Phonon-Limited Transport in Carbon Nanotubes Using the Monte Carlo Method.

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Carbon nanotubes (CNTs) are at the forefront of current research in nanoelectronics. At the present many questions still exist regarding the transport properties of these materials. The mobility of long (~325 μm) single-walled carbon nanotubes (SWCNTs) agrees very well with semiclassical transport simulations involving inelastic phonon scattering [1-2]. Such a transport model is likely to be valid when the tube length is longer than the momentum relaxation length (L_m), but may give insights into the electronic and phonon properties of nanotubes of all lengths. One may investigate the dependence of L_m, or other important transport properties such as the phonon-limited mobility, on the tube diameter, on surrounding fields, and on the temperature.

Monte Carlo simulations require models for the electron and phonon energy as a function of wavevector. The wavevector space of a nanotube is discretized into a large number of 1-D zones, each corresponding to a single electron subband or a single phonon subbranch. Considering electron transport in the three lowest conduction subbands, the important k-space is shown in Figures 1-2 for a highly symmetrical zig-zag SWCNT. The lattice structure of the zig-zag tube is described by the indices (n, m=0), with the tube diameter (d) proportional to n. Two equivalent band structure valleys are found near the zone edges. Important phonon branches are identified based on the conservation of momentum around the circumference of the tube. Phonons may be acoustic(LA) or optical(LO) and lead to intravalley or intervalley(IV) electron transitions. Analytical models for the electronic and phonon energy spectrum, shown in Figure 3-4, are designed to agree with the results of tight-binding [3] and force constant [3] calculations respectively. Within the Monte Carlo simulations, mobile electrons are considered to scatter inelastically with phonons according to Fermi's Golden Rule. This rate is collision broadened and the deformation approximation is assumed. Following the theoretical work of Anantram et al. [4], a deformation potential of D=9eV is used for zig-zag SWCNTs, independent of the tube diameter.

Steady-state, homogeneous simulations of the room temperature SWCNT mobility are given in Figure 5. Here the electric field is uniform and directed along the tube axis. The mobility is found to increase with increasing tube diameter for tubes with $d \leq 5$nm. Simulation results are found to agree closely with the low-field mobility of a 325 μm long, 3.9 nm diameter SWCNT measured by Fuhrer et al. [1]. The mobility, in Figure 6, was found to be very large ($\approx 1.5X10^5$ cm^2/Vs at 300K) and agreed with simulation at all but the lowest temperatures where defect scattering likely becomes dominant. Furthermore, the simulations appear to support the theoretical result for the deformation potential [4]. In Figure 7 the MC results show that L_m increases with increasing tube diameter. The relaxation length peaks and then decreases with increasing axial field. It is interesting that the simulations predict L_m to be only a few nanometers at low fields in the very small diameter tubes.

[1] T. Durkop, S. A. Getty, E. Cobas, and M. S. Fuhrer, *Nano Lett.*, Vol. 4, pp. 35, 2004.
[2] G. Pennington and N. Goldsman, *Phys. Rev. B*, Vol. 68, pp. 45426-45437, 2003.
[3] R. Saito, M. S. Dresselhaus, and G. Dresselhaus, *Physical properties of carbon nanotubes*, Imperial College Press, London 1998.
[4] L. Yang, M. P. Anantram, J. Han, and J. P. Lu, *Phys. Rev. B*, Vol. 60, pp. 13874-13878, 1999.

A full journal publication of this work will be published in the Journal of Computational Electronics.

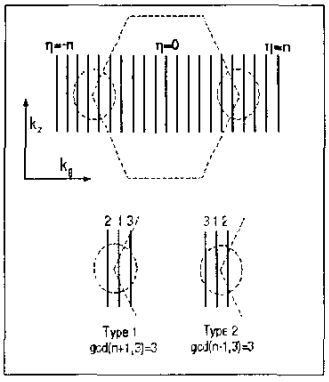

Figure 1: Electron k-space

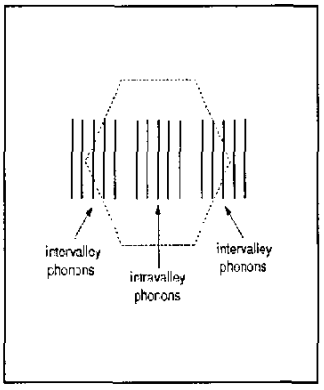

Figure 2: Phonon k-space

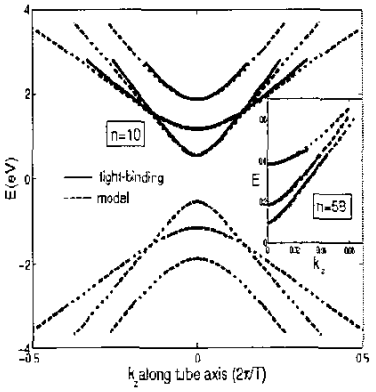

Figure 3: Band Structure

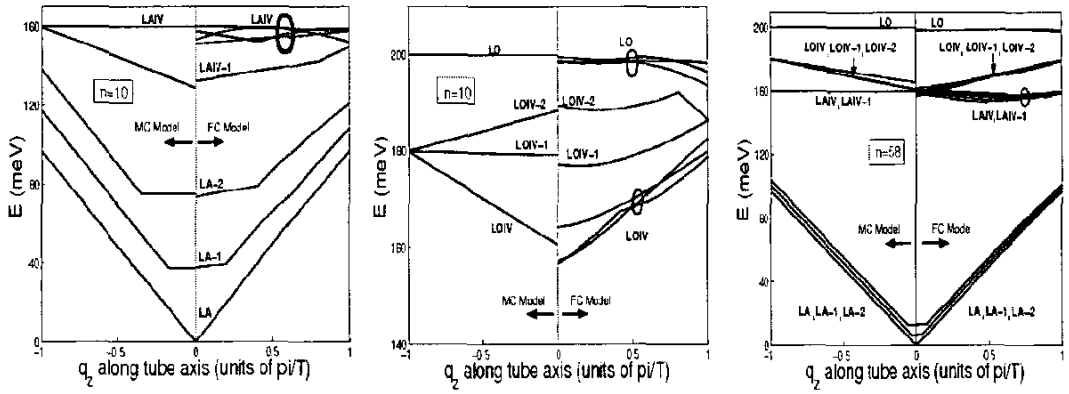

Figure 4: Phonon spectrum of an n=10 (a,b) and an n=58 (c) tube. The results of a force constant (FC) calculation And the Monte Carlo (MC) analytical model are shown.

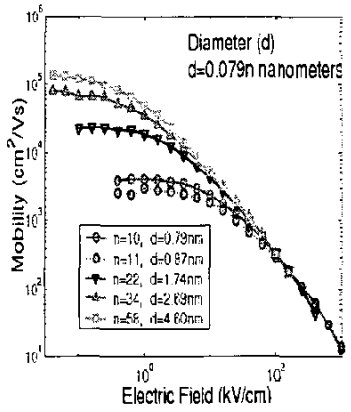

Figure 5: MC Mobility

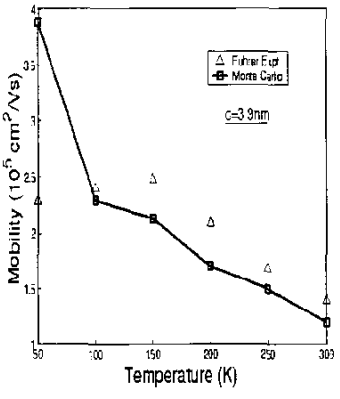

Figure 6: Low-field mobility

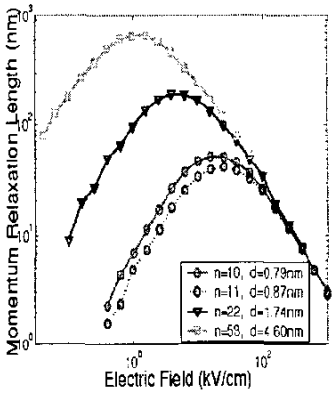

Figure 7: MC relaxation length

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