Electronic Structures and Band Gap of Doped Germanium Nanowires (GeNWs)

Rashid Nizam¹, Mirza Mohd Sehban², Shabina Parveen³
¹,²Department of Physics, IFTM University, Moradabad, India
³Department of Botany Pt.L. M. S. Govt. Autonomous P. G. College, Rishikesh. India

Abstract—The electronic properties of Germanium nanowires (GeNWs) for different crystal orientation, cross-sectional size and shape are calculated with the help of empirical tight binding method. The calculation used parameters to the nearest neighbor sp³d⁵s* atomic orbital basis. The three different color Germanium atoms are used to form three different Germanium nanowires. The nanowire is grow in the direction of x such that the wire is into (or out of) the paper. The cross section of Germanium <100> wire is seen rectangular from the cross section while the <110> nanowire looks hexagonal. It has been estimated that for circular Ge nanowire the conduction band minima = 2.10011eV; Valence band maxima = 0.0392472eV; and the band gap of Ge nanowire = 2.31077eV. Likewise for triangular Ge nanowire the conduction band minima = 2.01078eV; Valence band maxima = 0.406183eV; and the band gap of triangular Ge nanowire = 1.6046eV.

Keywords – Empirical Tight-binding approach, Germanium Nanowires and Band structure

I. INTRODUCTION

Self-assembled semiconducting nanowires are one of the best candidates for applications in nanoelectronics, optoelectronics, in addition to sensors [1-4]. Progress are doing in designing more complex structures, such as branched or compositionally modulated wires which requires a clear understanding of nanowire growth mechanisms. Nanowires are normally assumed to grow via the vapor liquid-solid (VLS) process [5] through which material from the vapor is incorporated via a liquid catalyst, commonly a low-melting point eutectic alloy.

GeNWs has been applied in as a Field Effect Transistors (FETs), logic gates and sensors [6]. Atomic orbital basis has been used to study tunneling as well as quantum confinement in electronic properties of GeNWs at material level [7, 8]. The bulk crystal symmetry is not conserved in GeNWs due to quantum confinement in the transverse directions that is why the bulk effective mass approximation fails for nanowires of smaller diameter [11]. One bulk effective mass approximation has been investigated at device level using ballistic top of the barrier model [16] that do not take into accounts the tunneling current. Wang et al. [16] have calculated the band structure plus nanowire confined masses with the help of sp³d⁵s* tight binding orbital basis. He used the Schrodinger's equation in continuum basis using for both the bulk and nanowire masses. He observed the bulk effective mass approximation expect too much for the threshold voltage for wire width < 3 nm and the on current for wire width < 5 nm. Later on, Nehari et al. [17] have calculated the sub-band position and transport effective masses using tight binding calculations. He has also solved Schrodinger's equation and has estimated current using mode space approach with his input parameters. His study revealed that the bulk effective mass overestimates the on/off current ratio for wire width < 3 nm as well as the thermal current too but underestimates the tunneling current.

II. COMPUTATIONAL DETAILS MODEL

A mathematical model is build up by generating the atomic positions of a Germanium nanowire is same as given [9]
Figure 1 cross section of (a) Circular nanowire (b) Rectangular nanowire (c) Triangular Ge nanowire

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

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

The Germanium nanowire nanowires are created in the direction ⟨100⟩, ⟨110⟩, ⟨111⟩ etc. First of all, a square nanowire Germanium nanowire is made with the help of Matlab program. After that, this is customized to create nanowire of different cross-sectional shapes (e.g. circular, triangular, and rectangular). It is observed that the electronic properties depend a lot on crystal orientation and its dimension.

They also modify for different cross-sectional shapes. To produce a nanowire of the desired shape, a square nanowire is grown first, and then the outer atoms are eliminated to form the desired shape.

Algorithm to build Nanowire:

Once the unit cell is appearance then it is repeated along $R_b$ and $R_c$ directions till the desired cross-sectional area are achieved. This is the final set of co-ordinates is called super cell. The nanowire is a one-dimensional device as well as it is assumed to be infinite in the growth direction ($R_a$).
So the super cell is repeated along R_a only for once. It will help ones to build the bandstructure of the nanowire according to. Lastly hydrogen atoms are inserted at the open bonds at the wire boundaries. The Ge - Ge bond length is 2.44 Å while Ge - H bond length is 1.52 Å. The bond angle is the same on both occasions.

**Building the Tight-Binding Hamiltonian**

Here the basis of the system in Hamiltonian is \( sp^3d^5s^* \). If the system encloses like by 2 atoms then the Hamiltonian of the system will be a 20 x 20 matrix. Each of the elements of the matrix indicates the dealings between the orbitals. When two orbitals overlap the type of bond will be \( \pi, \sigma \) or/and \( \delta \) depending upon the type of orbitals involved. For example, when the orbitals are \( s \) or \( s^* \) are involved then only \( \sigma \) bond is possible.

If it is assumed that the two orbitals engaged are both \( s \) orbitals. In this case the interaction element will be just equal to \( V_{ss} \) and the coupling energy between these \( s \) orbitals is called orbital parameter. These parameters are adjusted to produce bulk Germanium behavior and one can work on very well for nanowires having dimension >0.5nm. If one of the orbital is changed to \( p \) orbital, then the expression will be \( \langle \phi | H | \phi \rangle = l(V_{pp}) \). For band structure computation, the Hamiltonian is created from

\[
H(k_x) = H_o(k_x) + t_{01}e^{ik_x\Delta x} + t_{10}e^{-(k_x\Delta x)}
\]

(12)

Here \( k_x \) is the one dimensional (1D) wave vector as well as \( \Delta x \) is the distance between the last layer of a unit cell plus the first layer of the next unit cell. The matrix elements of \( H_o(k_x) \) are created from

\[
H_o(i,j) = \langle \phi_{i,n} | H | \phi_{j,m} \rangle e^{ik_x(x_m-x_n)}
\]

(13)

While those of \( t_{01} \) are created from

\[
t_{01}(p,q) = \langle \phi_{p,u} | H | \phi_{q,v} \rangle
\]

(14)

Here \( n \) and \( m \) label the atoms in the given unit cell, and \( u \) and \( v \) label the atoms between adjacent to that unit cells. The basis, \( \phi \) is the \( sp^3d^5s^* \) atomic orbitals and \( \phi_{j,m} \) is the \( j^\text{th} \) orbital of the \( m^\text{th} \) atom. The Hamiltonian is generated under tight binding approximation method. The energy integral expressions [1], \( \langle \phi_{i,n} | H | \phi_{j,m} \rangle \) and \( \langle \phi_{p,u} | H | \phi_{q,v} \rangle \), are taken from Slater and then the orbital parameters are taken from Boykin and Zheng [10].

It should be noted that Spin-orbit coupling is not considered in this study. Thus the band structure is achieved by computing the eigen energies of \( H(k_x) \) defined in Equation (12).

### III. Calculations And Results

The electronic properties that are the band structure, the band gap, and the electron effective masses of GeNWs are studied in this paper. The GeNWs are applied in growth <100> and <110> directions. It is supposed during nanowire growth, the bulk bond length and the dangling bonds are passivated with hydrogen atoms. The cross sections of <100> and <110> GeNWs are shown in Figure 1. The three different color atoms are Germanium and at the end the black atoms are hydrogen and 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 <010> and <001>, respectively for the <100> wires, and <110> and <001>, respectively for the <110> wires. The cross section of <100> wire looks rectangular. The unit cell is 0.565 nm long and has 4 atomic layers. The <110> nanowire looks hexagonal. It has 2 atomic layers in a 0.469 nm unit cell.

It has been calculated that for circular Ge nanowire the conduction band minima = 2.10011 eV;

Valence band maxima = -0.230495 eV so the band gap of circular Ge nanowire = 1.86962 eV as shown in figure 3. Similarly for rectangular Ge nanowire the conduction band minima = 2.01078 eV; valence band maxima = -0.406183 eV; and the band gap of rectangular Ge nanowire = 1.6046 eV as shown in figure 4. Likewise for triangular Ge nanowire the conduction band minima = 2.35002 eV; Valence band maxima = -0.0392472 eV; and the band gap of triangular Ge nanowire = 2.31077 eV as shown in figure 5.

**Effects of Cross-Sectional Shape on the Electronic Properties**

Figures 3, 4, 5 show the band structure for three different Ge 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 Ge nanowire is the smallest in case than other two different Ge nanowire. This is because of biggest in cross-sectional nanowires. Further it is seen that the largest band gap is triangular Ge nanowire as it has the least cross-sectional dimension among them.
IV. CONCLUSIONS

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

REFERENCES


Email: - rashid.nizam@gmail.com