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Short Communication

Impact of Inter-Wall Distance on Physical Properties of Metal-Semiconducting Double Walled Carbon Nanotube Quantum Dot

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Here we report the effect of inter-wall distance of CNT on transmission probabilities of electrons and holes as well as their binding energies. The binding energies were calculated using the variational method within the effective mass approximation and confinement potential. The barrier transmission probabilities of electrons and holes were also calculated using varying potential barrier height and quantum mechanical tunnelling. The binding energy is found to be decreasing with inter-wall distance. We find the presence of outer wall causes a decrease in the transmission probability. For a given core radius, the transmission probability of hole increases linearly with increasing hole energy. CNT QDs of inter-wall distance 3 nm resembles to type II core-shell quantum dot (CSQD). The observed results were compared with the previous investigations. The inter-wall distance causes a decrease in the transmission probability.

Keywords: Quantum dot, Binding energy, Variational method.

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1. INTRODUCTION

Quantum dots are the best example of rare nanotechnology; changes in the size, shape, or topology of the nanostructure determine its unique properties [1]. The electronic structure of a CNT is dictated by its diameter, length, and chiral angle [2]. The tuneability of the properties of these low dimensional structures has led to a wide range of applications. Due to the quantization of energy along tube axis, nanotubes are usually considered as one dimensional structure. In actual experiment we measure nanotubes of finite length. Quantum effects arise due to short tube lengths. Under this condition nanotubes behave as quantum dots. When two metallic electrodes are deposited on top of a CNT, a potential barrier is developed naturally at the nanotube-metal interface. When potential barrier is extremely thin a conduction mechanism called quantum mechanical tunnelling of carriers is predominant in metal semiconductor junctions [3]. The coupling between the nanotube and the metal depends on the contact material, Nanotube diameter and metallic/semiconducting character of the nanotube. Certain materials, such as Ti or Au, make (generally) good contact to nanotubes. It has recently been shown that Pd and Rh are very good materials to contact NTs [4, 5]. The strength of the Nanotube-metal tunnel barriers determines the degree of confinement of electrons in the Nanotube QD. So in our theoretical model, we consider metal-semiconducting double walled carbon nanotube quantum dot. By varying the inter-tube distance, the carrier transmission probability can be tuned. In small carbon nanotube QDs, the confinement increases over the Columbic interaction due to which electrons/holes starts tunnelling through the nanotube-metal interface.

In the present work the transmisssion probabilities have been theoretically calculated for metal-semiconducting double walled carbon nanotube quantum dot using varying potential barrier, which depends on the inter-tube distance on the transmission probabilities. The inclusion of tunnelling property should be incorporated to include the effect of inter-tube distance on the transmission probabilities and energy level structures of the carbon nanotube quantum dot. Our results have significant role in nano devices using metal-interface nanotube quantum dots. Metal interface CNT quantum device can be designed to produce ballistic transport

The geometry of metal-semiconducting double walled carbon nanotube quantum dot is depicted in Fig. 1. Here a is the radius of the inner tube and b is the radius of the CNT as a whole and inter-wall distance is calculated as $d = (b - a)$.

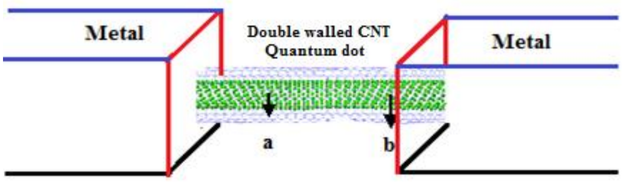

Fig. 1 – 3D geometrical view of metal-semiconducting double walled carbon nanotube quantum dot

2. RESULTS AND DISCUSSION

2.1 Theoretical Formulations

In order to calculate the transmission probabilities in metal-semiconducting double walled carbon nano-

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tube quantum dot, we use a potential function $V(r)$ with $V_0(e,h)$ as the potential barrier height 0.40 eV for hole and 0.30 eV for electron [6]. We divide the potential barrier into thin square barriers each of width dr, the transmission probability through a given barrier of width dr can be written as:

$$dT_p = e^{-2\sqrt{\frac{2m^*_{e,h}}{\hbar^2}\left[V(r)-E_{e,h}\right]}d\tau} \quad (1)$$

Therefore transmission probability (T_P) of charge carriers (electrons/holes) to the all thin square barriers can be calculated as:

$$T_P = e^{-8\pi\int_a^b \sqrt{\frac{2m^*_{e,h}}{\hbar^2}\left[V(r)-E_{e,h}\right)]}r^2 dr} \quad (2)$$

The potential function $V(r)$ for electron/hole is given by [7]:

$$V(r) = \frac{V_0(e,h)}{a^2}(r^2 - a^2) \text{ for } |r| \le a \quad (3)$$

Here a is the radius of the inner tube, $V_0(e,h)$ is the potential barrier height of electron/hole semiconducting double walled carbon nanotube [8]. The variation of confinement potential with inter-tube distance for electron/hole is depicted in Fig. 2.

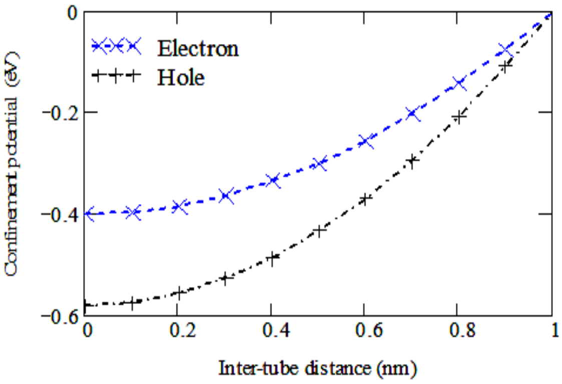

Fig. 2 – Variation of confinement potential as a function of inter-tube distance

Electron transmission probability as a function of inter wall distance is shown in Fig. 3. We have plotted the analysis for inter wall distance of 1.25 nm and 2.25 nm for semiconducting double walled carbon nanotube quantum dot, the inter wall distance is varied from 1 to 5 nm. It is interesting to note that the presence of outer wall causes a decrease in the transmission probability [9]. For two different values of the core radius of CNT, we find that transmission probability decreases sharply with increasing inter wall distance and is more cardinal to CNT quantum dots of smaller core radius (1.25 nm). So, small size semiconducting double walled carbon nanotube quantum dot provide greater possibility that carrier particles can tunnel through metal-semiconducting junction.

It can be depicted from the figure 4 that hole transmission probability decreases gradually as the

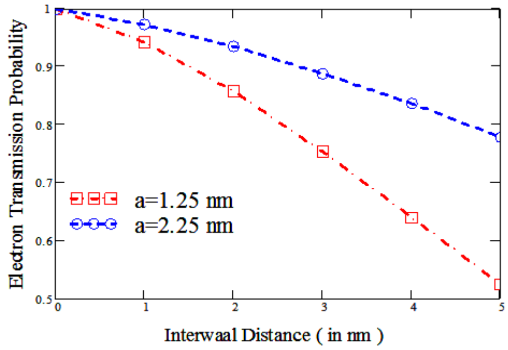

Fig. 3 – Variation of electron transmission probability as a function shell thickness in double wall CNT dot

inter wall distance increases. For inter wall distance of 3 nm and core radius of CNT of 2.25 nm, the hole may remain in the core region and the electron may tunnel to the metal-semiconducting junction. Therefore CNT QDs of inter wall distance 3 nm resembles to type II core shell quantum dot (CSQD) in which hole is confined in the core region and the electron may tunnel to shell region [5].

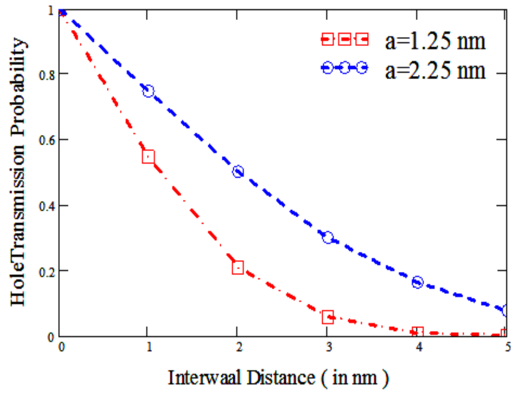

Fig. 4 – Variation of hole transmission probability as a function interwall distance

Fig. 5 and Fig. 6 shows variation of transmission probability as a function of electron and hole energy. For an electron, the transmission coefficient has been obtained for core radius 1.65 nm and 2.15 nm with inter wall distance of 0.5 nm. It has been observed from the graph that transmission probability of electron increases non linearly with increase in electron energy [9].The hole transmission

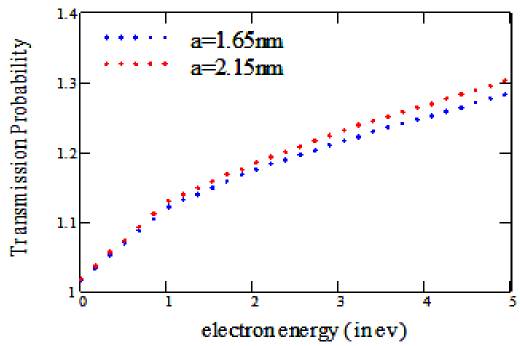

Fig. 5 – Shows variation of transmission probability as a function electron energy

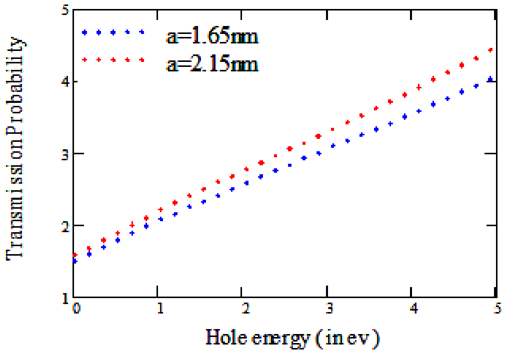

Fig. 6 – Shows variation of transmission probability as a function hole energy

coefficient is calculated for the same two core radius and same inter wall distance for comparison. For a given core radius, the transmission probability of hole increases linearly with increasing hole energy [9].

CONCLUSION

In summary, the calculated results have important implications in the fabrication of electronic devices using such types of interconnects, In the proposed model, we introduce, a double walled CNT channel for produce ballistic transport and the observed results were analytically derive using variation method with respect to inter wall distances

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