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Percolation in Carbon Nanotube Networks

William P. Grieder (Humboldt State University), Will Gannett (Humboldt State University), Ruth Saunders (Humboldt State University)

Abstract

Carbon nanotubes (CNTs) have become increasingly useful in different applications since they were discovered in 1991 by Sumio Iijima [1]. One of their many useful qualities is their electronic properties [2]. These CNTs, when formed into a network, can be used as transistors [3] or biosensors [4]. Transistors are devices that regulate either current flow or voltage and act as a switch; they are a crucial component of computers. Biosensors detect the presence of biomolecules. Efficient transistors and biosensors already exist; however, they are expensive to manufacture compared to these CNT networks. The ability of the CNT networks to be transistors or biosensors relies on the percolation properties of the networks. As long as these networks percolate, current can pass through the network from a source electrode to a drain electrode, which can then be modulated by an electrical or biological signal to make devices such as transistors useful.

Keywords: carbon nanotube, nano, nano networks, percolation, percolation theory

Introduction

Carbon Nanotubes are formed when sheets of graphene (carbon arranged in hexagonal structure) roll up to make a tube. Depending on the way that the graphene sheet rolls up, CNT's can be either metallic or semiconducting, as shown in Figure 1. When CNTs form, roughly 33% are metallicand the rest are semiconducting. This is determined by the placement of the electrons relative to each other. It is important to minimize the presence of metallic CNT's in the network, to make it easier to utilize these networks as transistors or biosensors, because metal-

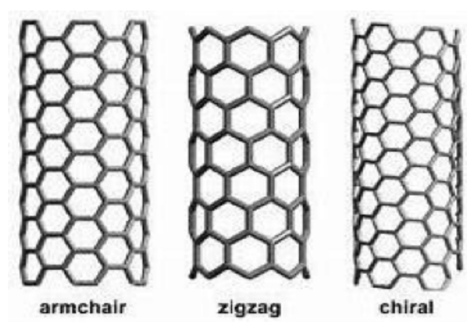


Figure 1: Diagram of Carbon Nanotubes showing different configurations: Armchair - Metallic, Zigzag and Chiral - Semiconducting [2]

lic tubes do not respond to external stimuli the same way semiconducting tubes do. Advancements in manipulating these CNT networks have made it possible for most metallic tubes to be stripped away, leaving only ~2% of the CNTs in the network as metallic [5].

Percolation

Percolation occurs when there is a pathway for something to travel through a given space, such as a forest fire traveling through a forest or using logs or rocks to cross a river [6]: only when there are enough connections can the fire spread through the forest or a person cross the river. In this case, percolation occurs when there is a pathway of CNTs that connects the source electrode to the drain electrode, allowing current to flow. In percolation theory, there is a useful value known as the percolation threshold. The percolation threshold is the lowest density that percolation occurs in an infinite network [6]. In finite networks, this is defined as the density where 50% of networks formed with that density will percolate. The percolation threshold of randomly placed sticks is ~6 sticks per square micron for 1 micron sticks, given by the Equation 1 [6].

$$\rho_{th}=4.26/(\pi l^2)$$

where ρ_{th} is the percolation threshold and l is the length of the sticks

(Equation 1)

It is crucial to fully understand the behavior of these networks in order to make reproducible devices. There is a balance between maximizing pathways for the current by having a high density and losing some of the sensitivity of the networks by being too far above the percolation threshold. The study of the percolation threshold for these networks will deepen our understanding of the behavior of these CNT network devices and allow us to provide experimentalists with information about optimal densities.

CNT Network Properties

Semiconducting materials are essential for transistors. Transistors behave like a switch turning on and off in response to an external electric field. Unlike metals, semiconductors have a resistance that can be changed when they are placed in an external electric field [7]. Most of the tubes in CNT networks are semiconducting and the relevant resistance for these networks are in the junctions between tubes. There are three types of junction: metallic-metallic (M-M), semiconducting-semiconducting (S-S) and metallic-semiconducting (M-S). The most responsive of these is the resistance between M-S junctions, which have a resistance on the order of 10^7 Ohms. The S-S junctions have a resistance on the order of 10^6 Ohms and M-M junctions have a resistance on the order of 10^5 Ohms [8]. For the network to function correctly, there cannot be a completely metallic percolation as the resistance of the network will not respond to the external field. When a percolating network is in an external electric field the resistance changes, allowing the network to have on and off states and act as a field effect transistor. The M-S junctions optimize the effectiveness of the transistor but also risk the possibility of metallic pathways [3]. Biosensors act in a similar way, where the electric field from charged particles affect the resistance of the network. The particle could then be determined from how the network resistance changes [4]. In order to determine the percolation threshold, which reduces the risk of metallic pathways, the percolation of these networks are simulated in a coding software, Python, for different network sizes and nanotube lengths. The output from the simulations are then compared to experimental results that show a percolation threshold of ~11 CNTs per square micron [9].

Method

The simulation sets an area for production of CNTs. The channel length is the distance between the electrodes where the width remains constant at 10 microns. The program then creates a stick to represent a CNT. An initial point is established within the channel, then another point is established at some specified distance (CNT length) and positioned at a random angle. The placement of these points are given by Equations 2 and 3, shown in Figure 2. These CNTs are giving a 2% chance of becoming metallic, while the rest become semiconducting. This production of sticks continues until there is a specified density of CNTs per square micron within the channel as shown in Figure 3.

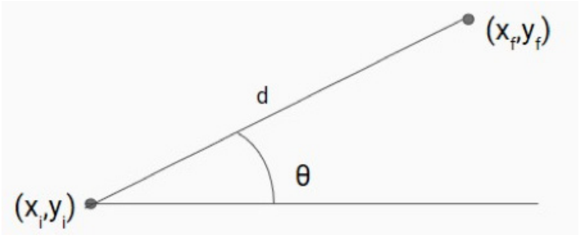
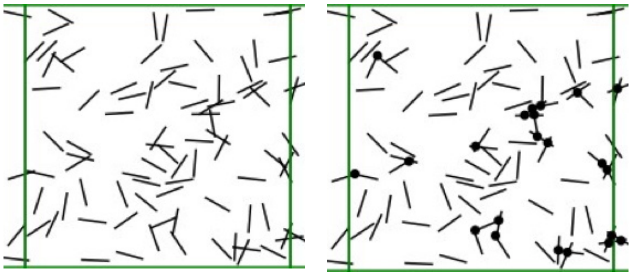


Figure 2:This stick represents a CNT where d is the length and θ is the random angle it is oriented in.

$$xf = xi + d\mathrm{Cos}(\theta) \qquad \text{(Equation 2)}$$
$$yf = yi + d\mathrm{Sin}(\theta) \qquad \text{(Equation 3)}$$



a) b)

Figure 3:
a. An example of a completed network
b. Same network with the junctions marked

Then the program analyzes the network to determine which CNTs are connected. The code stores the information of these connections in an adjacency matrix. Each component in the adjacency matrix is weighted with the value of conductance, given by Equation 4, between the respective junctions.

$$G = \frac{1}{R}$$

where G is conductance and R is resistance

(Equation 4)

The conductance of each junction is then used to find the conductance of the whole network. If there is zero conductance, then the network does not percolate between the electrodes. For a specific channel length, the simulation is run 100 times for increasing density. The fraction of the 100 networks that percolated is plotted as a function of density, as shown in Figure 4.

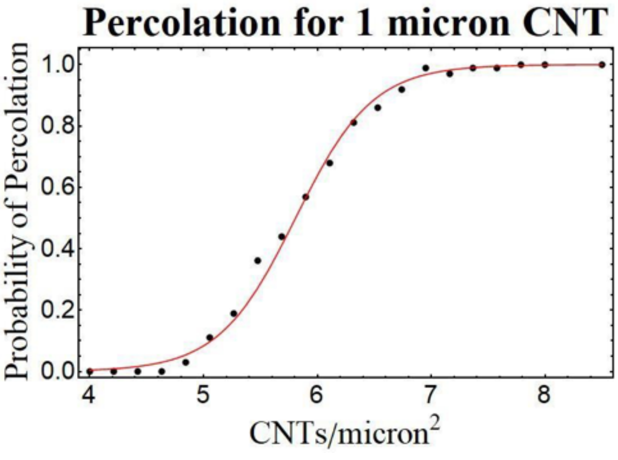


Figure 4: This plot shows the percolation progression for 10 micron channel length with 1 micron CNTs, where each point in this plot represents data from specific densities.
(Density is in CNTs per square micron , Fraction of percolating networks out of the 100 simulated networks)

Results

This simulation is run for channel lengths ranging from 5 microns to 70 microns with a constant width of 10 microns. It is also run for CNTs of lengths of 1 and 2 microns, as shown in Figure 5. In reality, the network is made up of tubes with lengths distributed between 1 and 2 microns. As the length of the of the CNTs were increased, the density of CNTs per square micron needed to achieve percolation quickly decreased. As the channel lengths increased, the density needed for percolation increased. The percolation threshold (the density when ~50% of the networks produced at that density will percolate) for networks with 1 micron long CNTs, are between 5 and 8 CNTs per square micron, while networks with 2 micron long CNTs needed densities between 1 and 2 CNTs per square micron, as shown in Figure 6. These results come from a simulation that uses any angle to orient the CNTs, but the CNTs tend to naturally align with each other, giving them a higher probability of being within certain angles, which is simulated as shown in Figure 7. This may explain why the above results disagree with the experimental percolation threshold. The needed density for percolation increases as the CNTs become more aligned, as shown in Figure 8. This happens since they are less likely to connect with other CNTs when they are parallel, as shown in Figure 7.

Figure 5: This figure shows a 10 micron channel length with density of ~ 3 CNTs per square micron using (a) 1 micron CNTs and (b) 2 micron CNTs. Red CNTs are metallic, black CNTs are semiconducting.

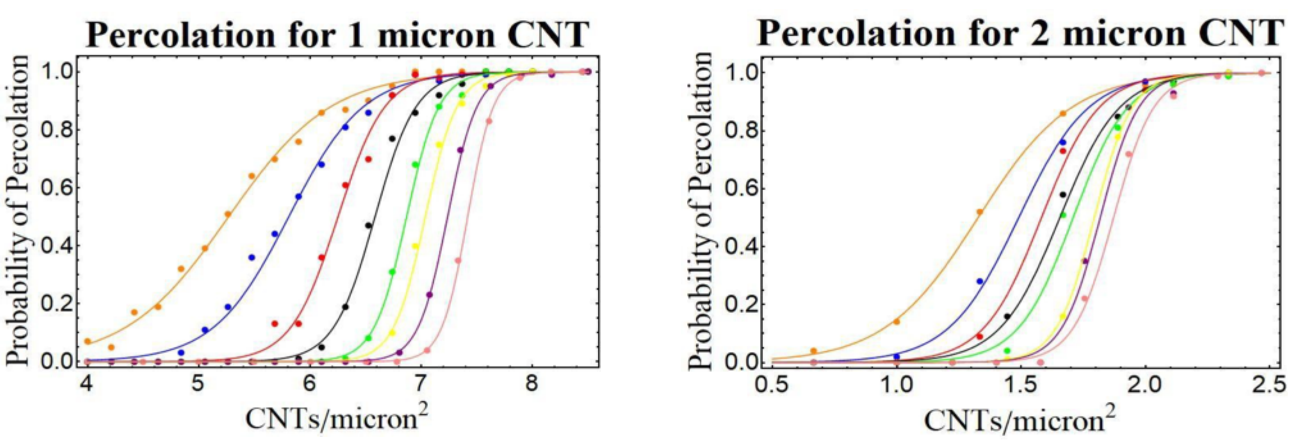
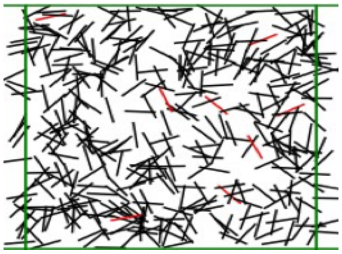
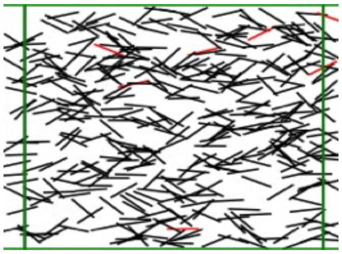


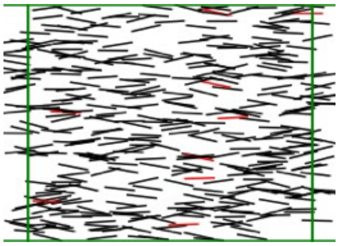
Figure 6: These plots show the progression of percolation as the channel length increases from 5 microns to 70 microns for (a) 1 micron CNTs and (b) 2 micron CNTs.



a)

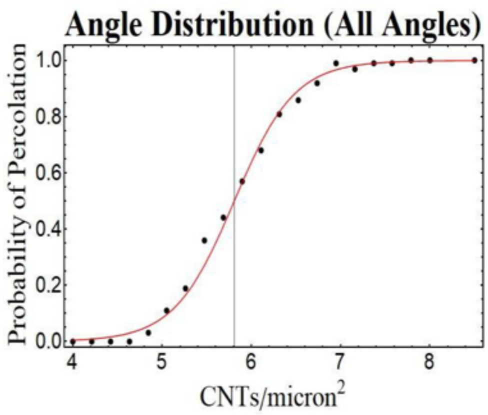


b)

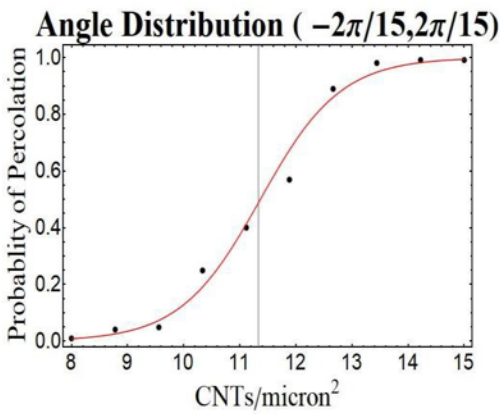


c)

Figure 7: The CNTs are oriented between (a) all angles, (b) -π/4 to π/4 radians, and c) -2π/15 to 2π/15 radians.



a)



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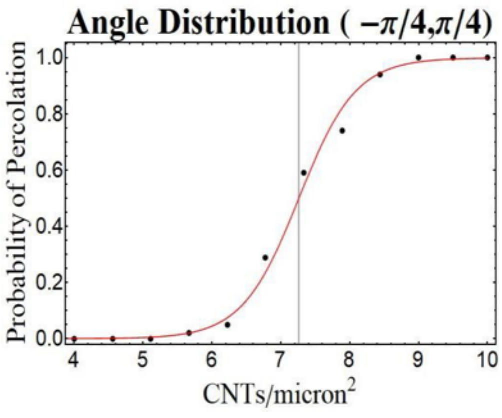

b)

Figure 8: Progression of percolation for 1 micron CNTs in 10 micron channel length (a) with all angles included, (b) with only angles between -π/4 to π/4 radians included, (c) with only angles between -2π/15 to 2π/15 radians included.

Future Work

Length Distribution

This code has been making networks with CNTs of a specific length of either 1 or 2 microns, when in the real nanotube networks, there are CNTs with lengths ranging from 1 to 2 microns long. Modeling this length distribution will affect the percolation threshold but will hopefully help bring the percolation threshold to the desired density.

Better Angle Distribution

Although there has been some angle distribution in the code, it doesn't include a distribution of probability for certain angles. The CNTs are much more likely to be parallel than they are likely to be at an angle to each other. Not only does this need to be changed but, since CNTs are so small, they don't have much effect on CNTs far away from them. This leads to localized groups of CNTs that could be aligned in one direction, while another localized group is aligned in another.

Curved CNTs

This code has been treating all the CNTs as though they are completely straight lines. Realistically, CNTs are curved, which might not have much effect on the percolation, but it is noticeable enough phenomena to include in the code.

Bundled CNTs

The same phenomena that causes the CNTs to align also causes them to bundle up together, which will greatly affect the percolation threshold of the networks. These bundles also tend to be mostly metallic, which will also greatly affect their use as transistors or biosensors.

Conclusion

The theory for percolation threshold for randomly placed sticks give a result of ~ 6 CNTs per square micron for a network of 1 micron CNTs [6], but our simulations produce results that still do not align with experimental results found in a previous study [9]. Without restricting the angles at which the CNTs lie, these simulations produced percolation thresholds at 5 - 7.5 CNTs per square micron for 1 micron CNTs and 1.25 - 2 CNTs per square micron for 2 micron CNTs. As the angles became more and more restricted, the percolation threshold increased much closer to the experimental results. However, in order to make the simulation represent real world CNT networks more accurately, some more modifications will need to be done to the code.

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