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APPLICATION OF GREEN'S FUNCTION APPROACH TO ELECTRONIC STRUCTURE OF CARBON NANOCYLINDERS

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The local density of states of the carbon nanostructures can be calculated in different ways. Here, we present the Haydock recursion method which, using the Green's function approach, transforms the given surface into a chain of equivalent sites. Then, using the continued fraction, we apply this procedure on the surface of the nanocylinders.

Keywords: graphene, carbon nanostructures, disclination, Green function, continued fraction.

1. Introduction

The local density density of states ($LDoS$) is one of the most important characteristics describing the electronic properties of the carbon nanostructures. Different methods were used for its calculation: The first exploits the form of the electronic spectra [1], the second deals with the gauge-theory model and the Dirac equation [2, 3], the third works with the Green function which can be calculated using different methods.

In this paper, we first describe the Haydock recursion method and the procedure of the calculation of the Green function. Then we apply this method to the calculation of the Green function and related quantities in the edge sites of the carbon nanocylinder and of the graphene nanoribbon perturbed by two heptagonal defects. Then we investigate the changes of the $LDoS$ for the changing distance of the defects and estimate the minimal and maximal distance of the defects on the perturbed surface of the nanocylinder.

2. Haydock recursion method

The $LDoS$ can be defined as

$$LDoS(E) = \lim_{\delta \to +0} \frac{1}{\pi} \mathrm{Im} G_{00}(E - i\delta), \tag{1}$$

where $G_{00}(E)$ is the Green function. It can be calculated using the recursion procedure which transforms an arbitrary surface into $1-$dimensional chain. This procedure is called the Haydock recursion method [5]. It divides the positions of the investigated surface into the groups of sites, each of them represents the site in the $1-$dimensional chain. Each site is represented by the state vector $|n\rangle$. Then, from the knowledge of the state $|1\rangle$, which corresponds to the usual state of the carbon atom, we can recursively compute the coefficients a_n, b_n corresponding to the particular sites of the chain using

$$|n+1\rangle = (H - a_n)|n\rangle - b_{n-1}|n-1\rangle. \tag{2}$$

The maximal value of n which is n_{max} determines the recursion depth. It is given by the size of the concrete surface, but in the case of infinitely large graphene, nanocone etc., it is up to our choice and it provides the rate of precision. Then we define $G_{00}(E)$ as [4]

$$G_{00}(E) = \frac{1}{E - a_1 - b_1 g_1(E)}, \tag{3}$$

where

$$g_i(E) = \frac{1}{E - a_{i+1} - b_{i+1} g_{i+1}(E)}, \qquad i = 1, ..., n. \tag{4}$$

3. LDoS of nanocylinder

In Fig. 1, we see the surface of armchair and zig-zag nanocylinder together with the labeling of the sites in accordance with the technique described in the previous section. The armchair form should be always metallic, the zig-zag form is mostly semimetallic and rarely metallic. The evidence of the metallicity is given by the peak in the $LDoS$ for the Fermi level [1].

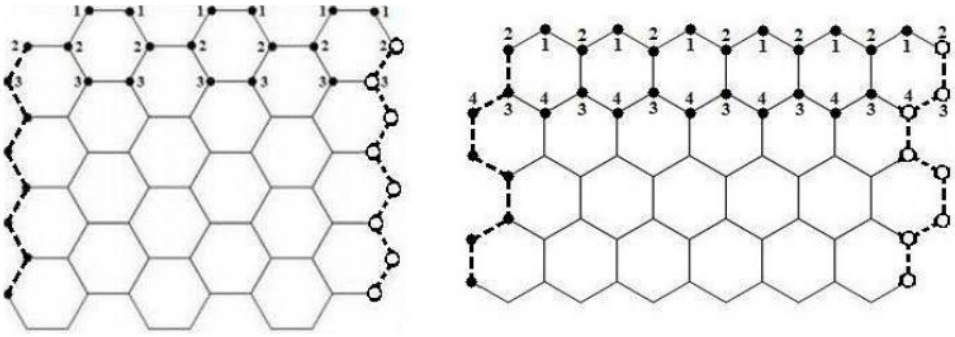

FIG. 1. Surface of two forms of the carbon nanocylinders: armchair (left) and zig-zag (right); the labeling of the sites corresponds to the technique described in the section 2; there are equivalent sites in each line parallel with the edge and that is why we label each line by the same number; the dashed lines consisting of sites denoted by black or white color are identical on the real surface.

To apply the Haydock recursion method, we have to choose the recursion depth n_{max}, which closely corresponds to the length of the nanocylinder. The $LDoS$ for different forms of the nanocylinder is shown in Fig. 2 together with the chosen values of the circumferential and the longitudinal number of atoms. The chosen value of the parameter δ in (1) is 0.1.

3.1. The case of perturbation

Let us investigate the $LDoS$ in the edge sites of a perturbed graphene nanoribbon of the sizes which have the same values as the above mentioned cylindrical surface (see Fig. 3). Because the structure of the surface is different from the previous case (Fig. 1), the placement and labeling of the equivalent sites is changed. For the chosen edge sites, the result is presented in Fig. 4. In this case, the chosen value of the parameter δ is 0.2.

To derive the limiting sizes of the disclinated nanocylinder, we investigate the $LDoS$ in the sites of the defects denoted by number 1 in the disclinated surfaces depicted in Fig.

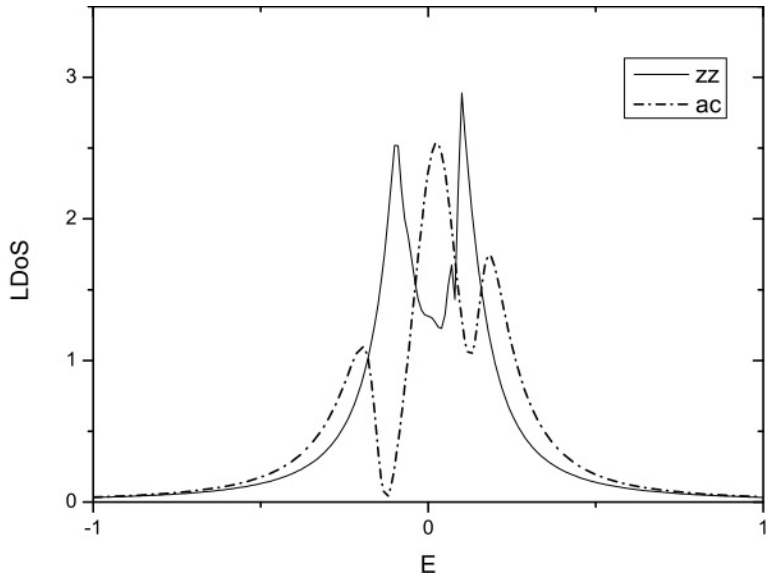

FIG. 2. $LDoS$ for armchair and zig-zag cylinder; longitudinal number of atoms: 12, circumferential number of atoms: 10 for armchair, 20 for zig-zag; here, $\delta = 0.1$.

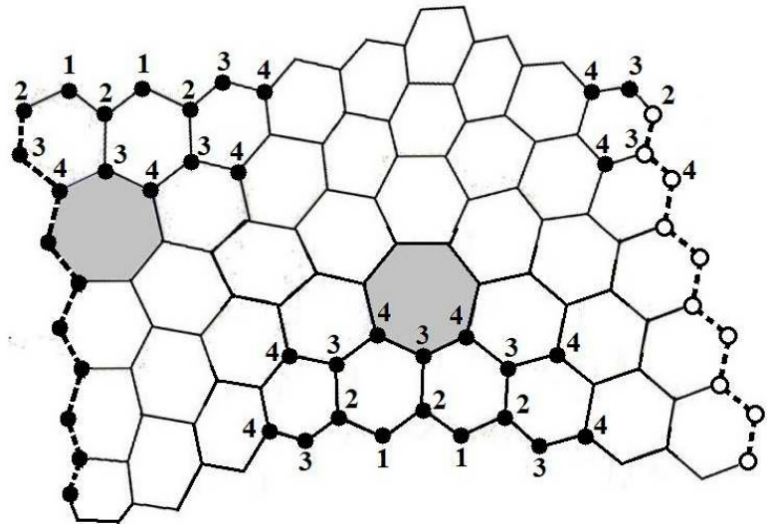

FIG. 3. Surface of the nanoribbon with a small perturbation; due to the mirror symmetry, we have pairs of equivalent sites in each line parallel with the edge, but there is not any line composed of equivalent sites only; so, we distinguish only the sites which are neighboring, next-neighboring etc. with the site 1 for which the $LDoS$ we calculate; the whole number of the sites in the chain is 9; in the case of the semi closed, nanocylindrical structure, the dashed lines consisting of sites denoted by black or white color are identical on the real surface.

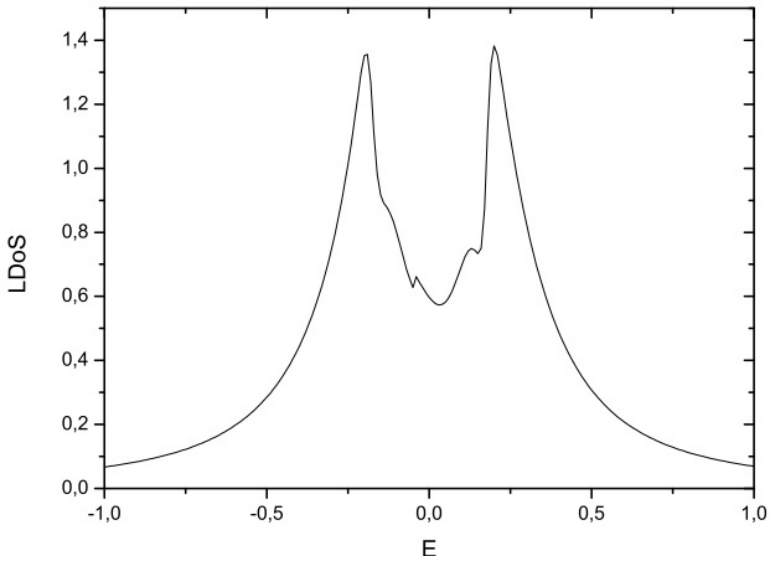

FIG. 4. $LDoS$ of the perturbed cylinder with surface depicted in Fig. 3; here, $\delta = 0.2$.

5 and we compare the results with the results presented in [1], where the $LDoS$ for the simple graphene was presented.

In Fig. 5, we define the distance of the defects in the units of the distance of the neighboring sites. Using the Haydock recursion scheme, we get the plots of the $LDoS$ outlined in Fig. 6. The acquired results should be similar to the $LDoS$ of simple graphene [1]. Then, we suppose the presence of the local minimum for the Fermi level in the corresponding plot.

Let us look through the plots of the $LDoS$ in Fig. 6. From these plots we see that the growing distance of the defects causes decrease of the $LDoS$ for the Fermi energy and violation of the peak. The case (d) in Fig. 6 corresponds to the expected shape of the $LDoS$ [1] and so, it corresponds to the minimal necessary size of the perturbed cylindrical surface.

4. Conclusion

We applied the Haydock recursion method on the calculation of the $LDoS$ of the carbon nanocylinder. We can compare the results presented in Fig. 2 with the calculation in [1], where the form of the electronic spectrum is applied. The results presented in this paper are close to our results. They are also similar to the plots presented in [6]. In both of these papers as well as in Fig. 2, the difference between the armchair and the zig-zag form is given by the peak for the armchair form at the Fermi level. But in Fig. 2, the peak at the Fermi level should be much closer. The inaccuracy is given by the choice of the values of δ and of the parameters a_n, b_n in the Haydock recursion method which does not provide a single solution.

Next, we derived that the minimal size of the disclinated cylindrical surface containing 2 heptagonal defects corresponds to the case (d) in Fig. 5 and that the maximal size corresponds to the surface which is twice longer.

The model of 2 defects can be also applied on a simulation of a dipole or a quadrupole present on a defect-free graphene surface: the dipole can be given by a combination of one pentagonal and one heptagonal defect and the quadrupole by two pentagonal and two

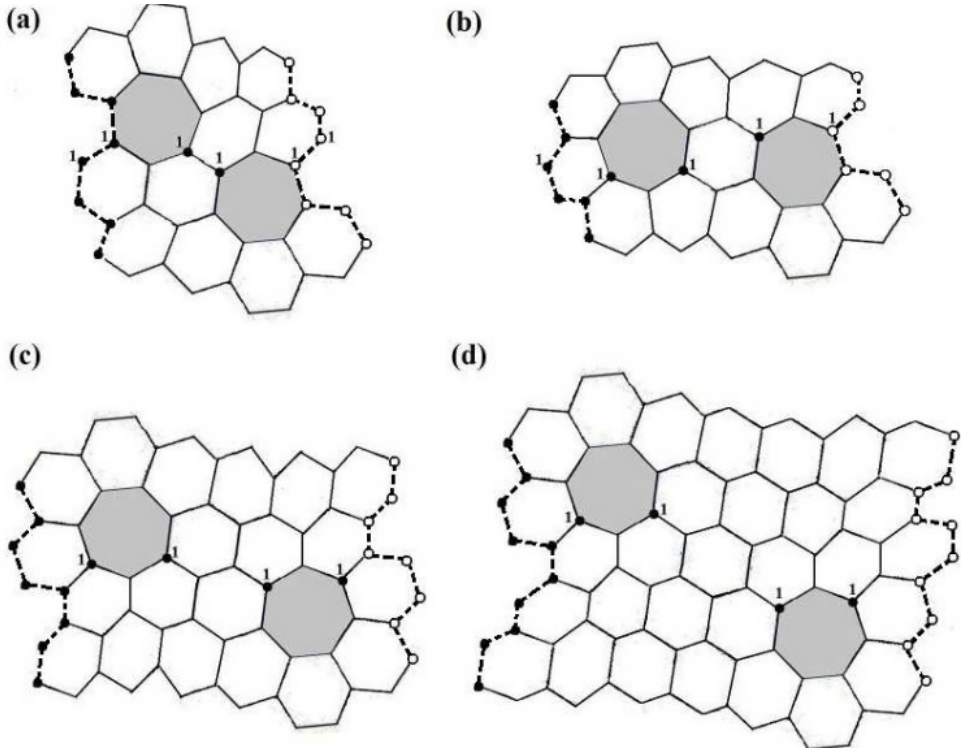

FIG. 5. Perturbed nanostructured surfaces with different distances of the defects. We calculate the *LDoS* for the denoted sites; in the case of the semi closed, nanocylindrical structure, the dashed lines consisting of sites denoted by black or white color are identical on the real surface.

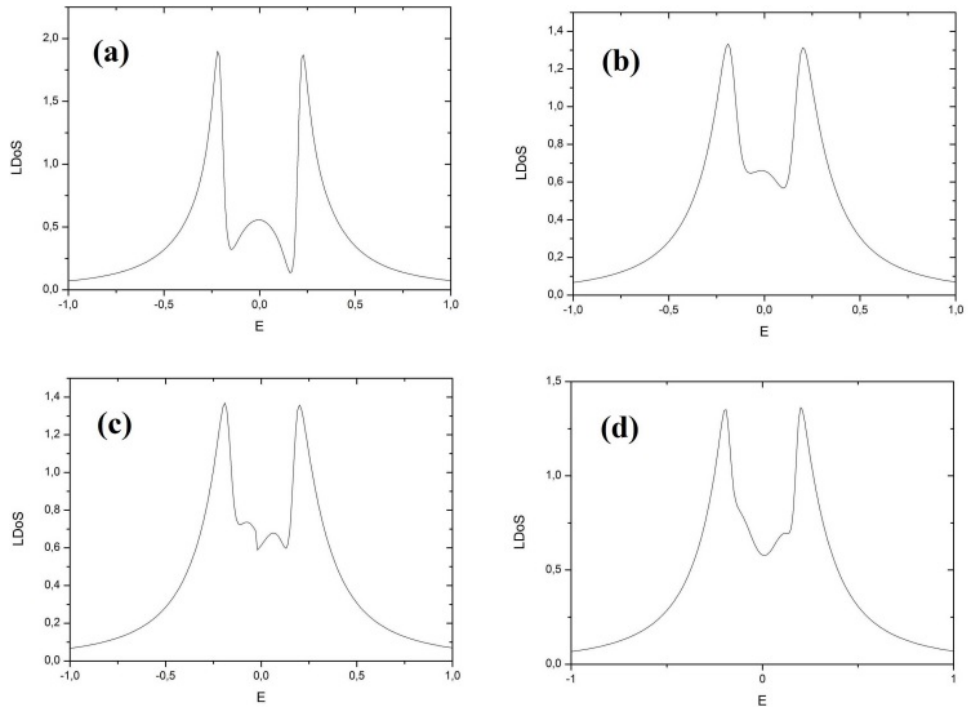

FIG. 6. *LDoS* for the particular cases of the perturbed cylindrical surfaces. The notation (a)-(d) corresponds to Fig. 5. The value of the parameter δ is 0.2.

heptagonal defects. Of course, higher number of defects can give much more possibilities. In the future, the calculations will be focused on these problems.

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