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Modeling and Simulation of CNT using VNL

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Abstract:
Modeling and simulation of metallic are performed through ATK and VNL by quantum wise. The simulation results for the voltage current of length of 17.32 shows more conduction if the length is 21.92 the simulation results for the current voltage shows less conduction.

Keywords: carbon Nanotubes, arm, chair, zigzag, VNL

I. INTRODUCTION

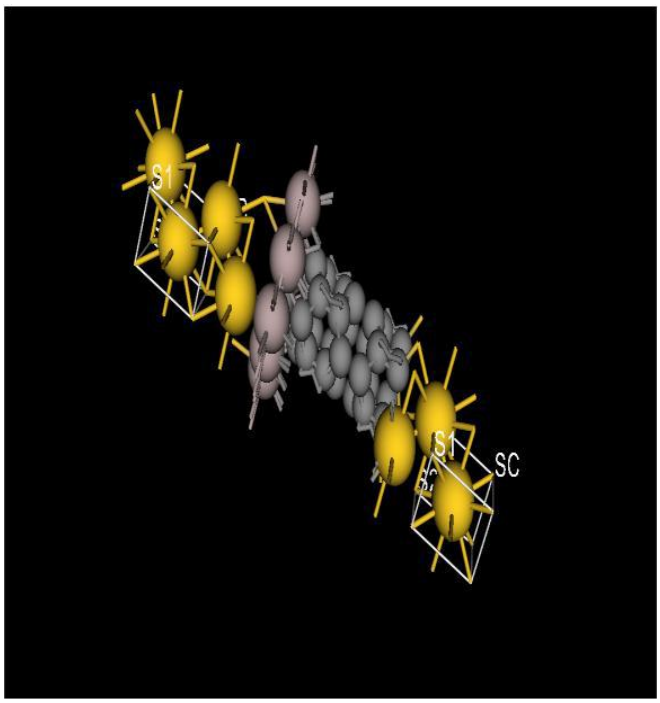
Virtual Nanolab (VNL) is a graphical interface that provides a group of modeling tools; the function of these tools is to set-up, investigate, and study nanoscale structures such as molecules, bulk and two-probe systems. The quantum mechanical equations that describe these systems are solved by VNL by using advanced software architecture and numerical methods to implement "ab initio" calculations. VNL simulates the electronic structure and the transport properties for the different systems based on two main techniques discussed before in this chapter; those techniques are density functional theory (DFT) and non-equilibrium Green's functions (NEGF). All the calculations performed in VNL are done by the Atomistix ToolKit (ATK) which is the main engine for computing the scripts.

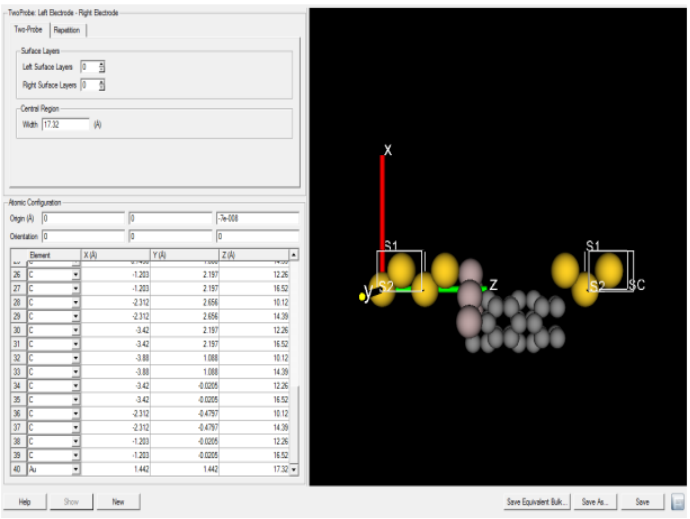
Following are the design specifications for CNT used to model CNT-metal contacts:

C-C bond length	1.422 Å
Type	Chiral
Radius	2.072 Å
Period	11.287 Å
Atoms in unit Cell	56
Band Gap	2.146 eV (Semiconducting)
Chiral Angle	19.1 degree

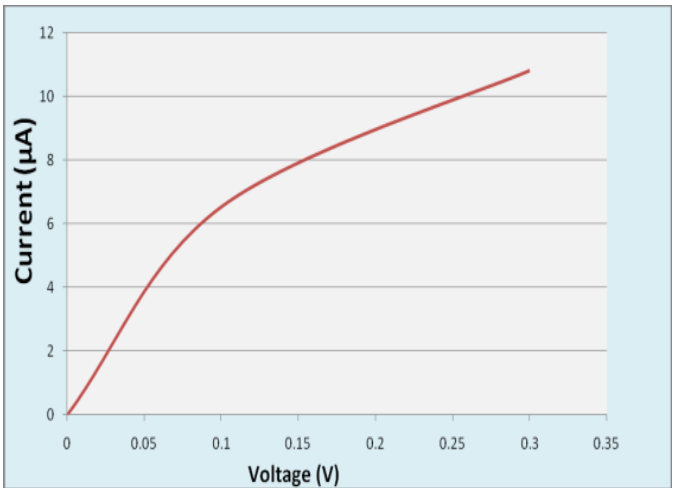
Model & Simulation 1: CNT – Al Contact Two

Probe System
Model of 17.32 Å



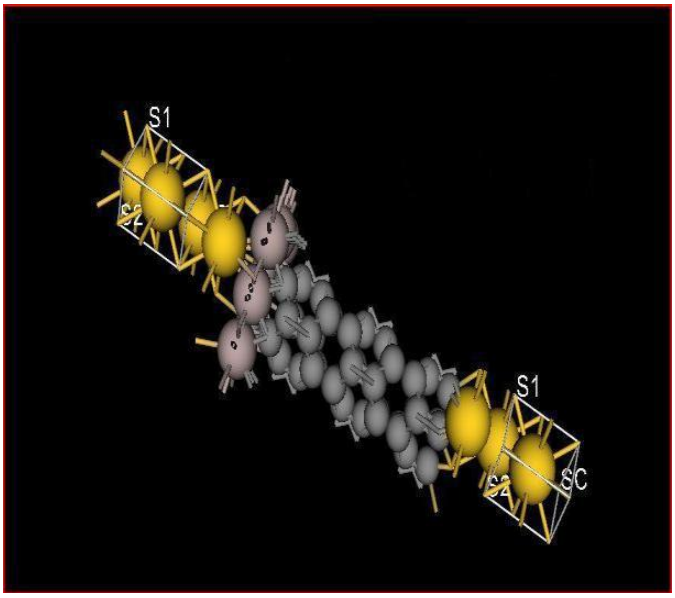


V-I Characteristic:

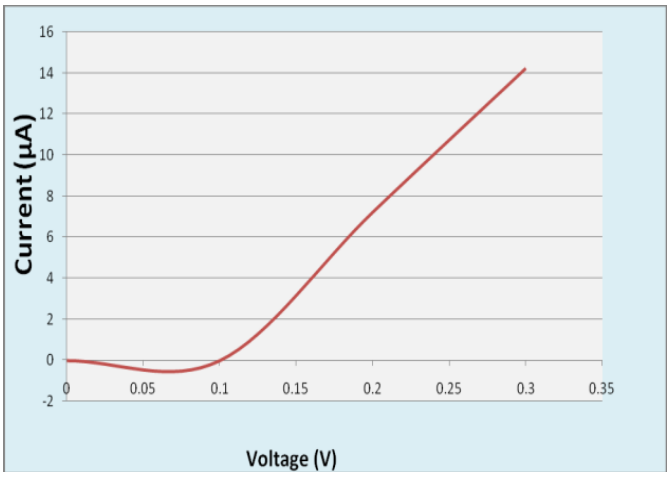


Model & Simulation 2 : CNT – Al Contact Two Probe System

Model of 21.92 Å



V-I Characteristic



SIMULATION METHOD:-

The quantum wise software with the first principles of ATK AND VNL allowsto focus on the properties of CNT of various (n,m) vectors.

II. SIMULATION RESULTS

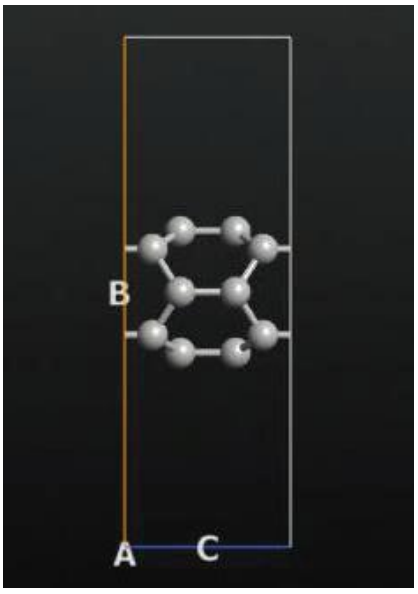


Figure.1.Bulk configuration of (4,0)

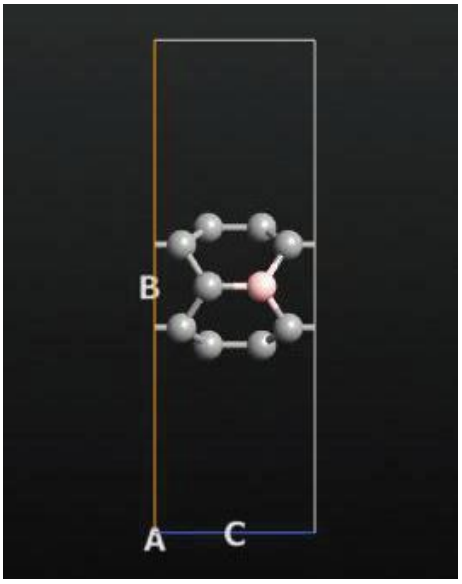


Figure.2.Bulk configuration of (4,1)

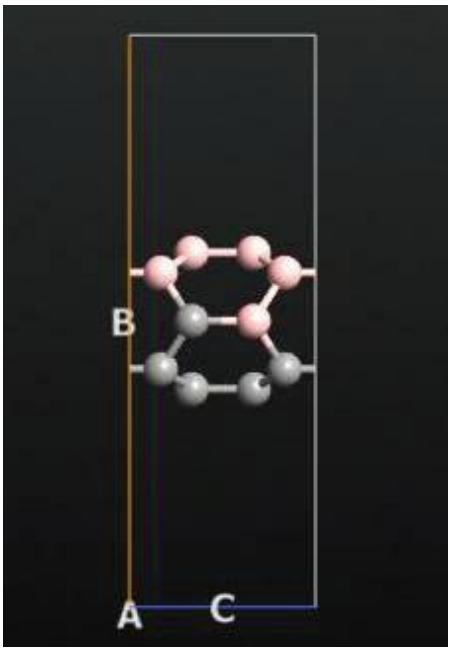


Figure.3.Bulk configuration of (4,5)

The band structure obtained using ATK of all the three configurations of carbon nanotubes is

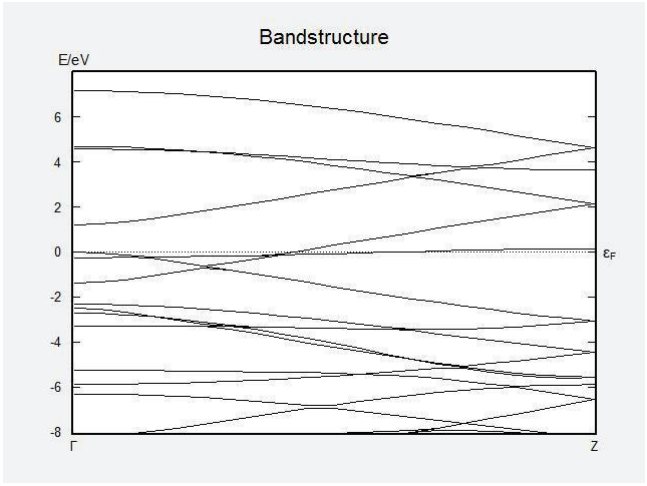


Figure.4.Band structure for (4,0)

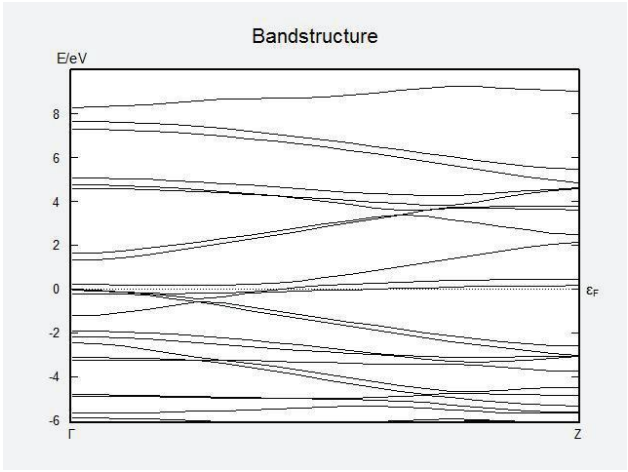


Figure.5. Band structure of (4,1)

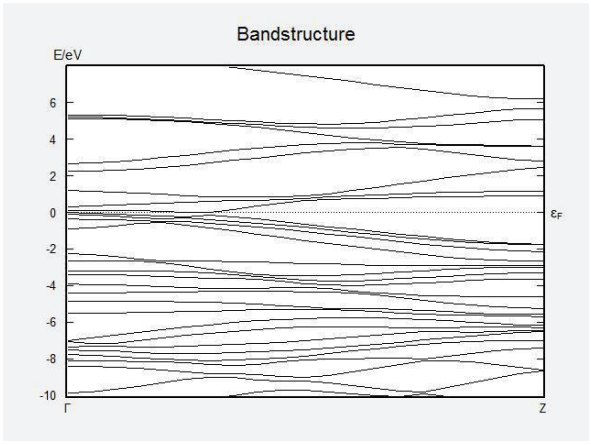


Figure.6. Band structure of (4,5)

III. RESULT & CONCLUSION

Reveals the computational studies of I-V characterstics of CNT-Metal by changing some various parameters. The Simulation results for the Voltage Current of different lengths (11.96 & 17.32 Å) shows conduction more of Ohmic kind, although the CNT used for the simulation is of Semiconducting in Nature. This is due to the direct transport as the CNTs are of very short lengths. The Metal-CNT contact for the length of 21.92 Å, the simulation results for the Current-Voltage are Close to the behavior of Shottky Diode. Computational analysis has been concluded and is proposed in the future work. So for getting the more satisfactory results, we need to perform the simulations of CNTs of longer lengths in order to avoid direct transport.

IV. FUTURE ASPECT OF THE WORK

Modeling and Simulations for Metal-CNT contact by varying the CNT Diameter. Modeling and Simulations for Metal-CNT contact by replacing the Carbon atoms in CNT by atoms of another element i.e. Si (For which the Model have been created and need to get the results) Modeling and Simulations for Metal-CNT contact on varying the temperature of the system**.**

V. REFERENCES

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