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Transport Properties and Applications of Graphene Nano-Ribbon-BN

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Abstract:
Two-dimensional (2D) graphene characterized by a unique electrical properties such as high mobility of electrons and ballistic transport at room temperature. In this research, graphene was used, which is considered a "miracle material" to build new technologies because of its strong and flexible structure, its electrical properties and chemical resistance. It is also characterized by its superconductivity and is made of only one carbon atom, and because of these unique specifications it is used as a sensor for gas in the oil industry due to the large surface area of graphene nano-ribbon (GNR). The properties of electronic transport, morphological and morphological of GNR and doped with B/N(GNR-BN) were studied using GOLLUM. The results showed that acceptable relaxation of graphene sheets was obtained as a result of useing B3LYP-DFT at the LDA/SZ DFT at SIESTA - trunk - 462 of program. The electrical conductivity of the uncontaminated graphene is greater than the doped and the highest value was 4.47 μs. The thermal conductivity, I-V characteristic and transmission were also studied. The graphene sheets were prepared using chemical vapor deposition technique and the study of structural and morphplogy properties of the samples through SEM images. Therefore, the uses of gas sensors are many and different, starting from homes and ending with giant plants, nuclear reactors and oil industries.

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1. INTRODUCTION

Graphene is a 2D atomic layer made up of carbon atoms, where graphene is the basic unit of 3D graphite construction. Graphite is a recognized and used material since the distant past, However, the possibility of isolating and studying a single layer of graphene has not been discovered until relatively recently [1,2,3]. The graphene sheets were manufactured using Various chemical techniques in the 1960s and 1970s, but the actual beginning was in 2004 when K. S. Novoselov, A. K. Geim, and colleagues at the Manchester University when they suggested a simple procedure based on mechanical graphite exfoliation(peeling) to segregate individual graphene layers [1,4,5].The accessibility of graphene exfoliate made the investigation of this material properties conceivable, leading to increased attentiveness in it and intensified effectiveness in graphene research currently progressing [5,6,7,8]. One of the most important features of graphene is its distinctive electronic transportability which is characterized by high Fermi speed as well as the super mobility of transport and high saturation speed of the carrier.

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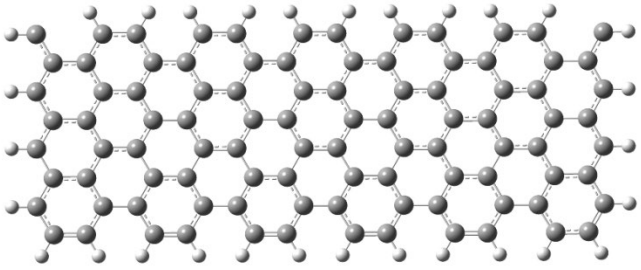
In addition to these properties, graphene is characterized by good mechanical strength, high thermal conductivity, flexibility and thinness. By having these characteristics, graphene can find many advanced applications in future electronics related applications [7,9,]. In addition, the other possibilities of graphene in high-speed analogue electronics are being explored extensively [3,6,8]. In this work, we will briefly identify and discuss the most important basic electronic descriptions as well as the I-V characteristics of graphene transport, features, attitude and transmission coefficient. When a GNR and GNR-BN is formed with heteroscedasticity, the complex manifestation its own unparalleled electrical properties; this domesticate to have spacious prospect in the nanoelectronics devices fabrications and development.

2. COMPUTATIONAL DETAILS AND EXPERIMENTAL METHODS

The calculation of the molecules properties in Fig.1, have been calculated using Density functional theory LDA/SZ fundamental group method, All these computation were accomplished by utilizing the SIESTA – trunk - 462 program [10] , GOLLUM program " version 1.0 " [11] and Gaussian View 5.0.8 [12].



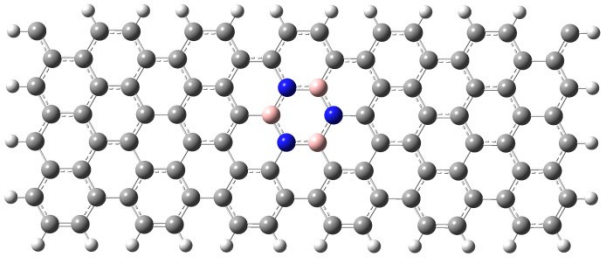


Figure 1: The optimized structures of (A) GNR and (B)GNR-BN at LDA/SZ density functional theory.

(C: B: N: H:)

All Deposition experiments were performed by using the hot walled chemical vapor deposition (HWCVD) implements. Temperature of reaction and the carrier gas flow rate were precisely controlled. OTF-1200X-4-NW is a compacted CVD furnace was used in this work, which was designed for growing various nano coatings on substrate up to 3 diameter. Four channels gas inlet are built in flange. Working Temperature: Max. heating temperature is 1150˚C (<2hour). uninterrupted cooperative temperature is 200-1100˚C, with a max. heating and cooling rate of 20˚C/min.

3. RESULTS AND DISCUSSION

The SEM images in Fig.2 show the morphology of the graphene deposited layer that was produced on Silicon wafer (100) substrate coated with thin multilayer of B-N that was produced by thermal evaporation process. As a number of substrates have been shown to be catalytically active using this approach, Ni is one of the most popular substrates for CVD of high-quality graphene production. Examination of these deposits by SEM revealed dense deposited film of graphene preferably flakes that was produced simultaneously as arrival growth process through a vapor–solid (VS)growth mechanism. Depending on the catalyst–substrate interaction strength, when the catalyst–substrate interaction is weak growth occurs by the ‘‘tip-growth mode’’, where

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carbon diffuses from the top of the catalyst to the catalyst–substrate interface causing the catalyst to lift off from the substrate; where the catalyst remains anchored to the substrate during growth. Thinner sheets (20–50 nm) were suggested to grow via a root growth pathway, as seen in Fig.2. The geometrical analytics for the proposed framework in this research is shown in Fig.1, two species are included for these structures; the first one (A) represent GNR and the second (B) is GNR-BN constructed by adding B/N compound in place of carbon atoms in phenylene rings. Successful calculation for The LDA/SZ has shown in this figure for the electronical properties like electrical conductivity expressed in (µs), thermal conductivity expressed in (W/m.K), I-V characteristic and the transmission coefficient.

The Chart represented in Fig. 1 demonstrate the relaxation construct of Graphene Sheet layout at Gauss View 5.0.8. and relax by utilizing the B3LYP/DFT at SIESTA – trunk - 462 of program.

As seen in Fig.1 there is no effect from adding B and N atoms in GNR to construct graphene grafts on fundamental properties of the arrangement, the bonds for C-C and C=C for these structures continue in the same identical range [5,13,14].

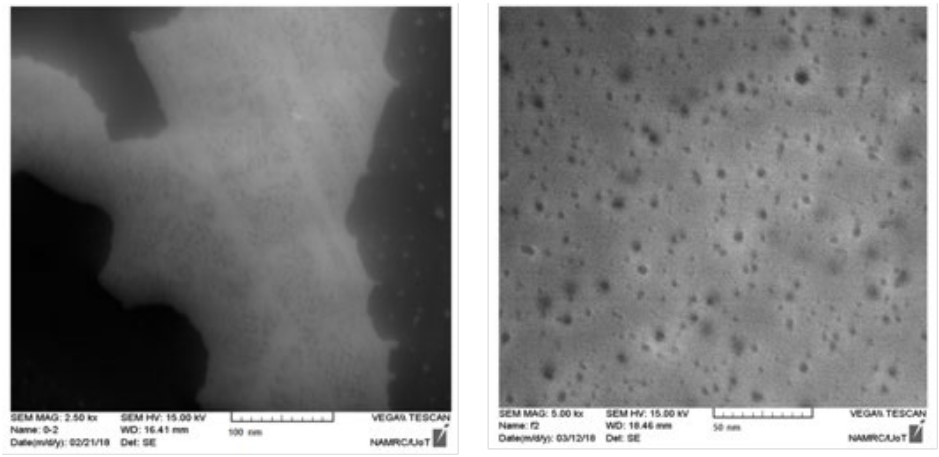

Figure 2: the SEM images of the GNR thin that was produced on Silicon wafer substrate.

The graphene sheets electrical conductivity that was considered in this work in Fig.3 shall be in the order of GNR > GNR-BN. The highest value of electrical conductivity of GNR is 4.47 µs. This is the result of the multi channels found in the pure graphene. The GNR-BN have an electrical conductivity that is equal to 4.47 µs. The source for this conductivity is caused by the value of the prohibitive gap of energy, as the greater the energy gap value, the lower the electrical conductivity [2,15].

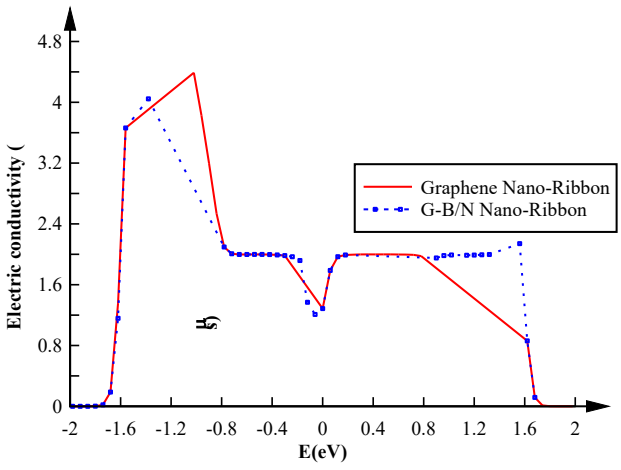

Figure 3: The electric conductivity in (µs) of the GNR and GNR-BN.

The similar behavior can be seen in Fig.4 for the Pure Graphene Sheet thermal conductivity and it is adducts, in which the thermal conductivity value decreases from 3.28*10-9 W/m.K for Pure Graphene Sheet to 3.01*10-9 W/m.K for GNR-BN.

In short words, The presence of the B / N compound in the GNR reduces the quantity of passages the electrons will pass across . As a result, the electrical and thermal conductivity of the GNR decreases significantly [16,17].

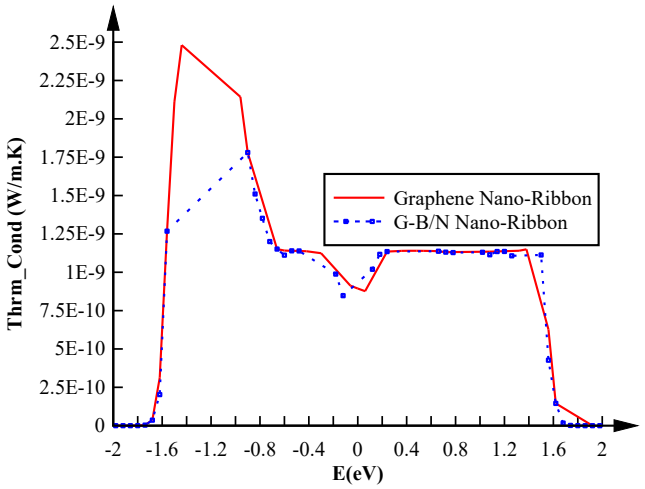

Figure 4: The thermal conductivity in (W / m. K) of the GNR and GNR-BN.

In this work, the analysis of the Voltage and Current for the uncontaminated sheets of graphene was accomplished by using LDA computation and then executed by performing of Gollum software. In these calculations, graphene is placed between two electrodes of contact carbon with an appropriate connecting atom between the sheet and the working electrode. The bias voltage (2V) is employed then in the axis connecting orientation with each other of the positioned atoms. Our computation propose also that the proportional interaction that take place with the electrodes have influence that is restricted on the sensing attitude of the GNR and its adducts. As we see in Fig.5 [5,15,16,18].

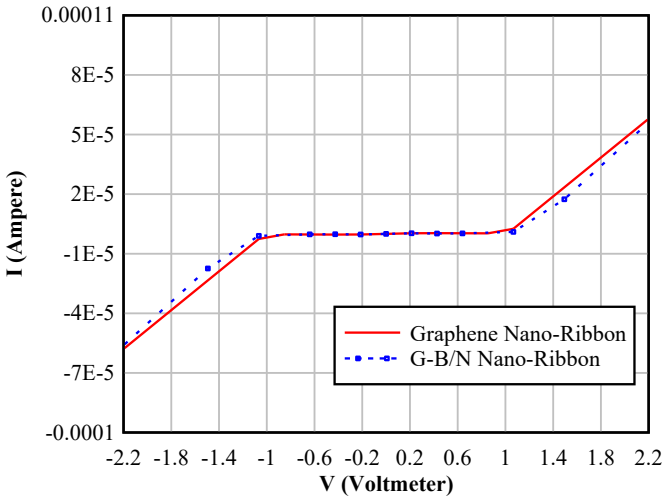

Figure 5: The I-V characteristic of the GNR and GNR-BN.

Fig.6 shows the transmission coefficient result of the two Sheets used in this work. There are several points are seeming promptly. The GNR transmission value is higher than that of the GNR-BN, where this value could be a result of the B and N atoms effect, since these atoms existence will cause turning of the located phenylene circle and distortion the ribbon of the GNR [17-18].

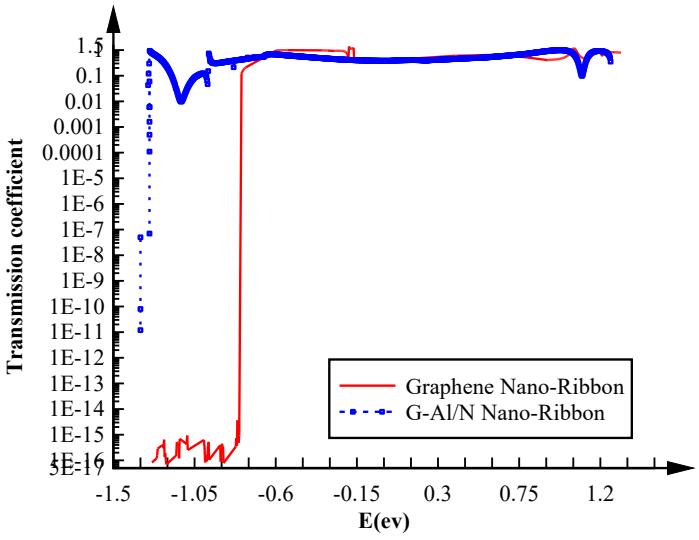

Figure 6: The coefficient of transmission for the Graphene Sheet and G-BN.

4. CONCLUSIONS

Good relax of the GNR was purposed at Gauss View 5.0.8. and relax by utilizeing the

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LDA/SZ DFT at SIESTA – trunk - 462 of program. The GNR have an electrical conductivity that is larger than that of GNR-BN, this was conducted to the multi channels of electron transport that characterized in the GNR, where the number of passages that the electrons can exceed decreases due to the presence of B/N compound in the Sheet. On the other hand, for the same reason, the thermal conductivity of the Graphene Sheet was reduced. The studied Graphene Sheets show voltage and current (I-V) that features are very much identical to realizing type. The conveyance value of the GNR is stronger than that of GNR-BN. The SEM results showed that the prepared sheets were well crystallized and had a large surface area and therefore had a gas sensitivity.

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