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Thermal Radiation from Metallic Single Walled Carbon Nanotubes of Different Shapes

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ABSTRACT We have considered two terminal devices for the study of electroluminescence from the conducting channels of metallic single walled carbon nanotubes of different size and shapes under the influence of the single vacancy defect and the single walled defect. The metallic carbon nanotubes which were considered for the study the restriction of gapless armchair nanotubes were used. We have considered electron transport in the ballistic regime without electron-phonon interaction. It was found suitable when the length of the conducting channel was smaller than the electron mean free path of metallic single walled carbon nanotube. By turning off the applied bias in the device, we have studied the thermal radiation from perfect and defected carbon nanotubes. We have studied electroluminescence and thermal radiation from metallic armchair single walled carbon nanotubes having defects in the ballistic transport regime based on tight binding method. It was found that single vacancy defect and Stone-Wales defect have enhanced the electroluminescence which increased exponentially in the low bias range, while for the perfect nanotube only thermal radiation contributed and the electroluminescence was neglected. The strong radiation due to transition between high energy bands became dominant. Due to confinement of thermal excitation in the transverse direction, the intensity of the thermal radiation was independent of the nanotube diameter. We have studied the thermal radiation of perfect and carbon nanotubes with different defects. The obtained results were found in good agreement with previously obtained results.

KEYWORDS Electroluminescence, Conducting Channel, Metallic Carbon Nanotubes, Armchair, Vacancy Defect, Gapless, Thermal Radiation, Tight Binding Method, Transition, Thermal Excitation.

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INTRODUCTION

Misewich et al. [1] studied the electroluminescence and photo luminescence from the single walled carbon nanotubes. Chen et al. [2], Lefebvre et al. [3] and Avouris et al. [4] studied the electrical properties of semiconducting carbon nanotubes experimentally. Sveningsson et al. [5], Li et al. [6] and Wei et al. [7] presented that emission spectrum was found different from black body like emissions in nanotube bundles and multiwalled carbon nanotubes. Xie et al. [8] and Essing et al. [9] studied that a side peak close to the main transition peak due to phonon assisted emission appeared in the radiation spectrum. Shtogun et al. [10], Partovi-Azar et al. [11] and Wu et al. [12] studied that carbon nanotubes have significant influences on very properties of carbon nanotubes as electric and magnetic properties, transport properties [13-16], field emission [17], mechanical and optical properties [18-22]. Brozena et al. [23] studied the defects engineering for tuning the optic properties of carbon nanotubes. Piao et al. [24], He et al. [25] and Ishii et al. [26] presented the case of enhancement of photoluminescence and tuning of the single photon emission by sp^3 defects. Katano et al. [27] studied experimentally that a local defect was induced by injecting tunneling electrons from a scanning tunneling microscope tip to a multiwalled carbon nanotube and corresponding changes of electroluminescence due to the defect were seen. We have considered a two terminal device for the study of electroluminescence from the conducting channels of metallic single walled carbon nanotubes under the influence of the single vacancy defect and single Stone-Wales defect. The radiation from device was calculated using non equilibrium Green function method by Zhang and Wang [28].

METHOD

The study of bias induced light emission and thermal radiation was studied considering nonequilibrium Green's function method based on tight binding model. The Hamiltonian of the electrons in the carbon nanotube using the nearest neighbour tight binding model as

$$H_0 = -\sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j$$

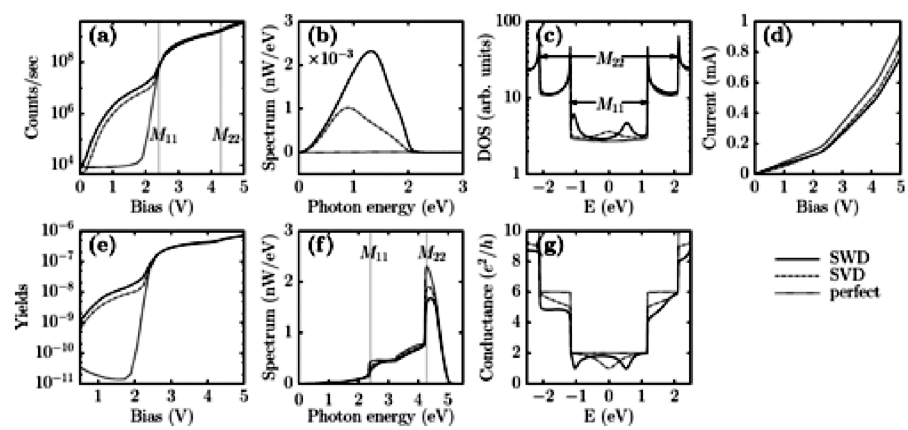
Where t_{ij} is the hopping parameter, $c_i^\dagger\left(c_j\right)$ is the electron creation or annihilation operator on site i or site j, the angular bracket $\langle i, j \rangle$ is the nearest neighbour sites. The coupling of the electrons with the electromagnetic field in free space by using the Peirls substitution via $t_{ij} \to t_{ij} e^{i\theta_{ij}}$ with phase factor $\theta_{ij} = \frac{e}{\hbar}\int_{r_j}^{r_i} A.dl$ was used. Here $e = -|e|$ is the electron charge, $\hbar$ is the reduced plank constant, A is the vector potential for describing the free space electromagnetic field. The coupling of the electrons with the electromagnetic field in the lowest order approximation was obtained by expanding θ_{ij} in terms of A to the linear term is represented as

$$H_{\text{int}} = \sum_{\langle ij \rangle}\sum_{k}\sum_{\mu=x,y,z} M_{ij}^{k\mu} c_i^\dagger c_j A_\mu\left(r_k\right)$$

Where the electron-phonon coupling matrix is $M_{ij}^{k\mu} = i\frac{e}{2\hbar} t_{ij}\left(r_i - r_j\right)\mu\left(\delta_{ki} + \delta_{kj}\right)$. The electroluminescence from a single walled carbon nanotube was considered by two terminal device having bias voltage. The device contained left and right leads having semi-infinite extensions of the pristine carbon nanotube. The central part was the conducting channel which had a finite length. We have taken into the consideration interaction of electrons with the electroluminescence field only in the central region. When a bias voltage was applied an electric current was produced through the channel and photons were excited and emitted due to the inelastic scattering of electrons interacting with the electromagnetic field. The single vacancy defect was modeled by using a large onsite energy of 10^6 ev for the vacant atom and the Stone-Wales defect was created due to rotating carbon-carbon bond by 90 degrees. We have considered the nearest neighbour hopping parameter $t_{ij} = t$ as a constant. The Radiation was calculated using the nonequilibrium Green's function method. The important quantity was the current-current correlation function using the monopole approximation and neglecting the screening effect on current fluctuations, the radiation power and rate of the photon counts i.e. number of photons emitted per unit time in the far field was made. The geometry of a single walled carbon nanotube was taken through the tube chiral vector and determined by a pair of integers (n, m). The band structure of the metallic single walled carbon nanotube showed linear dispersion relation in the low energy range around the Fermi level. The optical transitions became forbidden in low energy range due to an external electric field along the tube axis. The obtained results were compared with previously obtained results.

RESULTS AND DISCUSSION

We have studied the thermal radiation using nonequilibrium Green's function in the case of conducting channels of metallic armchair carbon nanotubes with defects considering tight binding model. Graph (1) shows the plots of the two terminal device of the carbon nanotube with chiral index (7,7). This shows the results for each plot for the cases that the carbon nanotube channel contained a single walled defect, a single vacancy defect and no defect.



Graph 1: Plots for the two-terminal device of the carbon nanotube with chiral index (7, 7).

Graph (1) (a) shows a perfect carbon nanotube with increasing of bias voltage, the photon counts were very small and little changed in the low bias range until the onset of bias at about 2.4 v, which was implied the opening of M_{11} transition between the two Van Hove singularities presented by the density of states as shown in Graph (1)(c). It was found that thermal radiation was small and was dominant for the perfect carbon nanotube. Graph (1) (b) and (1) (f) show the spectrum of the radiation power. Graph (1) (b) shows that the average energy of the emitted photons from the carbon nanotube with single walled defect was larger than that from the carbon nanotube with single vacancy defect. The radiation spectra for the perfect carbon nanotube and the defect effected carbon nanotubes due to large bias showed little difference in Graph (1)(f), where the influence of the defects on the radiation was not obvious due to the strong transitions from high energy bands. Graph (1)(d) shows that electric current decreased more significantly for single vacancy defect than that of single walled defect in low bias range. Graph (1) (g) shows the localized states due to the defect in the low range which reduced the conductance by one quantum unit. Graph (1)(e) shows the enhancement of counts and decreasing the current due to defects. Graph

(2) shows the influence of the diameter of the carbon nanotube for the electroluminescence.
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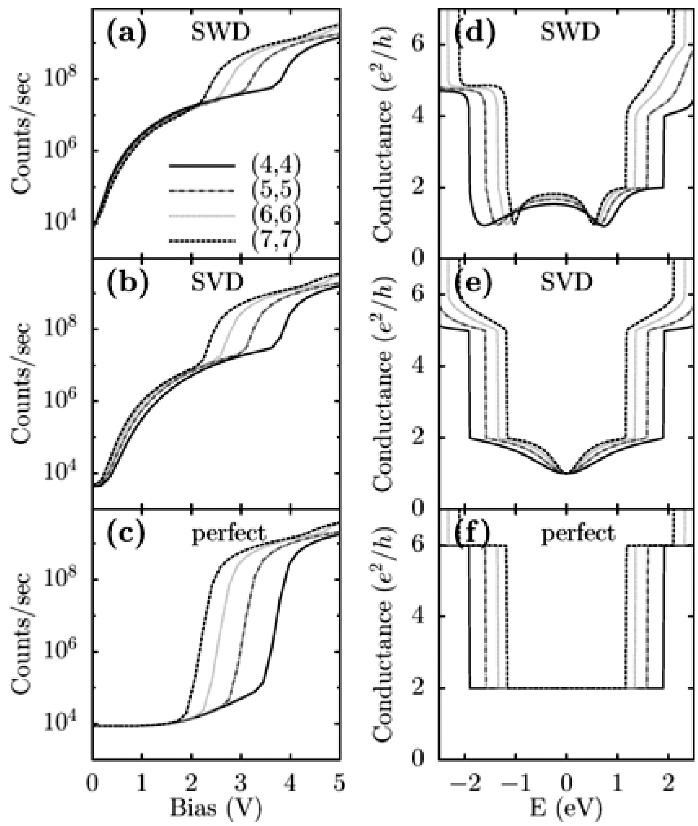
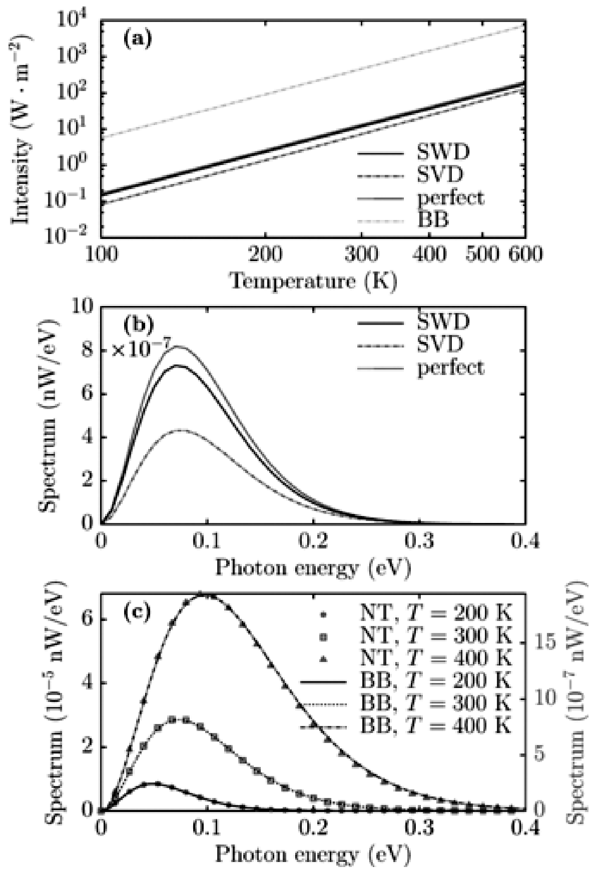


Graph 2: Plot of photon counts per second and conductance for the two-terminal device using carbon nanotubes with different diameter.

We have considered four different armchair carbon nanotubes with the chiral index (n,n) ranging from $n=4$ to $n=7$ and their diameters were $d = 5.42\text{Å}$, 6.78Å, 8.14Å and 9.49Å. Graph (2)(a), (2)(b) and (2)(c) show distinct features for the electroluminescences from the carbon nanotubes with different diameters through the overall trends. The counts from carbon nanotubes with different diameters created bubbles in the high bias range with defects. The plot of Graph (3) shows the thermal radiation from the carbon nanotube channel of the two terminal devices by tuning off the bias voltage.



Graph 3: Plot of thermal radiation from the conducting channel of the two-terminal device using (7,7) carbon nanotube under zero bias.

Graph (3) (a) also shows that the radiation power of the perfect carbon nanotube and the affected defects carbon nanotubes versus the temperature followed by scaling law as the black body radiation. Graph (3) (b) shows the spectrum of the thermal radiation. Graph (3 (c) shows the plot of perfect carbon nanotube case. This also shows the fitting of spectra of black body radiation with perfect carbon nanotube. The obtained results were compared with previously found results and were in good agreement.

CONCLUSION

We have studied thermal radiation from metallic single walled carbon nanotubes of different shapes. The study of thermal radiation from conducting channels of metallic armchair carbon nanotubes with defects using nonequilibrium Green's function method was made based on tight binding model. The effect of the diameters of carbon nanotubes with defects on the radiation was made. The radiations from metallic carbon nanotubes in thermal equilibrium presented black body like spectrum. It was found that for perfect nanotubes having small diameter their thermal radiation were independent of tube diameter because of confinement of the thermal excitations in the tube circular direction. It was also found that the single vacancy defect and Stone-Wales defect enhanced the electroluminescence and was increased exponentially in the low bias range. For the perfect nanotube only thermal radiation contributed. The obtained results were compared with previously obtained results of theoretical and experimental works and were found in good agreement.

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