Mechano-electrical properties of metallic carbon nanotubes

An Honors Thesis by:
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Advisor:
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Ball State University
Muncie, Indiana
Expected Graduation: May 2010
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Abstract

Single-walled metallic (4,4) nanotubes are simulated using proprietary density functional theory software. Current voltage curves and conductance are calculated for varying axial strains. Density of states calculations are then made in an attempt to understand the strain-conductance relationship.

Acknowledgements

This study would not have been possible without the tutelage and knowledge of Dr. Ronald Cosby. His exactitude and advise have been a constant benefit. I would like to acknowledge the Ball State Honors College for their financial support via the Undergraduate Fellowship. I would also like to thank Feras Alzubi for his advice when I was beginning my research.
**Introduction**

Carbon nanotubes (CNT’s) are allotropes of carbon that have received a great deal of attention in the past two decades because of their dizzying array of practical applications. CNT’s are so highly considered because they have some extraordinary properties. They can be semiconducting, or metallic, and have high flexibility and high strength. While all nanotubes are all essentially tiny cylinders of carbon, they can have remarkable variability in their structure. The most grossly visible property is that CNT’s come in single-walled and multi-walled varieties. In this study the nanotubes in question were single-walled. The next important structural variable in CNT’s is known as the chirality. Chirality in the context of carbon nanotubes is described by the chiral vector \((n,m)\). Three separate classes of nanotube are defined in this way. Armchair nanotubes have \(n=m\), zig-zag nanotubes are \(m=0\) and chiral nanotubes occur when \(0<m<n\) [1]. This may seem a bit abstruse. However, one can think of creating a nanotube by taking a sheet of graphene, which looks a bit like chicken-wire, and cutting out a section. It is easy then to visualize rolling this chicken-wire into a tube by joining the corners of our section. This yields an armchair chicken-wire tube. If one were to now put a twist on the mesh before rolling it up, such that the corners were joined to vertices other than the corresponding corners, a tube with a different chirality would be obtained. It should be noted that this is not in fact how CNT’s are constructed; rather it is a useful

![Figure 1: Shows the chiral vector and the chicken-wire like molecular lattice of graphene [2]](image-url)
mental artifice used for visualizing the difference in structure that occurs in these nanotubes. However, the chirality is not merely a matter of the geometry of the constituent atoms. It also determines the way in which the nanotube conducts electrical currents. Armchair nanotubes are exclusively metallic [3]. This study solely examines single-walled, (4,4), metallic nanotubes.

The purpose of this study is to examine the electrical properties of single walled armchair, (4,4) nanotubes under axial compression. Using proprietary modeling software, we examine the conductance-strain relationship for a 48-atom carbon nanotube segment between copper contacts. We also present density of states data in an attempt to fundamentally describe the conductance behavior.

Methods and Techniques

The software utilized for this study is the Atomistix ToolKit (ATK) that is produced by the QuantumWise company. This software is run on the Ball State University College of Science and Humanities Computing Cluster. ATK comes with a native graphical user interface for generating scripts to run called Virtual NanoLab(VNL). It can be used to develop whole systems for investigation or generating useful bits of codes for inclusion in one’s own scripts. ATK can simulate semi-infinite bulk systems, molecules or two probe systems. It can also perform complicated transport calculations to determine the electrical properties of a system. To do this, ATK implements two basic techniques, Density Functional Theory (DFT) and Non-Equilibrium Green’s Functions (NEGF) [4].

A central problem of quantum chemistry and condensed matter physics is that the equation which governs objects at the scale of molecules and smaller, the Schroedinger Equation is intractable when
dealing with a system of more than three or four particles. A solution in these cases is not difficult to achieve, it is impossible. Therefore several models and approximations exist to try to escape this difficulty. One such method is DFT. DFT uses the real space density of electrons in the ground-state in place of the many-body problem of N electrons and 3N coordinates. The downside of this approach is that the energies that result from this calculation are dependent on the electron density and the electron density is dependent on the energy configuration of the system. Therefore, the accuracy of the calculation depends on the degree to which this self-consistent calculation converges. ATK uses Density Functional Theory to calculate energies, electron densities, atomic forces and other properties. NEGF methods are the standard when constructing models of transport in systems where quantum effects must be accounted for. It is used in ATK to calculate properties like current. It too results in a self-consistent calculation of the electron density that must be iterated until it converges to some desired tolerance. A linear carbon chain was chosen as a test system from parameterization purposes because it was small, undemanding in terms of computation time, and bears a superficial resemblance to the carbon nanotube system that is of true interest. The specific parameters that the linear chain is used to probe are called the mesh cutoff, the energy shift, and the self-consistent field tolerance [4]. The mesh cutoff determines the fineness of the real space grid of points that ATK samples to perform the iterative self-consistent calculation. A larger mesh cutoff indicates a finer grid, requiring ATK to

Figure 2: A 10 atom linear carbon chain
calculate electron densities at more points and taking longer to calculate, but providing more accurate values for quantities like structure and energy. The energy shift determines the cutoff radius of electron wavefunctions. True wavefunctions extend outwards to infinity, though the magnitude of the wavefunction approaches zero. Practically we must designate a cutoff radius to avoid calculations that are not only time-consuming, but useless. The energy shift is inversely related to this radius, smaller energy shifts indicate larger radii. This costs calculation time, but can capture the effects of longer range, non-nearest-neighbor interactions. The self-consistent field tolerance is the degree of accuracy that we ask the self-consistent calculation to converge to [4]. To investigate the parameter space a script was written to calculate the total energy of the system as a function of the mesh cutoff and energy shift. During the investigation process the self-consistent field tolerance was found to have a negligible effect on the value of total energy. Complete parameter data is included in the appendix.

The primary system we are examining is a small segment of nanotube between copper contacts with three scattering layers. The segment is unrealistically small, only 48 atoms. This was chosen to reduce computation time to manageable levels.

Goals

If nanotubes become widespread as electrical components in devices, it is likely that the nanotubes will at some point be deformed or strained. Therefore, it makes good sense to understand the effects this will have on the device. This understanding may
also lead to knowledge that would allow the electrical properties of carbon nanotubes to be fine-tuned.

**Results**

Current-voltage (I-V) curves were calculated for varying strain. The slopes of these curves are the conductances of the nanotube under these strains. Figure 5 is an example I-V curve. It is linear and therefore has a simply defined conductance.

Figure 5: Example I-V curves

These conductance results were collected and are presented versus strain in Figure 7. The results were a bit unexpected. The conductance increases until 6% and then decreases. We believe this is due to two competing phenomena. First, the conductance tends to go up because we are reducing the distance electrons must travel under a given voltage. One may think of a classical wire: the resistance is inversely related to the length of the wire. Second, compressing the tube introduces a bandgap as has been experimentally shown by Minot et al [4]. It is worth noting that strains of more than a few percent may be unphysical as buckling and breakage may occur before then.
We have attempted to verify that this is indeed the mechanism by which the conductance decreases by examining the density of states (DOS) of the nanotube under zero and 10% strains. These DOS plots (Figures 8 and 9) are not particularly illuminating. To better see these changes we took the differences between the density of states for 10% and 6% and 10% and 0% respectively. These are shown as Figures 8 and 9. The data is very scattered. The difference between from 10% to 0% seems superficially larger than the difference between 10% and 6%. However, no strong conclusions can be drawn from this. We
now believe that perhaps the total density of states of the entire system too closely resembles that of the copper scattering layers rather than that of the CNT segment. To find out if the compressive strain is in fact altering the density of states of the CNT, a local density of states calculation will be required.

Conclusions

Conductance-strain data for the 48 atom CNT between copper contacts was presented. Our hypothesis about bandgap formation via strain remains unsupported until local density of states data can be calculated.

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[2] Image from Wikimedia Commons. File is a part of the public domain.


Appendix: Parameterizations

The results of the parameterizations using the linear carbon chain test case are shown below in Figure 10. The data is well converged in total energy except for a large jump at approximately 0.0006 Rydbergs. At this point, the jump in total energy is unexplained. However, this anomaly does not appear to affect the calculated quantities.

### Computational Parameters Used

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Mesh Cutoff</td>
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<tr>
<td>Energy Shift</td>
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<td>Exchange Correlation – Local Density Approximation</td>
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<td>SCF Tolerance</td>
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</table>

Figure 10: The complete parameter space for the linear carbon chain.
Figure 7: Multiple curves corresponding to multiple energy shifts; all have the same equilibrium lattice parameter that are of interest. Figure 11 shows multiple curves of lattice parameter versus total energy. Again the jump is visible, but each curve has the same total energy minimum and thus the same equilibrium lattice parameter. Therefore, as long as we avoid using the value of 0.0006, we feel that this anomaly will not affect results.