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Unique effects of incommensurability on transport properties of incommensurate double-walled carbon nanotubes

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Abstract

On the basis of the multichannel Landauer formula, we investigated the effects of incommensurability on the electron transport properties of clean incommensurate double-walled carbon nanotubes (DWNTs). The results obtained clearly show that electron transport in incommensurate DWNTs can be either ballistic or non-ballistic depending on the energy region. In the lower energy region, the conductances remain at $2G_0$ (where $G_0 = 2e^2/h$ is the conductance quantum) except for at a very few positions, at least up to the system length of about 1.4 μm. And with increasing length, the conductances tend to change from $2G_0$ to $1G_0$ due to the antiresonances. This offers a possible explanation for the measurement results reported by Frank *et al* (1998 *Science* **280** 1744) and by Urbina *et al* (2003 *Phys. Rev. Lett.* **90** 106603). In the other energy regions, electron transport is non-ballistic and the conductances show a power law decay.

(Some figures in this article are in colour only in the electronic version)

Carbon nanotubes (CNTs) have attracted much attention due to their remarkable electronic and mechanical properties, and seem promising for nanoscale electronic device use [1]. One of the most interesting characteristics of the single-walled carbon nanotubes (SWNTs) is that their electronic properties are strongly dependent on their geometry [2, 3]. Moreover, combined systems formed from SWNTs, such as multi-walled carbon nanotubes (MWNTs) and bundles of closely packed SWNTs, show many unique physical properties [4–18]. Due to their complex lattice structures, there are more mechanisms which may affect their physical properties significantly [4, 6, 12–18]. Until now, these complicated physical properties, such as transport properties, have remained poorly understood and even controversial; much evidence for a diffusive regime [7, 8] and quantum interference effects has also been found [9, 10], and

it is also undecided why the observed ballistic conductance of MWNTs can be either $1G_0$ [9] or $2G_0$ [10].

A number of studies have been carried out to demonstrate the effects of incommensurability on electron transport properties of incommensurate MWNTs. For example, Roach *et al*, on the basis of the calculated spreading properties of wavepackets, infer that, in incommensurate MWNTs, electronic propagation follows a non-ballistic law [16]. Recently, Ahn *et al* made a spectral analysis of the energy levels of clean incommensurate MWNTs, and found that the level statistics is similar to that of the Anderson metal–insulator transition [17]. Very recently, Uryu [18] directly calculated the conductance of DWNTs with length shorter than 2000 nm; the results obtained show a clearer picture of the incommensurate DWNT transport properties: scattering in the bulk is negligible and the number of channels determines the average conductance. In addition, Uryu found that in some cases antiresonances with edge states in inner tubes cause an anomalous conductance quantization $1G_0$, near the Fermi energy.

In this paper, we calculate conductances of the longer incommensurate DWNTs, and pay further attention to the properties of antiresonance induced by the quasi-bound state and its effects on conductances of the longer incommensurate DWNTs. We find that the quasi-bound states are sited not only near the edges of DWNTs but also in other places. Hence, with increasing length of the tube, the probability of a $1G_0$ dip induced by the antiresonance may be enhanced, thus influencing the conductance of the longer incommensurate DWNTs significantly.

In the calculation of conductance, the whole system is considered as composed of a left-hand lead plus a DWNT and then a right-hand lead (L–D–R). Experimentally, one makes electrical contacts mainly with the outer tube and the coupling with the inner tube is very weak due to the very large anisotropy of the graphitic material [7]. For simplicity, here, the two leads are taken as SWNTs which are of the same type as the outer tube of the corresponding DWNT. This problem is most conveniently treated by the Green function matching method [19, 20]. The conductance is expressed using the Landauer formula:

$$C = (2e^2/h)\,\mathrm{Tr}[\Gamma_\mathrm{L} G_\mathrm{D}^\mathrm{r} \Gamma_\mathrm{R} G_\mathrm{D}^\mathrm{a}], \tag{1}$$

where

$$G_\mathrm{D} = (\epsilon - H_\mathrm{D} - h_\mathrm{LD}^\dagger g_\mathrm{L} h_\mathrm{LD} - h_\mathrm{RD}^\dagger g_\mathrm{R} h_\mathrm{RD})^{-1}, \tag{2}$$

and

$$\Gamma_\mathrm{L,R} = \mathrm{i} h_\mathrm{L,RD}^\dagger (g_\mathrm{L,R}^\mathrm{r} - g_\mathrm{L,R}^\mathrm{a}) h_\mathrm{L,RD}. \tag{3}$$

Here, H_D is the Hamiltonian of the DWNT; $h_\mathrm{L,D}$ ($h_\mathrm{R,D}$) is the matrix of the coupling between the DWNT and the left (right) lead. g_L and g_R are the Green functions due to the semi-infinite left and right leads, which are calculated using an iterative procedure [21].

Our model Hamiltonian is a tight binding one, which successfully describes the electronic structure of the MWNTs [16, 17]. In this model, one p_π orbital per carbon atom is retained, with zero on-site energies, whereas constant nearest neighbour hopping on each layer n (nn) and hopping between neighbouring layers (mn) are considered; the Hamiltonian is written as follows:

$$H = \gamma_0 \sum_{ijnn} (c_{in}^\dagger c_{jn} + \mathrm{H.c.}) - \beta \sum_{ijmn} (\cos(\theta_{ij}) \mathrm{e}^{(a-d_{ij})/\delta} c_{im}^\dagger c_{jn} + \mathrm{H.c.}), \tag{4}$$

where c_{in} ($c_{in}^\dagger$) denotes the annihilation (creation) operator of an electron on a C p_π orbital at site i and n is the SWNT index. γ_0 is the parameter for hopping between intra-layer nearest neighbour sites, i and j, and β is the strength of interwall interactions between interlayer sites,

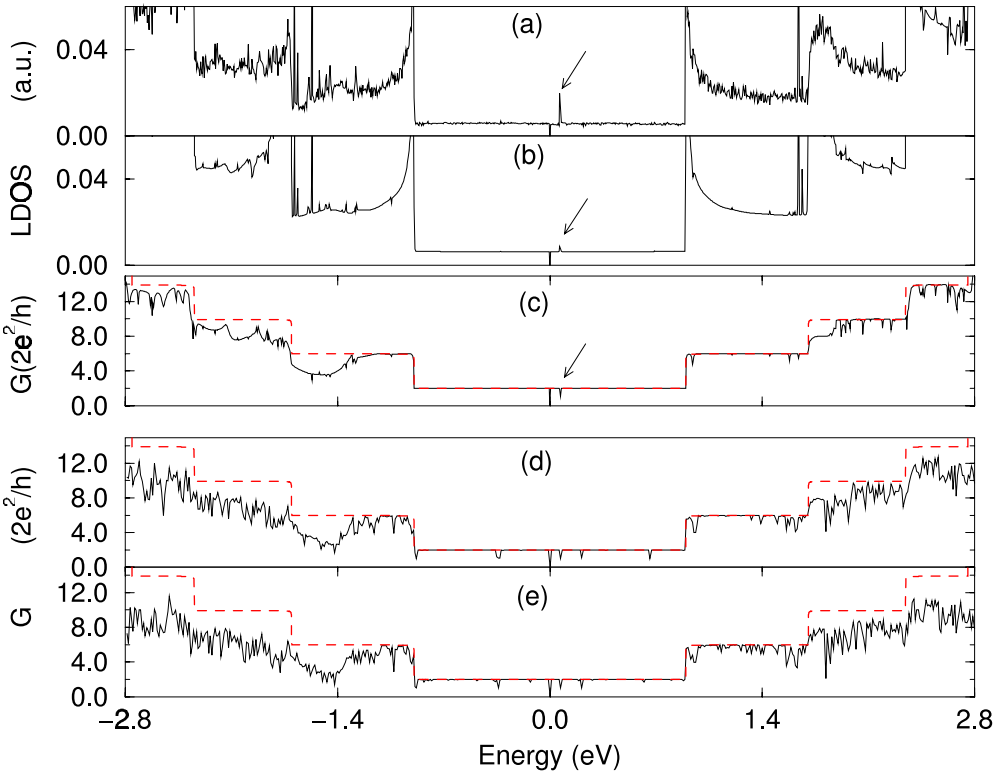

Figure 1. ((a), (b)) LDOSs at different space positions near the boundary of the (9, 0)@(10, 10) DWNT with the length of 7.38 nm. ((c)–(e)) The conductance of (9, 0)@(10, 10) DWNTs with different lattice lengths, of 7.38 nm, 246 nm and 1.48 μm, respectively. The dashed curves represent the conductance of an individual (10, 10) tube.

i and j, at the distance d_{ij} and with a cut-off for $d_{ij} > 0.39$ nm. θ_{ij} is the angle between the two p_π orbitals. The parameters used here are $\gamma_0 = 2.9$ eV, $\beta = \gamma_0/8.0$, $a = 0.334$ nm and $\delta = 0.045$ nm.

We have studied some finite-sized incommensurate DWNTs, such as (9, 0)@(10, 10), (8, 1)@(10, 10), (8, 2)@(10, 10) and (5, 5)@(18, 0) DWNTs, and found that they have similar electron transport properties. Therefore, below, we choose the incommensurate (9, 0)@(10, 10) DWNT as a typical case to study. We will show the energy dependence of the conductance and investigate the system size dependence of the conductance.

Some local densities of states (LDOSs) and conductances obtained for the incommensurate (9, 0)@(10, 10) DWNT are shown in figure 1. From figures 1(c)–(e) we found that the conductances of the (9, 0)@(10, 10) DWNT strongly depend on the energy region. In the energy region from −0.9 to 0.9 eV (i.e., between the two first van Hove singularities (vHss) of the outer (10, 10) tube), the value of the conductance is equal to that of the individual (10, 10) tube except at a very few energy positions. However, in the other energy regions, conductances fluctuate and decrease with respect to that of an individual (10, 10) tube. Correspondingly, the LDOS curves (see figures 1(a) and (b)) in the energy region from −0.9 to 0.9 eV seem smoother than those for the other energy regions. This is similar to the case for quasicrystals [22]. These energy dependent behaviours may be due to the two bands near the Fermi level, for neutral metallic SWNTs, being protected against backward scattering due to a certain symmetry of the

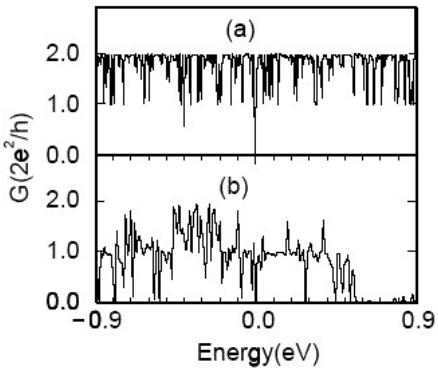

Figure 2. ((a), (b)) Conductances of (9, 0)@(10, 10) DWNTs with different lattice lengths, of 24.6 and 36.9 μm, respectively.

tube states, while the other bands are not [23]. It is also interesting to note that the value of the conductance near the 0.0 eV position is equal to zero, which is associated with the localized states near the sample boundary (see the LDOS near the boundary for the DWNT shown in figures 1(a) and (b)). Clearly, the above results are in good agreement with those reported in [17] and [18].

Now, we focus on the $1G_0$ dip of the conductance at the few positions in the energy range from -0.9 to 0.9 eV shown in figures 1(c) (indicated by the arrow), (d) and (e). We take the whole system as a quantum wire (the outer (10, 10) tube) attached to a resonator (the inner (9, 0) tube) [24]. In this energy region, the transmission probability of the outer (10, 10) tube is $T = 2$. This can be separated into $T_>$ and $T_<$, corresponding to more and less transmissive eigenchannels through the device, respectively; $T = T_> + T_<$ and $\mathrm{Tr}(tt^\dagger tt^\dagger) = T_<^2 + T_>^2$ [25]. It is found that, when $T = 1$ (i.e., the value of the conductance is equal to $1G_0$), $T_> = 1$ while $T_< = 0$. On the other hand, for the example shown in figures 1(a) and (b) indicated by the arrows, one of the LDOSs has a high peak shape in the corresponding energy position; however, the other only has a small peak, which indicates the existence of a quasi-bound state. Thus the $1G_0$ dip of the conductance may be due to the antiresonance produced by a destructive interference of the two transmissions via the bound and extended states [24, 25]. Our studies show that the quasi-bound states may exist both near the edge of the DWNT and in other places. Due to the complex lattice structure, it is hard to predict where antiresonances may arise; however, it is expected that the numbers of antiresonances will increase with increasing tube length.

Therefore, we study the length dependence of the conductance. From figures 1(c)–(e) we notice that, in the energy region from -0.9 to 0.9 eV, the conductances remain at $2G_0$ except at a very few energy positions, which indicates that the electron transport in this region is ballistic at least up to the system length of about 1.4 μm. Since the numbers of antiresonances may increase with increasing system length, we calculated conductances of longer (9, 0)@(10, 10) DWNTs; the results obtained are shown in figure 2. It is clear that, in the energy region from -0.9 to 0.9 eV, with increasing system length (see figure 2(a)) the conductances tend to be $1G_0$ at more and more energy positions, and there also exist a few energies at which the conductances become less than $1G_0$. On further increasing the lattice length to 36.9 μm (see figure 2(b)), there appear more zero conductances at a lot of energy positions, which can be seen clearly in the energy region from 0.6 to 0.9 eV. But the electron transport can remain ballistic.

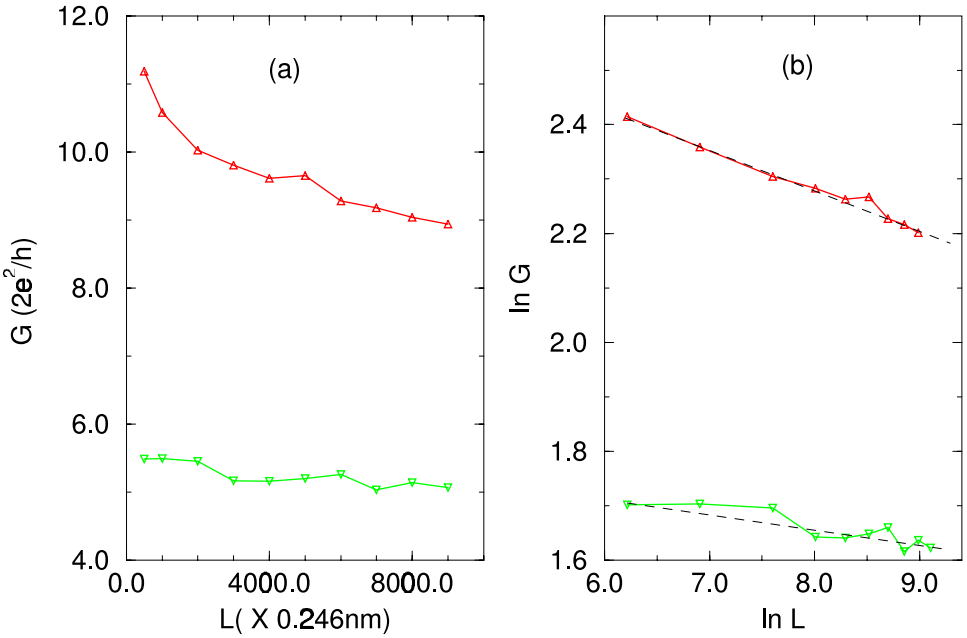

Figure 3. (a) The length dependences of the average conductances and (b) the log–log plot for different energy regions (upward pointing triangles: from −2.75 to −2.65 eV; downward pointing triangles: from −1.65 to −1.55 eV). The dashed lines fitting $g(L) \sim \alpha L^{-b}$ are superimposed in (b).

It is interesting to note that recently Urbina *et al* [10] reported that the conductance of the MWNTs remains fixed at $2G_0$ when the system length is about 1.4 μm. Meanwhile, some of their observed conductance steps show clear deviations from the quantized values even after taking into consideration the noise of the measurements, which is more pronounced at the end of the step. On the other hand, Frank *et al* [9] found $1G_0$ conductance in the MWNTs, where the measured MWNTs are embedded in fibres with a length of about 1 mm. Obviously, our results obtained for the conductance change with increasing system length, shown in figures 1 and 2, give a possible explanation for the measured conductances of the MWNTs reported in [9] and [10].

In the higher energy regions, from figures 1(b)–(d) we found that the conductances have a monotonic decreasing trend with increase of the lattice length. Due to the strong fluctuation of the conductance, here we have to employ the average conductance in a very narrow energy region in our detailed study. The length dependences of the average conductance obtained in the two energy regions (from −2.75 to −2.70 eV and from −1.45 to −1.40 eV) and a log–log plot are shown in figure 3. Obviously, although the value of the conductance fluctuates with change of the length, the conductance tends to decrease with increase of the lattice length, and the log–log plot shows a power law decay. Thus we may expect the wavefunctions to be power law localized in the thermodynamic limit, and the electron transport is hence diffusive [26]. The difference of the exponents of the power law decay in different energy regions indicates that the diffusive behaviour is also dependent on the energy positions—since in MWNTs on top of metallic gates the details of contacts, local excessive charges and depletion of charge carriers may change the position of the Fermi level [27, 28]. On the basis of our calculations, we guess that in conductance measurements [7, 8] the Fermi level is shifted to the higher energy region.

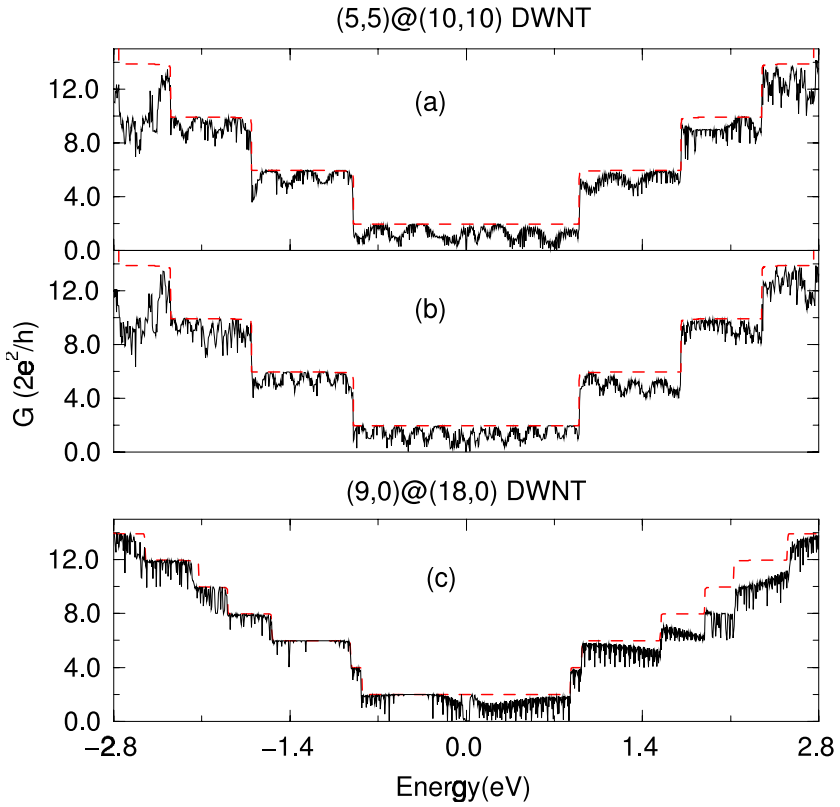

Figure 4. Conductances of finite-sized commensurate DWNTs: (a) the (5, 5)@(10, 10) DWNT with the length of 123 nm; (b) the (5, 5)@(10, 10) DWNT with the length of 246 nm; (c) the (9, 0)@(18, 0) DWNT with the length of 150 nm. The dashed curves represent the conductance of the individual outer tube of the corresponding DWNT.

Finally, for comparison, on the basis of the same model, we simply discuss electron transport properties of finite-sized commensurate DWNTs, such as (5, 5)@(10, 10) and (9, 0)@(18, 0) DWNTs. Some of the results obtained are shown in figure 4. Clearly, the conductances of the finite-sized commensurate DWNTs are very different from those of the incommensurate ones. The conductances of the finite-sized commensurate DWNTs have ordered fluctuation, but do not decrease monotonically with increasing system length in any energy region. Whereas, the conductance fluctuation properties are dependent on the tube helicity, the conductance of the (5, 5)@(10, 10) DWNT has slow and rapid fluctuations; however, the conductance of the (9, 0)@(18, 0) DWNT has no ordered slow fluctuation. References [29] and [30] have discussed the similar fluctuation behaviours occurring in SWNTs, which may be helpful for understanding the above-mentioned fluctuations in finite-sized commensurate DWNTs. Detailed study is beyond the scope of this paper however, so we leave this issue to future study.

In summary, our studies show that the incommensurability of the incommensurate DWNTs may produce significant effects on their electron transport properties. In the lower energy region, conductances remain at $2G_0$ except for at a very few positions at least up to the system length of about 1.4 μm. And with increase of the length, the conductances tend to change from $2G_0$ to $1G_0$ due to the antiresonances. In the other energy regions, electron transport

is non-ballistic and the conductances show a power law decay. These results offer a possible explanation for the experimental results.

It is important to point out that other factors, such as contacts between the sample and the leads, and electron–electron interactions, may also significantly affect the electron transport properties of the MWNTs. So, for a full understanding of the physical properties of the MWNTs, taking more factors into account is necessary.

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References

[1] Saito R, Dresselhaus G and Dresselhaus M S 1998 *Physical Properties of Carbon Nanotubes* (London: Imperial College Press)
[2] Saito R, Fujita M, Dresselhaus G and Dresselhaus M S 1992 *Phys. Rev.* B **46** 1804
Saito R, Fujita M, Dresselhaus G and Dresselhaus M S 1992 *Appl. Phys. Lett.* **60** 2204
Mintmire J W, Dunlap B I and White C T 1992 *Phys. Rev. Lett.* **68** 631
Hamada N, Sawada S-I and Oshiyama A 1992 *Phys. Rev. Lett.* **68** 1579
[3] Wildoer J W G, Venema L C, Rinzler A G, Smally R E and Dekker C 1998 *Nature* **391** 59
Odom T W, Huang J L, Kin P and Lieber C M 1998 *Nature* **391** 62
[4] Delaney P, Choi H J, Ihm J, Louie S G and Cohen M L 1998 *Nature* **391** 466
Delaney P, Choi H J, Ihm J, Louie S G and Cohen M L 1999 *Phys. Rev.* B **60** 7899
Kwon Y K, Saito S and Tomanek D 1998 *Phys. Rev.* B **58** 13314
[5] Ouyang M, Huang J-L, Cheung C L and Lieber C M 2001 *Science* **292** 702
[6] Kolmogorov A N and Crespi V H 2000 *Phys. Rev. Lett.* **85** 4727
[7] Langer L *et al* 1996 *Phys. Rev. Lett.* **76** 479
[8] Bachtold A *et al* 1999 *Nature* **397** 673
[9] Frank S *et al* 1998 *Science* **280** 1744
[10] Urbina A *et al* 2003 *Phys. Rev. Lett.* **90** 106603
[11] Maarouf A A, Kane C L and Mele E J 2000 *Phys. Rev.* B **61** 11156
[12] Kim D-H, Sim H-S and Chang K J 2001 *Phys. Rev.* B **64** 115409
[13] Klesse R 2002 *Phys. Rev.* B **66** 085409
[14] Sanvito S, Kwon Y-K, Tomanek D and Lambert C J 2000 *Phys. Rev. Lett.* **84** 1974
[15] Yoon Y-G, Delaney P and Louie S G 2002 *Phys. Rev.* B **66** 073407
[16] Roche S, Triozon F, Rubio A and Mayou D 2001 *Phys. Rev.* B **64** 121401
[17] Ahn K-H, Kim Y H, Wiersig J and Chang K J 2003 *Phys. Rev. Lett.* **90** 026601
[18] Uryu S 2004 *Phys. Rev.* B **69** 075402
[19] Nardelli M B 1999 *Phys. Rev.* B **60** 7828
[20] Chen J, Yang L, Yang H and Dong J 2004 *Chem. Phys. Lett.* **400** 384
[21] Lopez Sancho M P, Lopez Sancho J M and Rubio J 1984 *J. Phys. F: Met. Phys.* **14** 1205
Lopez Sancho M P, Lopez Sancho J M and Rubio J 1985 *J. Phys. F: Met. Phys.* **15** 851
[22] Tsunetsugu H, Fujiwara T, Ueda K and Tokihiro T 1991 *Phys. Rev.* B **43** 8879
Tsunetsugu H and Ueda K 1991 *Phys. Rev.* B **43** 8892
[23] Ando T, Nakanishi T and Saito R 1998 *J. Phys. Soc. Japan* **67** 2857
[24] Shao Z-A, Porod W and Lent C S 1994 *Phys. Rev.* B **49** 7453
[25] Sim H-S, Park C-J and Chang K J 2001 *Phys. Rev.* B **63** 073402
[26] Abrahams E, Anderson P W, Licciardello D C and Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42** 673
[27] Xue Y and Datta S 1999 *Phys. Rev. Lett.* **83** 4844
[28] Kociak M, Suenaga K, Hirahara K, Saito Y, Nakahira T and Iijima S 2002 *Phys. Rev. Lett.* **89** 155501
[29] Jiang J, Dong J and Xing A D Y 2003 *Phys. Rev. Lett.* **91** 056802
[30] Yang L, Chen J, Yang H and Dong J 2004 *Phys. Rev.* B **69** 153407