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Comparison of electron and phonon transport in disordered semiconductor carbon nanotubes

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Abstract Charge and thermal conductivities are the most important parameters of carbon nanomaterials as candidates for future electronics. In this paper we address the effects of Anderson type disorder in long semiconductor carbon nanotubes (CNTs) to electron charge conductivity and lattice thermal conductivity using the atomistic Green function approach. The electron and phonon transmissions are analyzed as a function of the length of the disordered nanostructures. The thermal conductance as a function of temperature is calculated for different lengths. Analysis of the transmission probabilities as a function of length of the disordered device shows that both electrons and phonons with different energies display different transport regimes, i.e. quasi-ballistic, diffusive and localization regimes coexist. In the light of the results we discuss heating of the semiconductor device in electronic applications.

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1 Introduction

Electron transport in carbon nanostructures, namely nanotubes and graphene nanoribbons, is in the focus of experimental and theoretical research during last years. In particular, the Anderson disorder model and localization of electrons in CNTs have been studied extensively in the past decade [1–4]. It is important to note that also *phonon* thermal transport in low-dimensional systems is of central importance for applications. By properly controlling thermal properties it is possible to enhance the device performance. In electronic applications, high values of both electronic and phononic conductances are desired. On the other hand a low phonon conductance is required in order to have efficient thermoelectric energy conversion. In this paper we focus on the phonon thermal conductivity in disordered systems and compare the effects of disorder on the phonon conductivity with the effect on the electron transport.

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In semiconductor materials heat transport is governed mostly by phonons and it is previously shown that the thermal conduction is strongly influenced by device dimensions [5]. For example, it was observed recently that phonon conduction can be reduced without effecting the electronic transport importantly in Si nanowires which leads to an enhancement in the thermoelectric figure of merit by two orders of magnitude compared to its bulk value [6–8]. This decrease in thermal conduction is mainly due to the scattering of phonons at disordered surface whereas electron transfer is maintained by bulk-like states. Thus, surface to volume ratio is a parameter to control the transport properties of these devices. Graphitic allotropes have the exceptional property that they are one atom tick. There is a growing interest in the field of phononic energy transport through carbon based materials. It is shown that thermal conductance of nanotubes can be tuned by sliding the inner shell inside the outer shell [9]. Disorder induced localization is believed to be a possible explanation of the exponential dependence of thermal resistance on the telescoping distance. Conductance is independent of the device length if the device is pristine. Real systems, on the other hand, always include disorder which we model with a distribution in force constants. Recently the effect of isotopic disorder on thermal conduction through nanotubes is studied theoretically [10, 11] and good agreement with experiment [12] is achieved.

In this paper, we analyze the effects of Anderson disorder in semiconductor CNTs on electron and phonon transport. First we summarize the atomistic Green function method in calculating the transport properties. Then we investigate the dependence on length of the device and on the operating temperature. The energy dependence of transport regimes are shown to coexist and their role on device performance depending on system parameters is discussed.

2 Model and Method

As it is common in transport calculations, we apply the partitioning scheme and divide the system into left electrode, center (scattering region) and right electrode subsystems ($\alpha = L$, C, and R respectively). Left and right electrodes are considered to be equilibrium, but with different electrical potentials φ_L and φ_R, as well as different temperatures T_L and T_R (Fig. 1).

2.1 Electron transport

We describe electron states in carbon nanotubes in the framework of the π-electron tight-binding model [13]. This approach is complementary to an ab initio one and allows to obtain

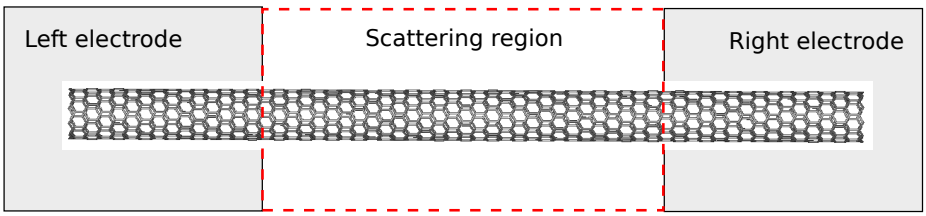

Fig. 1 Considered system: a carbon nanotube between electrodes.

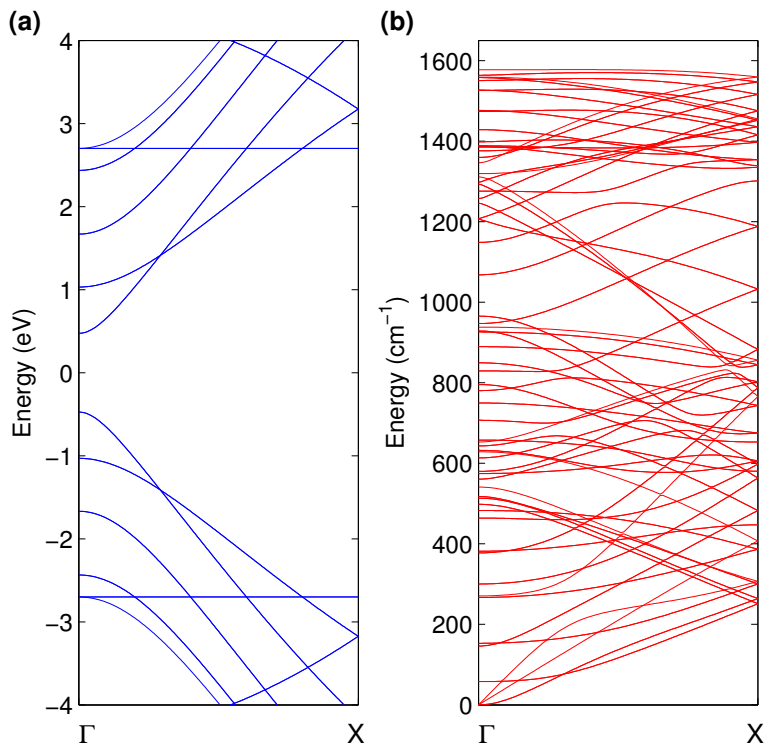

Fig. 2 Electron (a) and phonon (b) dispersions in pristine CNT(10,0).

physically transparent results. We write the first nearest neighbor single orbital tight-binding Hamiltonian of our system (for fixed spin $\sigma = \uparrow$ or $\sigma = \downarrow$, the spin index is omitted) as

$$\hat{H} = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{ij} t_{ij} c_i^\dagger c_j, \tag{1}$$

where hopping matrix elements t_{ij} between lattice sites are given by $t_{ij} = t$ for nearest neighbor sites and the on-site energies ε_i can be chosen zero for pristine structures. We take below $t = 2.7$ eV. As an example, the electron dispersion in ideal infinite CNT(10,0) is shown in Fig. 2a.

In calculating the transport properties, we follow an atomistic approach and employ nonequilibrium Green functions within the Landauer formalism, and a decimation technique [14, 15] to obtain transmission functions $\mathscr{T}_{ph}(\omega)$ and $\mathscr{T}_{el}(E)$ for phonons and electrons, respectively. We refer the reader to Refs. [16–19] for details of the Green function technique. We neglect the electron-phonon coupling in this work since it is shown that electron-phonon mean free path in nanoscale carbon tubes and ribbons is tens of μm even at room temperature [20].

The electron current is given by the Landauer formula

$$I = \frac{e}{h} \int_{-\infty}^{\infty} \mathscr{T}_{el}(E) \left[f_L(E) - f_R(E) \right] dE, \tag{2}$$

where $f_{L(R)}$ is the electron distribution function in the left (right) electrode and the transmission function $\mathscr{T}_{el}$ is defined as

$$\mathscr{T}_{el}(E) = \mathrm{Tr}\left(\hat{\Gamma}_L(E)\hat{G}_C^R(E)\hat{\Gamma}_R(E)\hat{G}_C^A(E)\right), \tag{3}$$

where the Green matrix functions in the central region $\hat{G}_C^{R(A)}$ and level-width functions $\hat{\Gamma}_{R(L)}$ are determined by the Hamiltonian of the central region $\hat{H}_C$ and the contact self-energies $\hat{\Sigma}_s$

$$\hat{G}_C^R(\varepsilon) = \left[(\varepsilon + \mathrm{i}0^+)\hat{I} - \hat{H}_C - \hat{\Sigma}_L - \hat{\Sigma}_R\right]^{-1}, \tag{4}$$

$$\hat{\Gamma}_{s=L,R} = i\left(\hat{\Sigma}_s^R - \hat{\Sigma}_s^A\right) = -2\mathrm{Im}\hat{\Sigma}_s^R. \tag{5}$$

While we use the tight-binding model, all Green functions are matrices in the atomistic basis.

2.2 Phonon transport

In the harmonic approximation the vibrational Hamiltonian can be written as

$$H_{ph} = \sum_\alpha H_\alpha + \left(u^L|\hat{K}^{LC}|u^C\right) + \left(u^R|\hat{K}^{RC}|u^C\right), \tag{6}$$

where in the first term

$$H_\alpha = \frac{1}{2}\left(\dot{u}^\alpha|\dot{u}^\alpha\right) + \frac{1}{2}\left(u^\alpha|\hat{K}^{\alpha\alpha}|u^\alpha\right) \tag{7}$$

is the Hamiltonian of the decoupled subsystem α, the second and third terms stand for the coupling between the central region and the reservoirs. Here $|u^\alpha)$ is the vector, and $(u^\alpha|$ is its transpose, of mass renormalized displacement coordinates $u_i^\alpha = \sqrt{m_i}x_i^\alpha$, x_i^α being the ith degree of freedom of subsystem α with m_i the mass associated to this degree of freedom. $K_{ij}^{\alpha\beta}$ is the matrix element representing the coupling between mass renormalized coordinate i of subsystem α with j subsystem β, and $K_{ij}^{\alpha\beta} = k_{ij}^{\alpha\beta}/\sqrt{m_i m_j}$ with $k_{ij}^{\alpha\beta}$ being the spring constant in direct coordinates. In our calculations, we use the fourth nearest neighbor force constant approximation (4NNFC), which yields phonon dispersions in agreement with density functional theory (DFT) calculations for graphene and carbon nanotubes [21–23]. For the case of GNRs, modification of force constants for the edge carbon atoms will improve the results, in the sense that it will result in a blue shift in the phonon density of states. Theoretical calculations show that hydrogenated and dehydrogenated ribbons have very similar phonon dispersions [24]. Therefore, we neglect the effects of hydrogenization in our phonon calculations. A subsequent reduction of lattice thermal conductance and a further but minor improvement to our results in reducing lattice thermal conductivity can be expected, but it is neglected for the sake of simplicity. As an example, the phonon dispersion in ideal infinite CNT(10,0) is shown in Fig. 2b.

Phonon heat transport in mesoscopic systems at low enough temperatures (lower than the Debye temperature T_D, which is about 2300 K in graphene and is of the order of 1000K in CNTs) is essentially quantum and at $T \ll T_D$ the heat flow is determined by coherent transport of noninteracting phonons. In this case the Landauer approach can be used. The thermal conductance in the limit of small temperature difference $dT = T_L - T_R$ is defined as

$$\kappa_{ph}(T) = \int_0^\infty \frac{d\omega}{2\pi}\hbar\omega\frac{\partial f_B(\omega,T)}{\partial T}\mathscr{T}_{ph}(\omega), \tag{8}$$

where $\mathscr{T}_{ph}(\omega)$ is the phonon transmission function, f_B is the Bose distribution with ω being the phonon frequency and T being the temperature [25, 26].

To actually calculate the phonon transmission function for nonideal nanotubes we use the atomistic single-particle Green function method [27–36], equivalent to the Meir-Wingreen method for electron transport [37].

$\mathscr{T}_{ph}(\omega)$ is determined by the matrix retarded phonon Green function in the central region $\hat{D}_C(\omega)$ and the phonon level-width functions $\hat{\Gamma}^{ph}_{L(R)}(\omega)$ of the left and right electrodes:

$$\mathscr{T}_{ph}(\omega) = \mathrm{Tr}\left[\hat{\Gamma}^{ph}_L(\omega)\hat{D}^{\dagger}_C(\omega)\hat{\Gamma}^{ph}_R(\omega)\hat{D}_C(\omega)\right]. \tag{9}$$

The retarded Green functions for subsystems in the absence of coupling between the central system with the electrodes are defined as

$$D^{(0)}_{\alpha}(\omega) = \left[(\omega + \mathrm{i}0^+)^2\hat{I} - \hat{K}^{\alpha\alpha}\right]^{-1} \tag{10}$$

with $\hat{I}$ being the identity matrix. The matrix inversion (10) can not be applied directly for semi-infinite electrodes and the surface Green functions are calculated numerically using the iterative method [14, 15].

The retarded phonon Green function for the central region in the presence of electrodes reads

$$\hat{D}_C(\omega) = \left[(\omega + \mathrm{i}0^+)^2\hat{I} - \hat{K}^{CC} - \hat{\Pi}_L(\omega) - \hat{\Pi}_R(\omega)\right]^{-1}, \tag{11}$$

where the polarization operator (phonon self energy) due to coupling to the reservoir α is

$$\hat{\Pi}_{\alpha}(\omega) = \hat{K}^{C\alpha}D^{(0)}_{\alpha}(\omega)\hat{K}^{\alpha C}. \tag{12}$$

Finally, the level-width function is determined by the relation

$$\hat{\Gamma}^{ph}_{\alpha}(\omega) = \mathrm{i}\left(\hat{\Pi}_{\alpha}(\omega) - \hat{\Pi}^{\dagger}_{\alpha}(\omega)\right). \tag{13}$$

3 Results for disordered nanotubes

Anderson disorder represents random small-scale fluctuations of system parameters. In this paper we consider simple local and uncorrelated disorder. For phonons we introduce Anderson type disorder by a random distribution of m_i at the C region, in the range plus/minus 10% of the original mass, which transforms to a distribution of disordered coupling matrix elements K^{CC}_{ij}. Green functions of the disordered region are obtained using decimation techniques and the transmission functions are obtained by averaging over 250 sample configurations. The results are presented in Fig. 3 and Fig. 4.

First of all we note that, unlike its electronic counterpart, phononic heat transmission takes place not only in a small energy window but phonons of all energy values contribute to the conductance. In this sense, low energy phonons play a special role in phonon thermal conduction in both pristine and disordered systems as it will be discussed below. We consider (10,0) CNT which is placed between reservoirs made of the same material [Fig. 3(a)]. The reservoirs are kept at different temperatures T and $T + dT$. We introduce Anderson type disorder in the central region and analyze the dependence of the transmission function and thermal conductance to disorder for CNTs with different lengths. The transmission function for the pristine CNT reflects the fact that each phonon branch is contributing to transport with unit probability.

Namely, the transmission function at energy ω is the number of phonon branches $N(\omega)$ crossing at this energy each acting as an independent transmission channel [Fig. 2(b)]. Increasing the length of the C-region, the transmission is reduced but the low energy transmission is almost unaffected by disorder [Fig. 3(c)]. On the other hand high energy phonons are extremely sensitive to disorder in the sense that the transmission is blocked to a great extend even for the shortest regions with disorder. We also note that disorder induced scattering is more important near van Hove singularities in the density of states. We observe that thermal conductance drops as the length of the central region is increased but this drop is significant only at high temperatures [Fig. 3(b)]. As the temperature increases the difference in conductance for different lengths increase and then saturates. The low temperature thermal conductance is insensitive to disorder because of two reasons. First, because the transmission of low energy phonons itself is insensitive to disorder. Second, the term $p(\omega,T) = \omega\,\partial f_B(\omega,T)/\partial T$ in the integrand of Eq. (8) is filtering out the contribution of

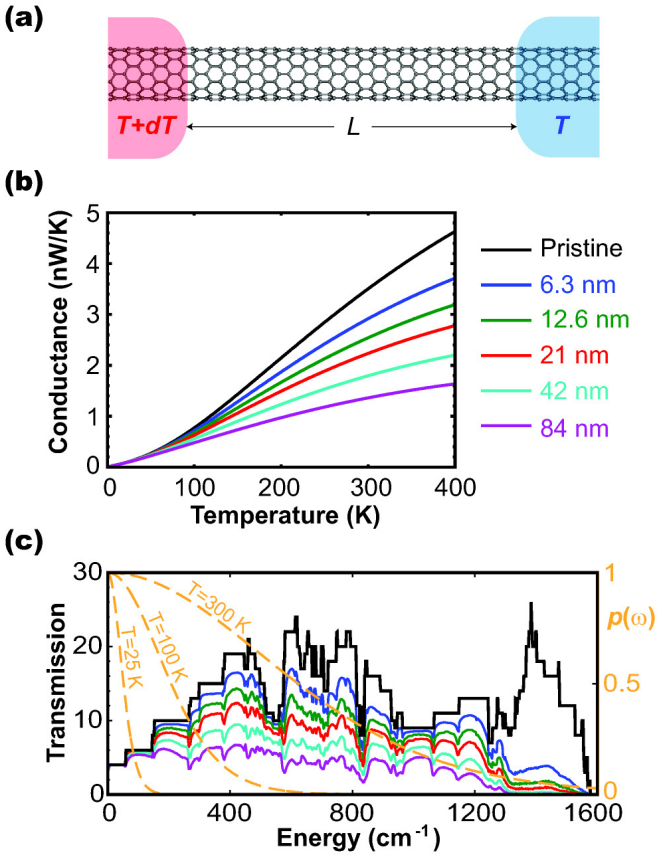

Fig. 3 (a) Schematics of the system under consideration. (10,0) CNT is placed between reservoirs which have a temperature difference dT. We include Anderson type disorder at the central region whose length L is varied. (b) Thermal conductance as a fnction of temperature T for (10,0) CNTs with diffrent lengths. (c) Transmission versus energy for CNTs with diffrent lengths L (solid curves). Black curve is the transmission function of pristine (10,0) CNT. Dashed curves are the prefactors $p(\omega,T)$ for T =25, 100, 300 K (see text). (Same color code is used in subplots (b) and (c)).

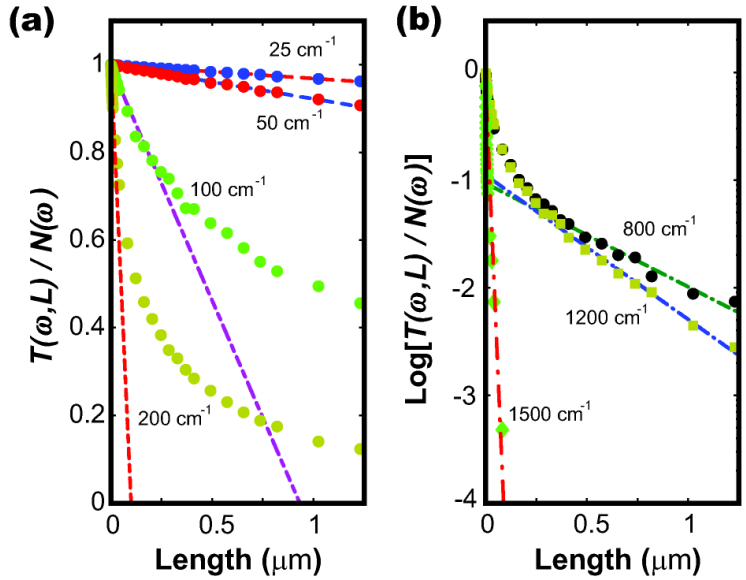

Fig. 4 Different regimes of phonon transport through (10,0) CNTs. Normalized transmission values are plotted as a function of length for various energies. At low energies (25 cm^{-1}, 50 cm^{-1}) $\mathscr{T}(\omega)/N(\omega)$ can be fit to a line (a). Intermediate energies like 100 cm^{-1} and 200 cm^{-1} deviate from the linear behavior and show $1/L$ behavior (a). High energy phonons are best described with an exponential law (b).

high energy phonons to low temperature conductance. At high temperatures $p(\omega)$ flattens and the filter effect diminishes.

In order to identify the different transport regimes, we analyze $\mathscr{T}_{ph}(\omega,L)/N(\omega)$ for a number of ω values, and as a function of L. Transmission amplitudes are normalized in this way using their pristine values $N(\omega)$ in order to enable comparison. In Fig.4(a), it is shown that low energy transmission (ω =25, 50 cm^{-1}) decreases linearly with L reflecting the fact that low energy phonons display a quasi-ballistic behavior. For higher energies (ω =100, 200 cm^{-1}) the transmission function deviates from the linear fit to short device transmission (see Fig. 4(a)) and a diffusive behavior is observed. On the other hand, energetic phonons (ω =800, 1200, 1500 cm^{-1}) experience localization at different lengths depending on their energies as it is shown in Fig. 4(b).

Different transport regimes coexist for phonons with different energies. Altough high energy phonons experience localization, a pure localization regime or an exponential dependence of thermal conductance on CNT length is not observed.

Therefore heating of the semiconductor CNT device in electronic applications is dependent on the length of the device and the frequency distribution of generated phonons. Low energy phonons will be discharged effectively while localization of energetic phonons may cause overheating of long devices. Localization induced heating becomes more dramatic at high operating temperatures.

The Anderson disorder for electron transport is introduced by random variation of the hopping matrix elements t_{ij}, which are sensitive to geometry fluctuations. We take the range of t_{ij} fluctuations to be plus/minus 10% of the average value (2.7 eV) corresponding to mass disorder. We average the curves over 50 configurations, the results are presented in Figs. 5

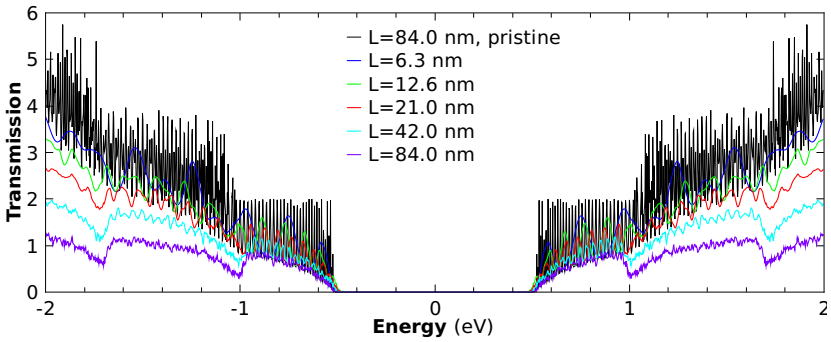

Fig. 5 (Color online) Electron transport through CNT(10,0) with Anderson disorder. Transmission as a function of energy is shown for different lengths.

and 6. As the model for electrodes we take the wide-band metal edge electrodes coupled to the edge carbon atoms of nanotubes, so that strong quantum interference oscillations of the transmission are observed in the pristine case (Fig. 5). Oppositely, transmission through disordered CNTs is more regular because of the self-averaging. The transmission as a function of length demonstrates exponential suppression at large lengths, which is a signature of localization in quasi one-dimensional system. In Fig. 6 the length dependence at three different energies is shown, it is clear that scattering increases and the localization length decreases at larger energies, when large number of electron bands is involved.

It is interesting to compare the energy dependence of disorder effect on electron and phonon transport. Phonon transport is not affected only at very low energies, so that at room temperature the thermal conductance is effectively suppressed. Electron transport at the energies within the first band of transverse quantization is not affected by moderately

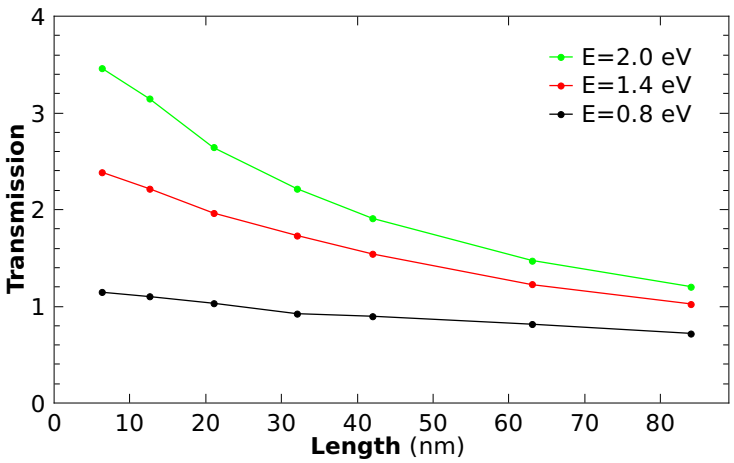

Fig. 6 (Color online) Electron transport through CNT(10,0) with Anderson disorder. Transmission as a function of length is shown for different energies.

strong disorder of the considered type. It means that the conductance of doped nanotubes (which are semiconducting with large enough gap) or finite-voltage conductance due to injection of carriers into the conduction band will not be changed essentially by disorder, while the phonon conductance can be suppressed.

4 Conclusions

In summary, we analyzed the effects of disorder on phonon thermal transport and electron charge transport in semiconductor CNTs. We show that different transport regimes for phonons of different energies coexist and their relative weight on thermal conductance depends on temperature. Long wavelength phonons are transmitted effectively, but short wavelength phonons are likely cause overheating and the effect of localization will be more pronounced at higher operating temperatures. On the other hand, electron transport is much less sensitive to disorder. One can conclude that disorder can be an effective mechanism of engineering the thermoelectric properties of carbon nanostructures, as was shown by two of us in Ref. [38] for graphene nanoribbons.

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