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Short Communication

I-V Characteristics of a Molecular Wire of Polyaniline (Emeraldine Base)

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Abstract:

In this study, Polyaniline molecule (emeraldine base) is modeled as a molecular wire and the effects of the metal/molecule coupling strength and the molecule length on the current-voltage (I-V) characteristics are numerically investigated. Using a tight-binding Hamiltonian model, the methods based on Non-equilibrium Green's function theory, Landauer formalism and Newns-Anderson model, our calculations indicate that the I-V curve has the step-like form and the current is very sensitive to the metal/molecule coupling strength. A negative differential resistance region is also exhibited after second voltage step in the I-V curves and the line slope at that region is studied as a function of two parameters, which are the metal/molecule coupling strength and the molecule length.

Keywords: *Molecular wire, Polyaniline (emeraldine base), Landauer formalism, I-V characteristics*

1. INTRODUCTION

Using of individual molecules as active components in nanodevices is a thriving area of research in molecular electronics in recent years. This is due to obtained various functionality and molecular devices such as diodes, negative differential resistance (NDR), field effect transistor and switches [1-6]. Nanodevices have been designed in such a way that a molecule is sandwiched between two electrodes (metallic or organic) [7,8]. Various methods such as template synthesis [9,10], template-free method [11 -13] and electrospining [14] have been widely used for the synthesis of polymer nanostructures.

Conjugated polymers are also a new class of materials which are of great potential for fabrication of molecular wires. They can be used to produce electronic devices such as Schottky diodes, field effect transistors, light-emitting diodes and nanosensors [15,16].

Among the various conducting polymers, polyaniline has seemed to be studied most and is an attractive and interesting conducting polymer for polymer-based devices because of its simple preparation technique, good environmental stability, its moderately high conductivity, excellent electrochemical properties, high redox reversibility and low cost [17-19]. The emeraldine base form of polyaniline (see Figure 1) is a semiconductor.

In this paper, following the above-mentioned interests and towards the modeling of a molecular wire, we use a model in which a polyaniline molecule in emeraldine base form (PAN) is connected to two metal electrodes. We numerically investigate the I-V characteristics of PAN in the Metal/PAN/Metal structure, where the nanocontacts

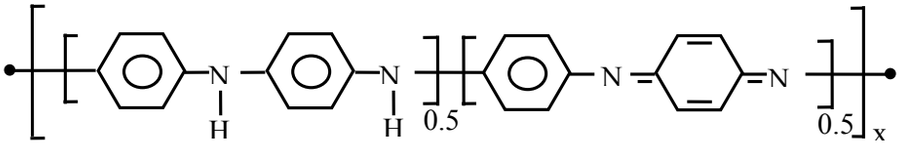

Figure 1: *A polyaniline molecule (in emeraldine base). x is a polymerization degree.*

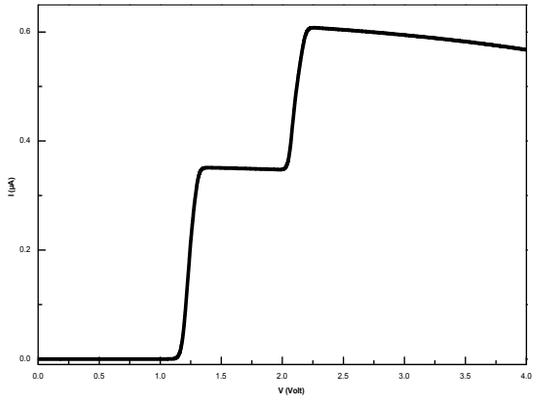

Figure 2: *The I-V characteristics of the Metal/ PAN/Metal structure.* t_c*=0.3eV, n=24.*

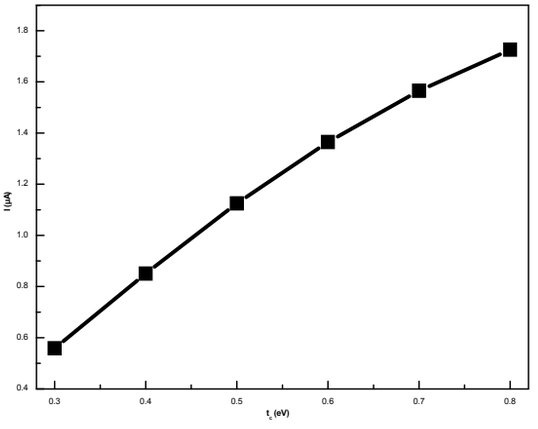

Figure 3: *The current vs. the metal/molecule coupling strength at V=1.3 Volt for n=24.*

are considered to be the Newns-Anderson model [20]. Using a tight-binding Hamiltonian model, the methods based on Green's function theory and the *Landauer* formalism, the effects of the metal/ molecule coupling strength and the PAN length in the I-V characteristics of the molecular wire are numerically investigated.

The model and description of the methods for investigation is introduced in section 2. The results and discussion are presented in section 3 followed by a conclusion in section 4.

2. METHODOLOGY

It could be shown that the Landauer transmission at certain energy can be expressed in the Green's function formalism by the following expression [20].

$$T(E)=Tr\ [\Delta_L(E)G^+(E)\Delta_R(E)G(E)]. \qquad (1)$$

The coupling matrices $\Delta_L(E)=\Delta_R(E)=\Delta(E)$ are minus the imaginary part of self-energy of the electrodes. E and $G(E)$ are the electron energy and the modified Green's function of the extended molecule, respectively. $G(E)$ is given as:

$$G(E)=(EI-H-\Sigma_L(E)-\Sigma_R(E))^{-1} \qquad (2)$$

Here, I, H and $\Sigma_L(E)=\Sigma_R(E)=\Sigma(E)$ are the unit matrix, the molecule's Hamiltonian and the self-energy of the electrodes, respectively.

The self-energy could be calculated via the Newns-Anderson model that its imaginary part is as follows:

$$\Delta_{L/R}(E)=\begin{cases}(t_c^2/\gamma)\sqrt{1-(E/2\gamma)^2} & |E/2\gamma|<1\\ 0, & \text{otherwise}\end{cases} \qquad (3)$$

t_c and 4γ =6eV are the metal/molecule coupling strength and electrode band width, respectively. The current, $I(V)$, is given as:

$$I(V)=(2e/h)\int_{-\infty}^{+\infty}dE\,T(E)[f_L(E)-f_R(E)] \qquad (4)$$

where the Fermi-Dirac distribution function, $f_{L/R}(E)$, is given in ref. [20].

$$H = \sum_i \varepsilon_i c_i^+ c_i + \sum_i t_{i+1,i} (c_{i+1}^+ c_i + c_i^+ c_{i+1}) \qquad (5)$$

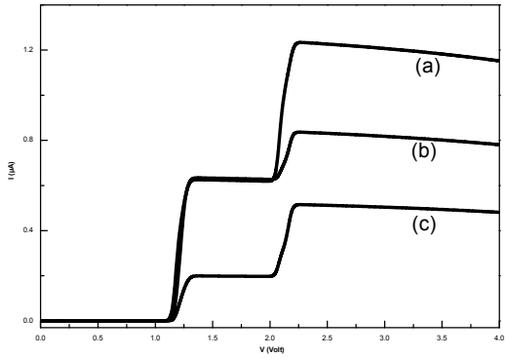

Figure 4: *The I-V characteristics for the different lengths of the PAN, t_c=0.3eV.(a) n=27 (b) n=60, (c) n=48.*

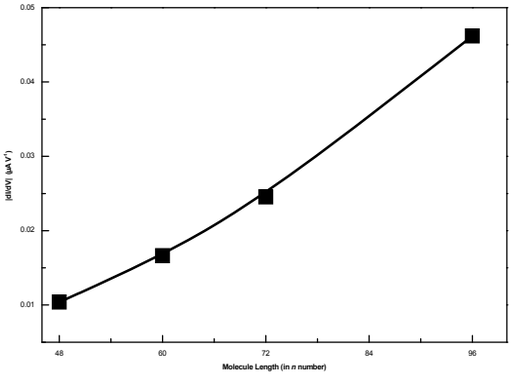

Figure 5: *|dI/dV| vs. the PAN length after second voltage step in the I-V characteristics t_c=0.3eV.*

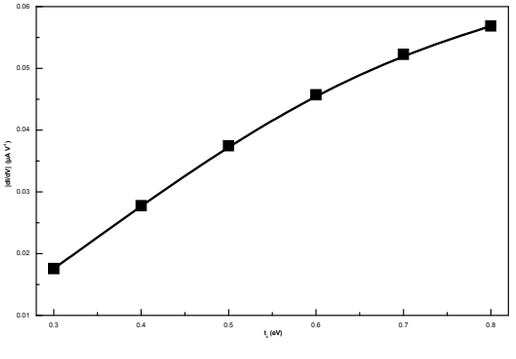

Figure 6. *|dI/dV| vs. t_c for n=24.*

The PAN is modeled within the tight-binding Hamiltonian with only one π-orbital per atom based on orthogonal basis sets as ref. [21]. The Fermi level, E_F, is chosen to be zero in this case. where c_i (c_i^+) is the annihilation (creation) operator of an electron at site i. ε_i and $t_{i+1,i}$ represent the on-site energy and the nearest-neighbor hopping integral, respectively. The wire takes in n polyaniline loop.

3. RESULTS AND DISCUSSION

Based on the formalism described in the previous section, we have investigated the I-V characteristics of the Metal/PAN/Metal structure as a molecular wire at *T=77 °K*. The tight-binding parameters are mentioned in ref. [22].

Figure 2 illustrates the I-V characteristics of the model molecular wire which is as a step-like form. The on-voltage is at $v \approx 1.3\,\text{Volt}$. There is also a negative differential resistance region after second voltage step in the I-V curve. Moreover, the effect of two parameters, t_c and the PAN length, on the I-V characteristics of the model wire is studied. According to Figure 3, any increasing in t_c considerably gives rise to the enhancing of the on-voltage's current. Figure 4 illustrates the I-V characteristics of the model system for the different lengths of the PAN. As it is shown in Figure 5, when the PAN length increases the line slope (proportional to the reverse resistance) in the negative differential resistance region of the I-V characteristics, largely increases.

The |dI/dV| value in that region is also very sensitive to the metal/molecule coupling strength, t_c (as shown in Figure 6). Our results suggest that this device could be used as an Esaki diode [23]. The Esaki diode shows a great promise as an oscillator and high-frequency threshold (tigger) device. It would operate at frequencies for greater than the tetrode would, well into the microwave bands.

4. CONCLUSIONS

To summarize, we numerically investigate the I-V

characteristics of the model Metal/PAN/Metal molecular wire. We have carried out some well-known approaches and methods based on Green's function theory, the Landauer formalism and the Newns-Anderson model for the metal electrodes as well as tight-binding Hamiltonian model to study the I-V characteristics of the wire.

The I-V characteristics exhibit switching behavior and are similar to characteristics of an Esaki diode. The current is very sensitive to the metal/molecule coupling strength. A negative differential resistance region is also indicated after second voltage step in the I-V characteristics and the line slope at that region is studied under the change of two parameters, the metal/molecule coupling strength and the molecule length.

Our results could be used to model some nanoelectronics elements and possible manufacturing technologies of considered structures.

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