



Characteristics of Carbon Nanotube Networks: The Impact of a Metallic Nanotube on a CNT Network

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Technical Report Abstract Page

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Characteristics of Carbon Nanotube Networks: The Impact of a Metallic Nanotube on a CNT Network

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The impact of metallic carbon nanotubes on a carbon nanotube (CNT) network structure is evaluated. Metallic tubes reduce the mobility of CNT networks, thus reducing their switching speed in electronic devices. It is anticipated that certain CNT network layouts or topologies will be more resilient to the impact of metallic tubes. Classes of networks have been identified such as regular, random, and scale-free. This study considers the performance of a variety of network classes in the presence of a metallic tubes. *Mathematica* commands are included in this report to demonstrate the operation of the software tool implementing the analysis as well as the theory behind its operation. While these results provide direction for possible nanotube topology design rules, more work needs to be done to verify and extend these results.

Electron and hole mobility provide a measure of the rate of current flow as a gate voltage is applied. The higher the mobility, the faster the gate can switch; this leads to faster computation and faster processors, e.g. faster routers, wireless links, computers, etc. Mobility is relatively easy to predict for a single carbon nanotube. Unfortunately, mobility becomes extremely complex for networks of tubes. Thus, given a network of tubes with varying degrees of randomness in their interconnections, what can be said about mobility? Are there network structures that yield better mobility results than others? Some network structures may be more resilient to the impact of metallic "short

circuits". The nanotube modeling technique described in Ref. 1 is used to evaluate such networks. A network topology that is least impacted by metallic edges may be ideal for use in production. This report attempts to identify ideal CNT topologies by generating networks with various properties and examining their resilience to randomly selected metallic tubes. Nanotubes are positioned to form pre-determined graph structures in order to determine the characteristics of an ideal network structure.

First, consider the impact of metallic tubes on the current on/off ratio of a randomly generated nanotube network. Figure 1 shows the current on/off ratio as the proportion of metallic tubes increases over a range of tube densities (tubes/square micron).

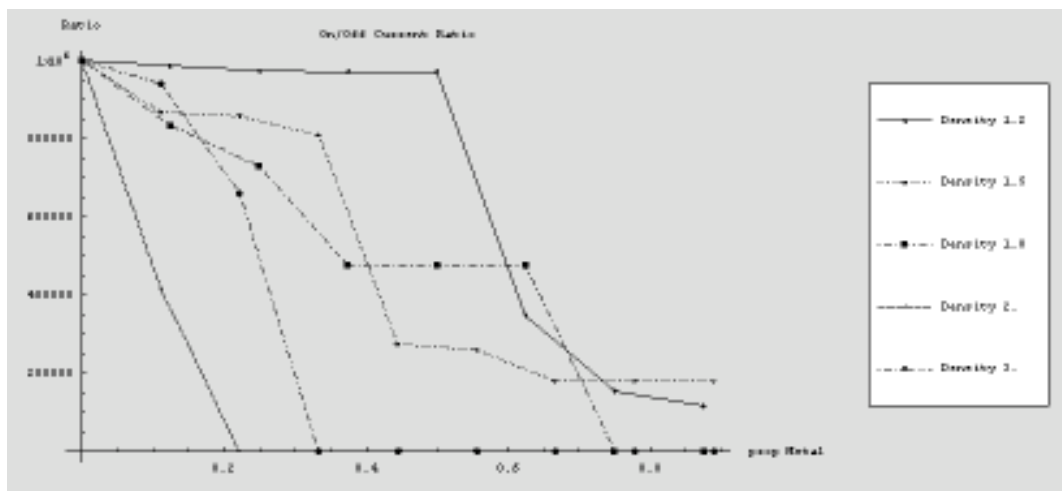


Figure 1 Channel widths are 3 microns and length is 1.5 microns. Tubes are 2.0 microns in length.

For the same conditions as shown in Figure 1 consider the impact of metallic tubes on mobility. While relatively easily controlled parameters such as channel area and tube density have an impact for a given proportion of metallic tubes, a more difficult variable to control and understand is the topology of the CNT network with respect to randomly positioned metallic tubes.

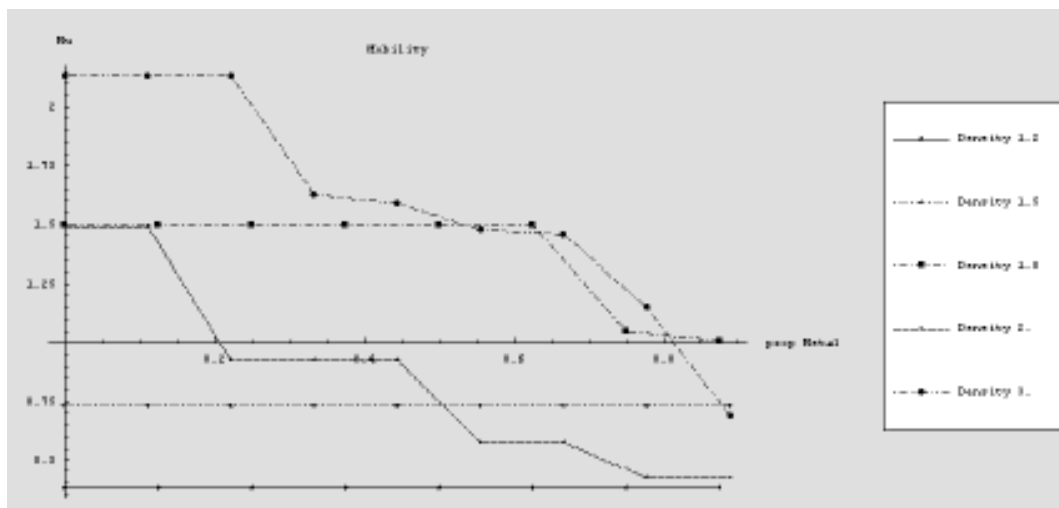


Figure 2 Mobility as a proportion of metallic tubes and tube density. Channel widths are 3 microns and length is 1.5 microns. Tubes are 2.0 microns in length.

A key component of the tube layout is the overall directionality of the tubes, that is, the angle of each tube relative to all other tubes. Isotropy quantifies the directionality of the tubes and is defined as $\frac{\sum l \cos a}{\sum l \sin a}$ where l is the tube length and a is the tube angle. Tubes that are nearly aligned have a high isotropy and tubes that are randomly oriented have a low isotropy. Figure 3 shows the isotropy of a set of CNT networks with constrained tube angles. The tube density is 1.2 per micron and lengths are constant at 3 microns. The angles range from being constrained between -1 through $+1$ degrees to -90 through $+90$ degrees.

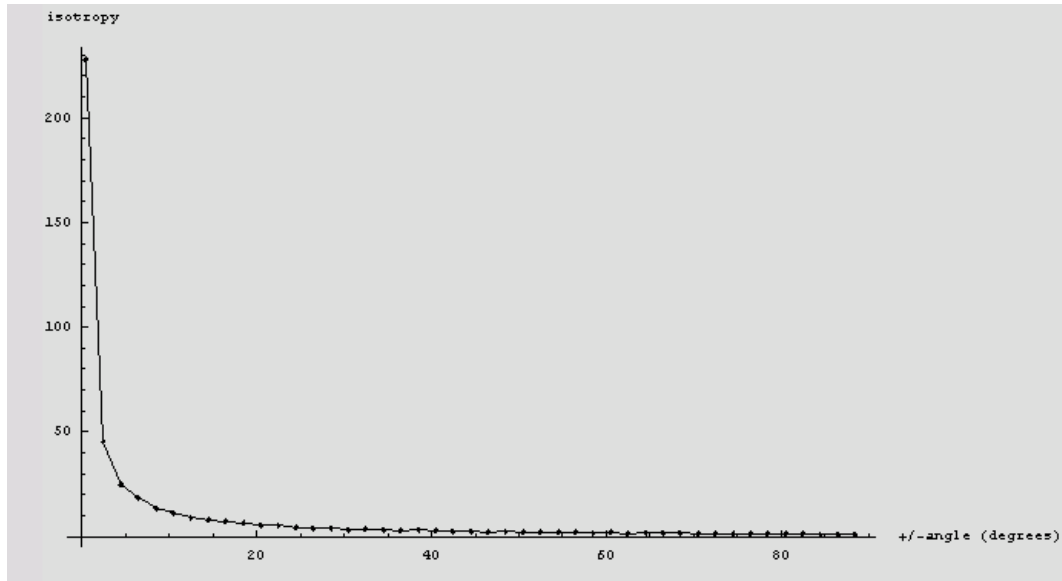


Figure 3 Isotropy as a function of tube angles.

The angle of each tube can be considered to encode information. Entropy, from an information theoretic viewpoint, measures the amount of information. Angle entropy is defined in this paper as $-\sum \Pr(a) \log_2(\Pr(a))$ where a is the tube angle and Pr is the probability of a tube with angle a given the network under analysis. The angle entropy of the network analyzed in Figure 3 is shown in Figure 4. The more random the angle, the more angular entropy exists and thus there should be a relationship between isotropy, angular entropy, the type of networks that are formed, and ultimately, their performance and resilience to metallic tubes.

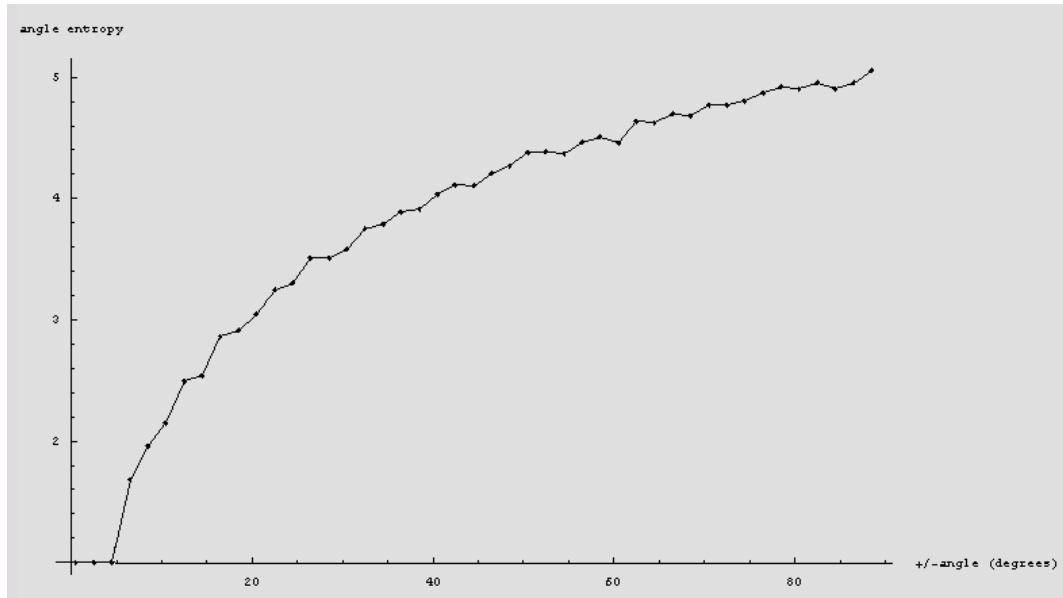


Figure 4 The angle entropy as a function of tube angles.

Clearly there is a relationship between isotropy and angle entropy as shown in Figure 5 for the same networks analyzed in the previous figures. High angle entropy means that the directionality and thus the isotropy are low. Information can be stored in tube angles; reading the information from the change in resistance of tube angles is simulated later in this paper.

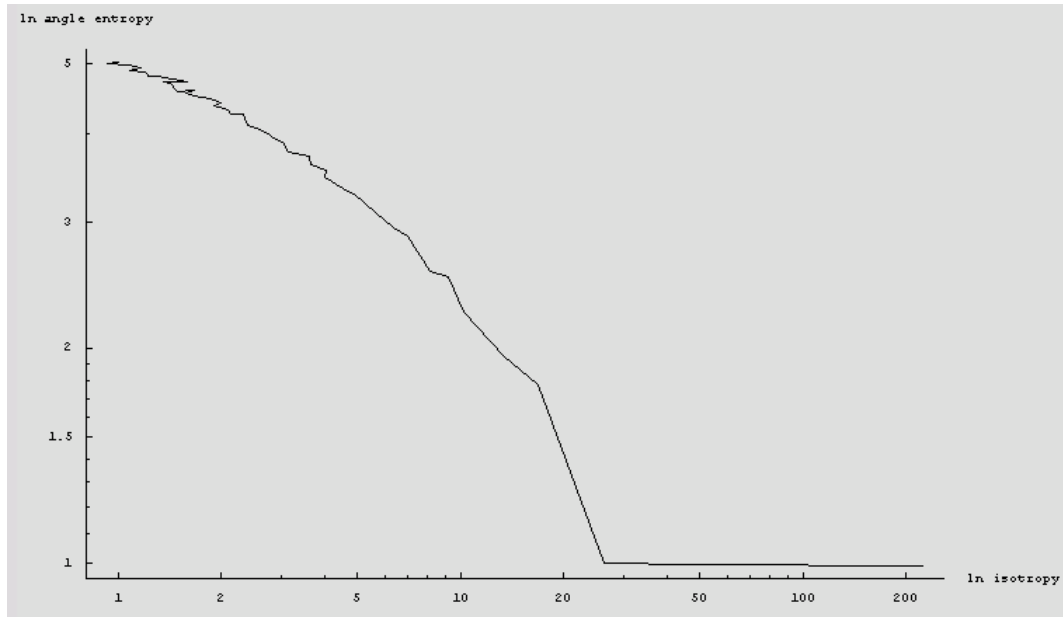


Figure 5 Natural Logarithm of isotropy versus angle entropy.

As isotropy increases and entropy decreases, the density of tube intersections increases. Greater angular variation enables the tubes to intersect nearer to one another. The inter-tube contact resistance has a greater impact as intersection density increases. There is also an impact on the probability of percolation, which will be considered in detail in a future paper.

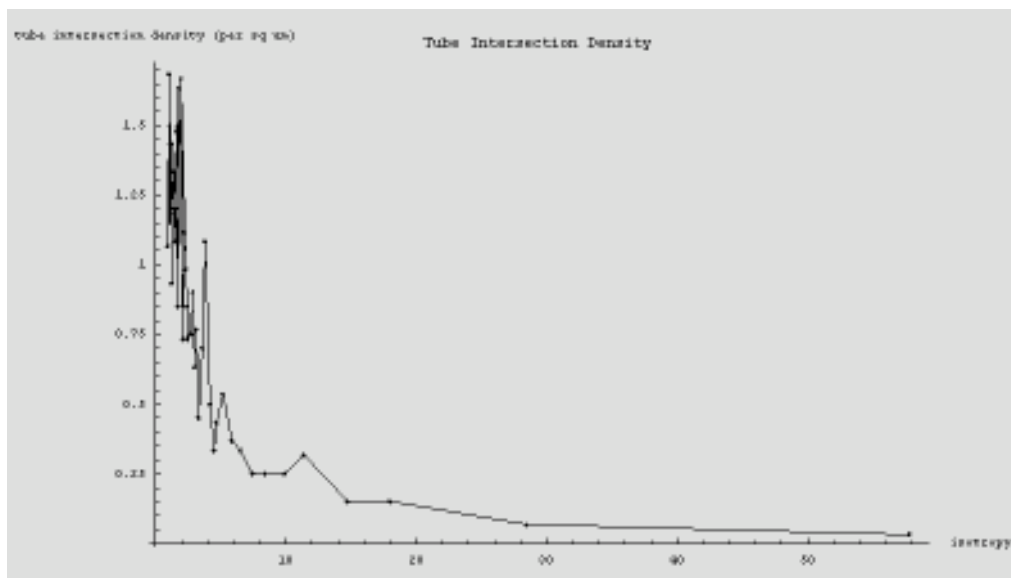


Figure 6 The density of tube intersections varies inversely with isotropy.

Consider next the specific types of graphs that are formed from the intersection of tubes. A random graph, $G(n,e)$, is comprised of n nodes and e edges. The probability that an edge exists between any of the $\binom{n}{2}$ possible node pairs is p . As an example,

Figure 7 shows tubes positioned to form a random graph with 10 nodes located in a circular pattern and a connection probability between any pair of nodes of 0.2. Note that while the random graph that generated this layout is comprised of 10 nodes, the corresponding CNT network may have more vertices because edges may overlap along the path from one node to another. Tube lengths and angles are shown in Figure 10.

One third of the tubes are randomly chosen to be metallic, shown in red in Figure 7. The metallic contacts are shown as the vertical lines on either side of the network and a number labels each tube as well as the contacts.

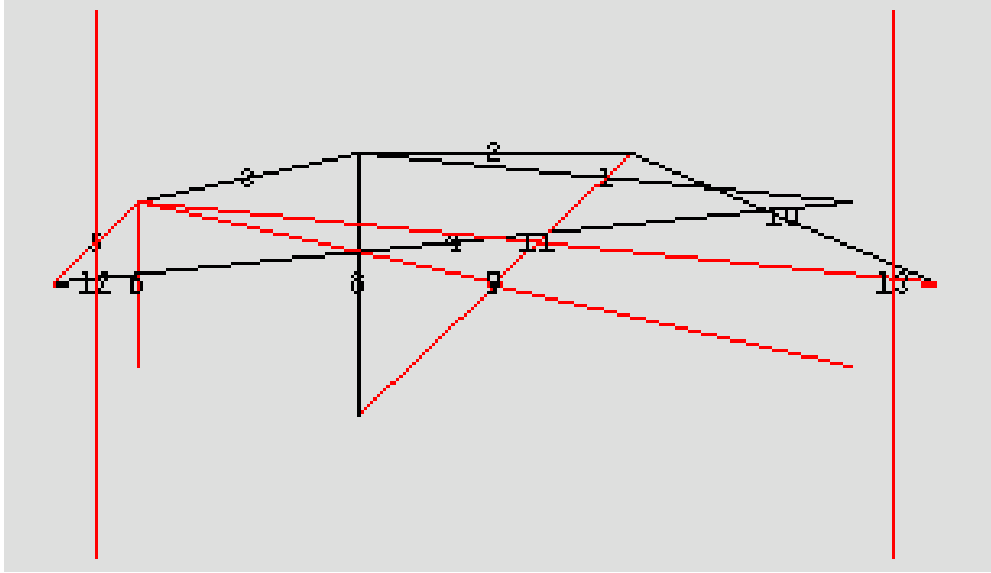


Figure 7 Tube layout generated from a random graph with 10 nodes and a connection probability of 0.2.

A regular grid graph is shown in Figure 8. It is a 5 by 2 node grid pattern. In both the random graph and the grid graph, 0.3 tubes are randomly selected to be metallic in 10 trials.

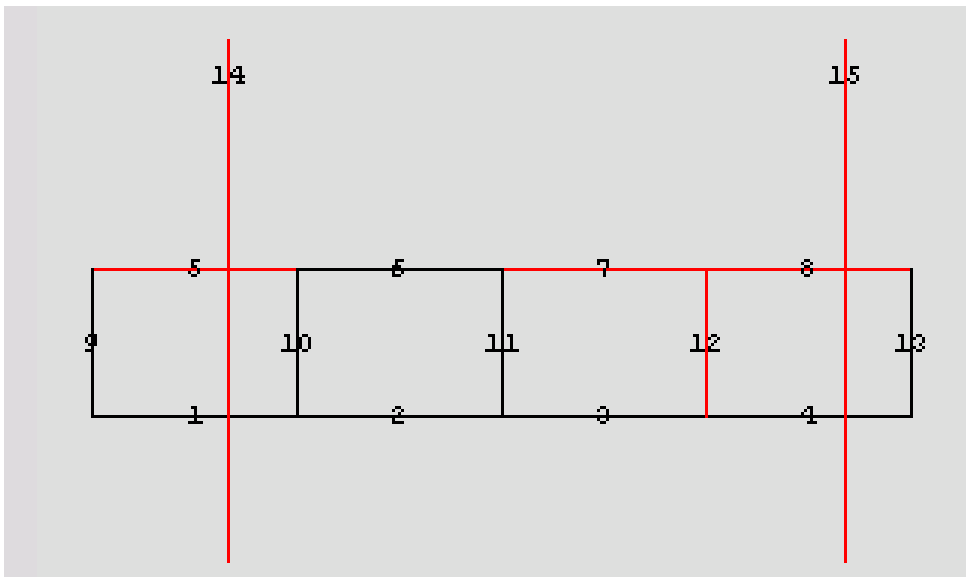


Figure 8 A 5 x 2 grid graph with 10 nodes.

Next the impact of a scale-free network of tubes is examined, that is, one in which the tube layout generates a scale-free graph.² In a scale-free graph the probability $P(k)$ that a node in the network connects with k other nodes is proportional to $k^{-\gamma}$. Such networks appear to be common in nature and the degree exponent γ depends on the detail of a particular network structure. Numerical values of the exponent γ for various systems are diverse but most of them are in the range $2 < \gamma \leq 3$. In Figure 9 a scale-free network of nanotubes is shown. The same percentage of nodes are metallic as in the previous random and grid graphs.

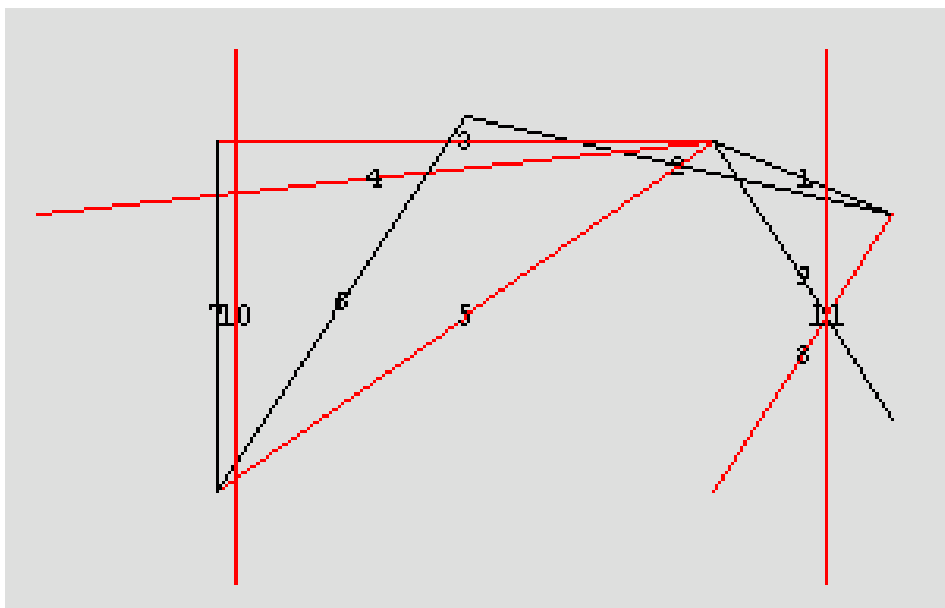


Figure 9 A scale-free structure of nanotubes.

Figure 10 shows the log variance in tube lengths (red) and angles (blue). The grid graph has the lowest variance in length since it is comprised of equal length edges. The random graph has the next greatest variance in length, while the scale-free graph has the greatest variance in length. It is expected that scale-free graph would have greatest variance in length since its graph edges tend to form small clusters with long connections among clusters. The isotropy of the random CNT network is 1.19, the

isotropy of the grid CNT network is 1.6 (the most aligned), and the isotropy of the scale-free CNT network is 0.75 (the least aligned).

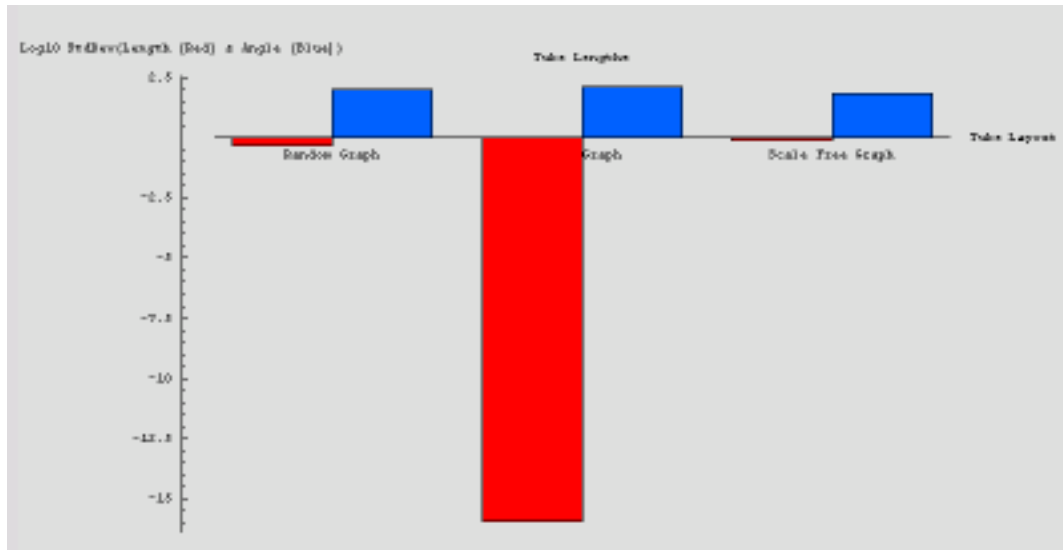


Figure 10 Log of the standard deviation of tube lengths (red) and tube angles (blue) for random, grid, and scale-free graphs respectively.

As shown in Figure 11, the logarithm of the variance of the resistance of the random and grid tube layouts are shown. The variance is significantly smaller for the grid graph. This leads one to suspect that ‘regular’ structures may be more resistant to the random appearance of metallic tubes.

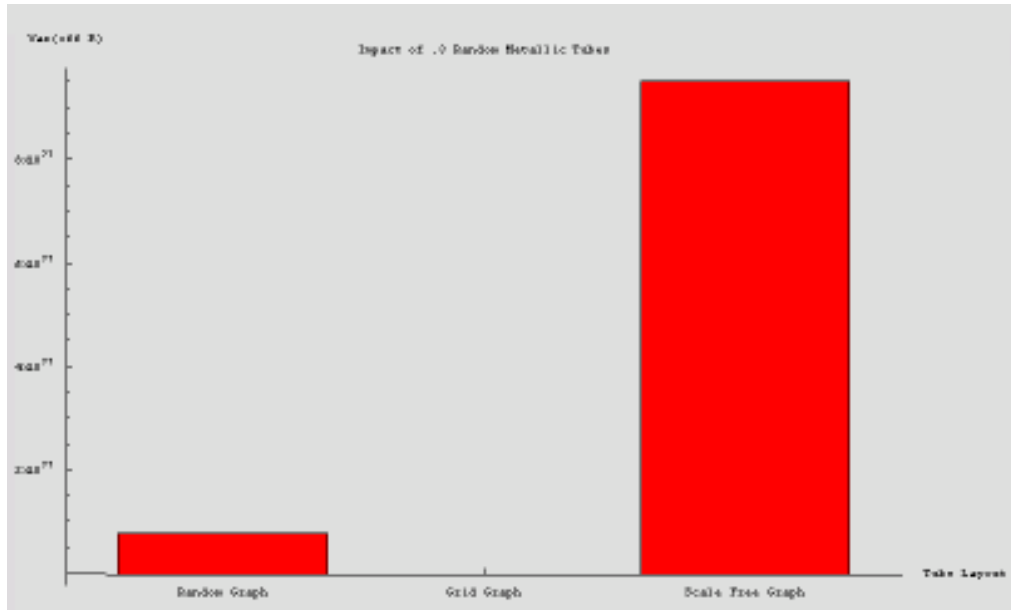


Figure 11 Variance in resistance with 0.3 random metallic tubes of the random and grid graph tube layouts.

In order to determine the contribution that each tube makes to the total resistance in the CNT network, a tube is removed from the CNT network and the network resistance is computed. The tube is then placed back into the network in its original location and a new tube is removed. This is repeated for each tube in the network. Figure 12 shows this process applied to each tube in the three network structures that were examined.

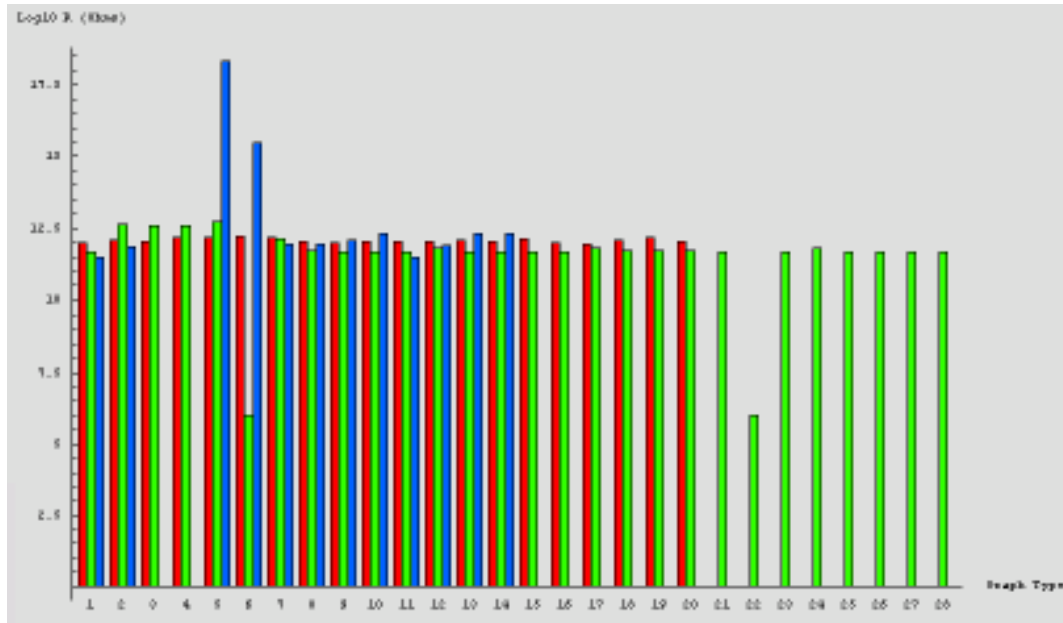


Figure 12 Base 10 logarithm resistance of the CNT network with each tube removed. The random graph tubes removed are shown in red, the scale-free graph tubes removed are blue, and the grid graph tubes are green.

The next experiment examines the impact of tube angle on resistance. Three randomly generated tube layouts were generated with increasingly greater variance in their tube angles as shown in Figure 13. The tube density and length are constant among all three layouts. These specific tube layouts are examined for the impact of the tube angle variance on resistance.

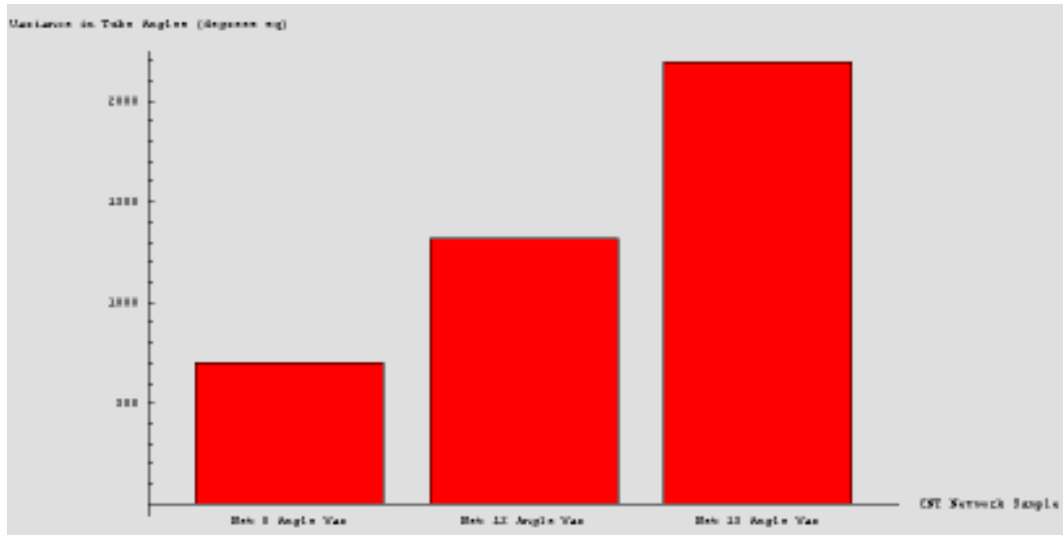
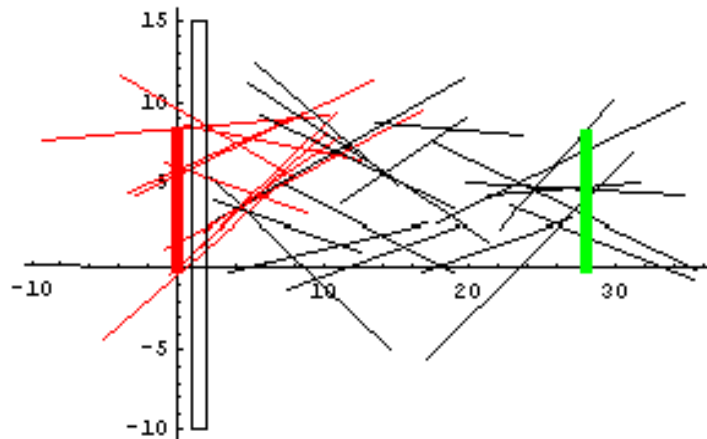


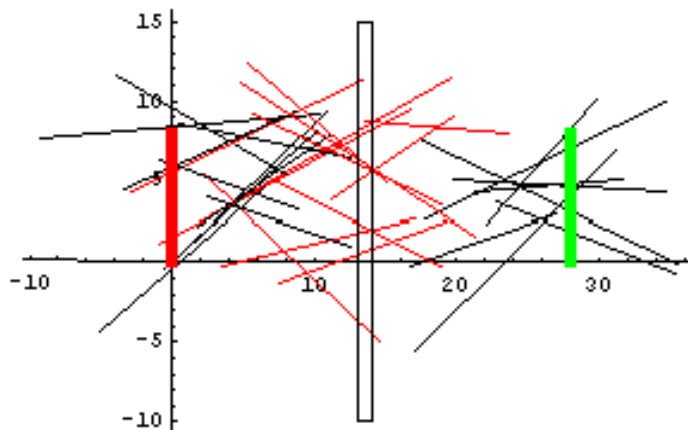
Figure 13 Three network layouts with the same density and tube length, but different angle variances are used as inputs for an experiment on the impact of tube angle on resistance.

This examination of the impact of tube angle uses a hypothetical gate whose position can change relative to the network structure. The concept is to view the gate as always turned on and sliding across the CNT network. Semiconducting tubes in contact with the gate are turned on; otherwise, they remain semiconducting at one teraohm resistance. There is no effect on metallic tubes. This may also be considered as a test of sensitivity to gate position. The gate slides continuously from left to right across the network structure, however, only three snapshots are shown in the following tables, namely the initial position of the gate, the middle position, and the ending position of the gate. Table 1 shows the tube network with the lowest angle variance as a gate sweeps over the tube network. The gate is narrowly constructed and only makes adjacent tubes semi-conducting (metallic conduction) while the remaining tubes are in an off state.

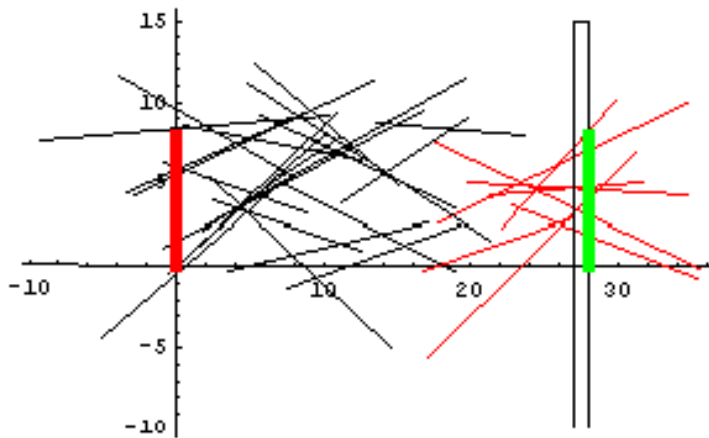
Table 1 Nearly-aligned, moderately-aligned, and unaligned tube networks as a gate passes continuously from left to right across the network structure.



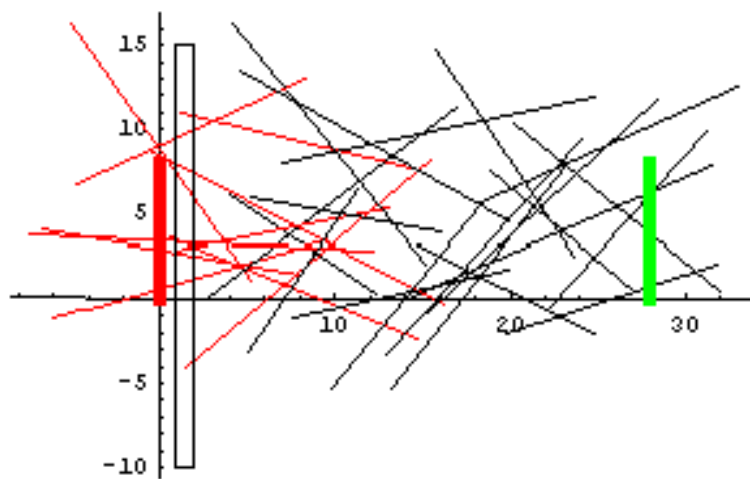
Gate near starting point. Tube angle is measured in degrees; the angle variance is 700.



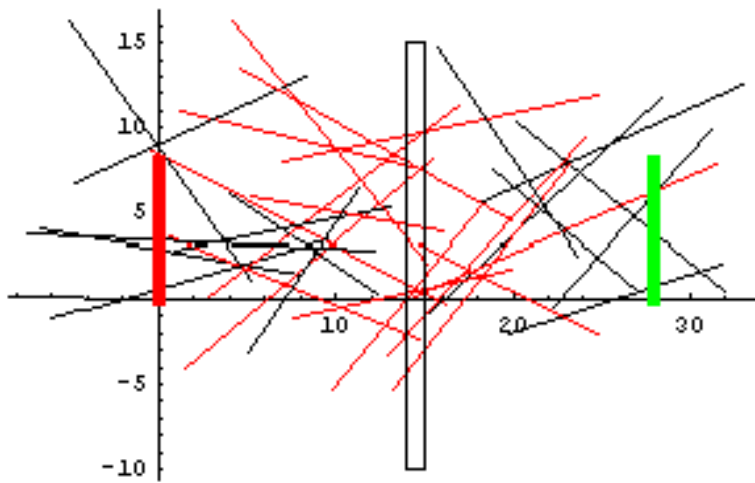
Gate near middle of simulated area. Same network as in previous figure.



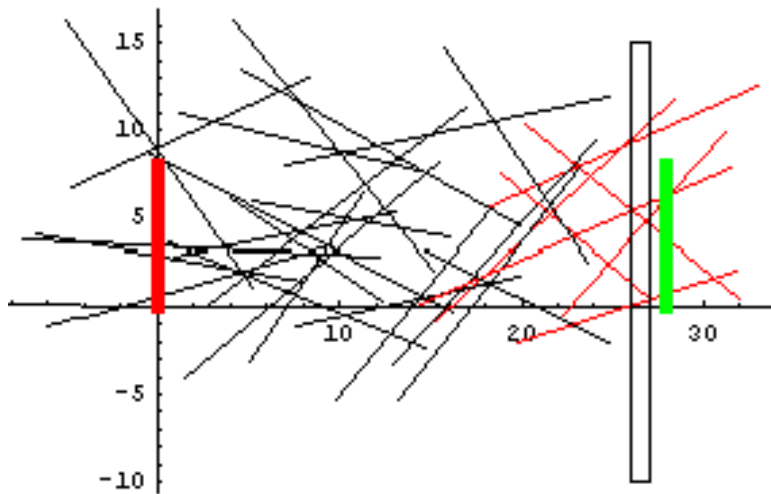
Gate at end of simulated area. Same network as in previous figure.



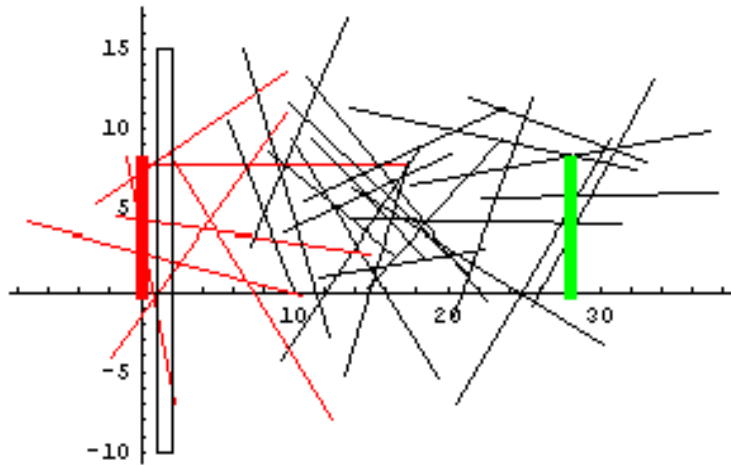
Tube angle is measured in degrees; the angle variance is 1320. Gate at starting position.



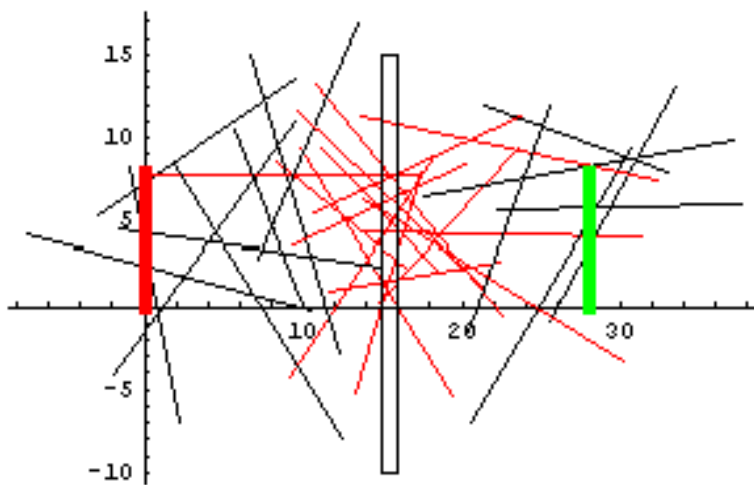
Gate in middle of simulated network. Same network as in previous figure.



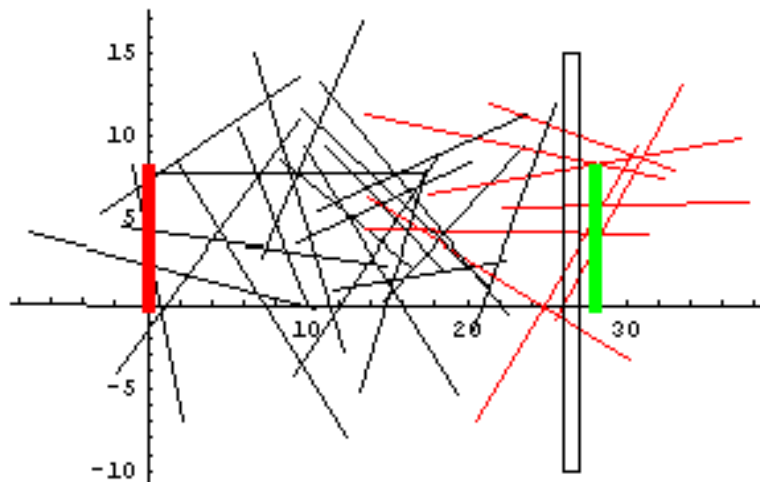
Gate at end of simulated network. Same network as in previous figure.



Tube angle is measured in degrees; the angle variance is 2194. Gate at beginning of simulated network area.



Gate in middle of simulated network area. Same network as in previous figure.



Gate at end of simulated network area. Same network as in previous figure.

Figure 14 plots the resistance for each tube layout as a function of the gate's position. The resistance is at a minimum as the gate passes over the middle of the network structure and is greatest at the ends.

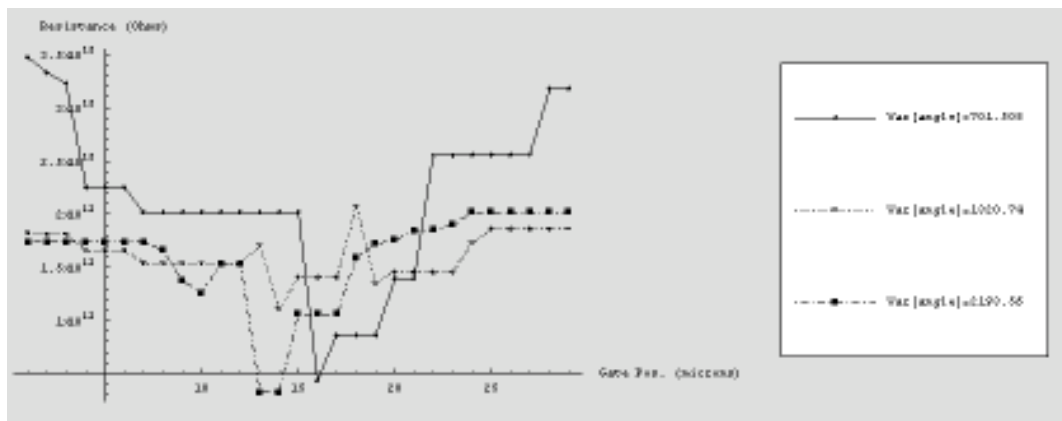


Figure 14 Resistance versus gate position.

The variance in the resistance is shown for each network in Figure 15. The moderately angled tube networks consistently have the least variance in resistance. This is a consistent outcome over many runs using different randomly generated network;

moderately angled tubes are show the most resilience to metallic tubes as shown later in this paper.

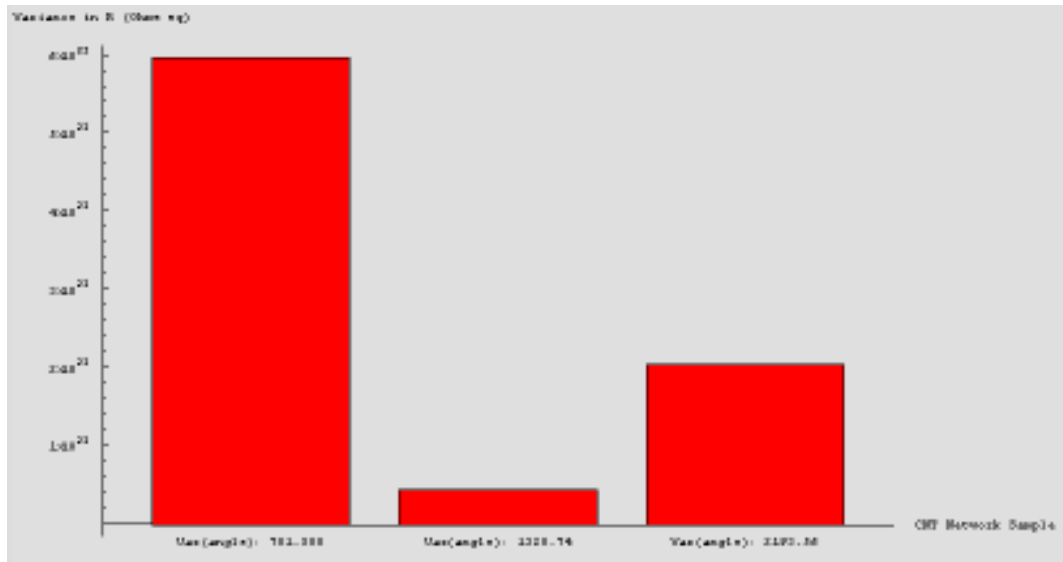
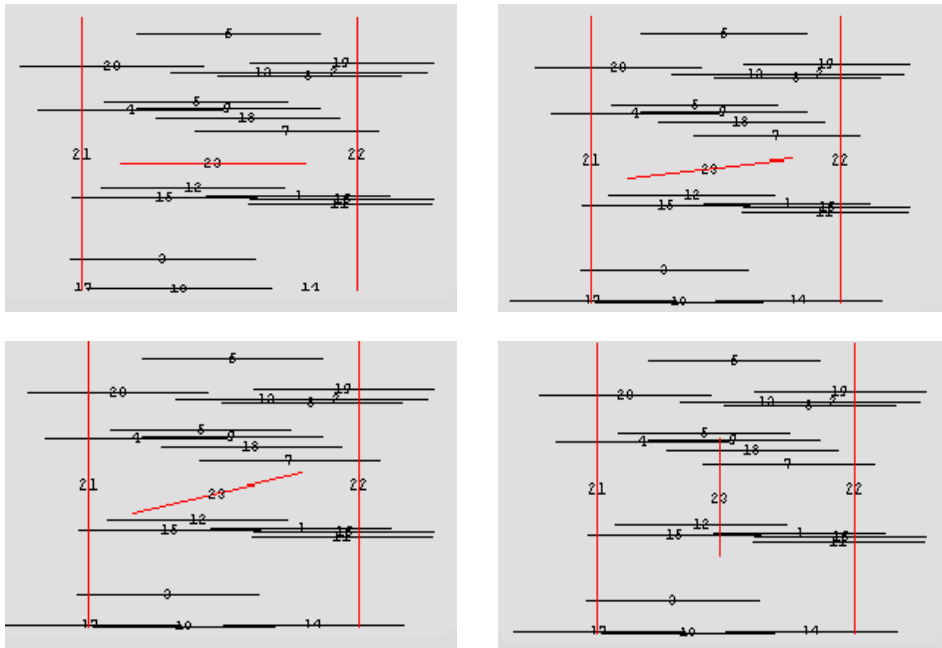


Figure 15 Variance in resistance as a function of tube angle variance.

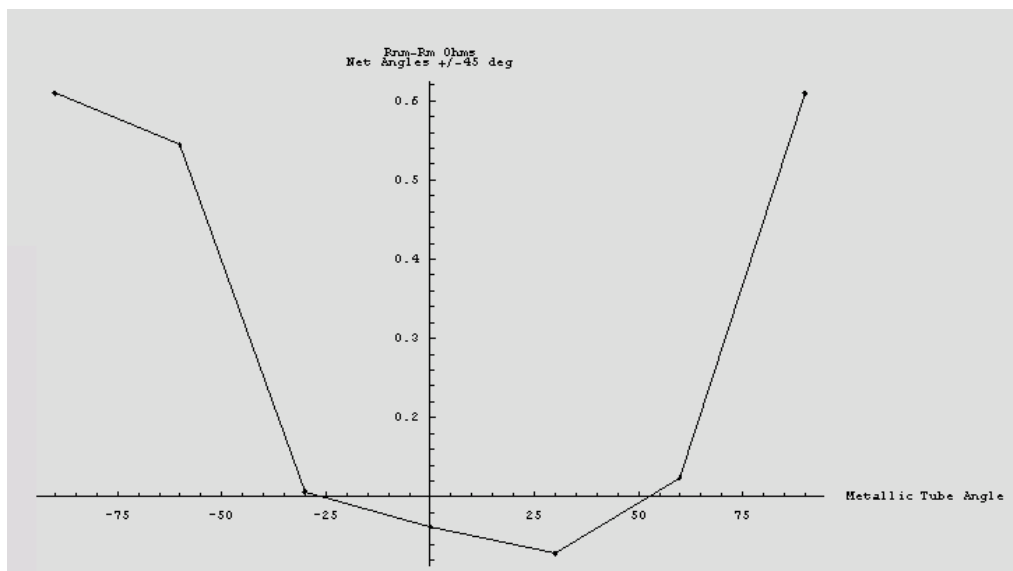
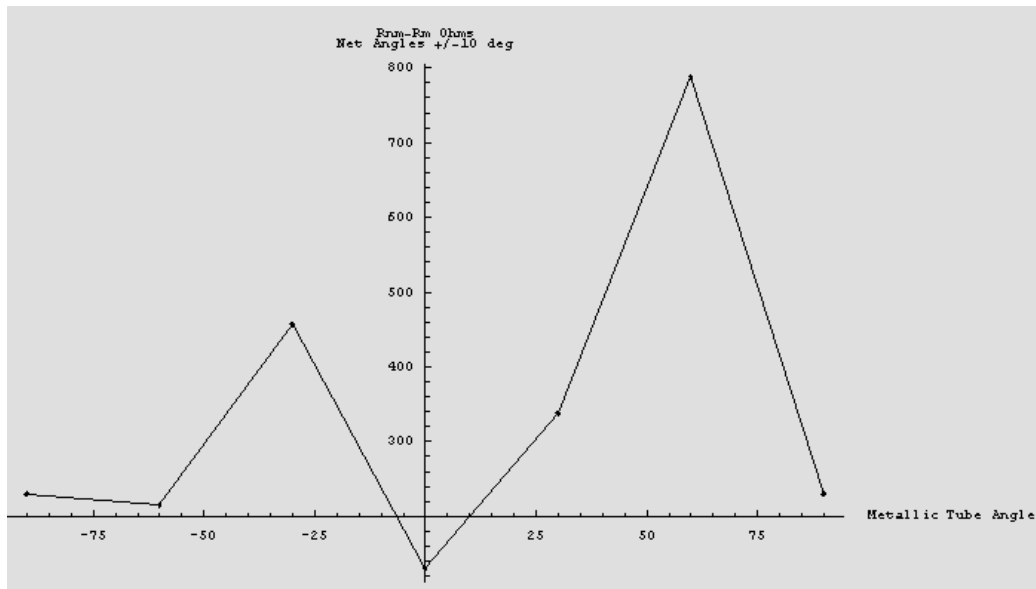
Another test of tube network angles and the impact of a metallic tube is shown in Table 2. A single metallic tube is placed in the center of a tube layout and rotated 180 degrees. The impact of the rotation is measured. This examines the impact of random metallic tube alignment with respect to a particular tube layout. In other words, how resilient is the network layout to a single random metallic tube alignment. In the example shown in the table below, the tube angles are zero degrees and there is no percolation.

Table 2 Rotating a single metallic tube within a tube layout.



In Table 3, the results are shown for uniform random layouts in which 20 tubes have angles that vary from -10 thru 10 degrees to -90 thru 90 degrees while the metallic tube is rotated from -90 thru 90 degrees in increments of 20 degrees. The plots show the difference in resistance without the metallic tube from the resistance with the tube at each of the specified angles. Addition of a metallic tube either decreases resistance or has no effect if it is not located in the percolation path. Thus, the difference in resistance is always greater than or equal to zero. From these graphs, it is clear that when tubes are most closely aligned, i.e. from -10 to 10 degrees, the metallic tube has a significant impact. As the tubes become more randomized in orientation, the impact of the metallic tube is greatly reduced at every angle.

Table 3 Angle versus difference in resistance with and without the metallic tube.



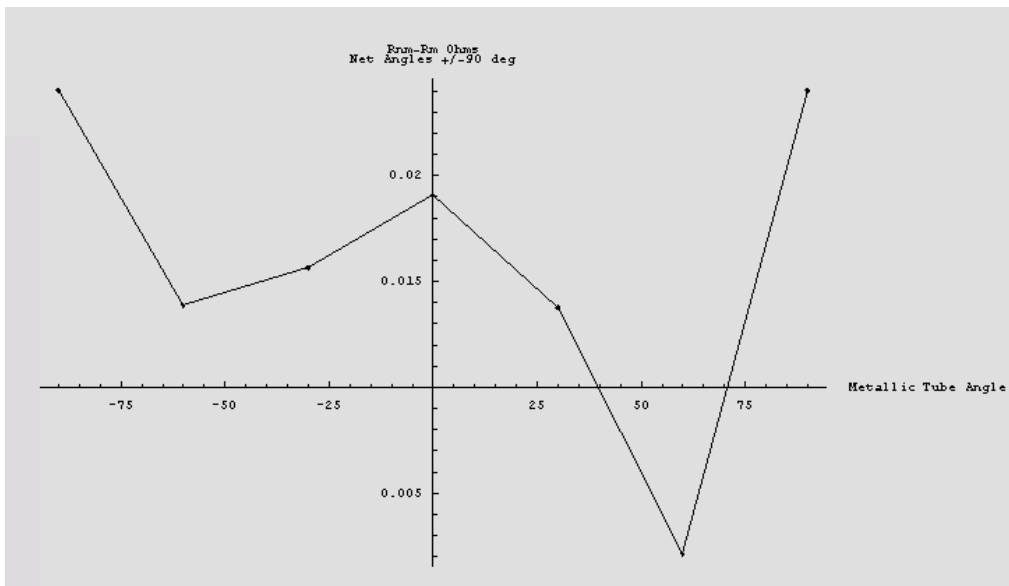
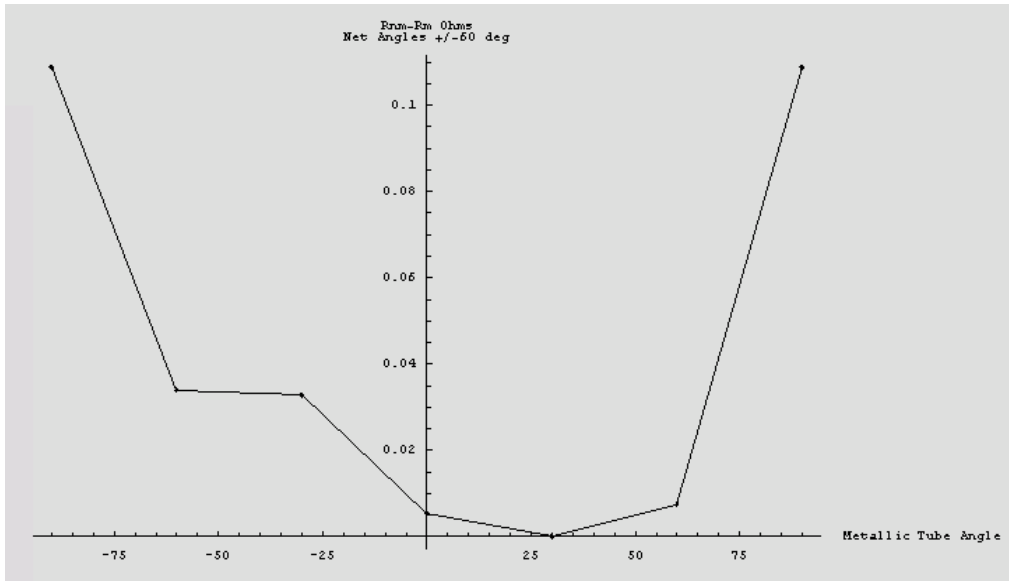
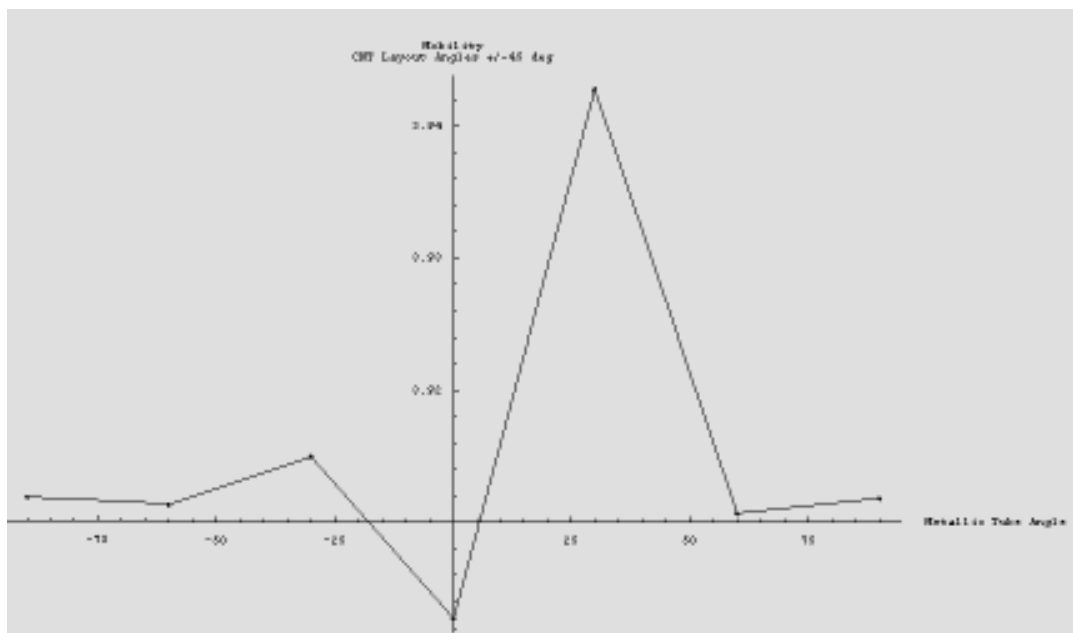
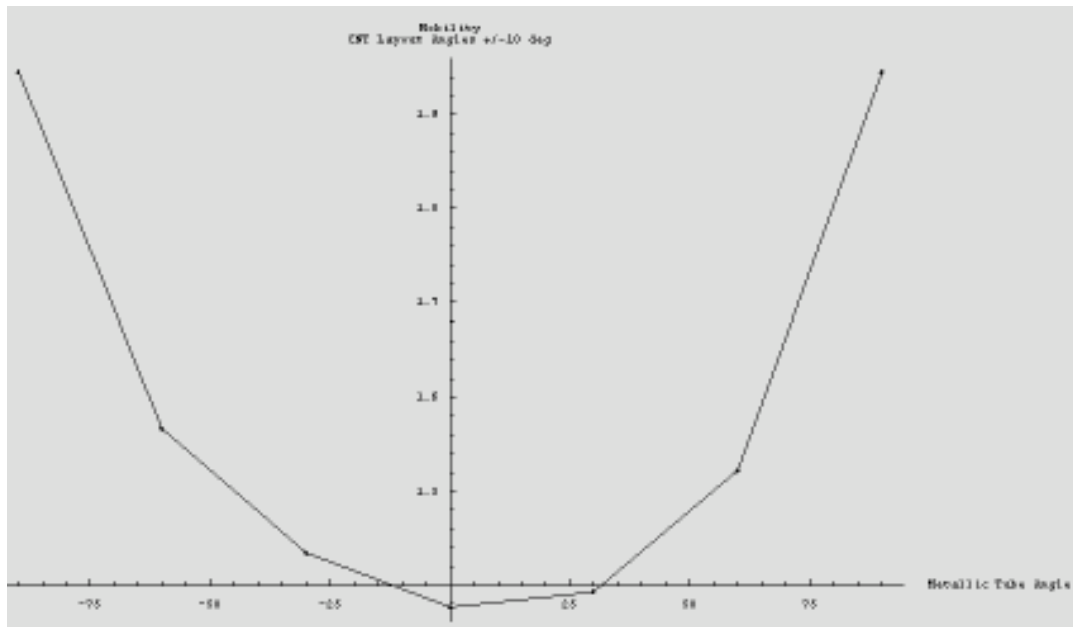
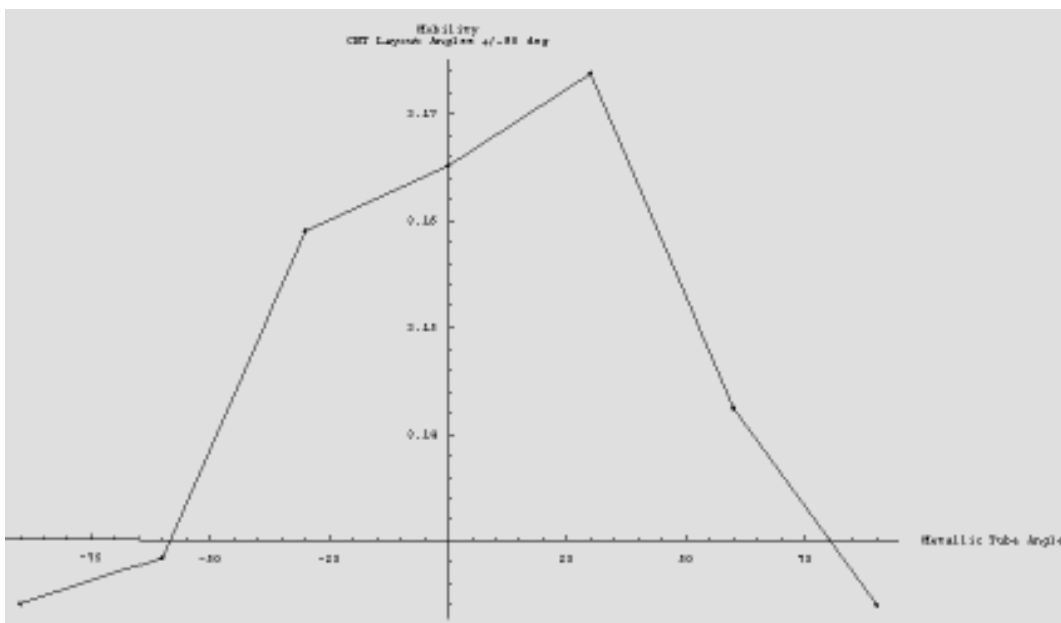
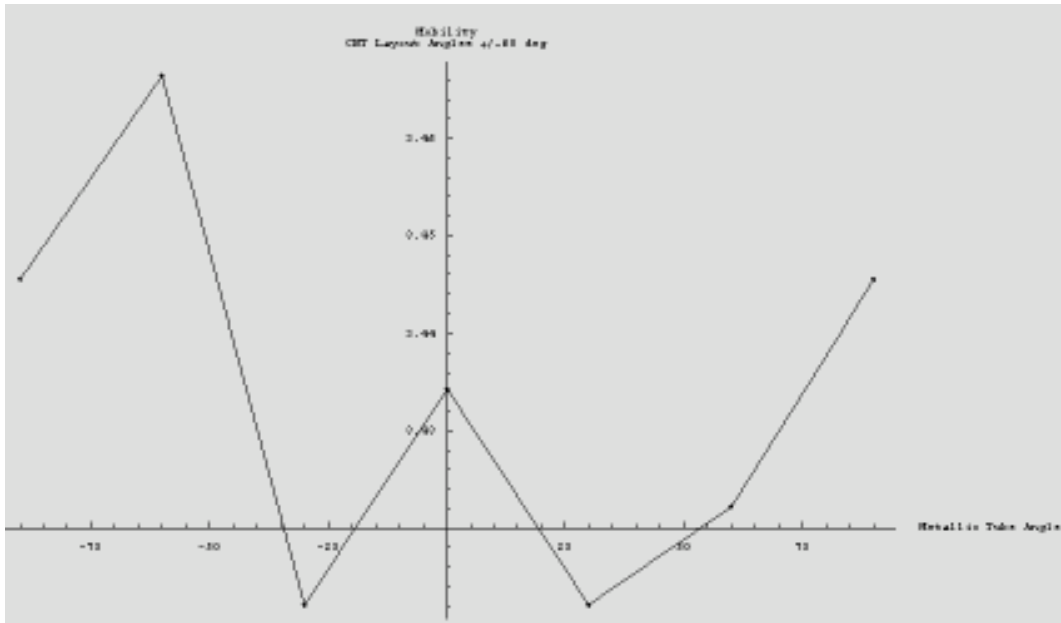


Table 4 shows the mobility as a function of metallic tube angle. When the semiconducting tubes are nearly aligned (first graph below) there is a convex bowl shape to the mobility with a minimum near the zero metallic tube angle. This is contrasted with the random semiconducting tube angles (last graph) where the mobility curve has a concave shape and the maximum is near the zero metallic tube angle. Also note that mobility was highest at the +/-45 degree semiconducting tube angle range regardless of the metallic tube angle.

Table 4 Mobility of the CNT network as a function of metallic and semiconducting tube angles.





Conclusion

The impact of metallic tubes on the current ratio and mobility of a random network has been characterized. Isotropy and angle entropy were introduced as a means of quantifying network structure. Three classes of network topologies were examined with respect to their resilience to metallic tubes, namely random, regular, and scale-free

nanotube networks. Initial evidence demonstrated that the regular graph had the least variance in resistance as tubes were randomly replaced with metallic tubes. The scale-free graph had the most variance in resistance. Finally, additional evidence shows that closely aligned tubes appeared to be most vulnerable to the metallic tube, that is, had the lowest mobility. Tubes at +/- 45 degrees from one another had the most resilience to the metallic tube (highest mobility). Note that while these results provide direction for possible nanotube topology design rules, more work needs to be done to verify and extend these results.

1. Bush, S.F., Li, Yun. "Network Characteristics of Carbon Nanotubes: A Graph Eigenspectrum Approach and Tool Using Mathematica," GE Global Research, Technical Report, 2006GRC023, January 2006.
2. Barabási, Albert-László and Reka, Albert. "Emergence of scaling in random networks". *Science*, 286:509-512, October 15, 1999.

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