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Computer simulation of electrical characteristics of single-walled carbon nanotube (9,0) with Stone-Wales defect

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Abstract. In the framework of the density functional theory, using the method of nonequilibrium Green's functions and in the local density approximation, the electrical characteristics of different configurations of a single-walled carbon nanotube with Stone-Wales defects are investigated. The calculation is implemented in the Atomistix ToolKit with Virtual NanoLab program. The current-voltage, \(dI/dV\)-characteristics and the density of states of the nanostructures under consideration were calculated. It is shown that the nature of the current flowing through defective carbon nanotubes depends on the extent of the Stone-Wales defects. It was found that a carbon nanotube with two consecutively connected Stone-Wales defects at a bias voltage of ± 2.6 V has a negative differential conductivity of -170 µS. The obtained results can be useful for calculations of new promising electronic devices of nanoelectronics based on a carbon nanotube.

1. Introduction

Investigation of the electrophysical properties of nanomaterials is one of the most important tasks of the modern solid state physics and materials science. The conduct of such studies is caused by the need to create radiomaterials with new, modified properties and their application for further miniaturization of elements of micro- and nanoelectronics [1-3]. In this regard, one of the intensively studied nanomaterials are carbon nanotubes (CNTs) [4, 5]. CNTs, combined with good electrical conductivity, still have unique properties like ultra-small dimensions, field emission, high chemical stability and the ability to attach a variety of chemical radicals that are favorable for the creation of promising electronic devices for transferring, transforming and processing of information.

It is known that the lattice defects CNT arising at the stage of its production or intentionally introduced have a significant effect on its electrophysical properties. Thus, it was shown in [6] that by changing the chirality of a single-walled CNT (SWCNT) by introducing a defect into its structure (pentagon-heptagon pairs), its electronic properties can be changed, for example, SWCNT with chirality (8,0) is a semiconductor with a band gap of 1.2 eV, while the SWCNT with chirality (7,1) appears as a semimetal (with a bandgap equal to zero). And in work [7] by introducing a defect into the structure of SWCNTs, heterojunctions semiconductor – semiconductor with different values of band gap were obtained. Similarly, subminiature semiconductor – metal heterojunctions can be obtained. Such CNT-based transitions are used to develop a transistor, as well as solar cells and...
One of the simplest topological defects contained in carbon nanomaterials is the Stone-Wales (SW) defect [9]. It is formed by a simple rotation of a pair of carbon atoms C-C by 90° (SW transformation), a result of which the symmetry of the hexagonal lattice is violated with the appearance in its structure of two pentagonal and two heptagonal elements. Such defect arises during quenching at high temperature even at the stage of obtaining a carbon nanomaterial or when it is exposed to irradiation.

In this paper, an attempt was made to determine the electrical characteristics of a single-walled carbon nanotube (9,0) with a Stone-Wales defect using computer simulation using the Atomistix ToolKit with Virtual NanoLab.

2. Description of the object and methods of research
Model-researched SWCNTs were obtained from a graphene sheet by twisting in the program Atomistix ToolKit with Virtual NanoLab using the Tube Wrapper operator. And the defects of Stone-Wales were formed in graphene sheets before twisting. The geometry of the investigated SWCNT (9,0) with various configurations of the Stone-Wales defect is shown in Fig. 1 a-e. (For ease of description, letters A, B, C, D, E for each configuration are conventionally assigned). The length of the electrodes along the C axis varies from ~ 7.1 Å to ~ 8.53 Å, and the length of the researched SWCNT is ~ 41.2 Å. The size of the quasiparticle scattering region (central region) is ~ 20 Å.

Computer simulation of the electrical characteristics of defective SWCNTs was performed within the framework of the Density Functional Theory (DFT) theory using the method of nonequilibrium Green's Functions (NEGF-Non-Equilibrium Green's Functions) in the local density approximation (LDA) [10, 11]. Modeling of quantum-transport characteristics of SWCNTs is implemented on the Atomistix ToolKit with Virtual NanoLab program. (The basic equations of this method are described in more detail in [12-14]). The CVC of a nanotube is calculated on the basis of the well-known Landauer equation:

![Figure 1. Geometry of SWCNTs with SW defects:](image)
where $e$ – electrons charge, $h$ – Planck’s constant, $\varepsilon$ – energy, $D(\varepsilon)$ – density of states, $U$ – self-consistent potential, $\gamma_1$, $\gamma_2$ – right and left electrode Luttinger parameters, $\gamma = \gamma_1 + \gamma_2$, $f(\varepsilon)$ – Fermi energy distribution function of quasiparticles, $k_B$ – Boltzmann’s constant, $T_R$, $T_L$ – current temperatures and $\mu_R$, $\mu_L$ – electrochemical potentials of the right and left electrodes.

To describe the interatomic interaction and optimization of defective carbon nanotubes, the Brenner potential was used [15], which describes well the carbon nanostructures.

### 3. Results and discussion

The results of calculating the density of states (DDOS – Device Density of States) of defective SWCNTs configurations are presented in Fig. 2 a-e. In [16], DOS of graphene with SW defect was investigated, where it was shown that SW defects lead to the appearance of a defect band $\sim 0.5$ eV above the Fermi level, when there is no such band in graphene without a defect. The origin of the defective strip is explained by structural instabilities in defective graphene. With increasing defect concentration, both the width and density of states of the defective band increase. Consequently, this defective band is useful for identifying SW defects and determining their concentration in a graphene film.

In this case, a defective band is observed near the energy $\sim 0.5$ eV, since the studied SWCNTs are obtained from a SW-defective graphene sheet by twisting. The defective SCWT band with two merged longitudinal SW defects (configuration B) appears at an energy of 0.5 eV with an intensity 24 eV$^{-1}$, and in the SWCNT with two merged transverse defects (configuration C), the defective band arises at an energy 0.54 eV with an intensity of 70.68 eV$^{-1}$. The presence of two SW defects in the structure of the SWCNT in the form of D and C configurations leads to a shift in the defect energy band to 0.42 eV with intensities 21.5 eV$^{-1}$ and 24.16 eV$^{-1}$, respectively. Features of DDOS of B- and C-configurations are the appearance of a band at an energy of -1.92 eV with intensities of 162.5 eV$^{-1}$ and 70 eV$^{-1}$, respectively. Let us assume that the band arising at an energy of -1.92 eV can be useful in identifying SW defects of SWCNTs.

The DDOS of D-structure differs from the other structures under consideration. The presence of two coupled longitudinal SW defects in the D-configuration of the SWCNT leads to the appearance of DOS intensities of 409.58 eV$^{-1}$, 198.25 eV$^{-1}$, 116.8 eV$^{-1}$ at energies of -2.64 eV, -1.68 eV and -1.14 eV, respectively.

The results of modeling the current-voltage characteristics (CVC) and differential conductivity are shown in Fig. 3. Introduction to the structure of SWCNT of Stone-Wales defects, leading to the formation of B-, C-, E-configurations, does not radically change the CVC and the differential conductivity of the carbon material. In these structures, a zero current is observed in the voltage range from -0.3 V to 0.3 V, then the current monotonically increases (Fig. 3a).

In the presence of two coupled longitudinal SW defects (configuration D) in the SWCNT, a completely different behavior of the CVC is observed. In the voltage range of 0-0.3 V, the current rapidly increases to a value of 15 $\mu$A, followed by a slow quasilinear increase in the current to 70 $\mu$A at $V_{bias} = 2.3$ V. In the range of $V_{bias} = 2.3 \div 2.8$ V, the current falls from 70 $\mu$A to zero.

The peculiarities of CVC of the examined carbon nanotubes are clearly manifested in their differential conductivity (Fig. 3b). Due to the symmetry of the $dI/dV$ spectra, we consider the differential conductivity of nanostructures only at positive values of the bias voltage.

The differential conductivities of A- and E-structures are similar and have peaks of 150 $\mu$S and 135 $\mu$S for $V_{bias} = 2.2 \div 2.3$ V, respectively, and at a near-zero value of the bias voltage, the $dI/dV$ spectrum assumes a zero value.

The $dI/dV$ characteristics of B- and C-configurations are similar, they have three local maxima and minima (Fig. 3b). The maxima of the differential conductivity of these structures of 100 $\mu$S and
120 µS are manifested at \( V_{bias} \approx 2.5 \) V; 115 µS and 130 µS at \( V_{bias} \approx 1.5 \) V; 90 µS and 88 µS at \( V_{bias} \approx 0.7 \) V, respectively. And the minima of 70 µS, 100 µS are observed at \( V_{bias} \approx 1.9 \pm 2 \) V; 10 µS and 30 µS at zero bias voltages.

The differential conductivity of the E-configuration differs greatly from the previous structures with the presence of three minima of -170 µS for \( V_{bias} \approx 2.6 \) V, 25 µS for \( V_{bias} \approx 1.8 \) V, 10 µS for \( V_{bias} \approx 0.6 \) V and for two expressed maxima of 50 µS at \( V_{bias} \approx 2 \) V and 66 µS at a near-zero value of the bias voltage.

**Figure 2.** The density of states of single-walled carbon nanotubes of A-, B-, C-, D-, E-configurations, respectively.
In the authors’ opinion, the similarity of the electrical characteristics of the A- and E-configurations, as well as B- and C-configurations of SWCNTs, is related to the dimensions of the generated SW defects. The defect of the E-structure is two separate SW-defects without fusion with dimensions of 7.1 Å × 4.92 Å. It is known that at low temperatures the main mechanism of electron transport in SWCNT is quantum subbarrier tunneling. In this case, the probability of overcoming the barrier formed by single SW defects, quasiparticles is large. As a result, the electrical characteristics of SWCNTs with parallel located SW-defects resemble the characteristics of SWCNTs without a defect.

The same picture is observed between the characteristics of the B- and C-configurations of SWCNTs. The size of the SW defects in B configuration is 5.42 Å × 10.96 Å, and in C configuration is 12.3 Å × 7.1 Å. We assume that the length of the quasiparticle jump allows to overcome the defective barrier in the structures under consideration.

The length of the D-configuration defect, existing as two successively connected SW defects, along the Z axis is 15.63 Å. The presence in the lattice of an extended defect degrades the electrical characteristics of the SWCNT. This explains the decrease in current in the D-structure in the voltage range of 2.3 ÷ 2.8 V (Fig. 3a). Let us note that the conductivity in such structure is an order of magnitude lower than in the others (Fig. 3b).

![Figure 3](image-url)

**Figure 3.** Current-voltage (a) and dI/dV-characteristics (b) of SW-defective SWCNTs (the letter designation corresponds to the structure shown in Figure 1).

Similar changes in *I(V)*; *dI/dV* characteristics should be taken into account when calculating electronic devices based on carbon nanomaterials, since one can not always obtain ideal single-walled carbon nanotubes.

4. **Conclusion**

Thus, in this paper, in the framework of the density functional theory, the main electrical characteristics (state density, CVC, differential conductivity) of SW-defective SWCNTs are modeled. The features of SWCNT density of states in the form of the appearance of a defect band of ~ 0.5 eV and ~ -1.9 eV above the Fermi level are found, identifying the presence of Stone-Wales defects and characterizing their concentrations in similar structures. It is shown that the transport current of SW-defective SWCNTs depends on the length of longitudinal defects. It was revealed that on the electrical characteristics of SWCNTs with two successively connected SW defects (D-configuration) at a bias voltage of ± 2.6 V, a negative differential conductivity region appears. The obtained results can be useful for calculations of new promising electronic devices of nanoelectronics based on CNTs.

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