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Electron transport properties of nanomaterials based on recursive Green's function method

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By using the recursive Green's function method, the electronic structure and transport properties of nano-band are calculated. The results show that the conductivity curves are also sensitive to the dependence of volume vacancies. The conductivity channel exists in both zigzag graphene nanoribbons (ZGNR) and armchair graphene nanoribbon (AGNR) when the concentration of methylene is 0.005. LDOS analysis shows that there are (quasi) localized states at the corresponding energy. With the increase of w, the suppression of conductivity becomes more and more obvious, and there is a conductance channel at $E = 0$ eV. The results show that a relatively stable conductance channel can be obtained when $w = 0.3$. When the vacancies are evenly distributed on the two boundaries, the ZGNRs has a stable transport hook, and the size of the transport ditch N oscillates down. That is, if the overall structure of the ZGNRs is symmetric, the transportation ditch is larger, and the transmission is mainly determined by its band gap.

Keywords: recursive Green's function, nano-scale, transport properties.

Используя рекурсивный метод функций Грина, исследуется влияние дефектов на электронную структурк и проводимость графена. Результаты показывают, что проводимость чувствительна к объемным вакансиям. Изменения проводимости существуют как в зигзаг графеновой наноленте (ZGNR), так и в графеновой наноленте (AGNR), когда концентрация метилена составляет 0,005. Анализ LDOS показывает, что существуют квази локализованные состояния при соответствующей энергии. С увеличением w подавление проводимости становится все более очевидным, и при $E = 0$ eV появляется канал проводимости. Результаты показывают, что относительно стабильный канал проводимости может быть получен при $w = 0{,}3$. Когда вакансии равномерно распределены по двум границам, ZGNR имеют стабильный транспортный крюк, и размер транспортного канала N уменьшается. То есть, если общая структура ZGNR является симметричной, транспортный канал становится больше, и передача в основном определяется его полосой.

Електронтранспортні властивості наноматеріалів на основі методу рекурсивної функції Гріна. *X.Mei, Z.Wu.*

Використовуючи рекурсивний метод функцій Гріна, обчислюються електронна структура та транспортні властивості нанодіапазону. Результати показують, що провідність чутлива до об'ємних вакансій. Канал провідності існує як у зигзаг графен-нанострічці (ZGNR), так і у графеновій нанострічці (AGNR), коли концентрація метилена становить 0,005. Аналіз LDOS показує, що існують (квазі) локалізовані стани при відповідній енергії. Зі збільшенням w подавлення провідності стає все більш очевидним, і при $E = 0$ eV з'являється канал провідності. Результати показують, що відносно стабільний канал провідності може бути отриманий при $w = 0{,}3$. Коли вакансії рівномірно розподілені за двома кордонами, ZGNR мають стабільний транспортний крюк, і розмір транспортного каналу N зменшується. Тобто, якщо загальна структура ZGNR є симетричною, транспортний канал стає більше, і передача в основному визначається його смугою.

1. Introduction

In research on nano-materials, carbon nanostructured materials have been paid more and more attention [1]. Carbon nanostructures include zero-dimensional fullerenes, one-dimensional carbon nanotubes and two-dimensional graphene [2]. Before the discovery of graphene, the properties of graphene have been studied theoretically. However, due to the instability of thermodynamics, graphene is considered to be unable to exist alone. In this paper, a recursive Green's function method is used to study the electron transport properties of graphene nanobeands in a tight bound framework. Because it is very difficult to fabricate perfect graphite thin nano-band experimentally, it is of great theoretical and practical value to study the physical properties of defective nano-band [3]. A large number of studies have shown that graphene has many excellent properties, which make it one of the most eye-catching carbon nanostructured materials [4]. Physicists believe that graphene can replace silicon, which contributes to the study of the properties of graphene and graphene-based nanomaterials [5] Graphene was prepared for the first time by mechanical stripping of Aljabali. The operation principle of this method is simple, but it is not easy to control. Therefore, after the discovery of graphene for the first time, various methods for the preparation of graphene, such as silicon carbide pyrolysis at high temperature, transition metal catalytic epitaxy, and chemical modification of dispersion / reduction, have emerged one after another [6]. In [7] studies show that chemical modification / reduction method is the most promising method for the preparation of graphene and is the most likely method for industrial preparation of graphene. For graphene, not only remarkable results have been obtained in its preparation, but also many properties of graphene have been well known. Son has considered the change of relative position and distance between Pz orbitals and he modified the interaction parameters and calculated the electronic structure and transport properties. The results show that the electron is scattered by the additional barrier, which is caused by the wrinkle and is proportional to the square of the weight curvature [9].

This paper is devoted to calculations of the conductivity of zigzag graphene nanoribbons (ZGNRs) with defects — absorbed by methylene and vacancies as such defects. The research objects are graphene nano-bands with boundary disorder and vacancy defects.

Recursive Green's function is often used to calculate the conductivity, charge density and current distribution of nanoscale devices after applied bias voltage. For larger systems, the recursive Green's function method uses the whole Green function method to calculate its Green function, and the matrix dimension is larger, so it will consume a lot of machine-time and computer memory [9]. The recursive Green's function method is to discretize the system into many parts and get the global Green's function by the recursive Green's function of each part. This method saves the computer resources by reducing the dimension of computing matrix and makes up for the deficiency of the full Green's function method. Following we will introduce the basic recursive process of recursive Green's function and the steps of solving the Green's function of two-electrode system by using recursive Green's function [10].

2. Experimental

Introduction of Recursive procedure

$$\underset{1}{\Big|} \xrightarrow{V_{12}} \underset{2}{\Big|} \xrightarrow{V_{23}} \underset{3}{\Big|} \xrightarrow{V_{34}} \underset{4}{\Big|}$$

For four discrete columns, $V_{ij} = (\mathrm{V}_{ij})^T$ ($i = 1, 4$; $j = 1, ,..4$) represents the interaction between column i and column j. The recursive Green's function is based on the Dyson equation:

$$G = G_0 + G_0 V G,$$
$$G = G_0 + G V G_0 ,$$

where G_0 is the Green's function before recursion, G is the recursive Green's function, and V is the interaction between recursive parts. According to the Dyson equation, recursion from column 1 to column 4 requires three recursive procedures: $1 \rightarrow 2$ column recursion:

$$\langle 1|G]1\rangle = \langle 1|G_0|1\rangle + \langle 1|G_0|1\rangle\langle 1|V|2\rangle\langle 2|G|1\rangle,$$
$$\langle 2|G]1\rangle = \langle 2|G_0|1\rangle + \langle 2|G_0|2\rangle\langle 1|V|2\rangle\langle 1|G|1\rangle,$$
$$\langle 2|G]2\rangle = \langle 2|G_0|2\rangle + \langle 2|G_0|2\rangle\langle 2|V|1\rangle\langle 1|G|2\rangle,$$
$$\langle 1|G]2\rangle = \langle 1|G_0|2\rangle + \langle 1|G_0|1\rangle\langle 1|V|2\rangle\langle 2|G|1\rangle,$$

where, in the case of $i = j$, $\langle i|G_0|j\rangle$ and $\langle i|G|j\rangle$ represent the Green's functions of number i column before and after recursion,

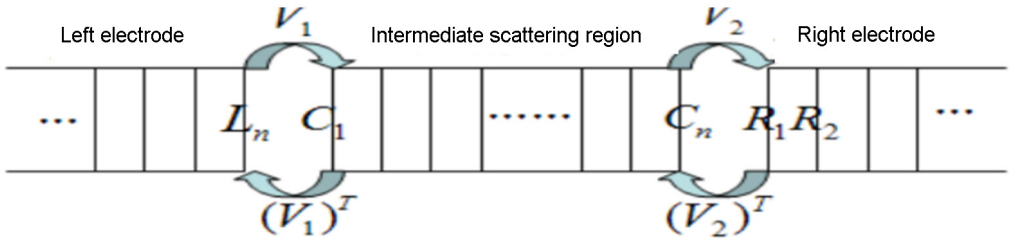

Fig. 1. Two-electrode system discrete into multiple columns

respectively. It can also be called a surface Green's function. In the case of $i \neq j$, $\langle i|G_0|j\rangle$ and $\langle i|G|j\rangle$ represent the Global Green's functions between j and i before and after recursion, respectively [11, 12]. Because column 1 and 2 are separated from each other before recursion. Therefore $\langle 1|G_0|2\rangle = \langle 2|G_0|1\rangle = 0$. Set $\langle i|G_0|j\rangle$ and $\langle i|G|j\rangle$ as ${G_0}^{ij}$ and G^{ij} respectively.

$1 \rightarrow 3$ column recursion: In this recursion, the whole column made up of the first and second column and third column are recursive, and the process is as follows:

$$\langle 1|G]1\rangle = \langle 1|G_0|1\rangle + \langle 1|G_0|2\rangle\langle 2|V|3\rangle\langle 3|G|1\rangle,$$
$$\langle 3|G]1\rangle = \langle 3|G_0|1\rangle + \langle 3|G_0|3\rangle\langle 3|V|2\rangle\langle 2|G|1\rangle,$$
$$\langle 2|G]1\rangle = \langle 2|G_0|1\rangle + \langle 2|G_0|2\rangle\langle 2|V|3\rangle\langle 3|G|2\rangle,$$
$$\langle 1|G]3\rangle = \langle 1|G_0|3\rangle + \langle 1|G_0|2\rangle\langle 2|V|3\rangle\langle 3|G|3\rangle,$$
$$\langle 3|G]3\rangle = \langle 3|G_0|3\rangle + \langle 3|G_0|3\rangle\langle 3|V|2\rangle\langle 2|G|3\rangle,$$
$$\langle 2|G]3\rangle = \langle 2|G_0|3\rangle + \langle 2|G_0|2\rangle\langle 2|V|3\rangle\langle 3|G|3\rangle.$$

The recursive Green's function method is used to calculate the Green's function for the two-electrode system. Fig. 1 is two-electrode system.

Where Ln, Cn, Rn represents the length of the left electrode, the middle scattering region and the right electrode, respectively. In order to obtain the Green's function of the whole system, we take the following steps:

First, the surface Green's functions of the left electrode and the right electrode are obtained by using the recursive Green's function.

From the surface of the left electrode to the last column of the middle scattering region, the Green's function which contains the left electrode and the intermediate scattering region is obtained

With the recursive of the Green's function obtained in the second step and the surface Green's function of the right electrode, the global Green's function of the two-electrode system is finally obtained.

3. Experimental

We have calculated the conductance of ZGNRs when N is 8 and ZGNRs is N = ll. In this study, the length of both samples was selected to be $M = 100$. All methylene groups are randomly distributed on two boundaries. For the sake of clarity, in Figure 2, we also draw the conductance of the perfect graphite bet nano-band. As expected, for graphene at this boundary, the conductivity curve decreases rapidly with the increase of the boundary adsorption concentration. In other words, the greater the number of methylene, the more obvious the suppression of conductivity. This means that it is difficult to observe quantized conductance in graphene nano-band. At the same time, we note that there are two conductance channels at $E = 1.0$ eV in the conductivity curve of ZGNRs when $w = 0.05$, but not in the vicinity of $E = 0.0$ eV. It means that there is only one methylene adsorbed on the boundary when $w = 0.05$, and the position of the methylene adsorption has no obvious effect on the conductivity curve. In order to analyze the cause of conductance channel, we calculated the local density of states (LDOS) of carbon atoms in methylene as shown in Fig. 2b. For ease of comparison, the figure also shows the LDOS on the carbon atom at the GNR boundary in the perfect case. It is very clear that there are two LDOS peaks in $E = 1.15$ eV. It implies that the electron state of energy $E = 1.015$ eV is a very strong localized state and is limited to a very small range, so it cannot open an electron channel, so there is no current formation.

In order to verify this local state, Fig. 3(a) is a panorama of LDOS, which describes the distribution of the electronic states of $E = 1.15$ eV at each lattice. It is clear that the probability amplitude of the electron state at the boundary methylene is much larger than that of other carbon atoms, that is, it is obviously localized on the methylene carbon atom and a few atoms around it, and the electron transport channel is completely

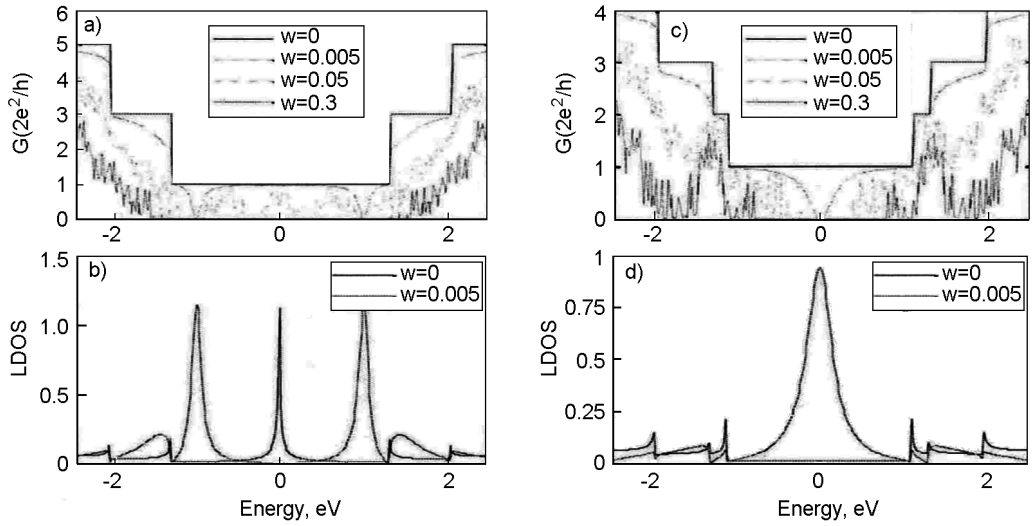

Fig. 2. a) Conductivity curves of ZGNRs obtained by different substitution probabilities (N = 8, M = 100); b) the LDOS when ZGNRs is perfect and when w = 0.05 respectively; c) conductivity curves of ZGNRs obtained by different substitution probabilities; d) the LDOS when ZGNRs is perfect and when w = 0.05 respectively.

blocked. Therefore, when the incident electron energy is about 1.15 eV, the nanoband cannot be passed. We have also calculated the LDOS, of another electronic state (E = 0.0 eV) as shown in Fig. 3b. It is clear that although this electron state is truncated at one edge of the nano-band, it is continuous at the other boundary, so it can open up an electron channel. On the conductivity curve, the conductivity did not decrease at E = 0.0 eV.

Unlike ZGNRs, ZGNRss only has a conductance channel when E = 0.0 e, and the concentration of methylene is 0.05, as shown in Fig. 2c. At the same time, the conductive step is smoothed. Similarly, conductive channels originate from localization of electronic states. To prove this-point, we calculate the LDOS, of the electronic state in E = 0.0 eV as shown in Fig. 2d. As you can see, LDOS also has a peak at E = 0.0 eV, which means it is a local state. To make a reasonable guess, as N increases, the transport gap will become smaller and smaller, because the larger N is, the weaker the boundary effect will be. In order to confirm this, we calculate the conductance of ZGNRs and ZGNRss and the transport channel with the change N when w = 0.3, as shown in Fig. 4. As we expected, whether it is ZGNRs, or AGNRs, the larger the N, the faster the conductivity curve rises. This is a very reasonable result, because with the increase of N, the more channels can be utilized. However, for AGNRs, we observed many conductive valleys on the conductivity

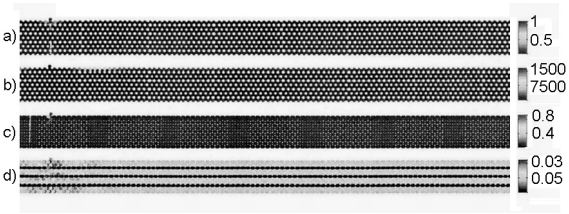

Fig. 3. a) and b) are panoramic images of LDOS with energy E = 1.15 eV and E = 0.0 eV, respectively. The structure of nano-band are the same of Fig. 2 b). c) and d) are LDOS panoramas with energy of E = 0.0 eV and E = 1.1 eV, respectively. And the structure of nan-band are the same of Fig. 2 d).

curve. It offers the possibility that we can change the energy of the incident electrons to regulate the conductance. In addition, from the conductivity curve, as the width of GNRs increases, the transport channel becomes narrower and narrower. This trend is shown in Fig. 4a. For ZGNRs, the size of the electric channel decreases exponentially with the increase of N, while for ZGNRss, we find that the conductance channel oscillates. This is not in line with our expectations. We also find that the oscillation of the species is related to the symmetry of the structure, that is, when AGNRs has a symmetric structure, its conductance channel is larger than that of its adjacent asymmetric structure. We are not clear about the physical mechanism behind this strange phenomenon.

The transportation channel is common in the GNRs with disordered boundary and gold attribute. In this section, we first con-

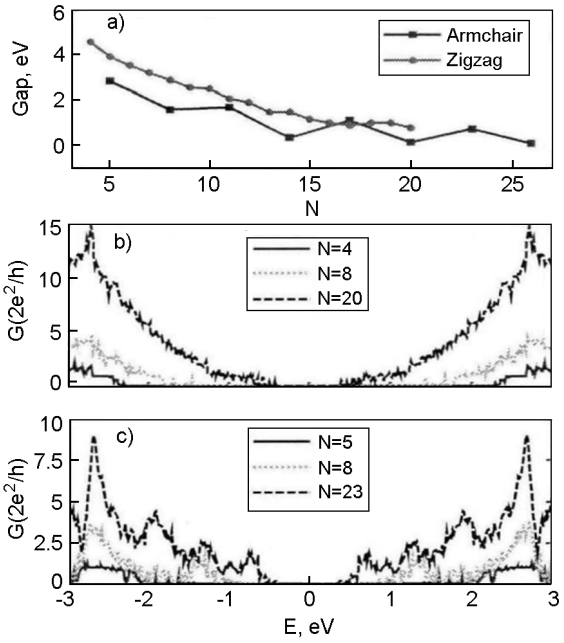

Fig. 4. a) The relationship between a) transport channel and nano-band width N. b) Conductivity curves of ZGNRs and ZGNRss with different width.

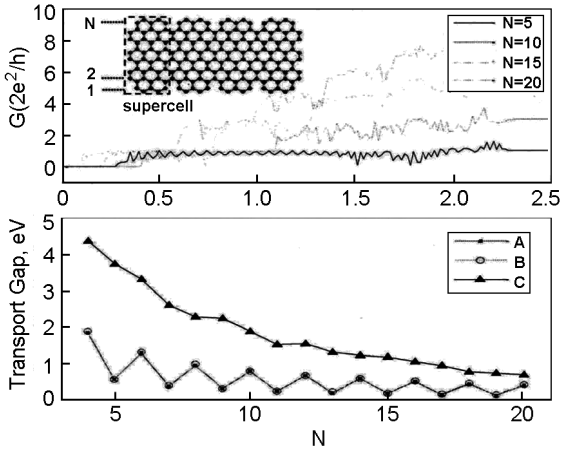

Fig. 5. a) ZGNRs conductivity curve of N with different width. Illustration: the corresponding structural schematic. b) Curves A and B are the variation of transport channel and gap with width N, respectively. And the structure is uniform and symmetric in terms of symmetric vacancies. When the vacancy is randomly distributed, the variation of transport channel with width N is shown in curve C.

sider the case where atomic vacancies are evenly and symmetrically distributed on the two boundaries, and the concentration of the boundary vacancies W is set to 1/3, which is explained below. In other words, an atomic vacancy appears in every three small blocks (the blue box in Fig. 5), and the distance between the vacancies is equal.

Fig. 5a is our calculation of the conductivity of nano-bands of different widths (N = 5, 10, 15, 20), in which the illustrations are corresponding structural diagrams, and it can be seen that the vacancies are symmetrically distributed on the two boundaries. There is no doubt that each conductivity curve has a transport channel at E = 0.0 eV, which is consistent with previous reports. Note that we only draw the conductivity curve when $E > 0$. It can be imagined that the size of the transport ditch should decrease with the increase of N, which is the inevitable result of quantum size effect [11, 12]. However, we can see from figure 5a that the transport channel of 15-ZGNRs is smaller than that of 20-ZGNRs and that of 5-ZGNRs is smaller than that of 10-ZGNRs. This is not in line with our earlier expectations. In order to reveal the variation rule, we have calculated the electronic transport channel of ZGNRs with width N = 1–20. The structure is shown in Fig. 5b. It is clear that the transport channel does not decline linearly or exponentially, but oscillates with the increase of N. It is found that when N is odd, the channel is larger, and when N is even, the channel is relatively small. When N is odd, it corresponds to symmetric structure, while N is even, which corresponds to asymmetrical structure.

4. Conclusions

The electronic structure and transport properties of the nano range were calculated using the recursive method of Green functions.

The results show that conductivity is sensitive to bulk vacancies.

The results show that a relatively stable conduction channel can be obtained when vacancies are evenly distributed over two boundaries. Thus, if the overall structure of the ZGNR is symmetrical, the transport channel becomes larger, and the transmission is mainly determined by its band. The results show that the band gap can be introduced by cutting graphene into a graphene nanozone. Preparation of nanoelectronic devices using graphene nano-strip has become a trend.

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