

# Computing Electronic Structures of Gallium Arsenide Nanowires

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**ABSTRACT:** Full band simulation studies are performed for Gallium Arsenide using  $sp^3d^5s^*$  orbital basis tight-binding approach. The electronic properties of Gallium Arsenide nanowires have been studied for different growth directions, shape and size of the cross-section. It has been calculated that for circular GaAs nanowire the conduction band minima = 2.169 eV; valence band maxima = -0.319 eV so the bandgap = 2.488 eV. Similarly for rectangular GaAs nanowire the conduction band minima = 2.069 eV; valence band maxima = -0.186 eV; and the bandgap = 2.256 eV. Likewise for triangular GaAs nanowire the conduction band minima = 2.444 eV; valence band maxima = -0.426 eV; and the bandgap = 2.871 eV. The band gap of rectangular GaAs nanowire is the smallest in case than other two different GaAs nanowire. This is because of biggest in cross-sectional nanowires. Further it is seen that the largest band gap is triangular GaAs nanowire as it has the least cross-sectional dimension among them.

**KEYWORDS:** Tight-binding approach, Gallium Arsenide nanowires and Band structure

## I. INTRODUCTION

The quantum wires manufacture have been a challenge for numerous decades [1-4]. The reports of successful growth of single crystal free-standing III-V nanowires have done in recent years [5-7]. The semiconductor nanowires (NWs) are attracting elements in the publication. They represent a unique system for exploring phenomena at the nanoscale as well as also due to their potential applications. The one-dimensional nanostructures are supposed to play a critical role in future electronic and optoelectronic devices. , Gallium Arsenide (GaAs) is one of the most significant materials used in semiconductor physics for making nanowires. This is due to the high electron mobility, it always carried a potential of being used in high speed electronic devices. It is possible to grow GaAs nanowires due to recent advances in fabrication technology. In the present paper a systematic study of the atomic and electronic structure of GaAs nanowires using Tight-binding approach calculations. We have considered three different types of nanowires with almost same diameters along [10] direction and reveal interesting band gaps in the nanowires.

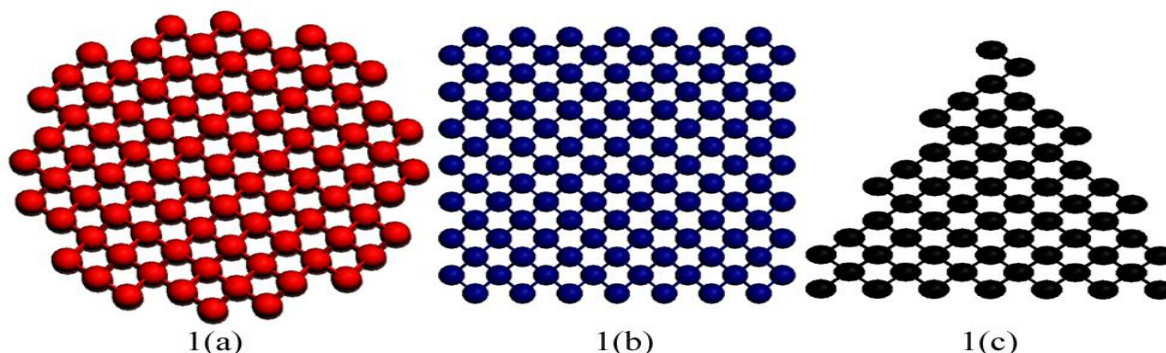


Figure 1 cross section of (a) Circular wire (b) Rectangular wire (c) Triangular GaAs nanowire

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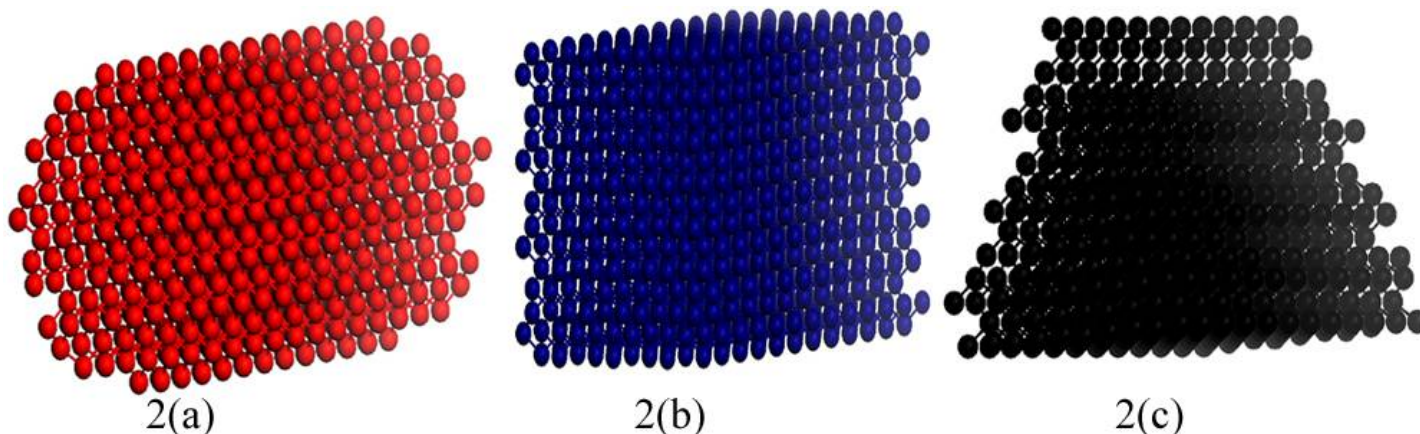


Figure 2 length wise of (a) Circular wire (b) Rectangular wire (c) Triangular GaAs nanowire

## II. COMPUTATIONAL DETAILS

### Model

A mathematical model is fabricated by creating the atomic positions of a GaAs nanowire and is given the following parameters

- ❖ Crystallographic orientation
- ❖ Nanowire cross-section in nanometer square
- ❖ Shape of cross-section

The direction of GaAs nanowire is  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ ,  $\langle 111 \rangle$  etc and formation of GaAs is symbolized as  $\vec{C}_1$ . First of all the model will make in the form of a square nanowire. This is done with the help of Matlab program is customized to create nanowire of different cross-sectional shapes (e.g. circular, triangular and rectangular) as shown in the above figure. The electronic properties of the GaAs nanowire depend upon a lot on crystal orientation and its dimension. To produce a nanowire of the desired shape of a square nanowire is grown first, and then the outer atoms are eliminated to form the desired shape according to [8]. The GaAs - GaAs bond length is 2.42 Å while GaAs -H bond length is 1.55 Å.

## III. RESULT AND DISCUSSIONS

The electronic properties that are the band structure, the band gap, and the electron effective masses of GaAs are studied in this section. The GaAs Nanowires are applied in growth  $\langle 100 \rangle$  and  $\langle 110 \rangle$  directions. It is supposed during nanowire growth, the bulk bond length and the dangling bonds are passivated with hydrogen atoms. The cross sections of  $\langle 100 \rangle$  and  $\langle 110 \rangle$  GaAs NWs are shown in Figure 1-2. The three different color atoms are Gallium Arsenide and at the end the black atoms are hydrogen atoms which are shown in any of the diagrams. The nanowire growth direction is x which is into (or out of) the paper. The other directions y and z are  $\langle 010 \rangle$  and  $\langle 001 \rangle$ , respectively for the  $\langle 100 \rangle$  wires, and  $\langle 110 \rangle$  and  $\langle 001 \rangle$ , respectively for the  $\langle 110 \rangle$  wires. The cross section of  $\langle 100 \rangle$  wire looks rectangular. The unit cell is 0.543 nm long and has 4 atomic layers. The  $\langle 110 \rangle$  nanowire looks hexagonal. It has 2 atomic layers in a 0.384 nm unit cell.

It has been calculated that for circular GaAs nanowire the conduction band minima = 2.169 eV; valence band maxima = -0.319 eV so the bandgap = 2.488 eV. Similarly for rectangular GaAs nanowire the conduction band minima = 2.069 eV; valence band maxima = -0.186 eV; and the bandgap = 2.256 eV. Likewise for triangular GaAs nanowire the conduction band minima = 2.444 eV; valence band maxima = -0.426 eV; and the bandgap = 2.871 eV.

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## IV. EFFECTS OF CROSS-SECTIONAL SHAPE ON THE ELECTRONIC PROPERTIES

Figures 3, 4, 5 show the band structure for three different GaAs nanowires cross-sectional shapes whereas keeping the cross-section area are almost same. It has been observed that the band gap increases with decreasing cross-section area as a result of quantum confinement. For example that the band gap of rectangular GaAs nanowire is the smallest in case than other two different GaAs nanowire. This is because of biggest in cross-sectional nanowires. Further it is seen that the largest band gap is triangular GaAs nanowire as it has the least cross-sectional dimension among them.

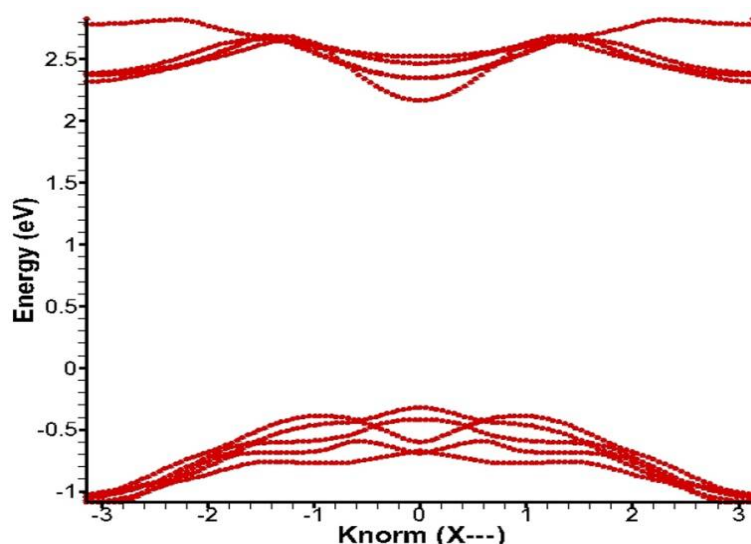


Figure 3 shows band gap of GaAs circular nanowire

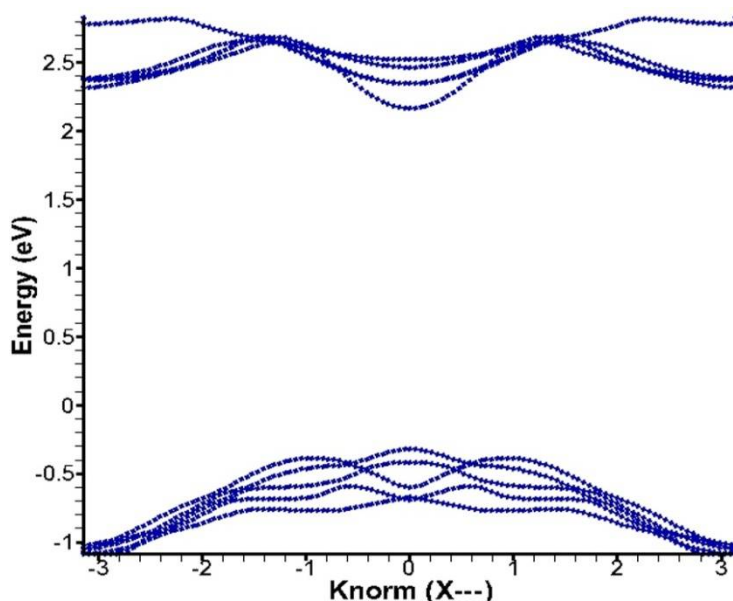


Figure 4 shows band gap of GaAs rectangular nanowire

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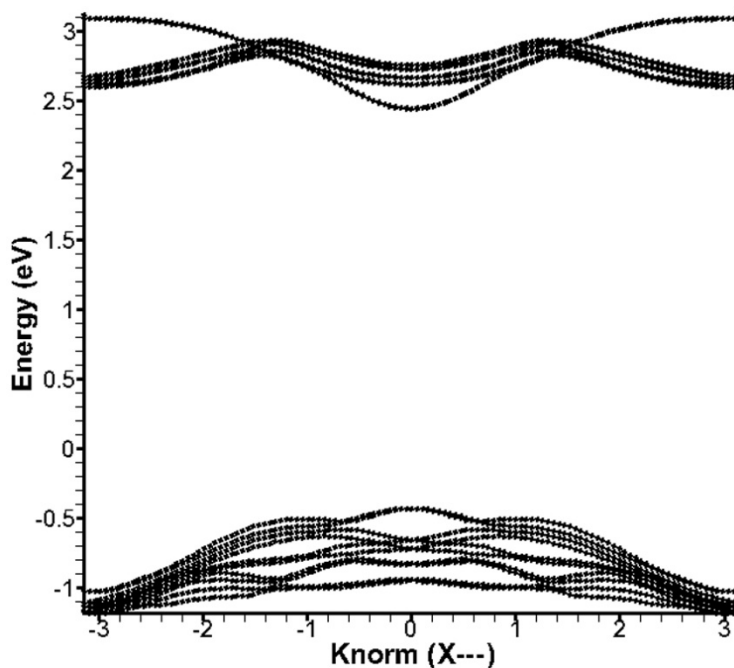


Figure 5 shows band gap of GaAs triangular nanowire

## V. CONCLUSION

Empirical tight binding parameters are utilized to find out the electronic properties of Gallium Arsenide nanowires for different crystal orientation, cross-sectional size and shape by using nearest neighbor  $sp^3d^5s^*$  atomic orbital basis. Band gap plus effective mass demonstrates strong variations as a result of quantum confinement. They are also diverging with crystal orientation. The smallest band gap is calculated for rectangular GaAs nanowire and the largest band gap for triangular GaAs nanowire.

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