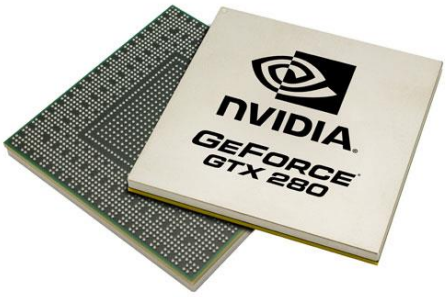

SIMULATION OF CARBON NANO TUBE AND ITS BEHAVIOR

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PROJECT OVERVIEW

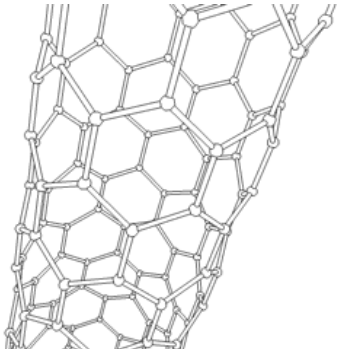
The main purpose of the project is to simulate and test the structure of carbon nanotube. Carbon Nanotubes are allotropes of carbon with cylindrical nanostructure and belongs to the structural family of Fullerene. Besides the simulation of structure of carbon nanotube the focus is also kept on the behavior of carbon atoms and their connecting bonds when a huge amount of physical force is applied on them.

Singled Walled carbon nanotubes with different arrangement of carbon atoms are simulated and forces are applied at the edges and at the center of the carbon nanotube. The resulting movement of carbon nanotube and the behavior of the bonds connecting between them is shown i.e the flattening and crushing effects are observed respectively.

INTRODUCTION

Carbon nanotubes (**CNTs**) are allotropes of carbon with a cylindrical nanostructure. Nanotubes have been constructed with length-to-diameter ratio of up to 32,000,000:1 significantly larger than for any other material. These cylindrical carbon molecules have unusual properties, which are valuable for nanotechnology, electronics, optics and other materials science and technology. In particular, owing to their extraordinary thermal conductivity and mechanical and electrical properties, carbon nanotubes find applications as additives to various structural materials. For instance, nanotubes form a tiny portion of the material(s) in some (primarily carbon fiber) baseball bats, golf clubs, or car parts.

Carbon nanotubes are categorized into:



- Single – Walled nanotubes (SWNT's)
- Multiple – Walled nanotubes (MWNT's)

Chemical Bonding in Nanotubes:

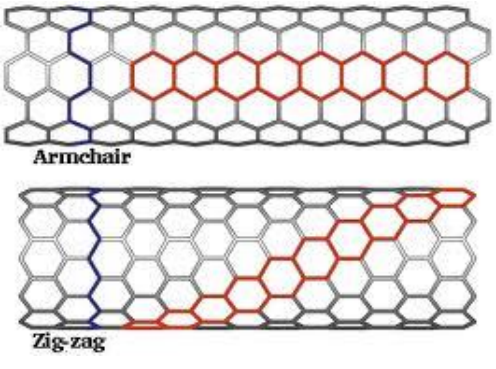
Hybridization of bonds present: sp^2 hybridization

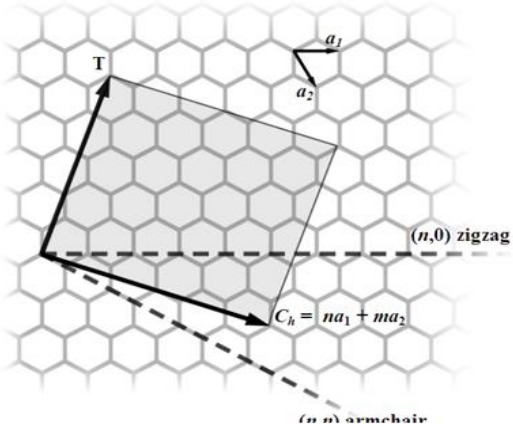
Types of Single walled nanotubes:

The structure of a SWNT can be conceptualized by wrapping a one-atom-thick layer of graphite called graphene into a seamless cylinder. The way the graphene sheet is wrapped is represented by a pair of indices (*n*, *m).*

The most important types of single walled carbon nanotubes are:

- Armchair SWNT's (n=m)
- Zigzag SWNT's (m= 0)





BEHAVIOR

The carbon nanotube physical structure can be demonstrated by considering carbon atoms as balls and the connecting bonds between them as springs connected in hexagonal manner and in turn forming a cylindrical structure.

Physical strength test:

When force is applied at the **center**:

The physical strength of the carbon nanotubes is tested by using the special setup shown below. The setup consists of platform and two boxes mounted vertically separated by a distance. These boxes acts as a support for holding the carbon nanotube in position. Then a box is dropped at the center of the carbon nanotube and as soon as the box hits the carbon nanotube it repels.

When force is applied at the **edge:**

To test the strength of the carbon nanotube in vertical direction, the scene is setup posing the carbon nanotube vertically stand on one surface edge. A box is dropped at the open ended edge and as soon as the box hits the edge of the carbon nanotube it repels. The box is dropped from various heights but it repels every time it hits the carbon nanotube in both cases.

Physics

This project includes cylindrical tube structure formed with hexagons. Carbon atoms are rendered as spheres and interatomic bonds as small cylinders.

- The interatomic bonding forces are represented by ideal springs with relaxed distance equal to bonding distance between carbon atoms.
- The angle between the neighboring atoms are again represented by ideal springs but the relaxed distance is considered in terms of angle. The relaxed angle is 120 degrees. The force is applied between the neighboring atoms if the angle is less than 120 degrees.
- To keep the nanotubes in a cylindrical structure another spring force is applied between carbon atoms in the cross-sectional cylindrical plane. The relaxed distance for this spring force is the diameter of the cylinder.

- To apply stress on the carbon nanotube, a cuboid is dropped on the carbon nanotube. The force for the cuboid is derived from the gravitational force.
- When the cuboid hits the nanotube it repels back due to opposition force by carbon nanotube (Structural force due to addition of bonding force and force from the neighboring atoms).

Graphics

- The color of the basement platforms is green and yellow.
- The yellow platform is the bigger than green platform and green platform sits on yellow platform.
- The vertical support blocks are blue in color.
- The balls are white in color and the connecting springs are yellow in color.
- The cuboid is pink in color.
- After cuboid hits the carbon nanotube the bonds between them expands in linear manner and returns to original shape after repulsion of cuboid.

Coding

- Creation of bonds between carbon atoms.
- Maintaining bonding angle between the neighboring carbon atoms
- Generation of cylindrical structure of carbon nanotube.

Code Repository in

EE470221

Path: home/cus-proj-base/boxes/boxes.cc

Simulation Results

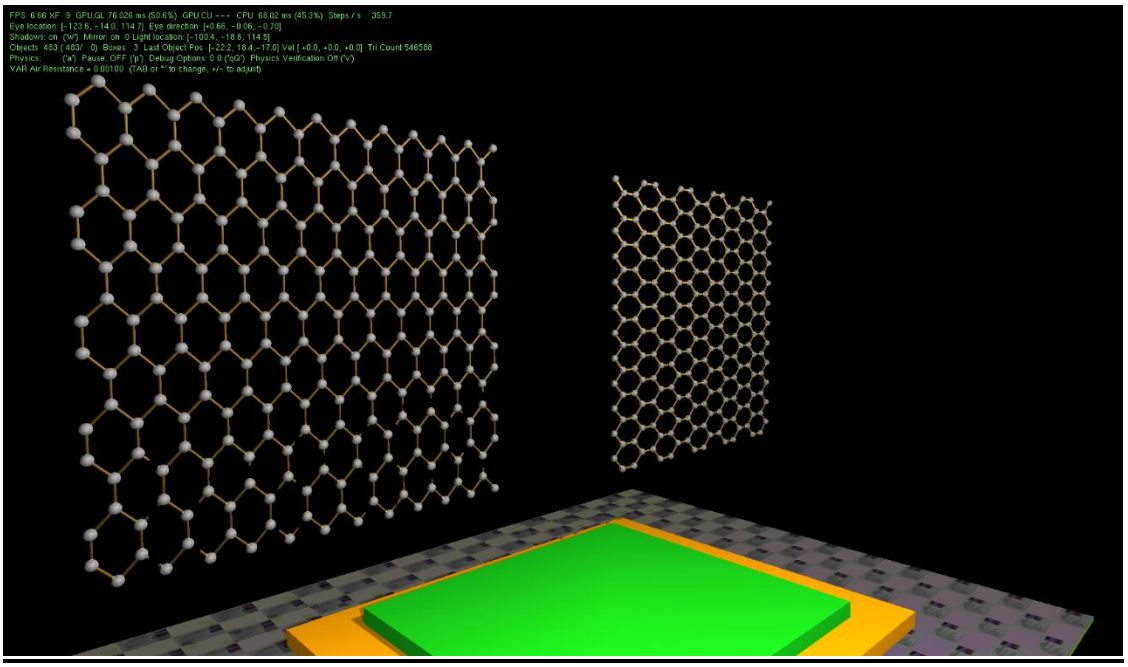


Fig 1: ZIGZAG AND ARM-CHAIR CARBON NANOTUBE

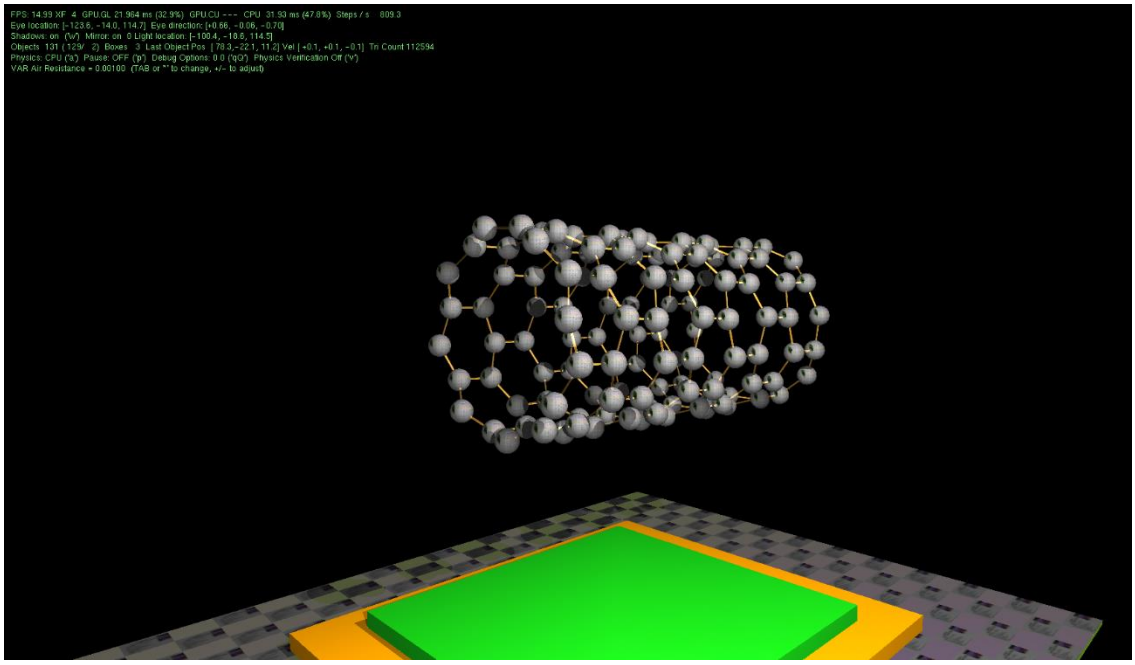


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FIG 2: ZIGZAG CARBON NANOTUBE (CYLINDRICAL STRUCTURE)

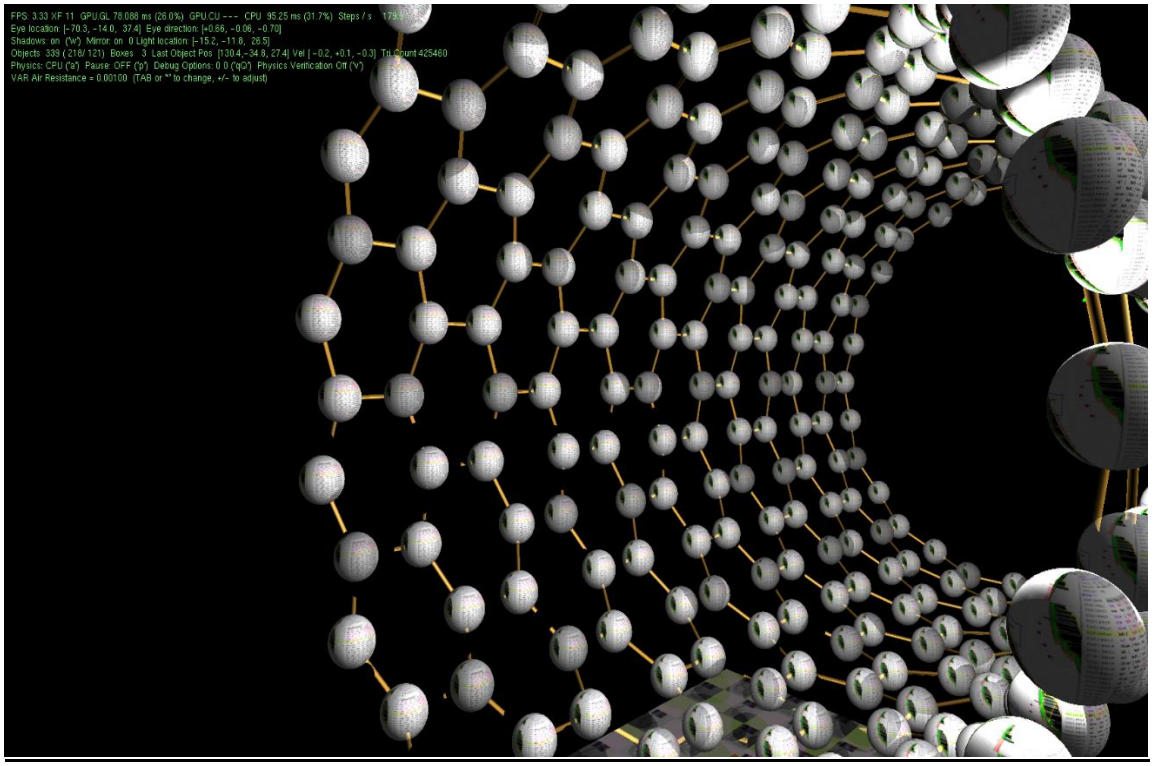

FIG 3: INTERNAL VIEW OF ZIGZAG CARBON NANOTUBE.

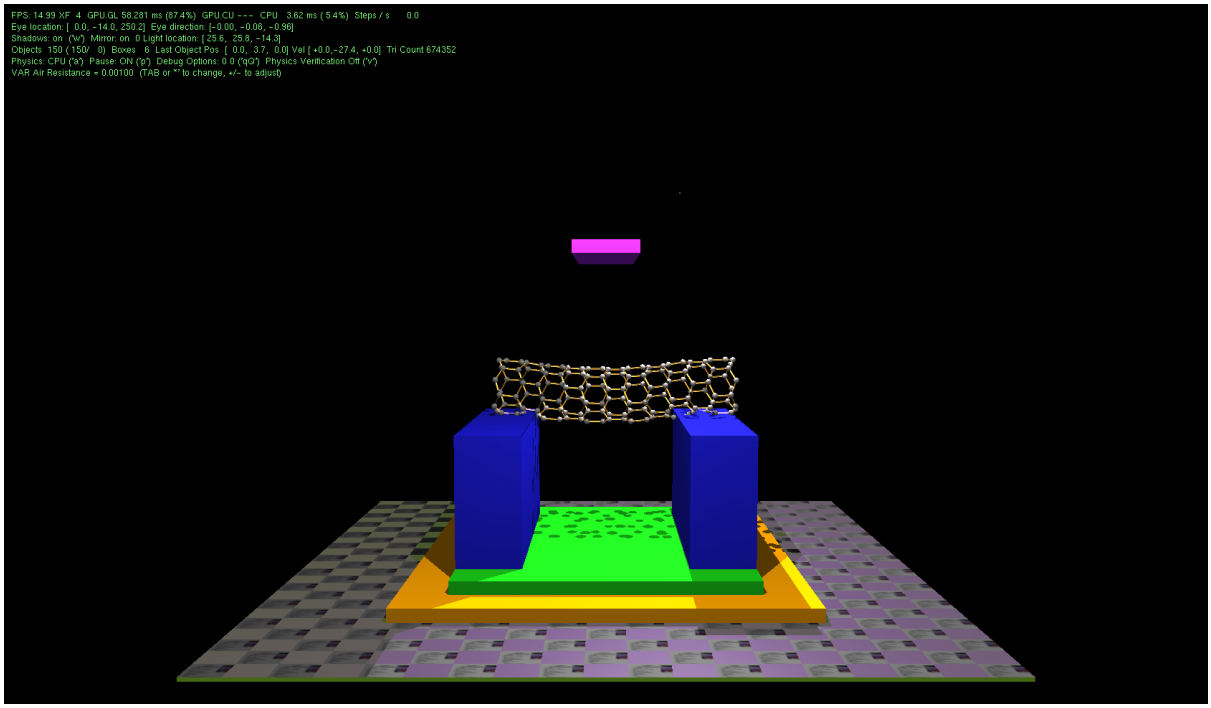

FIG 4: SCENE SETUP TO TEST CARBON NANOTUBE.

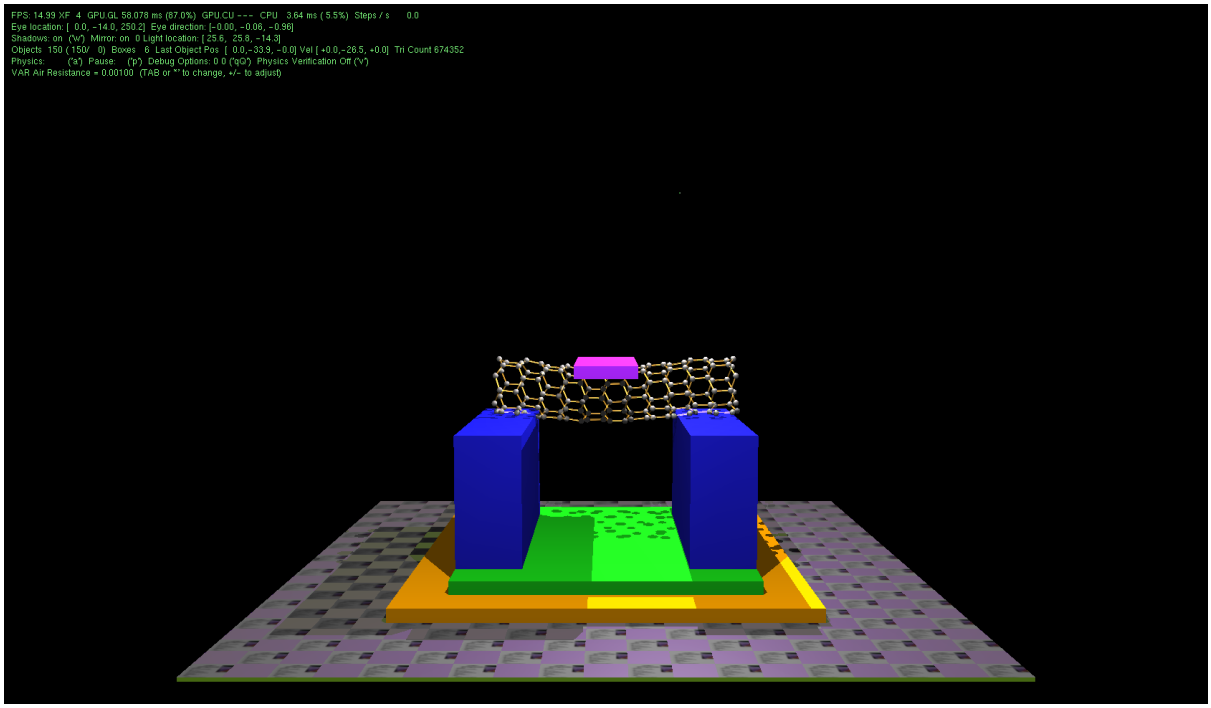

FIG 5: SCENE SETUP TO TEST CARBON NANOTUBE.

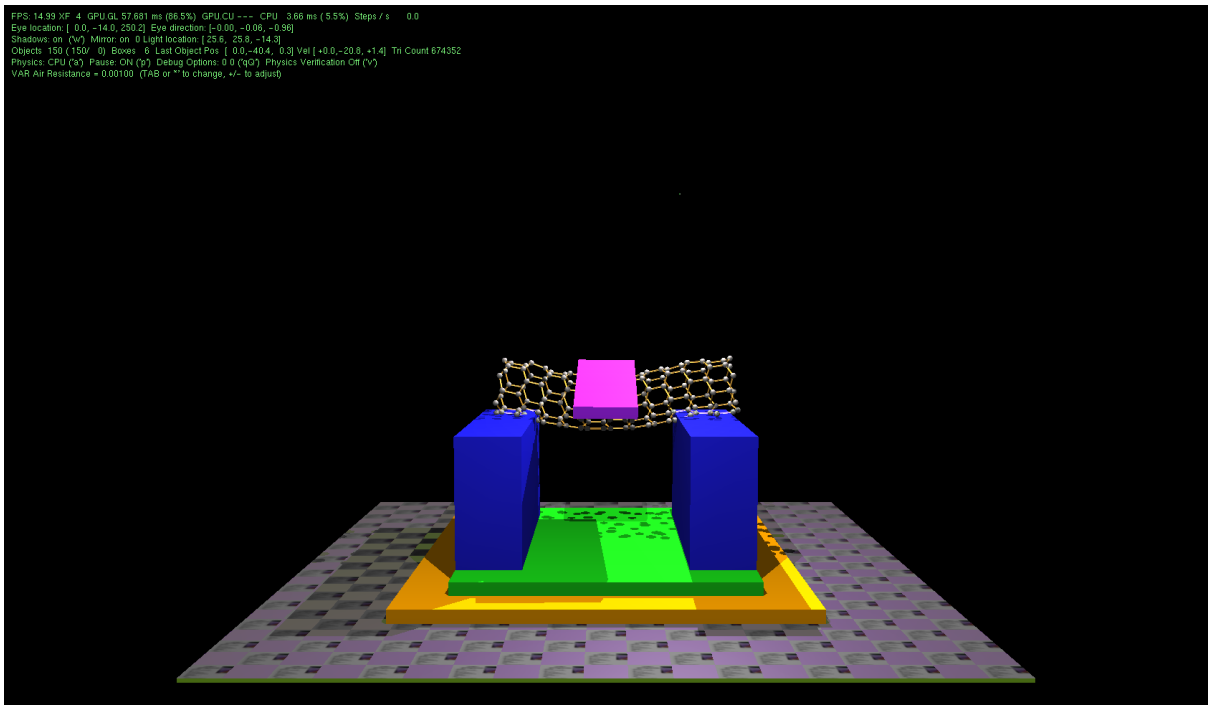

FIG 6: SCENE SETUP TO TEST CARBON NANOTUBE.

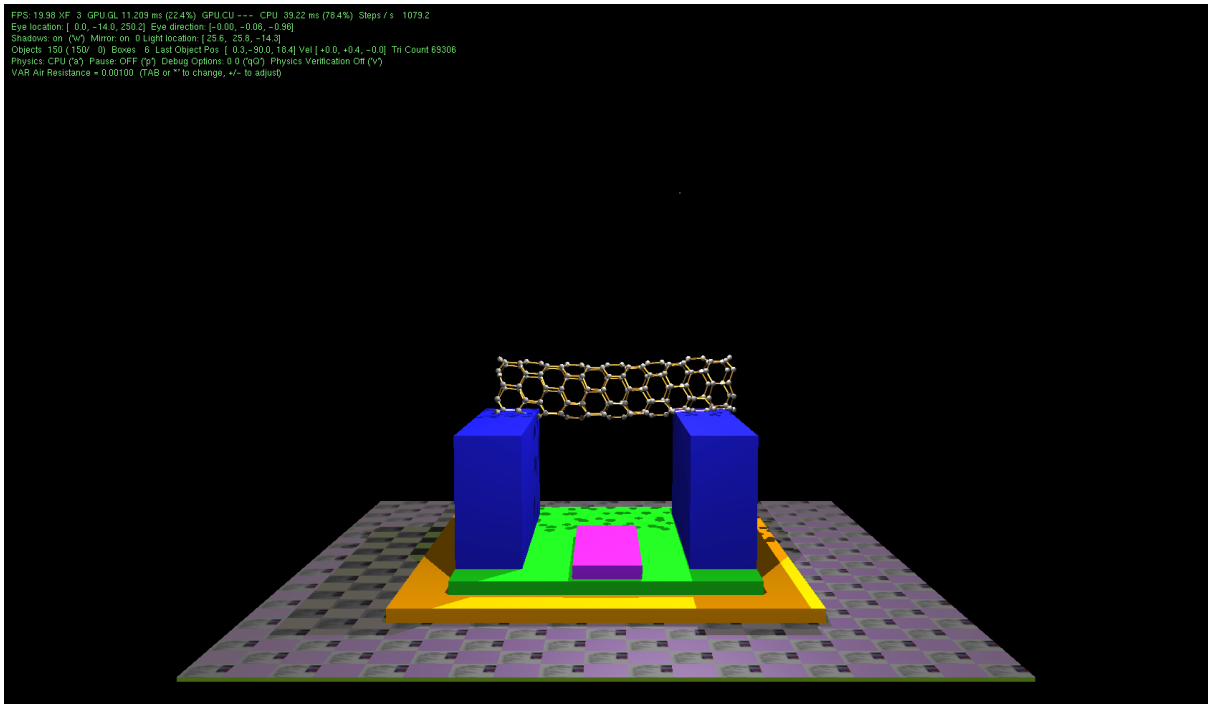

FIG 7: SCENE SETUP TO TEST CARBON NANOTUBE.

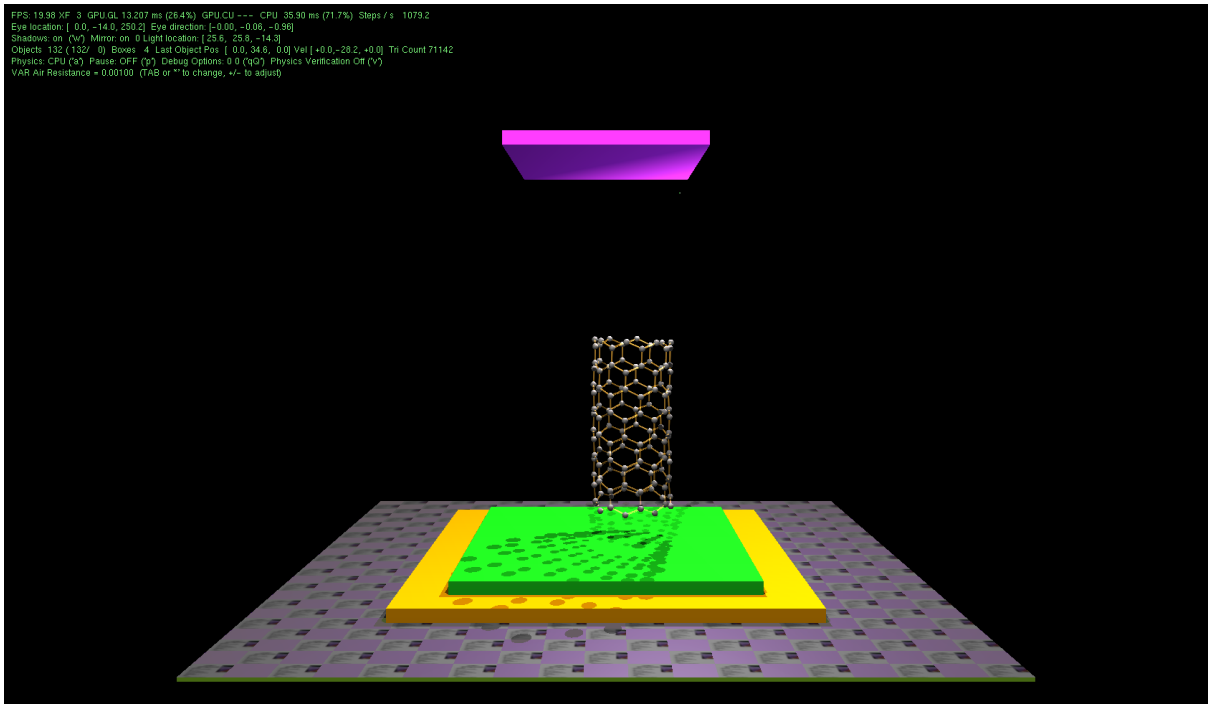

FIG 8: SCENE SETUP TO TEST CARBON NANOTUBE.

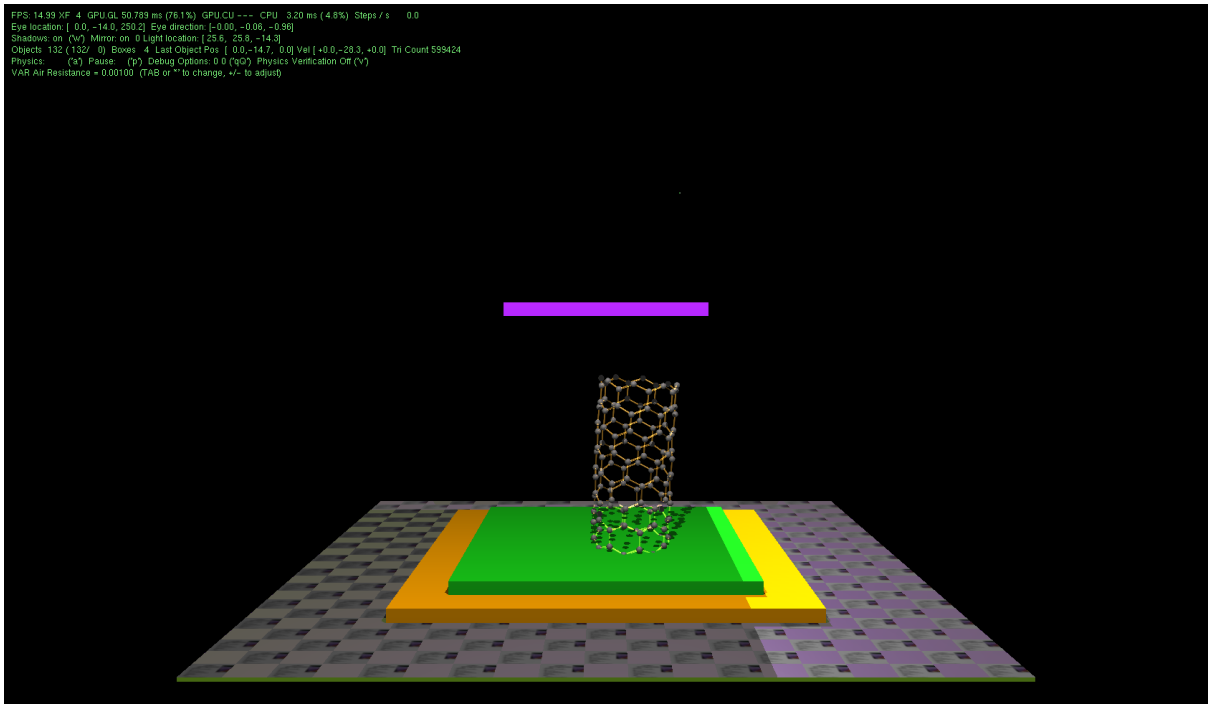

FIG 9: SCENE SETUP TO TEST CARBON NANOTUBE.

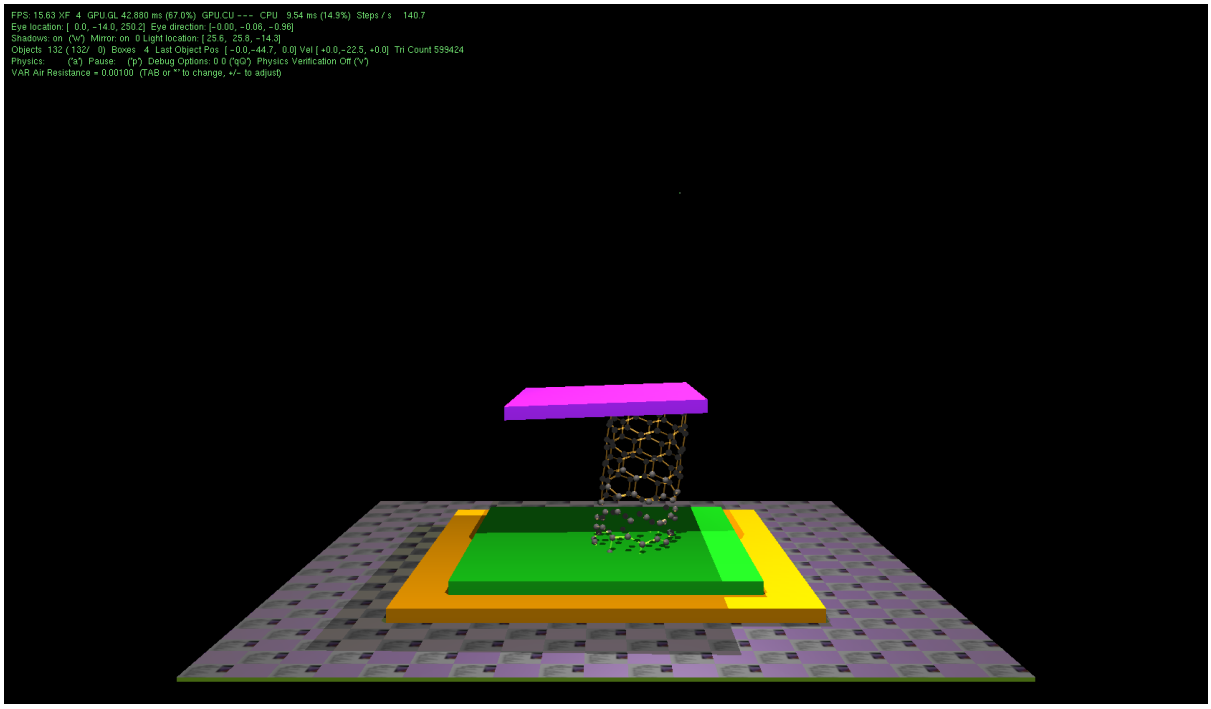

FIG 10: SCENE SETUP TO TEST CARBON NANOTUBE.

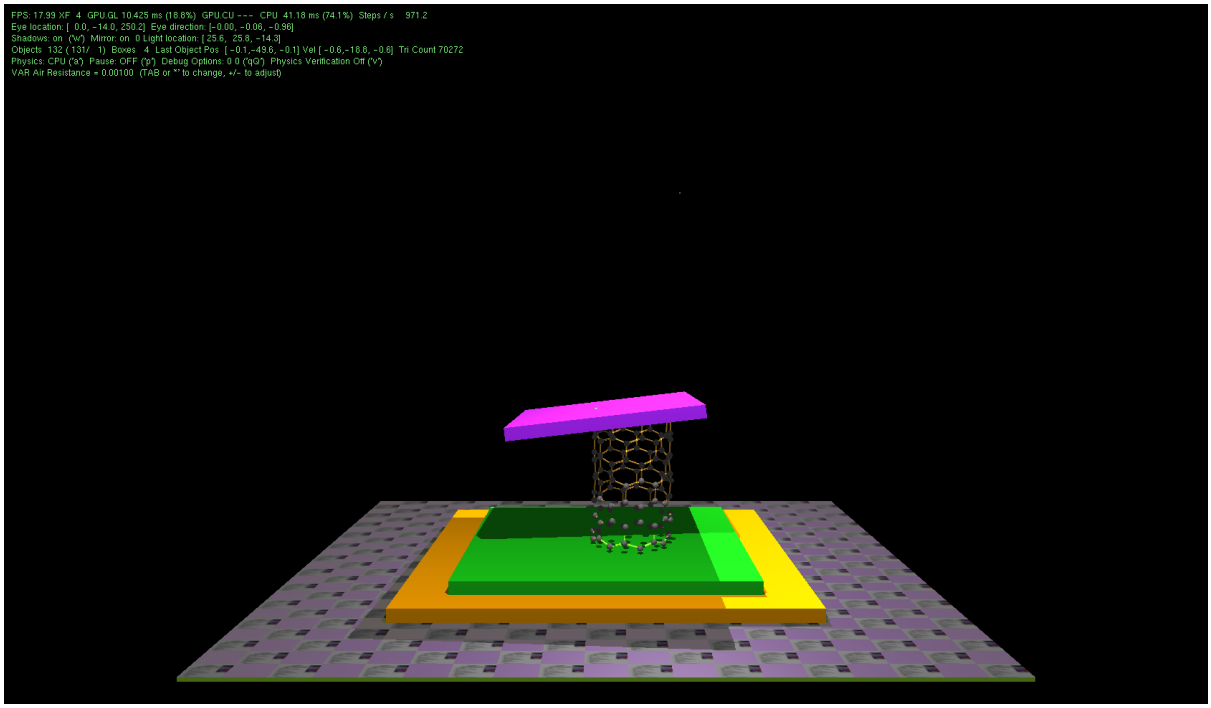

FIG 11: SCENE SETUP TO TEST CARBON NANOTUBE.