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Short Communication

Defects in Graphene Nanoribbons and Flakes: Influence on the Conductivity

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In this paper, we investigate the influence of topological defects in a crystal lattice of a graphene nanoscale and graphene flakes on their conductivity. By the direct Hamiltonian diagonalization for the graphene electrons, we obtain the density of states, which was recalculated into a tunneling current between the graphene nanoribbon and the contacting material (metal, quantum dots). We observe the effect of the defect type and its location on the tunnel current characteristics.

Keywords: Stone-Wales defect, Vacancy, Graphene structures, Conductivity.

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1. INTORDUCTION

As is well known, there are practically no crystals, all atoms of which would occupy a position with minimal energy. There are two types of deviations from ideal positions: a permanent and a temporary. In this paper, we study the permanent defects, and in particular point defects [1].

Such defects in the crystal lattice can be created intentionally or appear randomly at the synthesis. Such topological defects due to the rearrangement of interatomic bonds have a great influence on the properties of solids.

Although structural defects can degrade the performance of graphene-based devices, of-ten such deviations from the excellence can be useful in some applications, since they allow new functional capabilities to be achieved.

In graphene, which is a crystal with a hexagonal lattice [2], such defects are also observed. The simplest of these is the Stone-Wales defect [3-6], which occurs when one of the C-C bonds is rotated through an angle of 90◦, as a result we have that four hexagonal cells are transformed into two pentagons and two heptagons.

It should be noted, because the Stone-Wales defect violates the crystal lattice symmetry, this leads to the appearance of a dielectric gap in graphene [7]. This makes it possible to use graphene in nanoelectronics. At the same time, such defects are the centers of preferential adsorption of some chemical elements [8, 9]. This property can be useful in the impurity determining and the use of graphene as a highly sensitive detector of these gases.

In addition to the Stone-Wales defect, in this paper we also consider another zero-dimensional defect of the vacancy type [10, 11]. Such defects take a place in local changes in the interatomic distances and cause the distortions in the crystal lattice. In this case, an increase in the resistance of the lattice to a further displacement of the atoms is observed, which favors the increase in the strength of the crystal and their electrical resistivity.

2. METHODS

In The influence of above mentioned defects we evaluate with the help of the tunneling effect arising in the contact of a graphene nanoribbon/flake with a metal and quantum dots. The given approach has already been tested by the authors in studying the sensitivity of graphene flakes and nanorings to impurities [12].

The Hamiltonian for electrons in graphene nanoribbon can be written in the following form:

$$H = \gamma \sum_{\langle ij \rangle} a_i^+ a_j + c.c. \,, \tag{1}$$

where $\gamma = 2.7$ eV, the summation is over the nearest neighbors. A two-dimensional array of car-bon atoms is renumbered into a one-dimensional for the convenience calculations. One method of such numbering for the Stone-Wales defect (Fig. 1a) and for the vacancy (Fig. 1b) is presented in the Fig. 1 for graphene nanoribbon and graphene flake respectively.

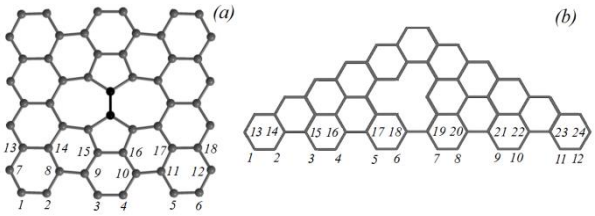

Fig. 1 – The geometry of the problem: a) the Stone-Wales defect; b) the vacancy

Further, we numerically diagonalize the Hamiltonian (1). Based on the Kubo theory we can write the expression for the current density of a contact [13]:

$$J_{tunnel} = 4\pi e |T|^2 \int_{-\infty}^{\infty} dE \sum_p \delta\left(E + eV - E_p^A\right) \sum_q \delta\left(E - E_q^B\right)\left(n_f(E) - n_f(E + eV)\right), \tag{2}$$

where $\delta(x)$ is the Dirac delta-function, the sum is described the tunnel density of states for contact A and B respectively; $n_f(E)$ is the equilibrium distribution of

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fermions with the energy E; V is the voltage between the contacts; E_p^A, E_q^B are the dispersion laws for contact materials A and B with the momentums (p and q). Here we use the "rough" contact approximation, when there are the restrictions on the geometry of the contact.

3. THE MAIN RESULTS

The dependence of the tunneling current (contact with metal and quantum dots) for the graphene flakes on the voltage for the vacancy defect is given in Fig. 2.

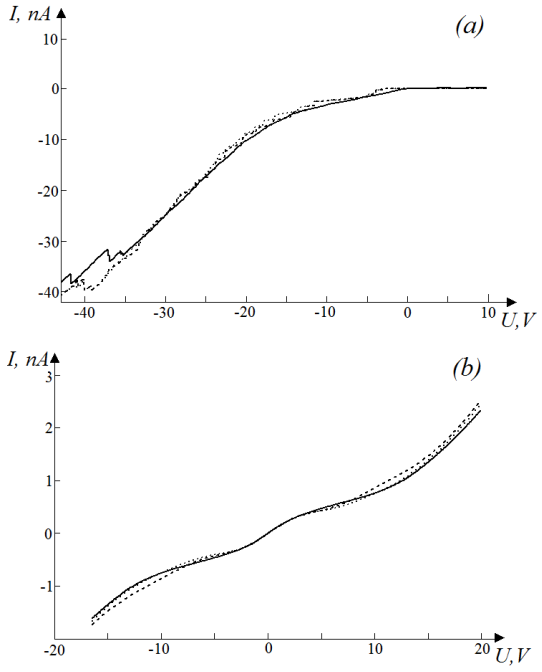

Fig. 2 – Dependence of the tunneling current (contact with the metal – Fig. a, contact with the quantum dots – Fig. b) for the flake versus the voltage in the case of the vacancy defect. The solid line – flake without defects; the dotted line – one vacancy; the dashed line – two vacancies nearby

The dependence of the tunneling current (contact with metal and quantum dots) for the graphene flakes on the voltage for the Stone-Wales defect is shown in Fig. 3.

The dependence of the tunneling current for the rectangle nanoribbon on the voltage is presented in Figs. 4 and 5.

In this work, we were able to estimate the effect of defects in graphene nanostructures on their conductive properties based on the obtained volt-ampere characteristics for tunnel contacts of nanoribbons and flakes with a metal and quantum dots. Within the framework of the proposed approach, the system is able to detect the presence of defects in it.

From given Figs. 2 and 3 it can be seen that the defect introducing rather change the current-voltage characteristics (CVC) of the contact with the metal and quantum dots. At the same time, a placement of the defect does not have so much influence on the CVC (the dotted line and the dashed line in Fig. 2 and 3).

For the metal case, we see a significant diodes effect.

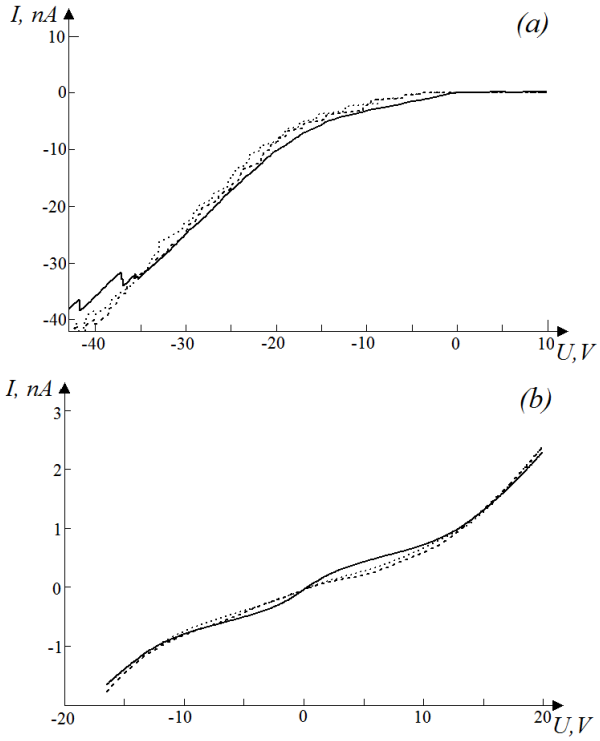

Fig. 3 – Dependence of the tunneling current (contact with the metal – figs. a, contact with the quantum dots – figs. b) for the flake versus the voltage in the case of the Stone-Wales defect. The solid line – flake without defects; the dotted line – defect in the middle of the flake; the dashed line – defect near the border of the flake.

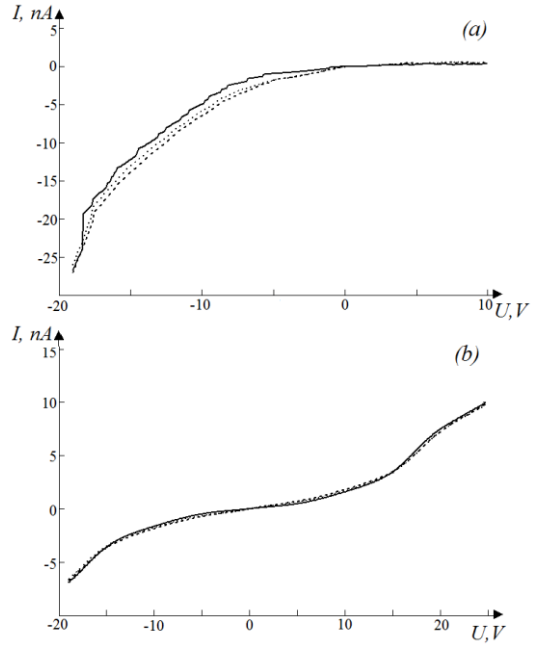

Fig. 4 – Dependence of the tunneling current (contact with the metal – Fig. a, contact with the quantum dots – Fig. b) for the rectangle nanoribbon versus the voltage in the case of the vacancy. The solid line – the graphene nanoribbon without defects; the dotted line – one vacancy; the dashed line – – two vacancies near-by

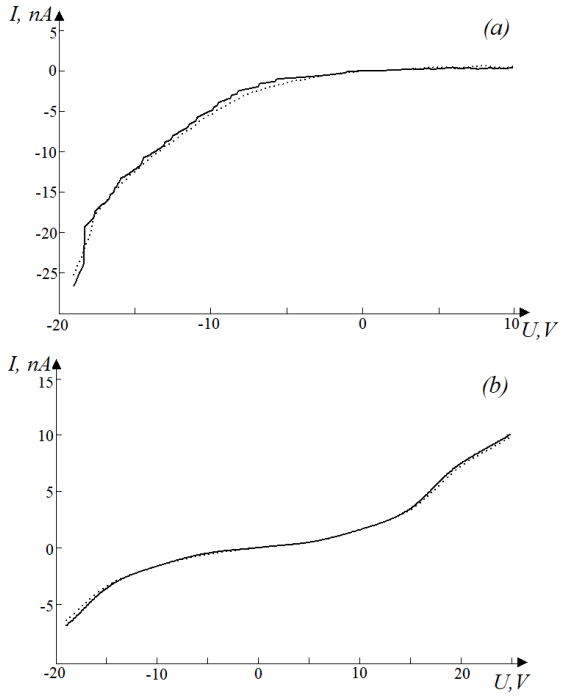

Fig. 5 – Dependence of the tunneling current (contact with the metal – Fig. a, contact with the quantum dots – Figs. b) for the rectangle nanoribbon versus the voltage in the case of the Stone-Wales defect. The solid line – the graphene nanoribbon without defects; the dotted line – defect in the middle of the flake

This fact allows us to apply the graphene nanoribbon and flakes (even with different defects) with the contact with metals as diodes. It can be useful for the practical applications. Because we can not always get the perfect graphene materials.

As the results of the calculations showed, the influence of both considered defect types for the contact with the quantum dots is less pronounced than for the contact with a metal (Figs. 4 and 5).

It must also be said that the presence of a defect like Stone-Wales and the vacancy defect is easier to detect in the graphene flake than in the nanoribbon.

4. CONCLUSION

In this section, we indicate the main results:

1. The influence of the defect type on the tunneling current was observed.
2. It was shown that neither the location of the Stone-Wales defect nor the number of vacancies leads to significant changes in the CVC of the tunneling con-tact.
3. The results of the numerical experiment allows us to conclude that for the defect detection the contact with a metal is the preferred option.

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