Modeling electron transport along carbon nanotubes

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A new hydrodynamic model suggests that as their radius increases, the semiconducting and metallic conductivities of carbon nanotubes become comparable.

Carbon nanotubes (CNTs) are innovative materials,\(^1\) proposed for a wide range of nano-electronic applications, including interconnects, passive devices, and antennas.\(^2\) CNTs consist of rolled-up sheets of a mono-atomic layer of graphite (graphene), which can be either single-walled or made up of several nested shells (multi-walled).\(^3\) Although graphene is a zero-gap semiconductor, once rolled up it may become either metallic or semiconducting, depending on its geometry.\(^1\)

The electrical, thermal, and mechanical properties of CNTs mean that they are increasingly used in nano-electronics. Their use may overcome some of the problems posed by conventional materials for technology nodes below 22nm, such as prevention of resistor-capacitor degradation by reducing the dielectric permittivity of interconnects and increasing their conductivity. CNT-based nano-electronics research has begun to mature, and the first practical examples of nanoscale devices integrating conventional materials with CNTs are appearing. Many attempts have been made to derive models of CNTs’ electrical propagation,\(^3\)\(^-\)\(^6\) but a complete description of how the conductivity depends on chirality (i.e., the way the nanotube is rolled up) has never been presented. We have developed a new hydrodynamic model of signal propagation along CNTs.\(^7\)

We rigorously evaluate the number of conducting channels, starting from the quasiclassical Boltzmann equation and taking into account the actual equilibrium velocity of the conducting electrons. Our model reveals, at low computational cost, the number of conducting channels and the conductivity’s dependence on CNT chirality and temperature.

The energy-dispersions relation of the conducting (\(\pi\)) electrons differ for semiconducting and metallic CNTs, at equilibrium and near the Fermi point (see Figure 1). To study a CNT’s electromagnetic response, one must describe the interaction of the \(\pi\) electrons with the fields produced by the \(\pi\) electrons themselves, external sources, and the lattice ions.

Both semiclassical and quantum-mechanical analyses have previously been used. The quantum-mechanical approach, based on first principles,\(^3\) imposes a high computational burden. To get analytically tractable results, quasiclassical models can be used, i.e., we assume that the electric fields associated with the \(\pi\) electrons and external sources are small compared to the lattice field and that they vary slowly on atomic lengths and timescales. We then treat the \(\pi\) electrons as quasiclassical particles and use the semiclassical Boltzmann equation to calculate their transport.\(^4\) We assume small perturbations of the electronic distribution functions around the equilibrium values, and take into account the actual equilibrium velocity of the \(\pi\) electrons.

Quasiclassical models require an estimate of the equivalent number of conducting channels, that is, the number of subbands around the Fermi level contributing to the conduction. One way of counting these is through the occupation probability of the states corresponding to the peak and valley of the valence- and conducting-subband energies, respectively. In an existing

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method, the velocity of the conducting electrons is assumed to be roughly equal to the Fermi velocity at the peaks and valleys. Our model rigorously evaluates the number of conducting channels, starting from the quasiclassical Boltzmann equation and taking into account the actual equilibrium velocity of the $\pi$ electrons.

We used this model to calculate the number of conducting channels as a function of the two integer indices $(m, n)$ that define the chirality of the CNT (see Figure 2). We also calculated the number of conducting channels as a function of CNT diameter and temperature (see Figure 3). The model we developed in terms of the conducting channels is applicable to any CNT, regardless of diameter. Our results are consistent with previous models for metallic single-wall CNTs with small radius.

We used our model to calculate the total axial conductivity and the CNT constitutive relation $\sigma(v)$, which locally relates, for any frequency, the axial electric field $E$ with the axial current density $J$, i.e., $J(z) = \sigma(v) E(z)$. We were then able to describe the propagation along a CNT interconnect. We derived a transmission line (TL) by coupling Maxwell’s equations to the constitutive relation, assuming quasitransverse electromagnetic propagation. We also presented equivalent propagation parameters, with the equivalent per length capacity, inductance, and resistance given in terms of the number of equivalent conducting channels. We found that we could, alternatively, derive this model by describing the CNT electron cloud as a fluid moving on its surface. We subjected the electron cloud to semiclassical transport equations, and applied quantum effects to the electron effective mass.

Despite its simplicity, a fluid model is physically meaningful. Its parameters can be easily associated with the main physical processes arising on characteristic lengths involving many unit cells, such as the collective effects. Fluid models can also be powerful: another model we have developed for CNT electron transport can account for chirality, diameter, and temperature, which affect the effective-mass dropoff, for example. (That model generalizes another that refers to metallic single-wall CNTs with small radius)

All of these semianalytical models are limited in frequency. The main assumption is that the frequency is sufficiently low

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**Figure 2.** Equivalent number of conducting channels versus CNT chiral indices $(m, n)$. (a) Small and (b) large radii.

**Figure 3.** Equivalent number of conducting channels versus CNT shell diameter, computed at $T = 273$ and $373\text{K}$. 

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for the electromagnetic response of CNTs to be mainly governed by intraband transitions of $\pi$ electrons with unchanged transverse quasimomentum. These transitions contribute to the axial (but not the transverse) electric conduction, exciting in fact an azimuthally symmetric electric current. Typically, the upper bound for these models is around 1THz. Another factor limiting the frequency range of fluid models is the high curvature effect, which violates the electronic symmetry of the graphene layer. A THz quantum transition with a large linewidth appears, which may have important effects in CNTs with radii smaller than 1nm.7

In summary, starting from the semiclassical Boltzmann equation, we have derived the equivalent number of conducting channels, and from there the CNT conductivity. Based on these results, we have proposed TL models of CNT interconnects. Our model yields, for low computational cost, the CNT conductivity dependence on chirality, showing in particular that, as the CNT radius increases, the semiconducting CNT conductivity becomes comparable to its metallic conductivity. We are now focusing our efforts on the scattering properties of CNT structures, and developing electronic-transport models able to take into account also the CNT curvature effects and interband transitions.

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References

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