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Electronic and transport properties of different boron-doped (12, 0)/(6, 6) carbon nanotube junctions

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Abstract

The local density of states (LDOS) and conductance of several $(12, 0)/(6, 6)$ carbon nanotube junctions (CNTJs) with two substitutional boron atoms have been calculated by the tight-binding model and the Green's function method. It is found that the conductance gap of boron-doped CNTJs changes differently, depending on the different boron positions. For some boron-doped positions, the large conductance gap of undoped CNTJ could disappear completely even if the rotational symmetry is still kept in the doped CNTJs. Our results clearly show that the transport property of a metal–metal CNTJ depends not only on the rotational symmetry of its interface but also on the doped impurity positions on the interface.

1. Introduction

Carbon nanotubes, discovered by Iijima in 1991 [1], have attracted great interest by virtue of their extraordinarily mechanical and electronic properties [2–4]. A single-walled carbon nanotube (SWCNT) can be either a metal or a semiconductor, depending on its diameter and helicity that are uniquely determined by its chiral vector, $\vec{C} = n\vec{a}_1 + m\vec{a}_2$, where $\vec{a}_1$ and $\vec{a}_2$ are two primitive lattice vectors of the graphite sheet and (n, m) a pair of integers [5–7]. Two segments of SWCNTs with different diameters and chiralities can be joined together by introducing the pentagon–heptagon (5–7) defects into the perfect hexagonal (6) network, creating the quasi-one-dimensional semiconductor/semiconductor (S/S), metal/metal (M/M), or metal/semiconductor (M/S) carbon nanotube junctions (CNTJs) that have been widely studied theoretically [8–12] and already synthesized in experiments [13, 14].

As is well-known, a metallic SWCNT has two linear electronic energy bands which cross at the Fermi level (E_F) and so contribute two conductance quanta $2G_0$ ($=4e^2/h$) to the conductance when the tube has no defect [15, 16]. However, some theoretical studies indicated that this conductance relation could be substantially modified by defects such as substitutional impurities and topological defects [10, 17–21]. On the other hand, Chico *et al* found that the transport properties of the CNTJs are very sensitive to the configurations of the topological

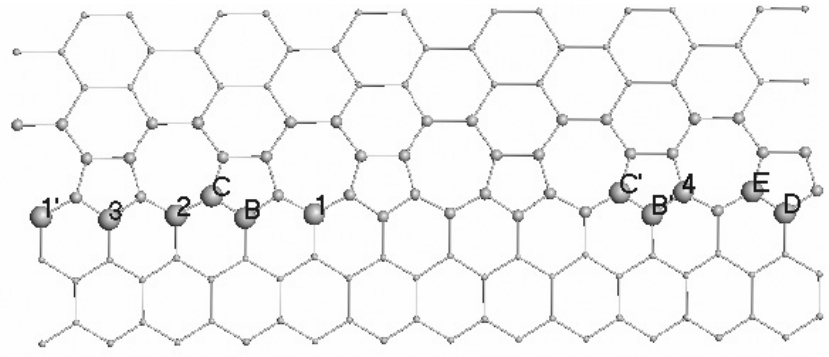

Figure 1. Two-dimensional representations of the $(12, 0)/(6, 6)$ junctions, in which the large balls represent the positions of the two boron atoms in the models (b)–(e).

defects [10]. This was well exemplified by two different $(9, 0)/(6, 3)$ M/M junctions, in which one interface has a threefold rotational symmetry and the other one is asymmetric, although both M/M junctions have the same number of pentagon–heptagon (5–7) pairs on their interfaces. It is the smaller structural differences (or different topological defect distributions) in their junction interfaces that make their transport properties differ greatly from each other, e.g., the symmetric one has a large conductance gap and the asymmetric one conducts. They also indicated that another $(12, 0)/(6, 6)$ CNTJ connected by six 5–7 pairs has an interface with sixfold rotational symmetry, making a conductance gap always appear in it. Chico *et al* further extended their conclusions, saying only the symmetry of the interface of the CNTJ is relevant to its conductance gap. Because the novel transport properties of the CNTJs are very important for fundamental research and potential applications of SWCNTs in future nanoscale electronic devices, further numerical and experimental efforts are needed to understand in more detail the effect of the defect arrangement at the interface of CNTJs on their electronic structures and transport properties.

Obviously, the substitution of another element for carbon at the interface can easily change the rotational symmetry of the junction and introduce new non-topological defects, leading probably to a large modification of its transport properties. Therefore, in this study, we have investigated the transport properties of boron-doped junctions based upon the π-electron tight-binding model, in which particular attention is paid to the effects of the boron impurities on the conductance gap of the symmetric $(12, 0)/(6, 6)$ CNTJ. It is found that the transport behaviours of the doped CNTJs are determined by both the symmetry of the matched junction and the positions of the doped impurities at the interface.

The models and calculation method are introduced in the following section. The results obtained and discussions are given in section 3. Some concluding remarks are offered in section 4.

2. Model and method

Based upon the symmetric $(12, 0)/(6, 6)$ junction with a ring of six 5–7 pairs around its circumference [10], denoted as model (a) in our paper, we substitute two boron atoms for carbon atoms at different positions of the junction interface, forming different models (b)–(e), respectively, for which a two-dimensional schematic diagram is given in figure 1, where the large balls represent the two boron atoms. Details of the substitutional positions and the symmetries of the doped junctions can be obtained from table 1.

Table 1. The positions of the two impurity atoms and the rotational symmetry of the models (a)–(e). Here, the letters correspond to those in figure 1.

Model	Positions of boron atoms	Rotational symmetry
(a)		C_6
(b)	B and B′	C_2
(c)	C and C′	C_2
(d)	B and D	No
(e)	C and E	No

The tight-binding (TB) Hamiltonian of the central junction with the on-site energies of the impurity atoms and the nearest-neighbour π-orbital hopping terms can be written as

$$H_{\mathrm{c}} = \sum_{q} \varepsilon_q a_q^{\dagger} a_q - t_0 \sum_{\langle ij \rangle} a_i^{\dagger} a_j + \mathrm{H.c}$$

where the sum over q is restricted only to the two impurity boron atoms due to the extremely short range of the impurity perturbation potential, and their on-site energy ε_q is taken to be $3t_0$ [17]. The on-site energies of carbon atoms are all taken to be zero. The sum over i, j is made to the nearest-neighbour atoms and the hopping parameter t_0 is set to be 2.75 eV [8] for all atoms since the boron atom is supposed to be 'carbon-like'. In the conductance calculation, the whole system is divided into three parts, i.e., the central junction and the two semi-infinite leads (left and right), which are taken as the (12, 0) and (6, 6) tubes, respectively. The problem can be conveniently treated by the Green's function matching method [16, 22], in which the conductance is expressed as

$$G = \frac{2e^2}{h} \mathrm{Tr}[\Gamma_{\mathrm{L}} G_{\mathrm{C}}^{\mathrm{r}} \Gamma_{\mathrm{R}} G_{\mathrm{C}}^{\mathrm{a}}],$$

where

$$G_{\mathrm{C}}^{\mathrm{r,a}} = \left(\varepsilon \pm \mathrm{i}\gamma - H_{\mathrm{C}} - h_{\mathrm{LC}}^{\dagger} g_{\mathrm{L}} h_{\mathrm{LC}} - h_{\mathrm{RC}}^{\dagger} g_{\mathrm{R}} h_{\mathrm{RC}}\right)^{-1},$$

$$\Gamma_{\mathrm{L(R)}} = \mathrm{i} h_{\mathrm{L(R)C}}^{\dagger} (g_{\mathrm{L(R)}}^{\mathrm{r}} - g_{\mathrm{L(R)}}^{\mathrm{a}}) h_{\mathrm{L(R)C}}.$$

Here, G_{C} is the Green's function of the central junction, $h_{\mathrm{L,C}}(h_{\mathrm{R,C}})$ is the coupling matrix between the central junction and the left (right) lead, and $g_{\mathrm{L}}(g_{\mathrm{R}})$ is the Green's function of the left (right) semi-infinite lead obtained from an iterative procedure [23]. The superscripts r and a on the G and g symbols represent restarted and advanced, respectively. The LDOS is calculated by using $\rho(j, \varepsilon) = -(1/\pi)\,\mathrm{Im}(G_{\mathrm{C}}^{\mathrm{r}}(j, j, \varepsilon))$, where j is the ordinal number of the carbon atom in the central junction, restarted (advanced).

3. Results and discussions

The calculated conductance and corresponding defect-atom-averaged (including the impurities and the 5–7 pairs) local density of states (LDOS) for all the models (a)–(e) are shown in figures 2(A)–(E), respectively. A large conductance gap exists in model (a), agreeing well with the results of [10]. According to the interpretation given by Chico *et al*, after doping boron atoms, the transport behaviours of models (b) and (c) should be similar since both of them have the same twofold rotational symmetry. However, it is clearly seen from figures 2(B) and (C) that the electronic and transport properties of models (b) and (c) are very different from each other. A small conductance gap still exists in model (b), but model (c) has a finite flat conductance without any gap.

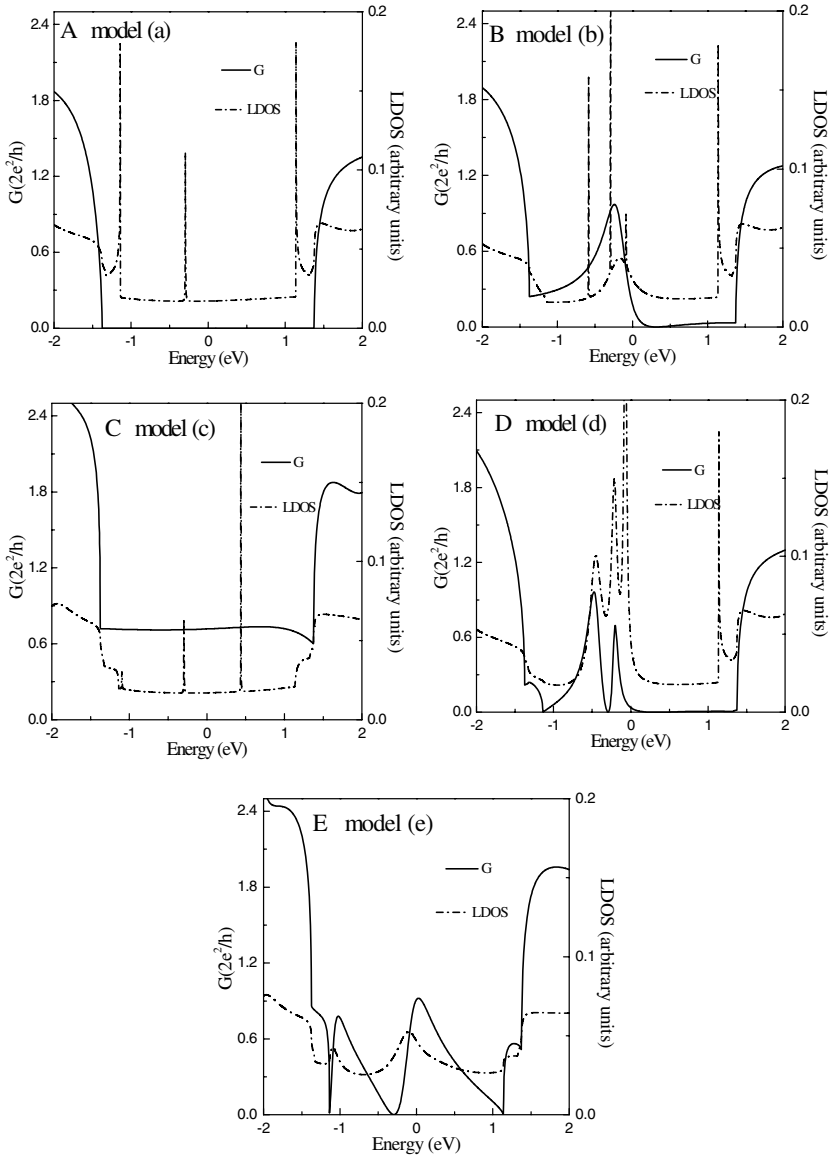

Figure 2. (A)–(E) give the conductances (solid lines) and defect-atom-averaged (including the impurities and the 5–7 pairs) LDOS (dashed lines), respectively, for the models (a)–(e).

In order to explore the reason why the conductance gap appears in model (b), we have calculated the spatial LDOS as a function of position z for the models (a)–(c) at energy $E = 0.312$ eV (where the conductance of model (b) is zero). Here, the position z is taken along a surface atom line parallel to the junction axis. In figure 3 are shown the results obtained along a straight line passing through the atomic site marked by the letter B in figure 1. The cases along other atom lines parallel to the junction axis, including those passing through the boron atom sites, have also studied and the results obtained are similar. It is found from figure 3(A) that, along this line, the LDOS minima equal zero at some positions, especially on the side of the

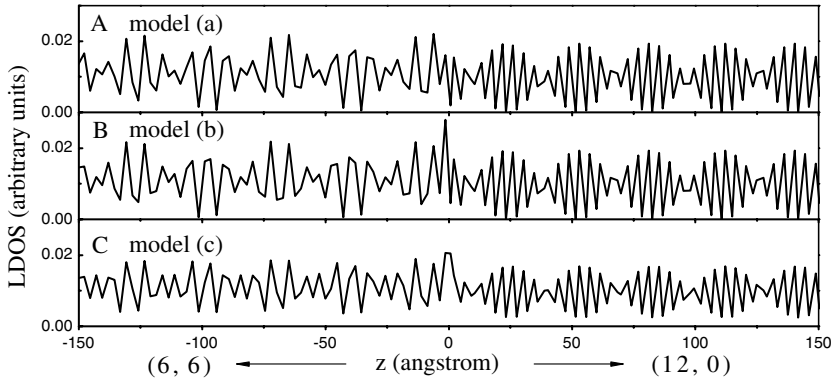

Figure 3. The spatial LDOS at energy $E = 0.312$ eV is shown in (A)–(C) as a function of the position z (its zero lies at the middle of the junction) for the models (a)–(c), respectively.

(12, 0) tube. Furthermore, the node position of the zero minimum LDOS depends only on the z positions, but not the azimuthal coordinates perpendicular the tube axis. This result indicates that at these special z positions the reflection coefficient is equal to 1. As a result, the incoming electron waves from one side cannot be scattered into the other side, making the transmission coefficients to be zero, which is coincident with its zero conductance at this energy. The result for model (b), shown in figure 3(B), is similar to that for model (a), and its zero LDOS at some z positions is obvious too, agreeing with its zero conductance at this energy. On the other hand, as we can see from figure 3(C), the LDOS of model (c) is distinctly different from the above two cases. Its LDOS minima are non-zero, indicating that the reflection coefficient is smaller than 1, and so it has a finite conductance at this energy. Based upon the above analyses, we can conclude that a small conductance gap in model (b) is also induced by the total reflection like in model (a).

We have also investigated the transport behaviours of the boron-doped systems when the two impurity atoms are located at other positions, making the system asymmetric. Two of the typical results are shown in figure 2(D) and (E), which corresponds to the cases of two boron atoms located, respectively, at positions of B–D (model (d)) and C–E (model (e)), as shown in figure 1. Based upon the conclusions in [10], the conductance gap should not exist in the asymmetric M/M junctions because their interfaces now have no rotational symmetry. However, it is clearly seen from figure 2(D) that there still exists a large conductance gap in model (d).

Both models (b) and (c) have twofold rotational symmetry, and the structural difference between them is the different positions of the two doped boron atoms, i.e., in model (b) the boron atom positions are not shared by the pentagon and heptagon but in model (c) they are. Although the interfaces in models (d) and (e) have no rotational symmetry, their structural difference is the same as that between models (b) and (c), i.e., whether the two boron atoms are shared by the pentagon and heptagon or not. By comparing the results shown in figures 2(B)–(E), it is clearly seen that in addition to the rotational symmetry of the interface, the impurity atom positions at the interface also play an important role in determining the transport behaviours of the CNTJs. When the impurity atom positions are not shared by the pentagon and heptagon, their effects on the transport behaviour of the CNTJ are smaller, making the original conductance gap of the undoped CNTJ still exist, although decreased somewhat.

The conductance and LDOS of the doped junctions are also calculated when the two impurity atoms locate at other positions, such as 1–1′, 1–2, B–3, 1–D, B–4, and C–4, etc,

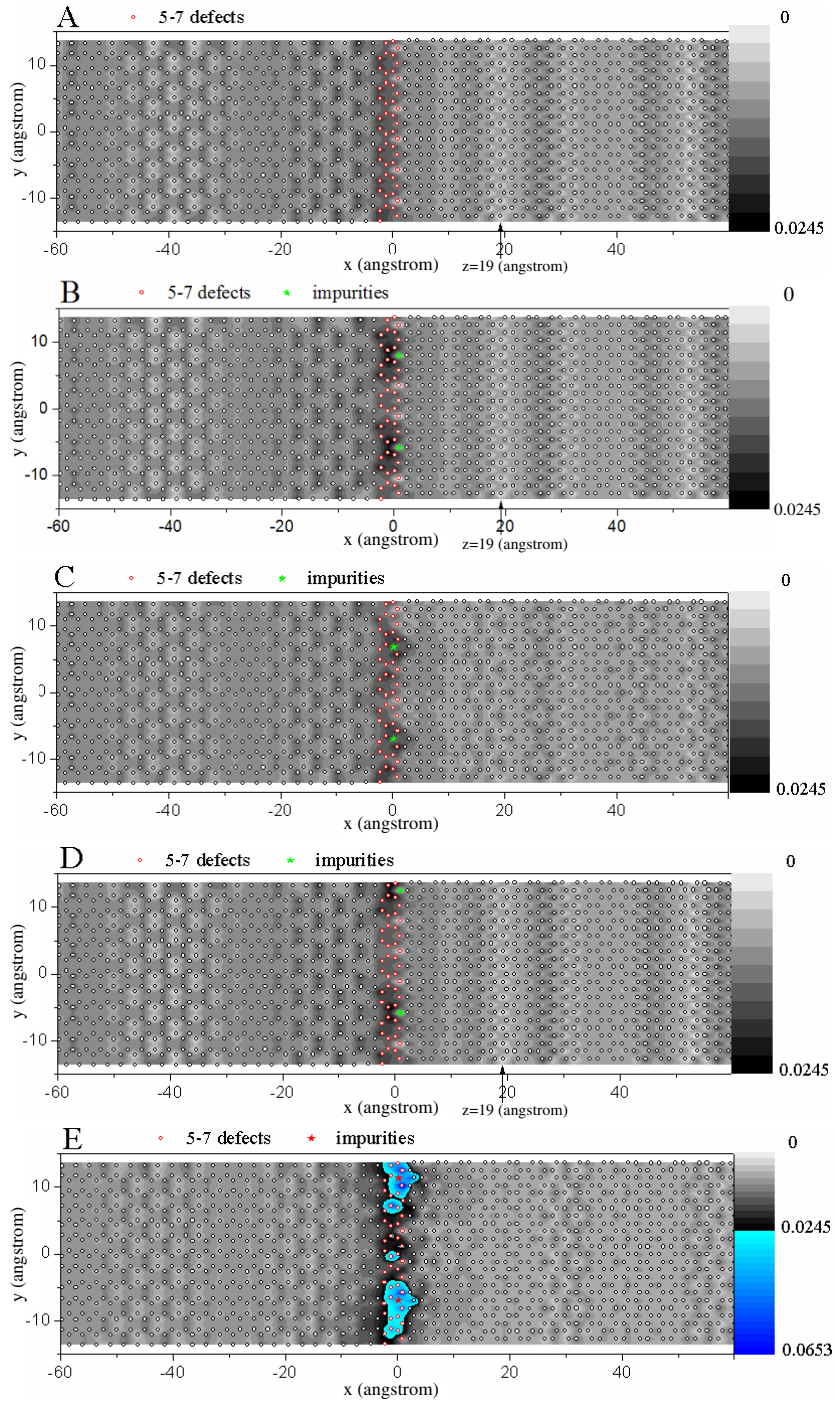

Figure 4. The 2D contour maps of the LDOS at $E = 0.312$ eV are given in (A)–(E) for all the models (a)–(e), respectively. The carbon and boron atomic positions are marked by the ∘ and the ⋆, respectively. The x, y axes are parallel and perpendicular to the tube axis, respectively.

(This figure is in colour only in the electronic version)

for which similar results to those above are obtained. If the impurity atom positions are not shared by the pentagon and heptagon, their effect on the transport behaviour of the CNTJ are smaller, favouring more appearance of the conductance gap within some energy range in the doped $(12, 0)/(6, 6)$ M/M junctions. And the gap is not induced by the quasi-bound states produced by the defects (including the 5–7 topological defects and the boron impurities), but on the contrary, it is induced by the quantum interference.

To further explore their electronic properties of the doped CNTJ and give more information along the tube circumference, the related LDOS contour maps at energy $E = 0.312$ eV are shown in figure 4 for all the models. It is clearly seen that the results for the models (a), (b), and (d) are very similar to each other. At some z positions, e.g., near $z \approx 19$ Å, shown by the arrows in figures 4(A), (B) and (D), the LDOS is equal to zero along the circumference in these three models, which is consistent with their zero conductance at this energy. Such results show clearly that the conductance gaps in both models (b) and (d) are indeed induced by the total reflection as in model (a), indicating that the distribution of impurity atoms at the interface also has an important effect on the transport property of the CNTJ in addition to the rotational symmetry of the interface in the doped cases. On the other hand, the difference between the LDOS contour maps in figures 4(A), (C) and (E) is obvious. It is found that the LDOS in figure 4(C) is extended, having no zero value anywhere. Furthermore, along the circumference, its LDOS minima are located at different z positions. So model (c) could have a finite conductance at this energy. The LDOS in figure 4(E) also shows a non-zero value everywhere and the different z positions of its minima along the circumference as in figure 4(C). But, in contrast to that in figure 4(C), the LDOS in figure 4(E) now shows clearly that its maxima are located mainly at the middle of the junction, near the boron atoms (much larger than elsewhere), obviously exhibiting the quasi-bound state induced by the impurities at this energy. As a result, the resonant conductance peak appears in figure 2(E).

By comparison of all these figures, we found that in models (a)–(d) at this energy, the combination of the interface rotational symmetry and the impurity atom distribution on the interface controls the electronic and transport properties of the doped CNTJs.

Finally, we should emphasize that for models (b)–(e), we have also studied the cases with two carbon atoms replaced by two nitrogen atoms, which could be more easily made experimentally. The results obtained are found to be similar to the cases of boron doping.

4. Summary

In conclusion, we have investigated the electronic and transport properties of several boron-doped $(12, 0)/(6, 6)$ junctions based upon the TB model. It is found that the transport properties of the doped junctions differ distinctly from each other. For example, for some boron atom positions, the large conductance gap of the undoped junction disappears completely, but for others, a smaller conductance gap still exists due to the total reflection. Our results clearly show that the transport behaviour of doped M/M carbon nanotube junctions depends not only on the rotational symmetry of the interface of the doped junctions but also on the impurity atom distributions on the interface.

Acknowledgments

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