Transport in a metallic nanotube at finite temperature

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We consider the effect of thermal phonon displacements on the coherent transport in carbon nanotubes. The atomic displacements are generated using tight-binding molecular dynamics simulations, and the conductances are computed using a nonequilibrium Green’s function technique. Atomic displacements due to lattice vibrations lead to different levels of conductance reduction and fluctuation on the massive and massless bands of a metallic nanotube. Different conduction regimes are studied by examining the resistance on different length scales. The temperature-induced displacements have a significant impact on the ballistic or diffusive transport in carbon nanotube.

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These phenomena, which will affect transport, cannot be captured in the present static approach. The effect of nonadiabatic effects on electron dynamics in the presence of moving nuclei is beyond the scope of this work. Acoustic phonon is operative in our investigation, while we have restricted ourselves to the low applied bias regime corresponding to the UCF value of 0.365\(e^2/\hbar\). This weak temperature dependence behavior is crucial for the applications of nanotubes as metallic quantum wires. From the bond length statistics in Fig. 2, different temperatures lead to different structural disorders and, thus, to the fluctuations of hopping energies in tight-binding model. The equilibrium carbon-carbon atom distances are single valued at 1.42 Å for the nearest neighbors, 2.46 Å for the second nearest neighbors, and 2.84 Å for the third (vertical lines in Fig. 2). In particular, we observe that the lengths of double \((r=1.31\ Å)\), conjugated \((r=1.42\ Å)\), and single \((r=1.54\ Å)\) bonds are all present in the radial distribution function. The radial distribution functions are all broadened increasingly as temperature goes up, with a corresponding decrease in height. Anyhow these dependences are relatively insignificant since carbon has a very high Debye temperature. We also note that the peaks in radial distribution function are not symmetrically distributed due to anharmonicity contribution captured in our TBMD scheme.

We see that near \(E_f\), the intrinsic conductance of nanotube only degrades slightly at room temperature or even up to 700 K. This weak temperature dependence behavior is crucial for the applications of nanotubes as metallic quantum wire. From the bond length statistics in Fig. 2, different temperatures lead to different structural disorders and, thus, to the fluctuations of hopping energies in tight-binding model. The equilibrium carbon-carbon atom distances are single valued at 1.42 Å for the nearest neighbors, 2.46 Å for the second nearest neighbors, and 2.84 Å for the third (vertical lines in Fig. 2). In particular, we observe that the lengths of double \((r=1.31\ Å)\), conjugated \((r=1.42\ Å)\), and single \((r=1.54\ Å)\) bonds are all present in the radial distribution function. The radial distribution functions are all broadened increasingly as temperature goes up, with a corresponding decrease in height. Anyhow these dependences are relatively insignificant since carbon has a very high Debye temperature. We also note that the peaks in radial distribution function are not symmetrically distributed due to anharmonicity contribution captured in our TBMD scheme.

To consider the disorder effect on tubes of increasing lengths, we randomly interconnect different segments of MD generated nanotube atomic coordinates to form longer tubes.
to study the transport scaling. This strategy is the same as a recent study on the doped silicon nanowires. Our coalescent longest nanotube is composed of 20 160 carbon atoms. In the calculation of conductance near the Fermi energy, a statistical average has been done over 300 coalescence realizations for each tube length. The results are shown in Fig. 3 in which we give the ensemble-averaged resistance as a function of tube length for atomic configurations generated at three different temperatures. If the electron transport is ballistic, the resistance should not depend on length. However, we found that the resistances grow as functions of length. It initially increases in a linear manner, indicating that the length of the tubes we considered is in the quasiballistic or diffusive regime. In such a regime, as the resistance is commonly analyzed with a linear relation in the form $R = R_c + (R_s)L/d$, where $R_c = 1/G_0 = (1/N)h/2e^2$ is contact resistance, $(R_s)$ is resistance of a single segment, and $L/d$ is the segment repeating number. If we take the mean-free path as the distance in which the resistance has become twice the value of the intrinsic contact resistance, the mean-free path is about 300 Å. For the even longer nanotube, the resistance starts to increase more rapidly above the initial linear scaling behavior, manifesting the so-called medium localization. Eventually the resistance should increase exponentially or superlinearly with length when one-dimensional localization effect emerges, as confirmed in the recent experiment. Further we can observe that as the temperature increases, the deviation from single segment linear scaling becomes larger and the onset length scale for localization is reduced.

We fitted the data with a power-law relation $R = a(L/d)^b$ and found the exponent $b$ values to be 1.10, 1.15, and 1.33 for 100, 300, and 700 K, respectively. For a given tube length, the intrinsic resistance of the freestanding one-dimensional metallic nanotube is found to increase with the absolute temperature. As the tube length increases, temperature starts to play a more dominant role, and the atomic displacements eventually cause localization effect to set in. This thermal effect is more clearly presented in the inset of Fig. 3 where we replot the scaling data in the main frame. For the longest tube $L/d = 35$ considered here, we can estimate the temperature coefficient to be about $\alpha = (1/R)dR/dT = 0.001/K$.

In conclusion, the quantum conductance in a metallic freestanding single-wall nanotube is studied at several temperatures. Substantial temperature dependence of the conductance in the range of 100–700 K has been revealed. We show that at a specific temperature the atomic displacements induce scattering, which in turn impose a length scale for ballistic transport along the metallic nanotube. Our method can be applied to investigate other carbon materials such as graphene where buckling effect is also important at room-temperature condition.

Recently, experimental work has been carried out to measure the individual metallic single-wall carbon nanotube’s resistance from room temperature up to 1000 K in vacuum. A relatively small linear temperature dependence of resistance is obtained. Their measured temperature coefficient $1.1 \times 10^{-3}/K$ is in good agreement with our long nanotube calculations. This value is also consistent with the results of $n$- and $p$-type silicon nanowires measured between 75 and 325 K.

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