# Effects of local structural defects on the electron transport in a carbon nanotube between Cu electrodes

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Using the first-principles approach with the Landauer formalism, we studied the effects of monovacancy and Stone–Wales defects on the electrical conductance of carbon nanotube (CNT) itself and its junction with copper electrodes. We found that the Stone–Wales defect has almost negligible impact on the electrical performance of the CNT(5,5) and its junction with copper at the Fermi level, while the monovacancy can reduce the electrical conductance of the CNT(5,5) significantly and that of the Cu/CNT(5,5)/Cu junction by more than 30%. © *2010 American Institute of Physics*. [doi:10.1063/1.3527918]

Carbon nanotube (CNT) is considered one of the most promising candidates for future nanoscale device.[1] Numerous studies have been conducted to explore the electronic structure of CNTs as well as the junction between CNT and electrodes.[2–6] In most of these studies, the CNT is considered perfect without any defect. In reality, however, defects are often inevitable during CNT fabrication. Several studies have found that the defects affect the electron transparent performance of CNT.[7–12] However, the effects of defects on the electron transmission at the metal/CNT/metal junction system have not been investigated.

In this letter, we report our studies on the effects of local structure defects such as monovacancy and Stone–Wales on the electron transmission in CNT and Cu/CNT/Cu junctions. The CNT considered here is (5,5) with open ends. The Cu/CNT/Cu junction consists of a CNT(5,5) in end-contact with a Cu electrode at each end. Two types of CNT defects, monovacancy and Stone–Wales (or pentagon-heptagon-pair), are considered.

Density functional theory and nonequilibrium Green's function methods are employed in this study. The general gradient approximation with double zeta basis sets was used in the calculation. For convergence, a tolerance of $1\times10^{-5}$ of the total energy was used as the criterion. For the CNT(5,5), the *k*-sampling set used is $1\times1\times100$. For the Cu/CNT(5,5)/Cu junction, the Brillouin zone parameter used is $3\times3\times100$. The computations were performed using the commercial software package QUANTUMWISE (ATK2008.10).[6] In what follows, results for the defective CNT will be presented first, followed by the results for the Cu/CNT/Cu junction.

To compute the electron transport in a CNT, we constructed a two-probe system by dividing the CNT into three regions, namely, left-electrode, right-electrode, and the scattering region in between the electrodes. A region of vacuum space is generated around each electrode. Their volumes are sufficiently large so that the CNTs can be considered as isolated individuals. The scattering region consists of four unit cells of the CNT(5,5) nanotube with a defect in the middle of the CNT. The Cartesian coordinate system used in the calculation is such that the *z*-axis is along the axial direction of the CNT.

Shown in Fig. 1 is the calculated electron transmission coefficient of CNT(5,5) with and without defect. It is seen that the electron transmission coefficient of the defect-free CNT(5,5) is equal to 2 around the Fermi level (0 eV), indicating that there are two transmission channels, $\pi$-bonding state and $\pi$-antibonding state. The CNT with the Stone–Wales defect shows two dips in the transmission spectrum, one at approximately 0.95 eV above the Fermi level, the other approximately 1.5 eV below the Fermi level. The reduction of transmission coefficient at these two energy levels is about 50% of that at the Fermi level. It has been reported that the dip above the Fermi level is attributed to the complete reflection of the $\pi$-bonding state, while the one below the Fermi level is due to the complete reflection of the $\pi$-antibonding state.[7] It is interesting to note that the Stone–Wales defect does not reduce the transmission coefficient at the Fermi level. In fact, the calculated transmission eigenvalues of CNT(5,5) with Stone–Wales defect at the Fermi level are 0.9997 and 0.9451, respectively. Therefore, one may conclude that the electron conductance of CNT(5,5) at the Fermi level is not affected by the presence of Stone–Wales defect.

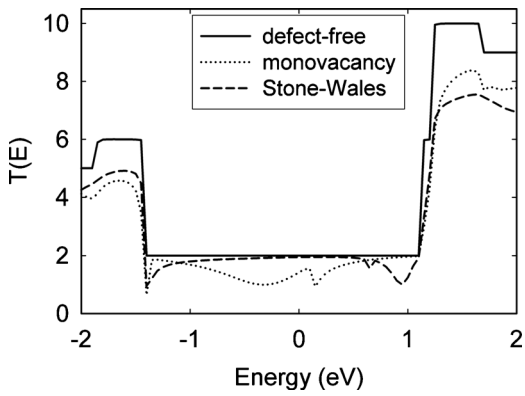


FIG. 1. Electron transmission spectrum of CNT(5,5) with and without defects.

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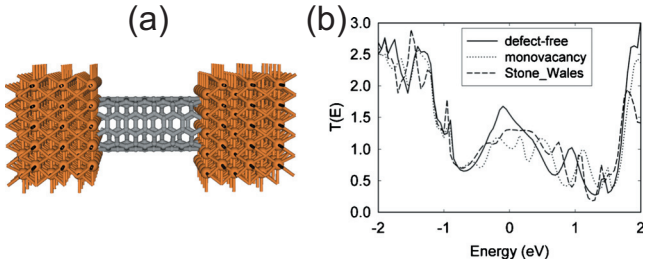


FIG. 2. (Color) (a) The geometry of the Cu/CNT(5,5)/Cu two-probe system and (b) the electron transmission spectra of all three systems.

These results are consistent with the study on a CNT(10,10) tube.[7–10]

Unlike Stone–Wales defect, the monovacancy shows significant impact on the conductance of CNT(5,5). In the vicinity of Fermi level, the monovacancy causes one broader tip below the Fermi level (about −0.3 eV) and a narrower dip above the Fermi level (about 0.15 eV). This is quite different from the results studied by tight-binding model,[13,14] which predicts only a single dip exactly at the Fermi level. In tight-binding models, only one $p$ electron per carbon atom perpendicular to the CNT surface is studied. The reduction of transmission coefficient at the broader dip (−0.3 eV) is approximately 50% of that of the defect-free CNT at the Fermi level. In addition, another dip far from the Fermi level (−1.4 eV) is also formed, which shows approximately 70% reduction of transmission coefficient. The narrower dip at 0.15 eV originates from resonant scattering by quasibound states derived from the broken $\sigma$ bonds around the vacancy. The original $\sigma$ bonds between the removed C atom and its neighbors are broken, resulting in dangling bonds, which are mainly composed of $p$ orbital parallel to the CNT surface.[7] Since $\sigma$-bond states are perpendicular to the $\pi$ valence band states, very little coupling can take place between them. The corresponding transmission eigenvalues at the Fermi energy level for the CNT(5,5) containing monovacancy defect were calculated as 0.9897 and 0.4279, respectively, which implies that one transmission channel is only slightly affected, while the other one is significantly reduced.

To study the Cu/CNT/Cu junctions, a copper electrode is attached to each of the open ends of the CNT(5,5), as shown in Fig. 2(a). The interface gap between CNT and Cu electrodes is determined by minimizing the total energy of the system.[15] The electron transmission spectra of the Cu/CNT/Cu junction are shown in Fig. 2(b) for the three systems. The solid line is for the defect-free CNT, the dotted line is for the CNT with a monovacancy, and the dashed line is for the CNT with a Stone–Wales defect. Clearly, near the Fermi level, the defect-free Cu/CNT/Cu junction shows the highest transmission coefficient, although it is still lower than that of the CNT itself, indicating that scattering takes place at the Cu/CNT interface. Both monovacancy and Stone–Wales defects reduce the transmission coefficient at the Fermi level, although the former seems to have a bigger effect.

Details of the electron transmission at the Fermi energy can be illustrated in the $k$-sampling space. Figure 3 shows the transmission probability contour as a function of $(k_x,k_y)$ zone. For all these cases, the lower values are all located around the $\Gamma(0,0)$ point. It has been shown that the property of junction states is dependent on whether or not they are

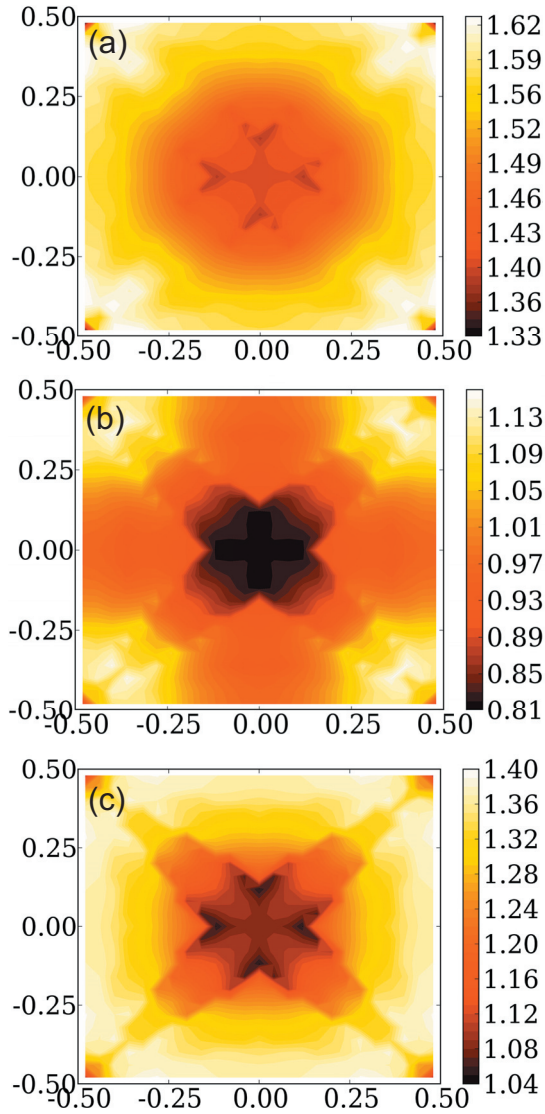


FIG. 3. (Color) Electron transmission probability as a function of $(k_x,k_y)$ points in Cu/CNT(5,5)/Cu systems: (a) defect-free, (b) monovacancy, and (c) Stone–Wales.

coupled with the bulk states.[16] As shown in Fig. 3, the presence of the Stone–Wales defect in CNT(5,5) does not alter the bonding mode in the junction, particularly around the $\Gamma(0,0)$ point, while the monovacancy changes the bonding mode in the Cu/CNT(5,5) junction significantly. Thus around the $\Gamma(0,0)$ point, the Cu/CNT(5,5) with a Stone–Wales defect shows a similar transmission behavior as the defect-free one. However, far from the $\Gamma(0,0)$ point, especially along the diagonal directions, the transmission mode is closer to that of the monovacancy. Furthermore, the amplitudes of transmission coefficient values at varies $k$ points for Cu/CNT(5,5) with monovacancy are the minimum. It is evident that the transmission ability for Cu/CNT(5,5) with Stone–Wales defect falls in between of other two systems.

Based on the calculated electron coefficient shown in Fig. 2(b), the current-voltage ($I$-$V$) relation of the Cu/CNT(5,5)/Cu systems can be determined using the Landauer–Buttiker formula.[17] Thus the total resistance of the systems can be obtained by averaging the values in the 0–0.1 V regime. The results are 9.1, 10.4, and 12.2 kΩ for the defect-free, Stone–Wales defect, and monovacancy cases, respectively, representing increased resistances of 14.3% due

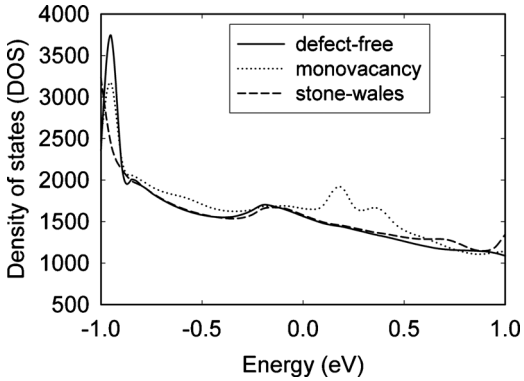


FIG. 4. DOS of Cu/CNT(5,5)/Cu systems.

to a Stone–Wales defect and of 34.1% due to a monovacancy defect.

To better understand the cause of such resistance increase, we calculated the density of states (DOS). Figure 4 shows the DOS of the CNT/Cu junction systems with and without the defect. It is seen that the Stone–Wales does not affect the DOS very much, while the monovacancy results in significant peak on the DOS curve in the vicinity of the Fermi level. At this particular energy level, we also calculated the local density of states (LDOS). Shown in Fig. 5 are the three-dimensional isovalue plots of the LDOS without defect [Fig. 5(a)] and with a monovacancy [Fig. 5(b)]. The color scales used in both figures are the same so that the same value of LDOS is represented by the same color in both plots. It is clear from these plots that the DOS is localized around the monovacancy defect. In addition, our calculations on the Stone–Wales defect show that the DOS localization around the defect is not as severe as in the monovacancy case. These results seem to indicate that DOS localization near the defect is the main cause of reduction in electrical conductance in the Cu/CNT/Cu junction.

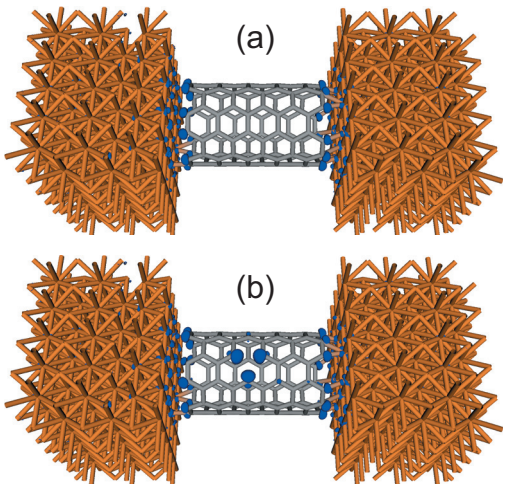


FIG. 5. (Color) Local DOS of the Cu/CNT/Cu system: (a) defect-free and (b) monovacancy.

In summary, Stone–Wales defect has negligible effect on the electrical conductance of CNT(5,5) at the Fermi level of CNT(5,5), while monovacancy defect significantly reduces the electrical conductance in CNT(5,5) by severely blocking one of the two transmission channels. Furthermore, monovacancy in CNT(5,5) results in more than 30% of reduction in the electrical conductance of Cu/CNT/Cu junctions, while the Stone–Wales defect decreases the conductance by only 14%. The localization of DOS around the defect is the main cause of the reduced electrical conductance of the Cu/CNT/Cu junction.

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