6 V to ~ 0.7 V. In our opinion, the nature of these series of equally spaced *dI/dV* spectra is associated with resonant tunneling of quasiparticles, and the main mechanism for the formation of data of the equidistant series of the *dI/dV* spectrum of the nanodevice under consideration is Coulomb interaction of quasiparticles. The second and third features of the *dI/dV* spectrum are manifested in the form of dips in both GNT and OGNT. The differential conductivity of the nanotubes under consideration is very different from each other at one resonant voltage, when a feature appears in the form of a peak in a GNT, it appears as a dip in an OGNT, and vice versa. A uniform exponential increase in the amplitudes of the *dI/dV* spectrum of the GNT and an exponential decrease in the *dI/dV* spectrum of the OGNT are observed.

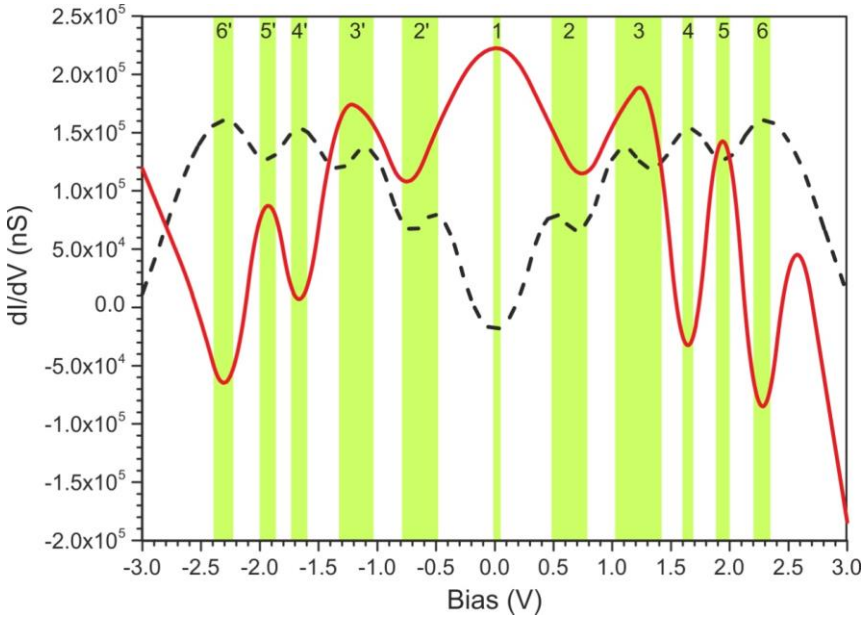

Fig. 6 – *dI/dV* characteristics of CNT: dashed line – GNT; solid line – OGNT

4. CONCLUSIONS

Thus, in this work, in the framework of DFT + + NEGF, we studied the main electrophysical characteristics (local density of states, transmittance spectrum, state density, CVC, differential conductivity) of nanodevices with identical geometrical parameters based on GNT and OGNT. It is shown that at the Fermi level, OGNT have a nonzero density, and in the energy range – 1.45 ÷ 0.68 eV the DDOS and transmission spectra of OGNT are two times higher than the analogous characteristics of GNT. It is shown that the CVC of GNT is of semiconductor type and CVC of OGNT – is of metallic type. It was revealed that the *dI/dV* spectrum shows equidistant series of differential conductivity of possibly Coulomb origin. It is shown that, at a resonant voltage, the features of the *dI/dV* spectrum of the GNT in the form of maxima appear in the OGNT in the form of minima, and vice versa, the minima of the GNT spectrum in the form of the maxima of the OGNT spectrum (at the same value of the resonant voltage). It was found that the amplitudes of the differential conductivity feature in the form of an equidistant series of GNTs decrease exponentially, while OGNTs increase exponentially.

The results obtained can be useful for calculating new promising switching devices of carbon nanoelectronics.

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Особливості електричних характеристик октаграфенових нанотрубок

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Електронний транспорт в графенових та октаграфенових нанотрубках приблизно з однаковими геометричними розмірами (діаметрами 7,08 Å та 7,15 Å та довжинами 41,2 Å та 39,92 Å відповідно) був досліджений у рамках функціональної теорії густини (у наближенні локальної густини) та методу нерівноважних функцій Гріна (DFT + NEGF). Розраховані спектри пропускання, густина станів, вольт-амперні характеристики *dI*/*dV* для графенових та октаграфенових нанотрубок. Показано, що за природою вольт-амперних характеристик, графенова нанотрубка має напівпровідникові властивості, а октаграфенова нанотрубка – металеві властивості. Було виявлено, що спектр *dI*/*dV* демонструє рівновіддалений ряд диференціальних провідностей кулонівського походження. Показано, що при резонансній напрузі особливості диференціальних провідностей у вигляді максимуму в графеновій нанотрубці супроводжуються мінімумом в октаграфеновій нанотрубці. Було встановлено, що амплітуди диференціальної провідності у вигляді рівновіддаленого ряду графенових нанотрубок зменшуються експоненціально, тоді як для октаграфенових нанотрубок вони експоненціально збільшуються. Результати можуть бути корисними для обчислення нових перспективних електронних комутаційних нанопристроїв.

Ключові слова: Вуглецева нанотрубка, Октаграфенова нанотрубка, Електронний транспорт, Спектр пропускання, Густина станів, Вольт-амперна характеристика, Диференціальна провідність.