Simulating of Oxygen Gas Sensor Based on Silicon Carbon Nano-Ribbon

Mohammad Reza Moslemi[1], Mehrnaz Fahami[2]

[1]Department of Electronics and Electrical Engineering, Zarghan Branch, Islamic Azad University, Zarghan, Iran
[2]Department of Electronics and Electrical Engineering, Sepidan Branch, Islamic Azad University, Sepidan, Iran
([1]Moslemi_mr@yahoo.com, [2]mehrnaz.fahami@gmail.com)

Abstract- In this thesis using non-equilibrium Green function with density functional theory, examined of the simulating of oxygen gas sensor based on silicon carbon Nano-ribbon and comparison to the conventional sensors. At first, test an oxygen molecule with several different decorated to find the best position relaxation (in this of gas deposition, sensor will be the least amount of total energy), and then to evaluate the behavior of sensor we re-examined process with two molecules of oxygen. In addition, we have shown that oxygen can alter the current-voltage characteristic of zigzag silicon carbon Nano-ribbon and create new fluctuations resistance. These alternations are made due to discontinuities in the combination of orbitals along the silicon carbon Nano-ribbon. This decoration alters the discontinuities and creates more visible fluctuations. Also, in low bias voltages, the changes are similar in all the cases. The study demonstrates that in the decorated zigzag silicon carbon Nano-ribbon, the edge states are the main states for transporting electron from one electrode to another.

Keywords- *Non-equilibrium green function, zigzag silicon carbon Nano-ribbon, Resistance*

I. INTRODUCTION

The need for gas sensors, which can work efficiently at high temperatures, has always been perceivable in many industries, aerospace science (for emission indication), finding fuel leaks, fire inspection and the supervision of exhaust fume in vehicles. Among all the sensors, the oxygen sensor is widely used for controlling the combustion procedure (the proportion of air and fuel) in car engines and in the industrial thermal kilns, for the detection of intended gases in some environments, such as underground mines and oilfields [1]. Not only these sensors must show fast responses to the Oxygen, their sensitivity in high temperatures should also be prompt. Nowadays, the production of almost every fragment in gas sensors is based on the semi-conductors. Above all, the Si based sensor can perform a cheap, and still reliable, function [2]. Despite this, a serious demerit of these sensors is their malfunction at the temperatures of 200°C or above, as a result of the short energy gap in Si [3]. This semi-conductor substance provides an equal Stoichiometric proportion and has many outstanding features, such as expanded bandwidth (3.02 eV), high thermal conductivity, low congestion of intrinsic carrier, wonderful mechanical persistence, enormous breaking field and high pace of electron buoyancy in saturation. With regard to the mentioned characteristics of SiC, it has an abundant function when it comes to need high power and in high frequency electronic devices [4]. Moreover, the strong chemical bonding and the consistency and roughness of the networks in SiC [5] have made a great candidate out of it for being used in high temperatures and harsh circumstances, in which other semi-conductors, such as Si, lose their function [6]. As analysis demonstrates, SiC can be used as a hosting platform for the production of thin atomic sub-layers at high temperatures [7]. With regard to the possible functions of Silicon-Carbide during the past few years, it is mainly preferred to focus on the structural and electronic characters of Silicon-Carbide's surface in this article.

One of the drawbacks of the gas sensors is their high responding time, which can be improved by the use of some nanostructure under layers. The inner crystal networks and the free bonding on the exterior surface of these semi-conducting layers consist of highly densified Oxygen. The presence of such free bonding, that can take part in the absorbance of the gases around them, makes the alteration of the layers' electrical resistance possible if they deliver the molecular bonding (receiving or delivering the free electron to the substance) [8]. According to the aforesaid advantages, it can be expected that the Si-based sensors would be suitable for the production of such sensitive materials, as their primary substance is both available and cheap. In spite of this, those sensors which are based on mingled semi-conductors show some other advantages, such as higher sensitivity, lower response rate and wider temperature range [9]. The recent studies also show that among the mingled semi-conductors, the accumulation of porous structures or substances with separated metal layers can increase the sensitivity of the sensors [9]. According to the mentioned benefits, in this article, we made decision to use the mono-layered SiC, which not only grants the already mentioned characteristics, it also carries the features of both Si and C [10].

The two major style of the Silicon-Carbide Nano-ribbons in nature are Zigzag and Armchair. As the energy status on the edges of the Nano-ribbon in Zigzag style causes some metallic characteristics in this substances, their function for the production of the gas sensors is more appropriate than that of the Armchair style. Despite this and with regard to the ideal electronic characteristics that were mentioned on the previous

sections, this structure has rarely been studied for the production of Oxygen gas sensor. In this article, it is attempted to analyze the electronic behavior of Silicon-Carbide Nano-ribbons with Zigzag style first, and then to simulate and inspect the accurate benefits of taking advantage of this substance for the production of the Oxygen gas sensor. For studying the transportation of the carriers on Silicon-Carbide Nano-ribbons in the present article, the Green unbalanced function method, is used. The provided content on this article is arranged as below.

In the second section, the considered style and the method of simulation are introduced. On the third section, the effects of Oxygen molecules on the electronic behavior of Silicon-Carbide Nano-ribbons with Zigzag style and the sensitivity of the introduced structure next to the Oxygen gas are scrutinized. As for the fourth section, the matters would be concluded.

II. THE INTRODUCTION OF THE CONSIDERED STYLE AND THE METHOD OF SIMULATION

A. Decoration with a oxygen atom

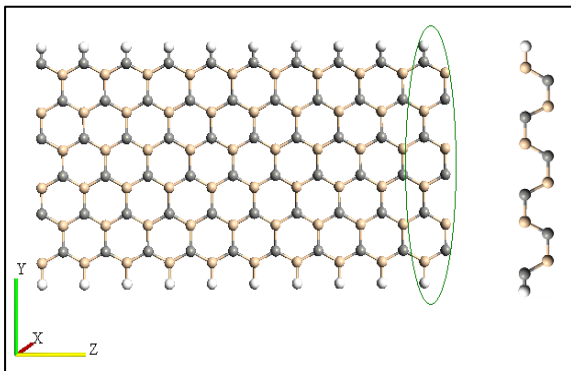The Fig. 1 represents some samples of Silicon-Carbide Nano-ribbons with Zigzag style.

Figure 1. A sample of Silicon-Carbide Nano-ribbons with Zigzag style and the width of n=12. The creamy balls, grey balls and white balls are representative of Si, C and Hydrogen atoms respectively.

As it is shown, Silicon-Carbide is a crystal, flat and single-layered substance, each of which single cells consist of 3 Carbon and 3 Si. These atoms are bond to each other on a honeycomb shape two dimensional surface, with the thickness of only one atom. On a Silicon-Carbide surface, each Carbon atom has been connected to 3 Sis. The angles among them in this situation are all equal and 120° [11]. Under the powerful Covalent bonds, Silicon atoms shape up a network of some regular hexagonal shapes [12]. On a surface of Silicon-Carbide, each Si and Carbon atom has a free bond out of the surface, which are perfect places for agent groups and Oxygen and Hydrogen atoms. With regard to the one extra free bond of the atoms that are located on the edge of the Nano-ribbons, in comparison to those located in the middle, and with the target to omit the edge impacts, Hydrogen has been used on edges as a choker element [13]. For ensuring the exactness of Hydrogen atoms' location inside the network and the placement of the

whole system in a tranquil status with low enthalpy, the mission for tranquilizing the system was accomplished with the accuracy of less than 0.02 eV per Angstrom.

For finding a better understanding about the foundation spot of the bonds among the Oxygen molecules and the Nano-ribbon, the simulation was done for the lowest rate of the system's enthalpy. From the simulation it was concluded that, regardless of their shape and their abundance of structure, Oxygen molecules have a tendency to occupy the spots that are as close as possible to the edges of the Zigzag Silicon-Carbide Nano-ribbons, which can be referred to as the well-known condition of the Zigzag Silicon-Carbide Nano-ribbon edge[14]. In Fig. 2, some possible spots for the settlement of the Oxygen molecules on the structure of Zigzag Silicon-Carbide Nano-ribbon are demonstrated.
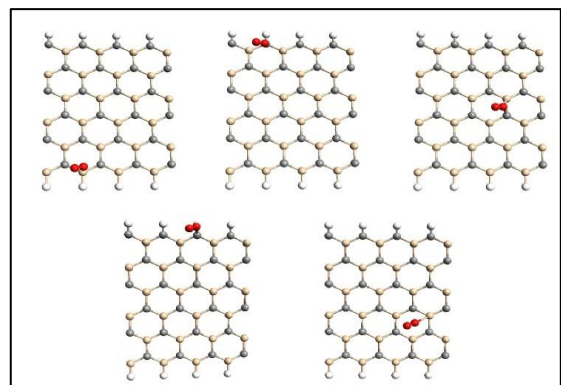

Figure 2. some of the possible points, through which the leakage of O2 on ZSiCNR is probable.

Here, the considered Nano-ribbon is placed in a structure as it is shown in Fig. 3, to help us analyze the impacts of the Oxygen bond on the electronic behavior of Silicon-Carbide Nano-ribbon. As it is shown on Fig. 3, the length of the sample canal is equal to 10 primary unit cells of Silicon-Carbide Nano-ribbon, which is connected to an exterior voltage source, like a resistance [14]. On the one hand, 10 unit cells can perfectly represent the electronic behavior of this substance at a transistor's channel, and on the other hand the time that is needed for simulation is optimized.
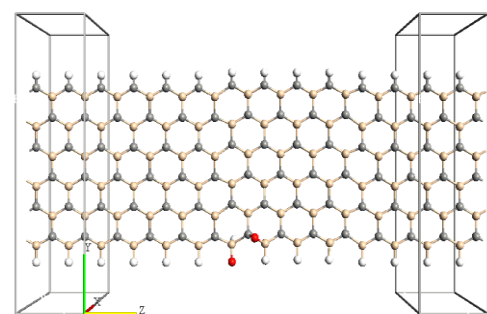

Figure 3. The complete structure of Oxygen - ZSiCNR consists of a canal, made of Carbon conductor and Si. White and red balls are Hydrogen and Oxygen atoms respectively.

Theory and method

As it is shown on this figure, the considered part is divided to three pieces. The part's two electrodes are actually two infinite semi-ribbons on both sides. In this case, the Hamiltonian Matrix can be written as below:

$$H = \begin{pmatrix} H_L & H_{LD} & \\ H_{DL} & H_D & H_{DR} \\ & H_{RD} & H_R \end{pmatrix} \qquad (1)$$

The sub-matrixes on the main diameter are representative of left connection Hamiltonian Matrix, Right Connection and the part's canal respectively. Moreover, the sub-matrixes on the sides of the main diameter demonstrate the coupling rate of each of the side connections with the canal. By having the aforesaid matrix, the Green function of the considered system can be achieved as below:

$$G = (ES - H)^{-1} \qquad (2)$$

Here, "S" introduces the orbitals overlap matrix. With regard to the Green function, the passing factor of the carrier can be calculated:

$$T(E) = Tr\left(\Gamma_L G_C^{ret} \Gamma_R G_C^{adv}\right) \qquad (3)$$

Here, G^{ret}, G^{adv} are the real and imaginary parts of the Green function. Furthermore, the ΓL, ΓR functions show the coupling among the canal with its side connections. Then, the conductivity rate of the considered canal can be written by the landa formula as below:

$$G(E) = \frac{2e^2}{h} T(E) = \frac{2e^2}{h} Tr\left(\Gamma_L G_C^{ret} \Gamma_R G_C^{adv}\right) \qquad (4)$$

Finally, the part's current can be written as:

$$I(V) = \frac{2e^2}{h} \int T(E,V)\left[f(E - \mu_L) - f(E - \mu_R)\right]dE \qquad (5)$$

III. CONCLUSION AND ARGUMENT

In this level, the passing current from the Nano-ribbon of the Fig. 3 under many different voltages, from 0 to 1, is calculated and drawn. For reaching a better understanding about the fluctuations of Nano-ribbon conductivity after the addition of Oxygen atoms, the current-voltage curve of a pure Nano-ribbon without the presence of Oxygen is drawn as Fig. 4.
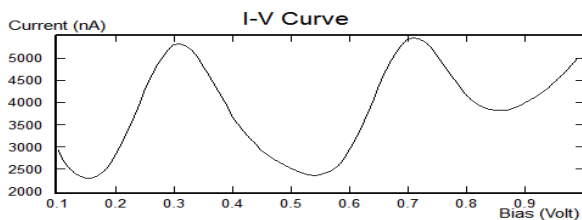

Figure 4. I-V curve for pur ZSiCNR without Oxygen.

As it can be seen in this figure, the current has some fluctuations between approximately 2 to 5 micro-ampere. In the simulated sample, some of the voltage scopes represent a negative resistance. The conductivity of this sample oscillates between 71.4 and 107 micro-Siemens, along the mentioned scope. As a result of the separation of the energy bond in canal and the consistency of the bonds on the electrodes connections, the load transportation would be deficient in some voltages, which can cause some changes in the conductivity of the considered part. Figure 05 represent the same current-voltage curve as the Fig. 2, but this time with the presence of Oxygen. As can be seen, the addition of one Oxygen molecule has had a noticeable impact on the conductivity of the Nano-ribbon. By taking a closer look at the curve, the conductivity rate of this sample fluctuates between 925 and 1000 micro-Siemens after the addition of the Oxygen molecule. This is equal to a change in conductivity for 960 micro-Siemens, which is about 23%.
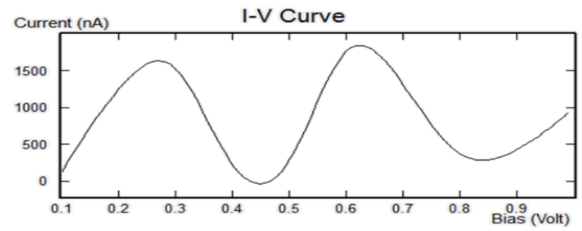

Figure 5. I-V curve for ZSiCNR with a single Oxygen molecule

For a better understanding about the fluctuating behavior, the current-voltage curve of the local status's density for the two biases of 0.1 and 1 volt are drawn as figures 06 and 07.
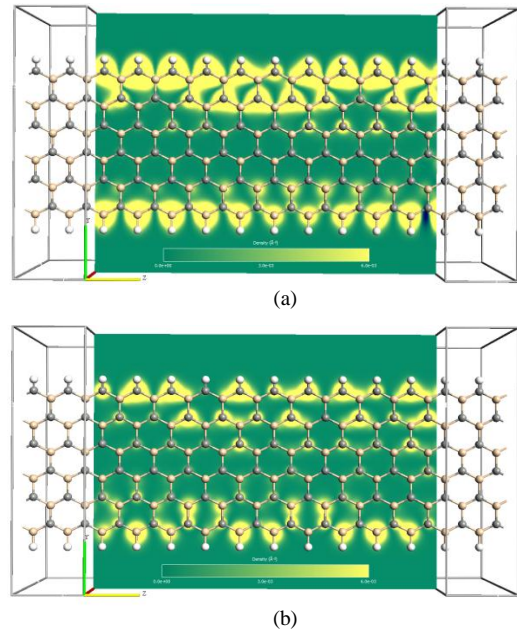

(a)

(b)

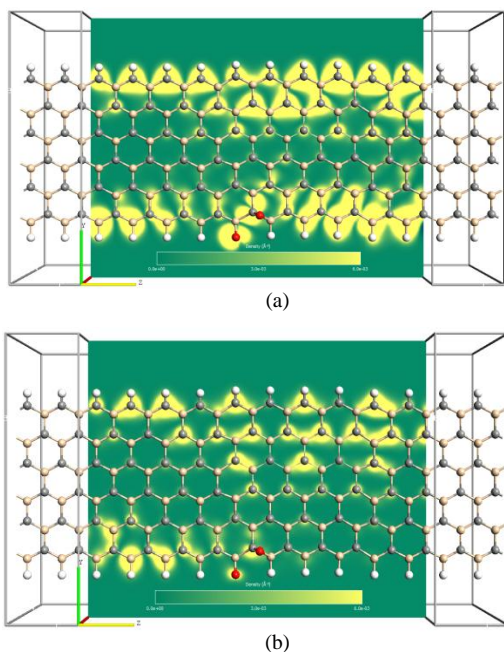Figure 6. Voltage reduction for the ZSiCNR structure, at the bias voltages of (a) 0.1, (b) 1.

(a)

(b)

Figure 7. Voltage reduction for the ZSiCNR – O$_2$ structure, at the bias voltages of (a) 0.1, (b) 1.

TABLE I. SENSITIVITY CHART

Bias voltage(v)	sensitivity in the presence of an Oxygen molecule (%)
0.1	2627.913
0.2	127.062
0.3	244.345
0.4	1476.202
0.5	865.736
0.6	65.923
0.7	308.046
0.8	1008.252
0.9	839.251
1	420.128

ACKNOWLEDGMENT

For the inspection of the transitional behavior of a ZSiCNR with a single O$_2$ molecule via NEGF-DFT, we succeeded to simulate the activated structure of O$_2$. The results illustrate that O$_2$ has a tendency to locate on the edges of the ZSiCNR. This can be attributed to the well-known edge status of ZSiCNR which cause considerable effects on the transportation of the electrons from the source to the drain. Selecting a condition that has the lowest level of energy and bonding the two Oxygen atoms with ZSiCNR can result in the consistency and resilience of the connection with ZSiCNR, which would lead to have the most consistent status on the edges of ZSiCNR. For finding a better understanding over the fluctuations in conductivity, we analyzed the I-V curve for the single O$_2$ molecule status. This curve is representative of some variables that can verify the validity of the output amounts for the suggested structures. As it can be seen on the Table.1, the sensitivity of the structure to the Oxygen gas is significantly high, which is a perfect proof for the suitability of choosing a sub-layer in our suggested structure.

REFERENCES

[1] F. Chaabouni, M. Abaab, and B. Rezig, "Metrological characteristics of ZnO oxygen sensor at room temperature," Sensors and Actuators B 100, pp. 200–204, 2004.

[2] I. Lundström, M. S. Shivaraman, and C. M. Svensson, "A hydrogen-sensitive Pd-gate MOS transistor," Journal of Applied Physics, vol. 46, pp. 3876-3881, 1975.

[3] E. Bekaroglu, M. Topsakal, S. Cahangirov, and S. Ciraci, "First-principles study of defects and adatoms in silicon carbide honeycomb structures," 2010.

[4] J. B. Casady, and R. W. Johnson, "Status of silicon carbide (SiC) as a wide-bandgap semiconductor for high-temperature applications," A review, Solid-State Electronics, Elsevier Science B.V. All rights reserved, vol. 39, pp. 1409-1422, 1996.

[5] W. C. Lien, "Harsh Environment Silicon Carbide Metal-Semiconductor Field-Effect Transistor,Phys," in Electrical Engineering and Computer Sciences in the Graduate Division. 2013, University of California. Rev. B 81, 075433 – Published 24 Februar, 2010.

[6] K. Emtsev, "Electronic, and structural characterizations of unreconstructed SiC(0001) surfaces and the growth of graphene overlayers," KATALOG DER DEUTSCHEN NATIONALBIBLIOTHEK, 2009.

[7] Z.Darmastuti, M.A. L.Ojamae, A.Lloyd Spetz, "SiC based Field Effect Transistor for H$_2$S Detection," IEEE sensors, pp. 770-773, 2011.

[8] A. Tiburcio-Silver, and A. Sánchez-Juárez, "SnO$_2$:Ga thin films as oxygen gas sensor," Materials Science and Engineering B 110, 268–271, 2004.

[9] M. Shafiei, "Investigation of Nanostructured Thin Film Based Schottky Diodes for Gas Sensing Applications," in Electrical and Computer Engineering, RMIT University, 2010.

[10] D. B. Lu, Y. L. Song, Z. X. Yang, H. R. Xu, C. Wang, Z. H. Ga, "Electronic and magnetic properties of SiC nanoribbons by F termination," 2011.

[11] F. M. Lopez, "Inkjet-Printed Multisensor Platform on Flexible Substrates for Environmental Monitoring," DOCTEUR ÈS SCIENCES, 2014.

[12] H. Sadeghi, "Electrical Transport Model of Silicene as a Channel of Field Effect Transistor American Scientific Publishers," Journal of Nanoscience and Nanotechnology Electrical 14(6), 2014.

[13] M.Berahman, M. Sanaee, and R.Ghayour, "A theoretical investigation on the transport properties of overlapped graphene nanoribbons," ELSEVIER carbon journa l, 2014.

[14] Berahman, M., Sheikhi, M.H, "Transport properties of zigzag graphene nanoribbon decoratedwith copper clusters," Applied Physics Letters, 116, 093701, 2014.