# Modeling & Simulation of CNT – Al Contact Two Probe System

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**Abstract:** *The purpose of this paper is to model next generation carbon nanotube cum metal based Schottky diodes. Modeling of semiconductor devices is critical in understanding factors which may affect their performance. This allows greater understanding of the underlying physics at atomic level and aids optimization in both materials and lowers development costs by reducing the time and effect between design and fabrication of working prototypes. It gives a threshold to make a revolution in VLSI design. Carbon Nanotube (CNT) Based devices present a bright future and promise to sustain FET scaling for the validation of Moore's Law. In Silicon based devices, the gate oxide thickness has already entered the nanometer range; channel scattering from the rough oxide interface and tunneling through the thin oxide are becoming prevalent problems. Carbon nanotube based devices do not have these difficulties due to their extra ordinary electrical properties. Simulation of CNT – Al Contact Two Probe System is studied.*

*Keywords: CNT, Chiral, linear atomic chain,VNL, aluminum, Two Probe System*

## 1. Introduction

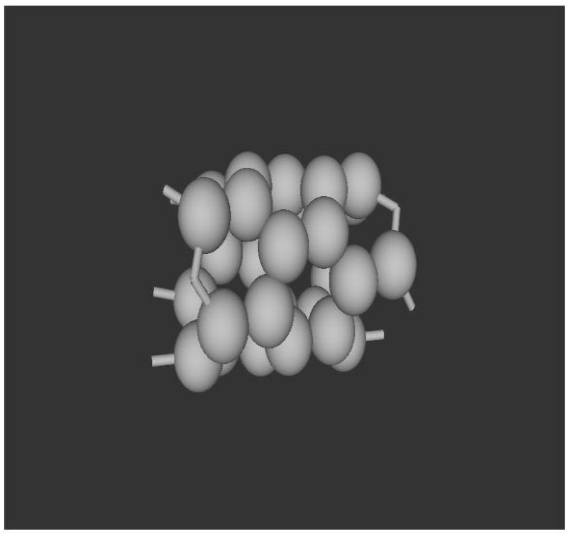
Nanotube Grower tool that can be used to construct and design carbon nano tubes A nanotube is characterized by two integer parameters, tube indices (4,2). The two-probe systems, in which two electrodes are in contact through a nano-scale piece of material the so called central or scattering region. In the following we will build three different two-probe configurations:

- A linear atomic chain
- A molecule between two metal surfaces
- A carbon nanotube

While setting up each of these systems, we will demonstrate different important and useful aspects of Virtual NanoLab (VNL). For a complete understanding, it is therefore important to go through all three cases. We will start with the linear chain[1-10].

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

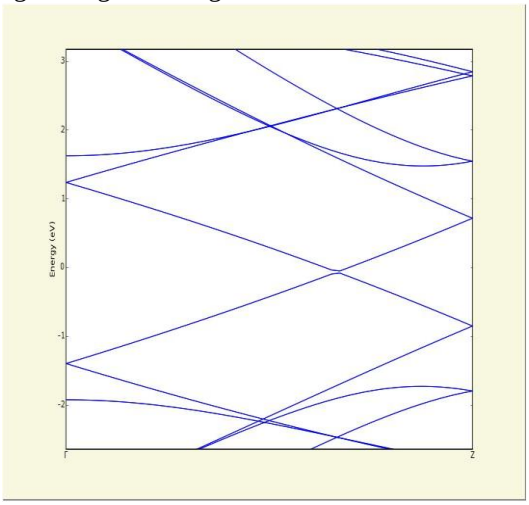
| | |
|---|---|
| C-C bond length | 1.422 Å |
| Type | Chiral |
| Radius | 2.072 Å |
| Period | 11.287 Å |
| Atoms in unit Cell | 56 |
| Band Gap | 2.146 eV (Semiconducting) |
| Chiral Angle | 19.1 degree |



**2. Tight-binding band structure of a (4,2) carbon nanotube.**

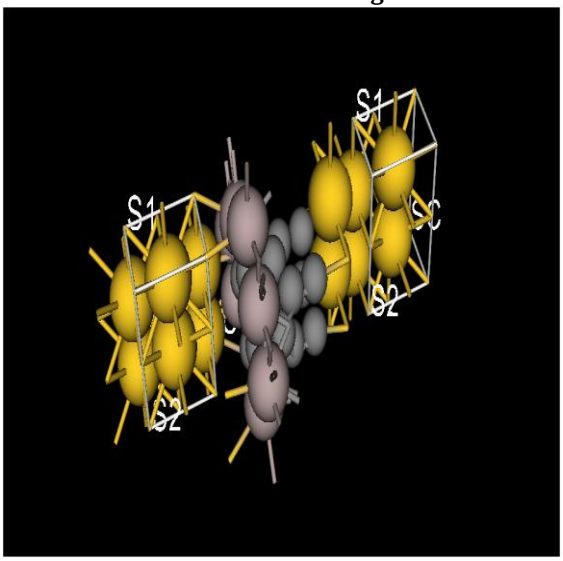
A Preview of the band structure of the nanotube in the energy area around the Fermi energy.
This plot is usually updates automatically when the tube indices are changed.

For the CNT (4,2) tube for the moment, VNL predicts that this particular tube is semiconducting. At the same time, the band structure plot appears to show a semiconducting structure. This is due to the fact that the preview of the band structure is generated on-the-fly using an analytic third-nearest-neighbor tight-binding formula.

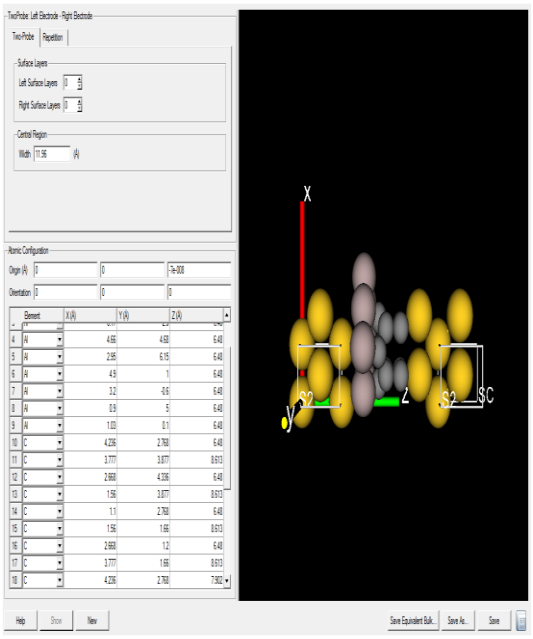



**3. Model & Simulation: CNT – Al Contact Two Probe System**

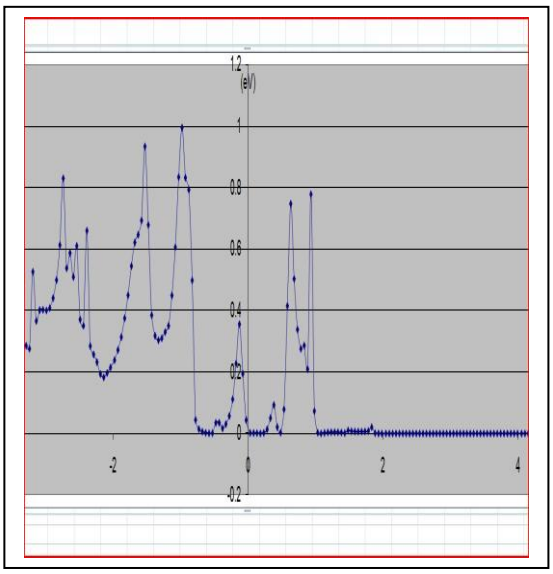
**Model 11.96 Å length**



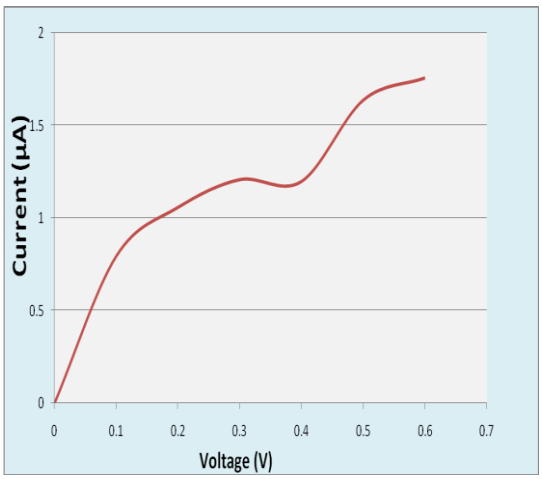

**Atomic Manipulator View of Model**




**Plot of Transmission Spectrum**




**I –V Characteristic**



## Conclusion

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 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.
So for getting the more satisfactory results, we need to perform the simulations of CNTs of longer lengths in order to avoid direct transport .

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