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AL-NANORIBBONS AS ELECTRODE FOR ELECTROCHEMICAL DEVICES: NEGF FORMALISM

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ABSTRACT

We are reporting here a study of Al-nanoribbons in armchair & zigzag configurations with and without, boron and nitrogen doping. A fully self-consistent nonequilibrium Green's function (NEGF) approach for electron transport has been implemented. The electronic transmission in Al, AlB and AlN nanoribbon molecular device are analyzed with two probe method. From the results, it is inferred that the AlN is a wide band gap semiconductor. Different trends in the I-V characteristics are observed for the three cases at various applied biases. The I-V curves of three configuration on comparison reveal that the order of maximum conduction current in forward direction is AlB (0.04-0.12 mA) , AlN(.025μA) and Al(0.33 μA). The transmission spectrum T(E, Vb), as a function of energy and applied biases have also been analyzed.

Keywords: Nanoribbon, NEGF, Transport property, Transmission spectra

I. INTRODUCTION

One-dimensional quantum wires and nanoribbons have recently attracted great interest because of the specific properties they exhibit and their potential applications as interconnects or functional components in future mesoscopic electronic and optoelectronic devices.[1,2] The discovery of carbon nanotubes[3] has significantly stimulated research activities into the syntheses and characterization of one-dimensional nanosystems.[4-16]In this paper we have tried to study electronic structures of pristine Aluminium nanoribbon along with boron and nitrogen doped Aluminum nanoribbons.

The perspective of a widespread use of clean but intermittent sources of electricity (wind and solar) as well as of hybrid electric vehicles calls for alternatives to ITO as electrode material for various optoelectronic devices. Aluminium being abundant, cheap and a relatively light and small atom have recently attracted much interest.

II. COMPUTATIONAL ASPECTS

The calculations are performed in all three model structures within the super cell approach with 20 atoms in each unit cell of respective structures with increasing the 5 unit cell in z- direction i.e. the structure is periodic along the z- axis. The relaxation and electronic transport calculations in the scattering region have been performed using respective super cells of Alznr 20.41x6.47x41.30, AlNanr 19.68x 5.81x 26.80 and AlBanr

21.97x 5.98x 30.95 while for the electrodes the unit-cell selected was 12.93x2.64x4.63 and 15.09x2.23x7.48 respectively. In the self-consistent potential and total energy calculations, the mesh-cutoff value taken is 250 Ry and the Brillouin zone is sampled by 1x1x1 special **k** points. We used the generalized gradient approximation (GGA) in the scheme of Perdew–Burke–Eruzerhof (PBE) [17] to describe the exchange and correlation potential, since the GGA is relatively more efficient to predict the energy gap of semiconductor than the local-density approximation (LDA) [18], which is well known to underestimate the fundamental band gap in semiconductors and insulators by 30–60% [19]. By adopting single zeta (SZ) basis set in the conjugate-gradient method, all atomic positions and unit cells are optimized until the atomic forces are less than 0.03 eV/ A^0.

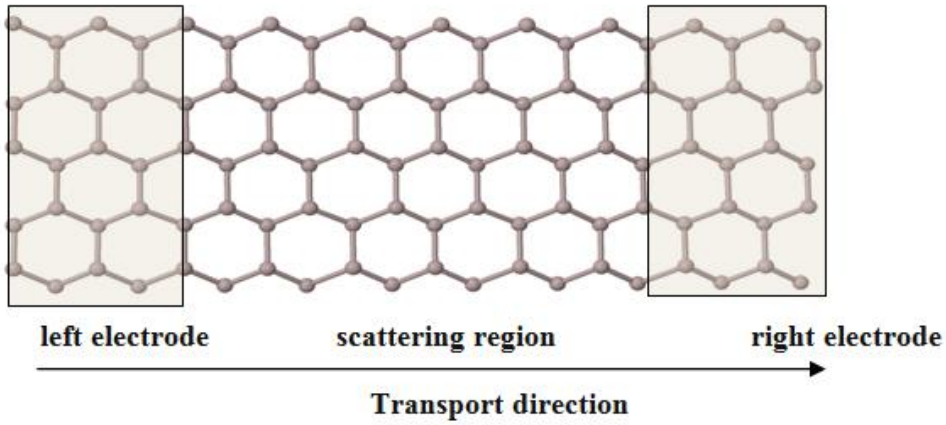
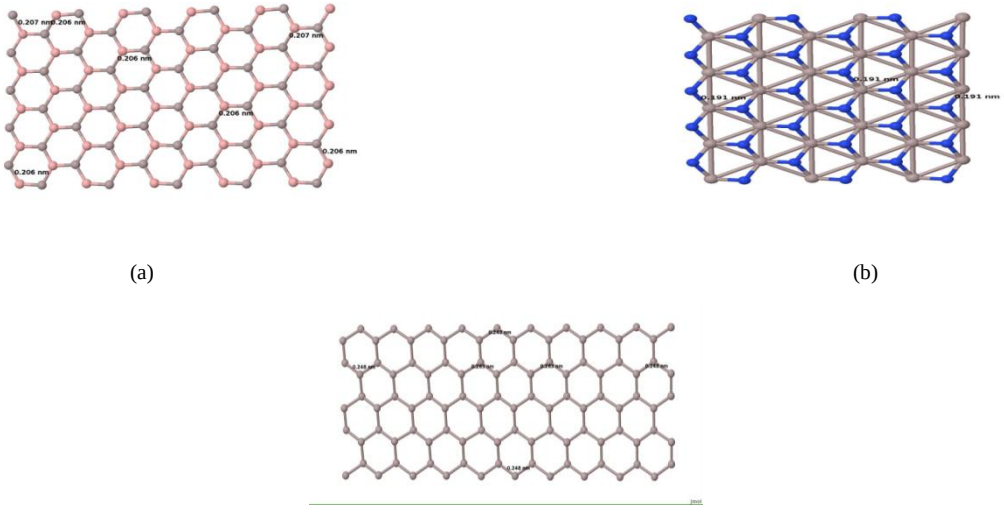


Fig 1: Schematic structure of the model device constituted by three parts: the left (L) and right (R) semi-infinite Alznr (electrodes) and scattering region

The principle idea of quantum transport calculations is to divide the system under investigation into three parts: two electrodes and a scattering region in between. The above model shown in Fig-1 depicts three parts mentionedabove, left semi infinite electrode, right semi infinite electrode and central scattering region. Central region



(a) (b)

(c)

Fig 2: Optimized structures of (a) AlBanr (b) AlNanr and (c) Al nanoribbon

constitutes the scattering region, left and right electrodes are extensions [20-22]. The size of scattering region has been considered sufficient enough to prevent the interaction between the left and right electrode. The junction is constructed so that the periodic replicas of the Alznr along with the direction parallel to the electrode edge are separated by nanometer range. The current through contact region was calculated using Landauer-Buttiker Formula [23].

III. TRANSPORT PROPERTY ANALYSIS

(I-V) Characteristics analysis

NDR (Negative differential resistance) is a property of electrical circuits; the current decreases with increasing bias voltage, which can be used for building bi-stable devices and highly functional components like latches, oscillators, memories [24-25]. Interestingly, the origin of NDR behavior in molecular electronics devices could involve different mechanisms [26-27] thus, the intensity of transmission peaks decrease at high bias voltage, resulting in NDR. Figure 3 shows the I-V characteristic curve of aluminium. As revealed from this curves up to 0.7 V there is no current flow with increase in bias voltage. The device is supposed to be in OFF state.

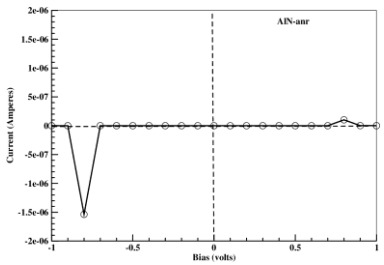


Fig 3: I-V characteristic curve of AlNanr showing very negligible curent in the forward bias region.

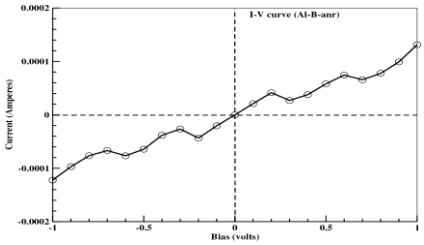


Fig 4: I-V characteristic curve of AlBanr showing curent in the forward and reverse bias region.

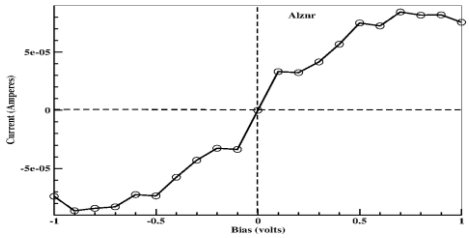


Fig 5: I-V characteristic curve of Alznr showing curent in the forward and reverse bias region.

At 0.8 V a current of 0.1µA has been observed for AlNanr and then there is a decrease in current. In the negative bias region also there is a sharp rise in current at 0.7 V and attains a maximum value of -1.6 µA at 0.8 V.I-V curves of Al and AlB show almost linear rise in current with voltage in positive and negative bias regions.

3.1 Transmission Curve Analysis

The behavior of I-V characteristics of AlNanr,AlBanr and Alznr mentioned in last section can be explained on the basis of their transmission curves. Electron transport characteristics for aluminum nanoribbon in the presence of an external bias voltage in two different configurations have been studied. As mentioned earlier basis sets comprised of linear combination of numerical type atomic orbitals and k-point sampling for the realistic modeling of the electrode has been performed in this study. In this study of aluminum nanoribbons, the role of the NEGF method is to describe the electronic structures of open systems composed of two bulk electrode parts and a device part.As we can see transmission curve of AlBanr continuous peaks which is close agreement with I-Vcurve as well.The transmission curve of AlNanr is not continuous which indicates that conduction has been reduced .The same behavior is reflected in I-V curves also.

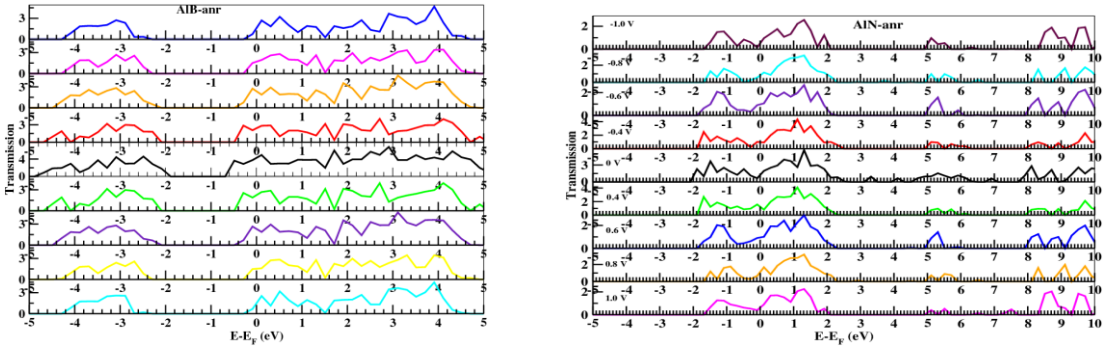


Fig6: Transmission curves of AlB-anr and AlN-anr

IV. CONCLUSION

We have studied the electronic transmission in Al, AlB and AlN nanoribbon and after comparison of I-V characteristic curve it has been inferred that the order of conduction current in forward direction is AlB (0.04-0.12 mA) > AlN(.025µA)> Al(0.33 µA. The bonds have more ionic character in AlN due to a charge transfer from Al to N.[28]. As reported by Menghao Wu et al. AlN nanoribbons are half metallic.[29]We have reached the conclusion that AlN is a wide band gap semiconductor.Transmission curve also imply that conduction is being enhanced in boron doped alminium. We also conclude that doping of Boron inceases the conductivity of aluminium nanorribbon.

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