Modeling & Simulation of CNT – Al, Model with Two layers of Al using VNL

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Abstract *Modeling and Simulation of Metal-CNTs contact are performed through ATK and Virtual NanoLab Packages by Quantum wise. The Simulation results for the Voltage Current of length of 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.*

Keywords— *CNT, Chiral, linear atomic chain,VNL, aluminum* Introduction

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1. Introduction

Virtual NanoLab (VNL), package of Quantumwise gives access to a powerful set of modeling tools for investigating nanoscale structures through a user friendly graphical interface. The VNL software uses advanced software architecture and numerical methods to find solutions of the fundamental quantum mechanical equations describing the electronic properties of nanoscale objects, such as molecules, bulk and two-probe systems by use of the technique[1-6]

• *Density functional theory (DFT)*

• *Non-equilibrium Green's functions (NEGF)*

Based on the these techniques, VNL can simulate the detailed electronic structure and transport properties of molecules, crystals, nanotubes, and two-probe devices. The way of working with VNL is in many

aspects similar to what it is done in an actual experiment:

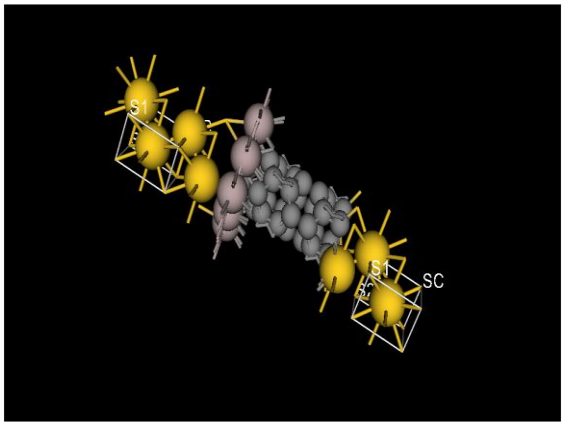
Nanotube Grower tool that can be used to construct and design carbon nano tubes A nanotube is characterized by two integer parameters, tube indices (4,2).

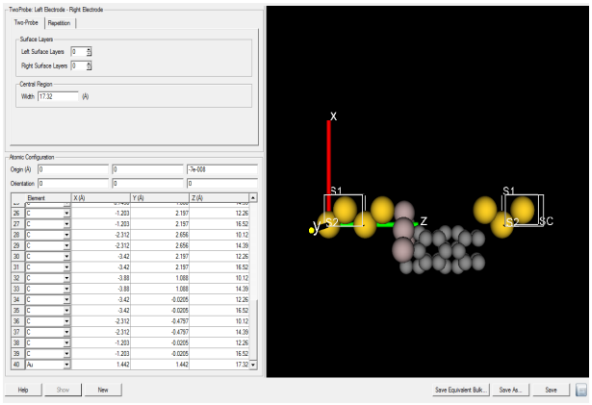
Following are the design specifications for CNT used to model CNT-metal contacts:

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

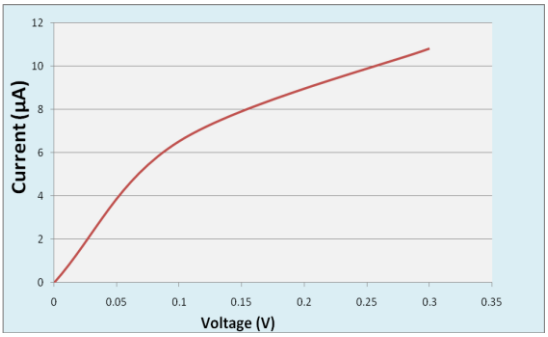
Model of 17.32 Å





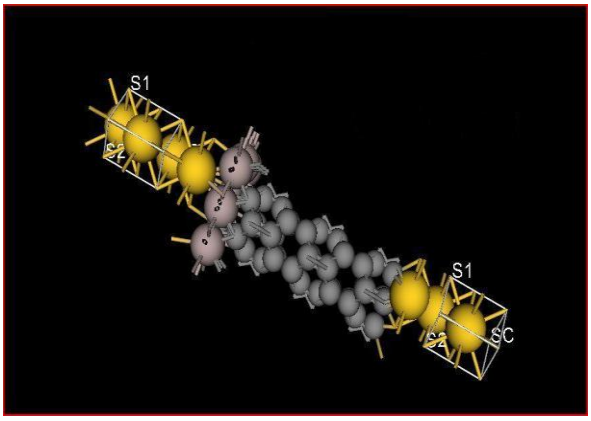
Executing the Python File Using the Job Manager of VNL .

I –V Characteristic

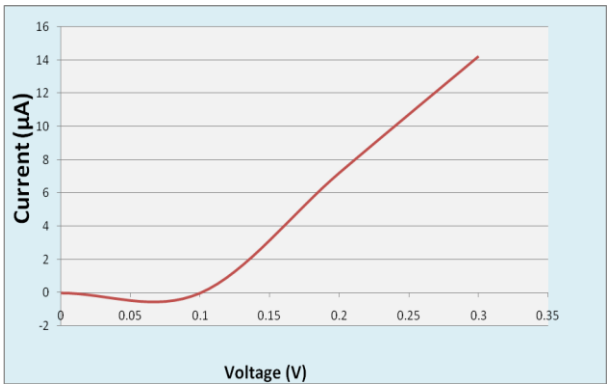


Model & Simulation 2 : CNT – Al Contact Two Probe System

Modelof 21.92 Å

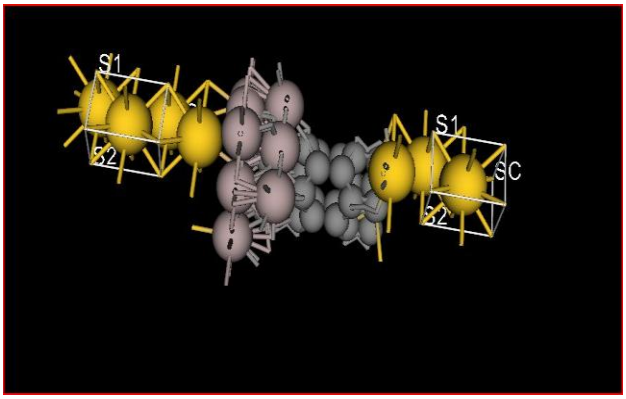


I-V Characteristic



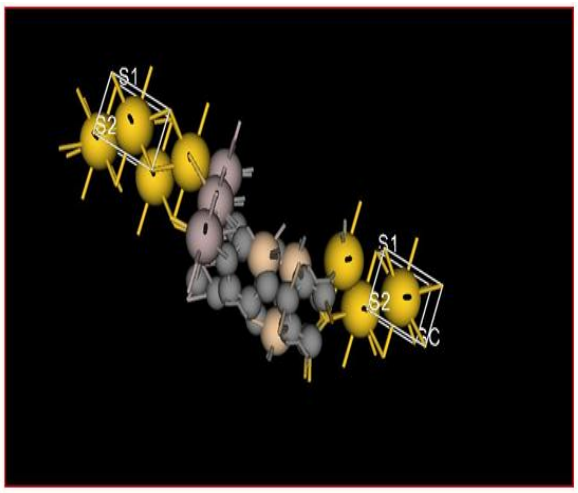
Model 1 : CNT – Al Contact Two Probe System

Model with Two layers of Al, 17.12 Å



Model 2 : CNT – Al Contact Two Probe System

Model by replacing Carbon by Si.



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 .

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**.**

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