Modelling the electrical conductivity of carbon nanotube films

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Abstract Submission

Carbon nanotubes (CNTs) are a fascinating material with very high electrical conductivity. In many practical applications, CNTs are deposited in a disorganized film. In order to model the electrical conductivity of such films, models of the electrical conductivity of individual CNT junctions must be combined with larger-scale models of their geometric structure. Such models elucidate the role that the CNT film structure has on electrical conductivity.

Introduction

Carbon nanotubes hold significant technological promise due to their extremely high electrical conductivities. This is due to metallic CNTs behaving as ballistic conductors, which enables highly energy efficient electrical devices to be constructed from them. One such example application is the use of a CNT film as resistance-changing element in non-volatile computer memory [1]. In such applications, the placement of individual CNTs is not directly controlled, and instead the electrical conductivity of a disorganized network of CNTs must be evaluated.

Methodology

The following steps were used to simulate the electrical conductivity of disordered CNT films:

(a) The intrinsic electrical conductivity of individual CNTs is high and the primary source of electrical resistance within CNT films is anticipated to occur at CNT-CNT junctions where electrons must tunnel from one CNT to another. In order to understand this tunneling resistance, a large library of CNT-CNT junction structures (Fig. 1) was simulated using density functional tight binding (DFTB) in combination with the non-equilibrium Green's function (NEFG) approach [2]. The results were used to generate an atomistic conductivity model (Fig. 2) which was found to include a radius dependance (Fig. 3).

(b) Mesoscopic models of nanoscale CNT films were generated using course-grained molecular dynamics (MD). The procedure used to generate these models is described in Fig. 4. A library of CNT films was generated, and an example structure is shown in Fig. 5.

(c) The developed atomistic conductivity model developed in (a) was used in combination with larger-scale DFTB calculations in order to parameterize electrical conductivities between the mesoscopic segments employed in (b).

(d) The structural models generated in (b) were then combined with the electrical parameters established in (c) in order to produce a large-scale electrical model of the conductivity of a nanoscale CNT film, using the method of nodal analysis. An example simulation is shown in Fig. 6.

Conclusion

A numerical model for simulating the electrical conductivity of nanoscale CNT fabrics has been developed, by combining atomistic electrical conductivity calculations with larger scale mesoscopic structure simulations. This will enable an enhanced understanding of the electrical conductivity of CNT films to be developed.

Acknowledgment

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References

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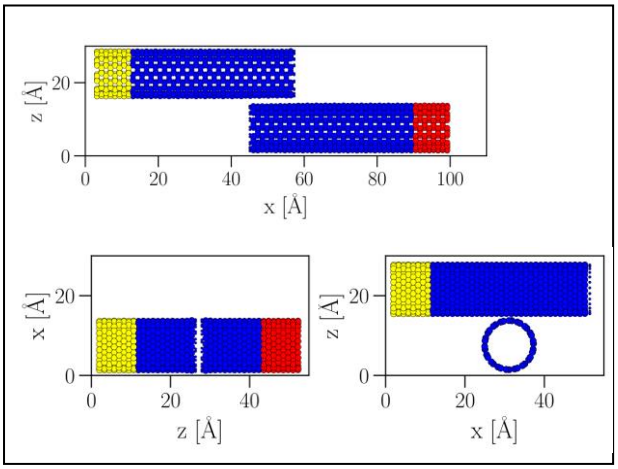

Fig. **1** Template CNT junction structures used to perform DFTB+NEGF electrical conductivity calculations. Red and yellow atoms denote the electrodes and blue the device region.

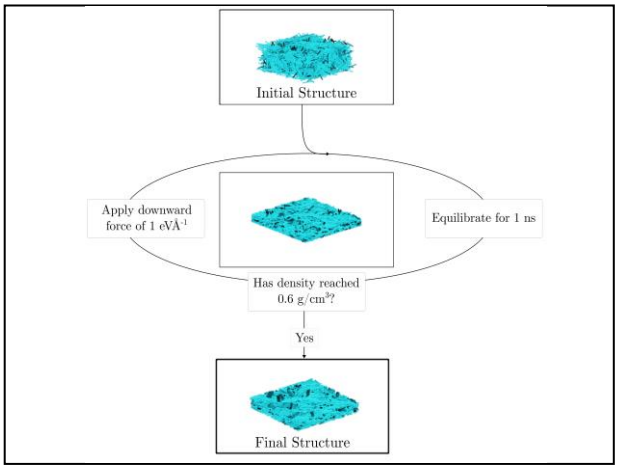

Fig. **4**. Procedure to produce mesoscopic CNT film models. An initial random structure is generated and then sequentially compressed and equilibrated in order to produce films of the target density.

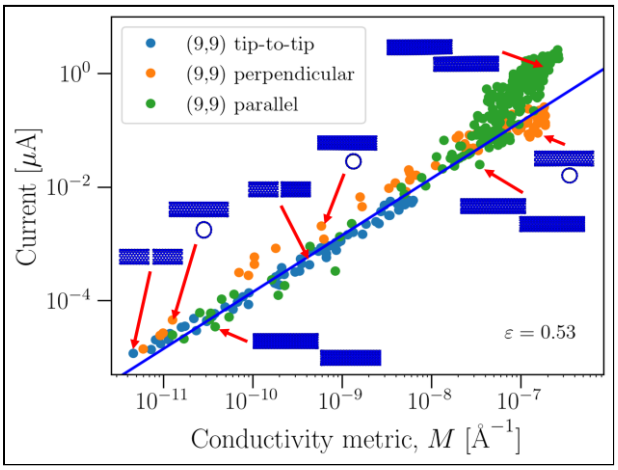

Fig. **2**. Atomistic calculations of the electrical conductivity of CNT-CNT junction structures, calculated using DFTB+NEGF (markers). A simple model is fitted to the available data.

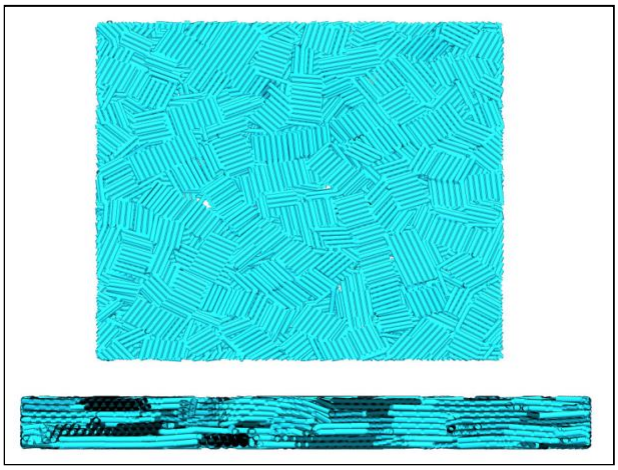

Fig. **5**. Example mesoscopic model of a dense CNT film. This film demonstrates significant bundling between the CNTs. The degree of bundling depends on the CNTs used.

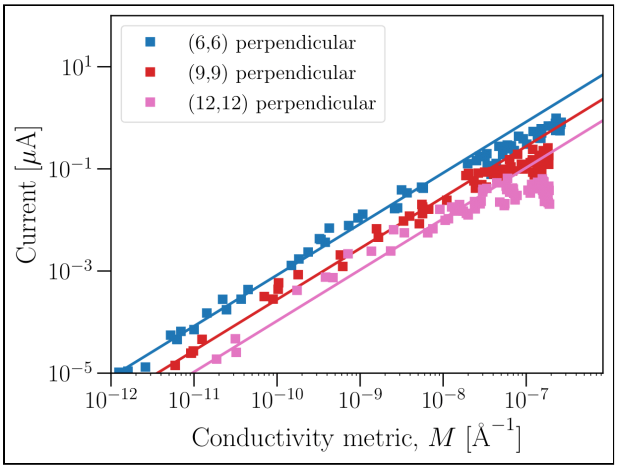

Fig. **3**. The electrical conductivity of CNT junctions formed from armchair CNTs decreases with increasing CNT radius.

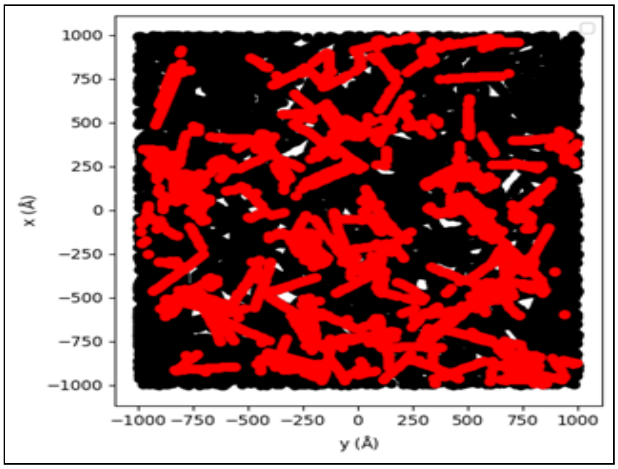

Fig. **6**. Example calculation of the electrical conductivity through a film model, highlighting current carrying CNTs.