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Bandgap Manipulation of Armchair Graphene nanoribbon (AGNR)

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Abstract: Bandgap Manipulation is very important for various applications. Optical Devices need smaller Bandgap where as Diode's need larger Bandgap. Armchair graphene Nanoribbon has a special property where if the numbers of atoms along the width is multiple of three or multiple of three plus one, they are semi metallic where as if the number of atoms is multiple of three plus two, it is Metallic that is band gap is zero. Here, it is shown that adding antidote can affect the Bandgap and Transport properties of material. I have used 11-AGNR and 9-AGNR to show that by adding antidotes the Bandgap can be increased or decreased to convert it from metallic to semi metallic. By doing this a significant change has been observed in the Current-Voltage characteristics of the devices where a negative resistance region is obtained which can be exploited in many applications. To simulate the structure, Tight-binding model and Non equilibrium Green's function method is used. The simulation was performed on MATLAB.

Keywords – AGNR, Armchair, Graphene, NEGF.

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1. INTRODUCTION

Graphene is a 2-Dimensional material which has very high electrical conductivity [7]. Graphene has the potential to be implemented in high frequency circuits, Integrated circuits and other electronic devices [8], [11]. Depending on the shape at the edges, GNR is classified into two types, Armchair GNR and Zigzag GNR. Studies in the past have shown that ZGNR are always metallic and AGNR can be metallic or semi-metallic [9], [10]. It is shown that electronic properties of ZGNR can be tuned by patterning the Vacancies [12]. Studies in the past have shown that the if the number of atoms along the width is multiple of three or three plus one the bandgap is semi-metallic and the bandgap is metallic if the number of atoms is multiple of three plus two [5], [13]. In [5], it is shown that the bandgap size can be controlled by adding antidotes and tuning the device dimensions. I have used the tight binding model as explained in [5] to simulate the band gap properties and understand the effect of introducing antidotes of various topologies on the bandgap. Studies done by [1] and [14], shows that introducing antidotes can raise the energy levels in the channel and it will lead to formation of a quantum well structure. This energy profile is used in a Tunneling field effect transistor where the electron tunnels by virtue of quantum mechanical tunneling [6]. I have used NEFG method as described in [1], [2], [3] to obtain the transmission parameter and hence the current transport properties. The objective here was to study the effect of introducing antidotes on negative differential resistance.

2. MODEL AND METHOD

a. Transport Properties:

To simulate the transport properties Non-equilibrium Green's function was used as discussed in [1], [2], [3]. The Hamiltonian matrix is used to describe the energy properties of the channel. The rows and columns of Hamiltonian consists of atoms in the channel, the diagonal elements of the Hamiltonian, tells us the on-site potential. As the input voltage changes the potential distribution in channel changes. The other positions represent the interaction potential between those atoms. As discussed in [1] the Hamiltonian is given by the following equation

$$H = \sum_i \varepsilon_i c_i^* c_i + \gamma_0 \sum_{i,j} (c_i^* c_j + H.c)$$

where ε_i is the on-site potential and γ_0 is the neighborhood interaction hopping parameter between neighboring atoms.

The equations used for simulation of Transport properties are as follows [1],[3].

$$\text{The current equation is } I = \int_{-\infty}^{\infty} \frac{e}{h} T(E) (f_L - f_R) dE$$

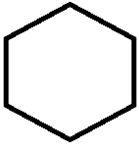
Where $f = 1/(1 + e^{(E-EF)/kT})$ is the fermi function and $T(E) = \text{trans}(\Gamma_L G(E) \Gamma_R G^*(E))$, Γ is broadening function which is the anti Hermitian part of self energies and $G(E)$ is the Green's function. More information can be found in [1] and [3].

b. E-k diagram:

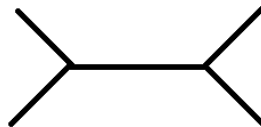
To simulate the E-k diagram tight binding model is used as discussed in [4] and [5]. The Hamiltonian matrix using this model is $H(k) = H_0 + H_1 e^{ika} + H_2 e^{-ika}$ where, H_0 is the Hamiltonian of a Unit in channel and H_1, H_2 are the Hamiltonian. Finding the eigen values for that specific wave vector in Brillouin Zone will give us the energy levels with respect to the wave vector.

Here, antidotes with various topologies are added as follows [5], the vertices are the atom sites:

1. First Topology



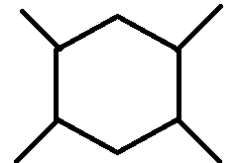
3. Third Topology



2. Second Topology



4. Fourth Topology



The lattice constant is 1.42 Angstrom and the Hopping parameters are taken from [1] and [5].

3. RESULTS AND DISCUSSION

a. Results from Tight Binding model.

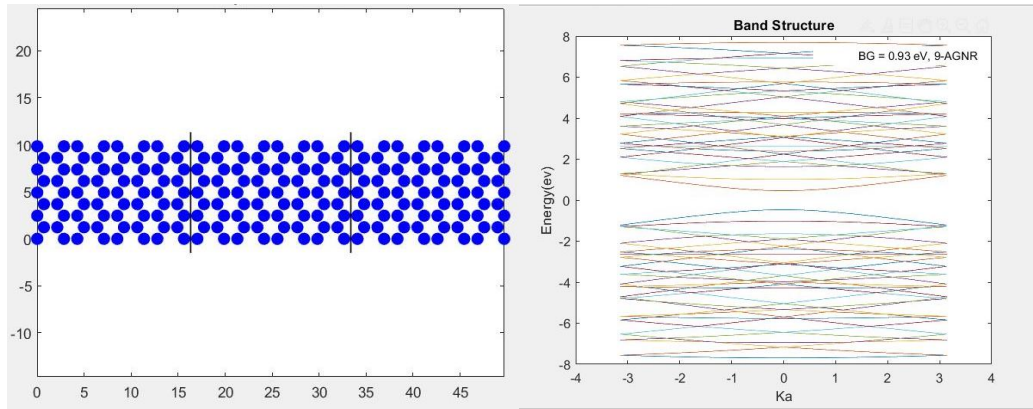


Figure 1- Visualization of 9-AGNR without antidotes and its band diagram

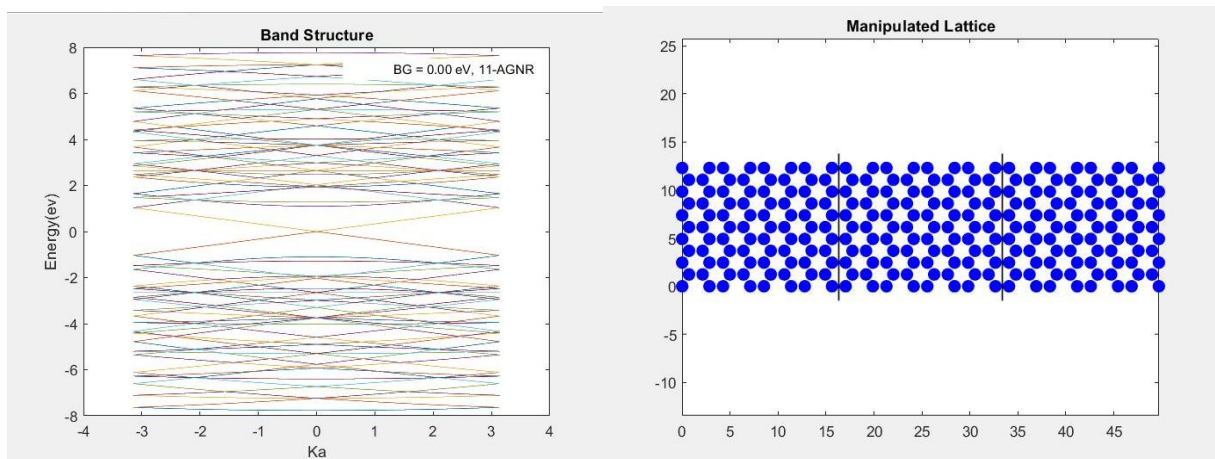


Figure 2- visualization of 11-AGNR without antidotes and its band diagram

Figure 1 and 2 represents the tight binding simulation results for the bandgap in 9-AGNR and 11-AGNR without antidote vacancy. 11-AGNR has a metallic bandgap whereas 9-AGNR has a semi-metallic bandgap. Introduction of antidote vacancy at different positions with different topologies affects the Hamiltonian of the channel. Therefore, the energy levels in the channel change thus affecting the bandgap. Figure 3 to 7 are the tight binding simulations for 9-AGNR and 11-AGNR with antidote vacancy of different topologies.

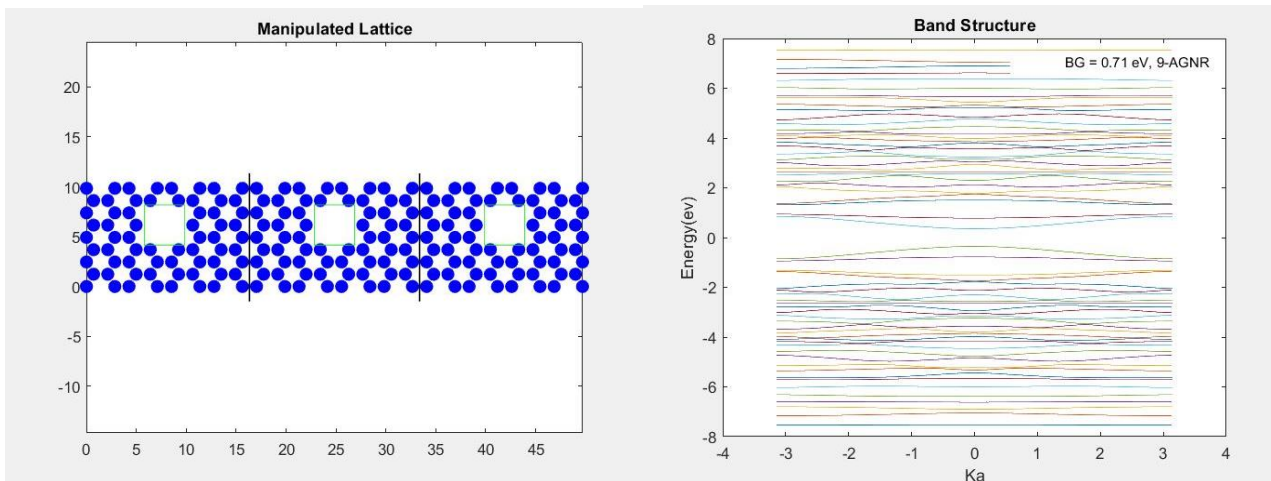


Figure 3- 9-AGNR with the first topology and its band diagram

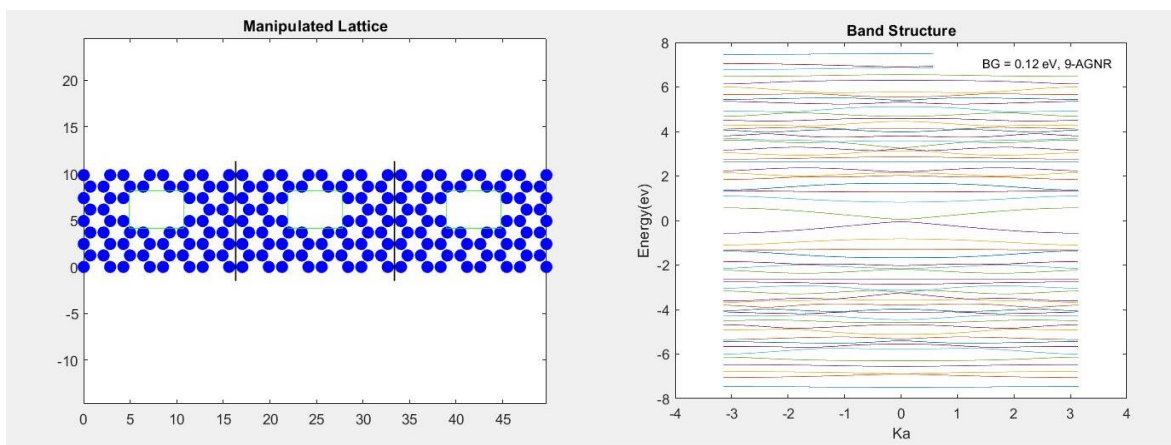


Figure 4- 9-AGNR with the Second topology and its band diagram

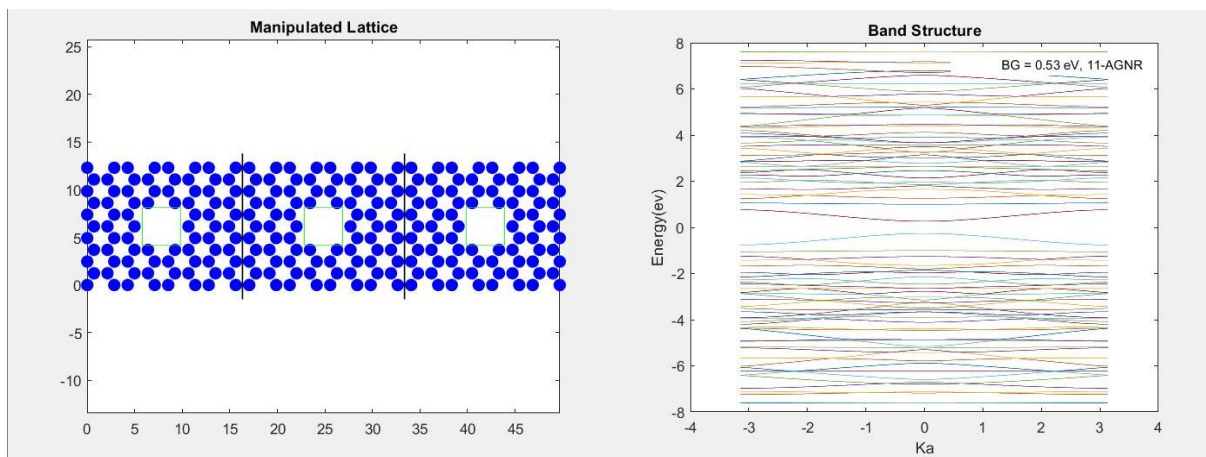


Figure 5- 11-AGNR with the first topology and its band diagram

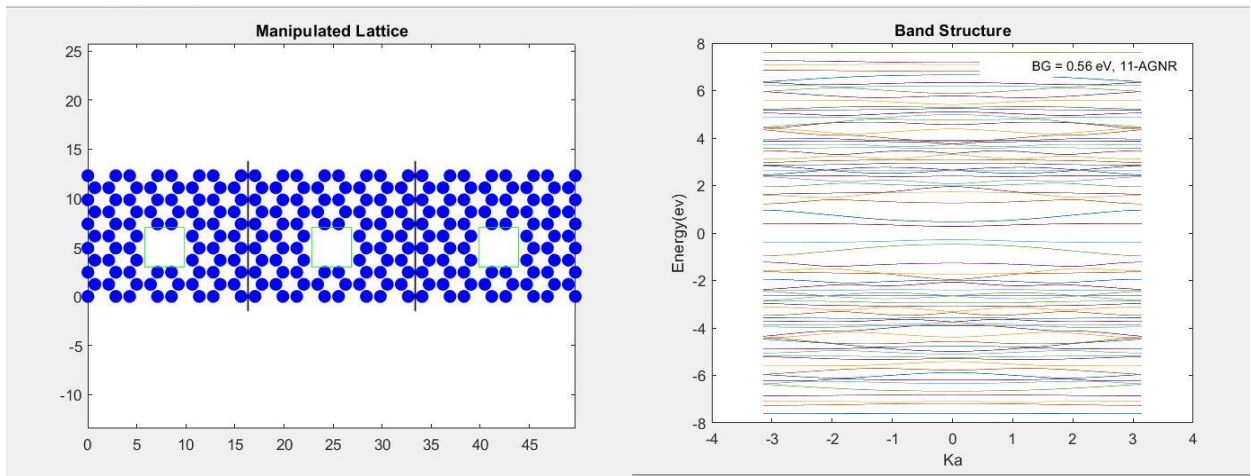


Figure 6- 11-AGNR with the third topology and its band diagram

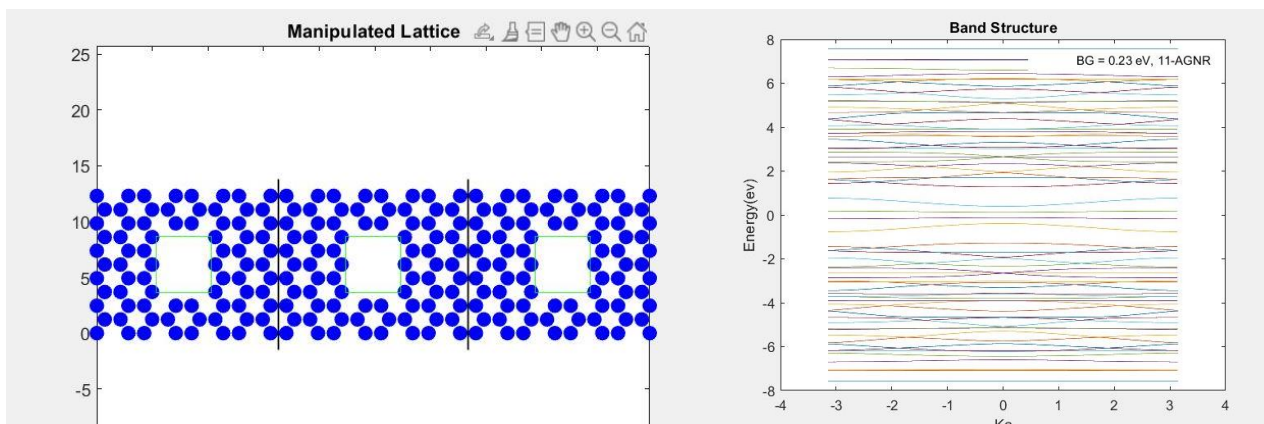


Figure 7- 11-AGNR with the Fourth topology and its band diagram

b. Results from NEGF formalism.

In the next section I will be showing the effect of antidote on current voltage relationships. As seen in [1] adding antidotes raises the energy levels in channel. The electrons can tunnel through some resonant states making use of quantum mechanical tunneling [6]. It was observed that by introducing antidotes in the channel a negative resistance region was found [1]. First topology is used here. Adding different number of antidotes results in different slope of negative resistance. I used Non equilibrium Green's function formalism to obtain the transport properties.

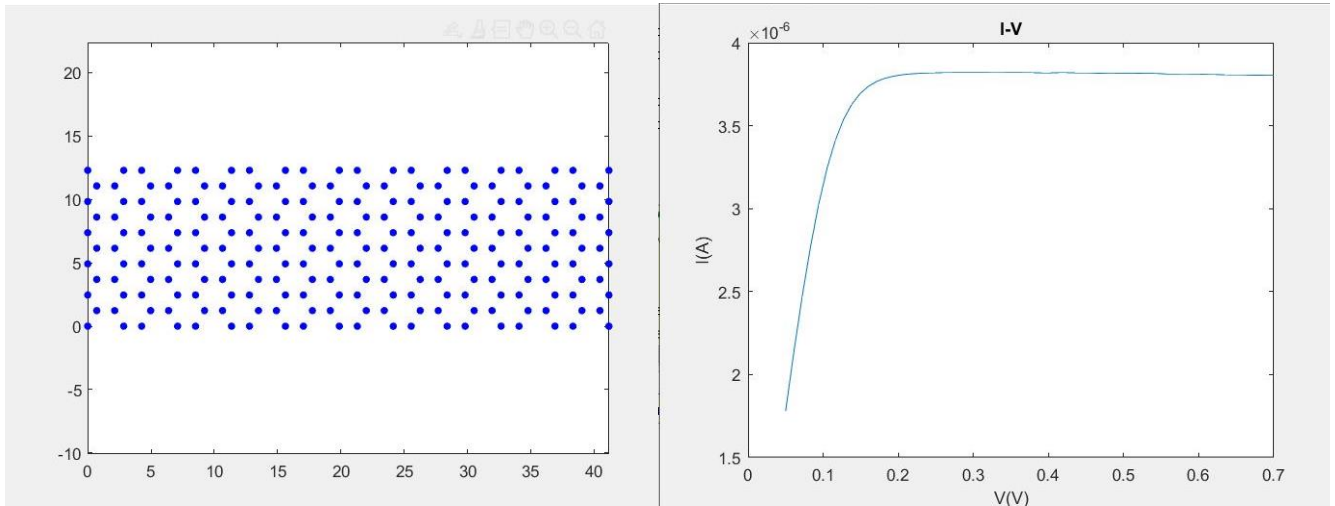


Figure 8- Current voltage relationship without antidotes in 11-AGNR

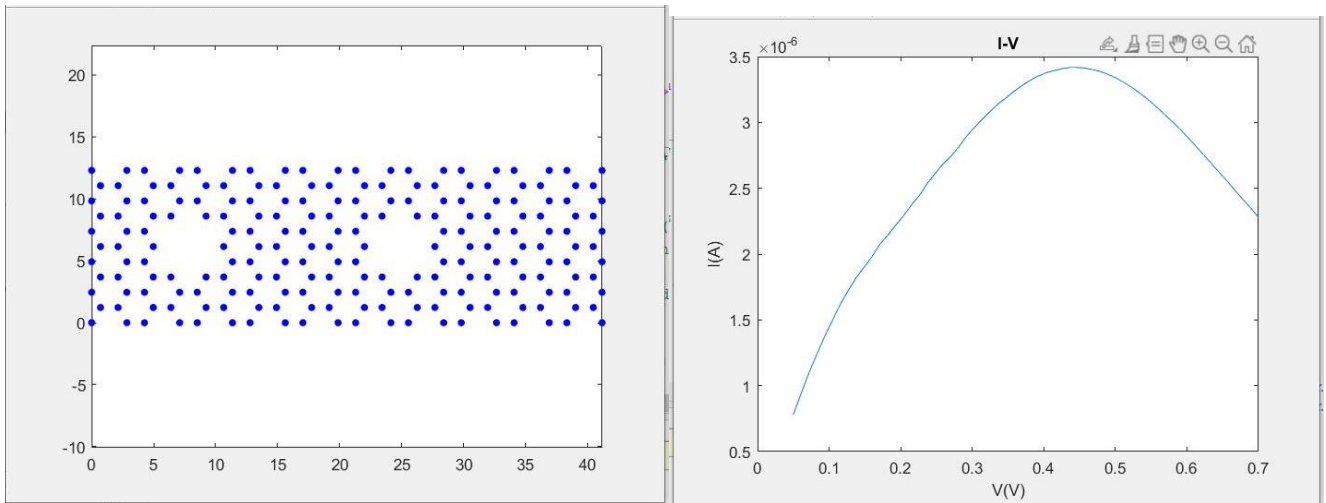


Figure 9- Current voltage relationship with 2 antidotes introduced at a specific location in the channel.

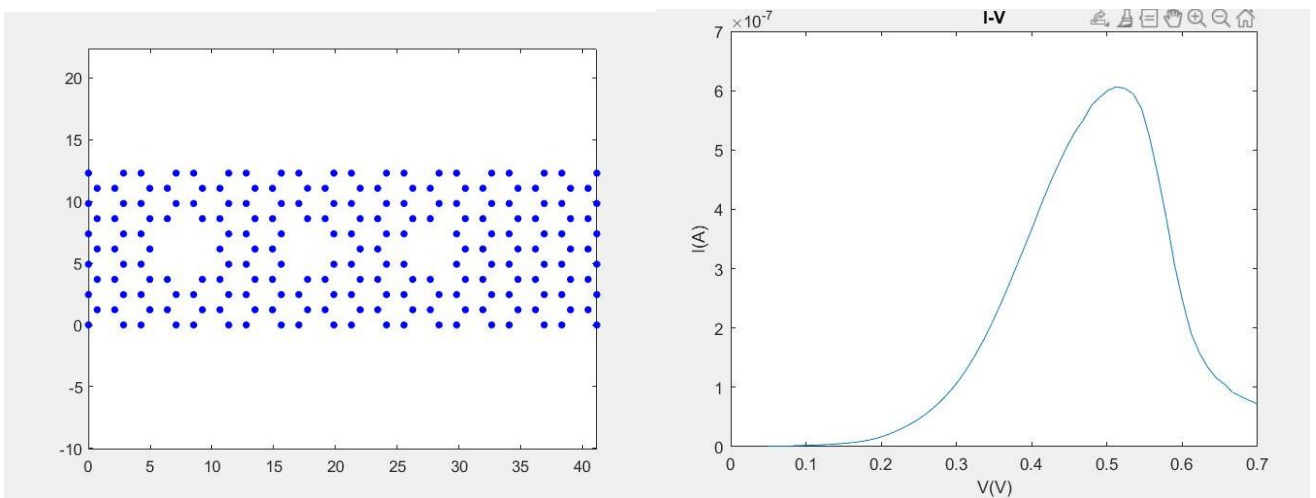


Figure 10- Current voltage relationship with 3 antidotes introduced at a specific location in the channel

4. CONCLUSION

In the above work, I used Tight binding model to simulate the Band Diagram properties of 9-AGNR and 11-AGNR. A significant change in Bandgap is obtained after introducing antidote vacancy in the channel. This is due to the fact that adding antidotes affects the channel Hamiltonian thus affecting the Eigen values and bandgap. It was found that adding antidotes in 9-AGNR decreases the bandgap and the bandgap increases in 11-AGNR. The change in bandgap is different for different antidote topologies. This approach is useful for designing novel nanostructures with different design requirements. I further used NEGF formalism to obtain the transmission parameter and hence the current with respect to the voltage applied. As seen in the simulation results, introducing antidote vacancy introduces the negative differential resistance which can be used for numerous application such as Oscillators, Microwave amplifiers, etc. As seen, increasing the antidotes in channel increases the negative slope. Different numbers of antidotes result in distinct negative slope which means different negative resistance can be obtained. Changing the location of antidote or Channel length or Barrier length will change the Transport properties as well which is not simulated here [5].

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