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ダンベル型グラフェンナノリボンの電気伝導特性解析

First Principle Calculation on the electrical Conductivity of Dumbbell-Shape Graphene Nano-Ribbon

○学　管　一兆（東北大）
Yizhao Guan ， Tohoku Univ.
学　工藤　拓也（東北大院）
Takuya Kudo ， Tohoku Univ.
正　鈴木　研（東北大）
Ken Suzuki ， Tohoku Univ.

Yizhao Guan[1], Takuya kudo[2], and Ken Suzuki[3]
[1]Department of Mechanical and Aerospace Engineering, School of Engineering, Tohoku University
[2]Department of Finemechanics, Graduate School of Engineering, Tohoku Univ.
[3]Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku Univ.

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1. Introduction

In order to develop the highly functional graphene-nano-ribbon (GNR) devices, it is indispensable for investigating methods for suppression of the Schottky barrier, which is a potential energy barrier that exists between metal-semiconductor junctions. The dumbbell-shaped graphene nanoribbon (DGNR) is proposed as a candidate for the highly sensitive strain sensor [1]. The DGNR consists of two important sections: center semiconduntive GNR with the width thinner than 70 nm, and the metallic GNRs at both ends with the width wider than 70 nm. The width of 70 nm is the critical length at which the electronic conductivity of GNR changes from mettalic to semiconductive. Since this structure consists of only carbon atoms, this dumbbell-shape GNR structure is the simplest structure for a strain sensor.

Thus, in this research, the authors focused on this DGNR structure which was made by armchair GNRs (AGNRs). In previous works, it was elucidated that the electrical properties of GNR changes with the total number of carbon atoms along its width and length directions, and both semiconductive and metallic behaviors occur as a strong function of the number [2]. The AGNR(N) are grouped into three families, N = 3m-1 family having smallest band gaps, the N = 3m family having medium band gaps, and N = 3m+1 family having the largest gaps, where m is an integer. Band gaps of each family decreases with increasing m and eventually goes to zero as m approaches positive infinite. Therefore, this research is going to pay attention to the idiosyncratic electrical properties of dumbbell-shaped GNR (DGNR) and probe the possibility of the suppression of the Schottky barrier by using this structure. Ab initio calculation is applied using SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) [3] for the simulation of dumbbell shape GNR and its electrons transportation calculation.

2. Model and Methodology

The electronic transport properties of GNRs and DGNR were studied by using density functional theory (DFT) with generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) functional implemented in SIESTA package. Current-voltage (I-V) characteristics of GNR and DGNR were analyzed by using nonequilibrium Green's function (NEGF) method implemented in the TRANSIESTA code. In this method, analysis model is divided three parts; conducting region and left and right electrodes. The current value under bias voltage from the right electrode to the left electrode is obtained from the transmission function, and then, the current through the contact region was calculated using Landauer-Buttiker formula,

$$\mathrm{I(V_b)} = \mathrm{G_0}\int_{\mu R}^{\mu L} T(E,V_b)dE$$

where $\mathrm{G_0} = 2(e^2/h)$ is the unit of quantum conductance and $T(E,V_b)$ is the transmission probability of electrons incident at an energy E through the device under the potential bias $\mathrm{V_b}$. The electrochemical potential difference between the left and right electrodes is $eV_b = \mu L - \mu R$.

Figure 1 shows the analytical model. The total number of carbon atoms along width direction in the electrode section is N_w, and that in the sensing section is N_n. In this study, the electronic conductivity of DGNR with N_w = 17 and N_n = 7 was analyzed. The 17 carbon atoms belong to 3m+2 family showing metallic property, while the 7 carbon atoms belongs to 3m + 1 family which shows semi-conductive property. Thus, there should be the Schottky

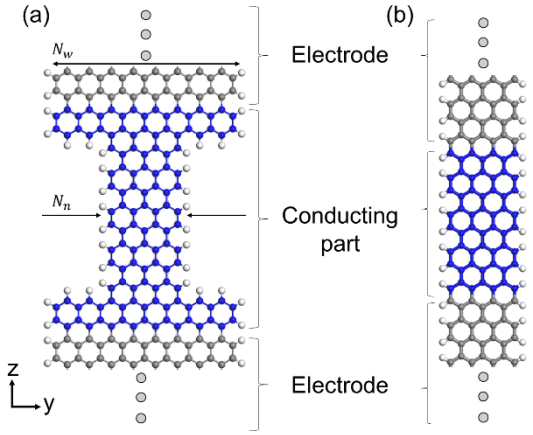

Fig. 1 (a) Analytical model of DGNR(17-7) and (b) AGNR(7). In these models, blue atoms indicate the conducting part and gray color atoms indicate the electrode region.

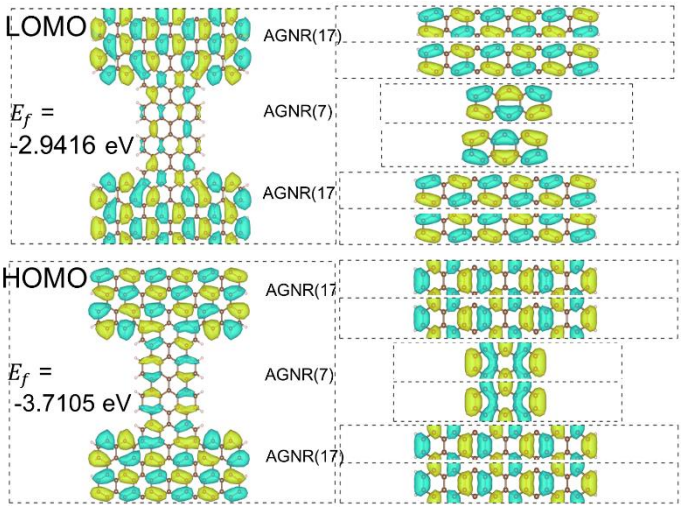

Fig.2 The Orbital Distribution of DGNR(17-7), AGNR(17) and AGNR(7), allied in electrode and conducting part order.

barrier between them. All the dangling bonds were terminated by hydrogen atoms for stabilization of the structure and helping convergence. The total number of carbon atoms in DGNR(17-7) was 232. For comparison, AGNR with 17 atoms along width and that with 7 atoms along width shown were also calculated in order to investigate the conductivity in the individual part of electrode and conductor part which are involved in the DGNR model.

3. Orbital Distribution and I-V characteristic

First, HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) distribution of DGNR(17-7), AGNR(7) and AGNR(17) were investigated as shown in Fig. 2. The two figures on the left-hand side are the orbital distribution of a DGNR and the figures on the right-hand side were the orbital distributions of two single GNRs. Both HOMO and LUMO distributions of the DGNR on the left-hand side were found to be significantly different from the single GNR on the right-hand side. Fermi energy in DGNR(17-7) was about -3.42 eV, AGNR(7) was -3.14 eV, and AGNR(17) was -3.39eV. The band gap of DGNR(17-7) was 0.87 eV, AGNR(17) was 0.19 eV and AGNR (7) was 1.44 eV, respectively. The DGNR(17-7) had a band gap almost equaling to the average value of the summation of AGNR(7) and AGNR(17).

The I-V curve (Fig.3) represented that the band gap strongly affected the current. Although the current flew through AGNR(17) with small band gap of 0.19 eV even at 0.5 V, in the AGNR(7) with band gap of 1.44 eV, current started to flow when the applied voltage raised up to about 2V. This agrees well with the previous works, figuring out the band gap is the key to the conductivity, which showing the metallic behavior for 3m + 2 family and semi-conductor behavior for 3m + 1 family.

4. Transmission Analysis

As shown in Landauer-Buttiker formula (eq.1), the current was a function of transmission probability integrated by different energy. It was indicated by previous work that the relation between transmission probability and bias energy is strongly related to band structure of the system. [4] From this relation, the mechanism of current variation

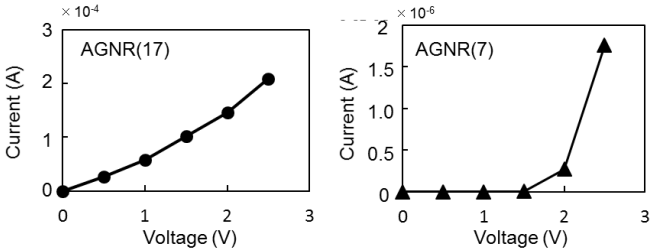

Fig.3 I-V characteristic of AGNR (17) and AGNR(7)

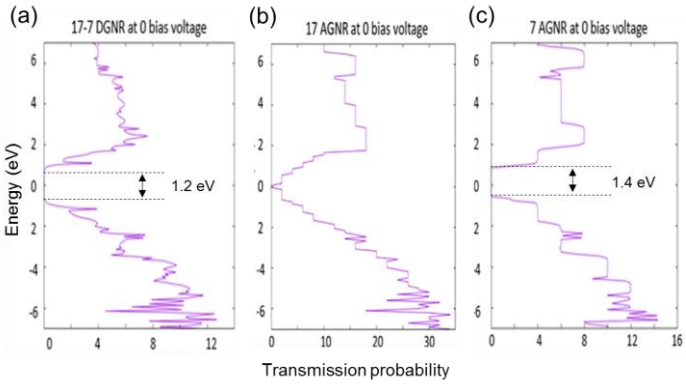

Fig.4 Transmission spectrum of (a) DGNR(17-7), (b) AGNR(17) and (c) AGNR(7) under zero-bias voltage.

between structures could be analyzed. The 0-bias voltage transmission spectrum is summarized in Fig. 4. It was found that the vertical line connects 0 transmission probability points on transmission spectrum of the DGNR(17-7) , which corresponds to the energy gap of about 1.2 eV, became larger than that expected from its band gap of 0.87 eV. This result suggests that the not only band gap but also the orbital distribution affected on the transmission property of DGNR. The current goes up monotonously when the band gap vanished with the increase of voltage, which is confirmed by previous study [4].

4. Conclusion

Electronic band structure of DGNR which consisted of a semi-conductive GNR and metallic GNRs at both its ends was analyzed by using Ab initio calculation. It was found that the not only band gap but also the orbital distribution affected on the transmission property of DGNR. In order to apply this stucture to a highly sensitive strain sensor, it is indispensable to find the DGNR structure with the minimum Schottky barrier.

5. References

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