Monte-Carlo Simulation of Carbon Nanotube Devices

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A Monte-Carlo (MC) simulator to model transport in carbon nanotubes (CNTs) has been developed. It can self-consistently simulate both metallic and semiconducting CNTs, assuming a coaxially gated geometry. Figure 1a shows the geometries assumed by this simulator. Simulated results successfully match experimental data for metallic tubes.

Like other MC simulators, the particle dynamics is based on a particle-mesh (PM) algorithm. A flux-based injection mechanism has been employed to model the contacts; both ideal and Schottky contacts can be handled, with the provision for both thermionic emission and tunneling in the case of the Schottky contact. After carriers get injected from the contacts at the source (S) and drain (D), a second-order spline interpolation scheme, known as the "triangular-shaped cloud" (TSC) scheme, is used together with the potential on mesh points to calculate the particle force, and this interpolated force is then used to calculate the ballistic free-flight of the particles by integrating the semiclassical equations of motion. After free flight, the same interpolation scheme is used to assign charge to the mesh points. This model, when combined with the Poisson equation, results in a self-consistent, *ballistic*, Monte-Carlo simulator. Figure 1b shows the potential profile of a ballistic MC simulation, with particles represented by dots. The separation of the S and D injected streams inside the device is a characteristic of ballistic transport.

In a real CNT, scattering is present, and to simulate it, the following scattering model has been used. It is believed that in a CNT, there is no surface-roughness scattering, and only acoustic-phonon (AP) and optical-phonon (OP) scatterings are present. The modeling of phonon scattering in metallic CNTs is particularly easy, since the density of states (DOS) in a metallic tube is constant, yielding a scattering rate that is independent of energy. However, the modeling of scattering in semiconducting tubes is more involved for two reasons: i) the DOS in a semiconducting tube is energy dependent, and ii) there are Van Hove singularities in the DOS at the band edges, leading to infinite scattering rates. The energy dependence of the scattering rate is modeled by incorporating the functional form of the DOS into the scattering-rate expression, $\Gamma_{ac,op} = \left(\upsilon_F \left|E_{final}\right|\right) / \lambda_{ac,op} \sqrt{E_{final}{}^2 - \Delta^2}$, which reduces to a constant at higher energies. The singularities can be removed by convolving this scattering rate with a Gaussian broadening function having a constant broadening factor, as shown elsewhere. This scattering model was added to the ballistic simulator. Figure 1c shows a snapshot of the self-consistent potential profile inside the device in the presence of scattering. As shown, some of the carriers are relaxed by emitting optical phonons and some are reflected backwards by acoustic phonons. Optical phonons have little effect in modifying the current in nondegenerate systems (Fig. 2a), and the biggest effect comes from backscattering by acoustic phonons (Fig. 2b). Figure 1d shows the complete output characteristics of a CNTFET having ideal MOSFET-like S and D contacts.

The above simulator has been applied to study the average mean-free path (MFP) of semiconducting tubes. It is found that due to the presence of the Van Hove singularity, the average MFP is much smaller than in metallic tubes and is bias dependent. It varies from 75nm to 275nm over a bias range of 50mV to 500mV, as shown in Fig. 2c. Taking 275nm as the MFP, we see that a 50-nm-long semiconducting tube operates at ~ 85% of its ballistic limit (Fig. 2d).

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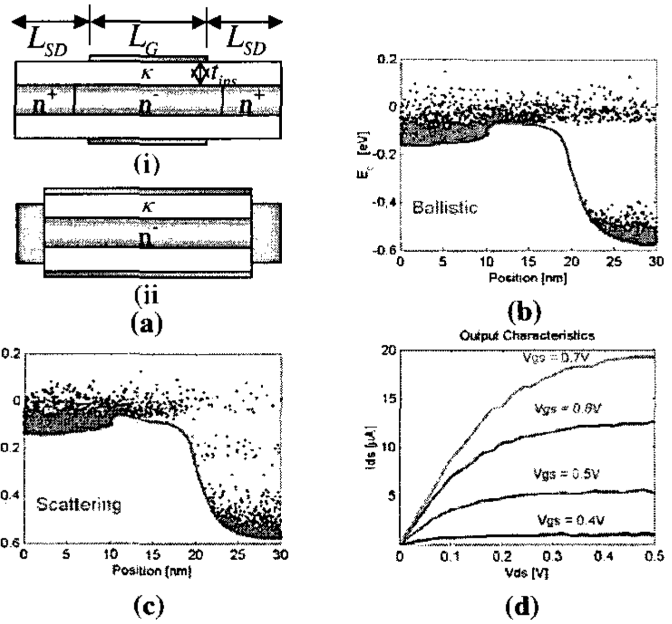

Figure 1: (a) Device geometry – coaxially gated CNTFET: (i) with ideal contacts to n^+ S, D; and (ii) with Schottky contact to S/D metal. The self-consistent potential profile of a MOSFET-type CNTFET with $L_{SD} = L_G = 10nm$, $t_{ins} = 2nm$, and $\kappa = 25$ is shown in (b) for ballistic transport, and in (c) for transport with scattering; part (d) shows the output characteristics of the device when scattering is present.

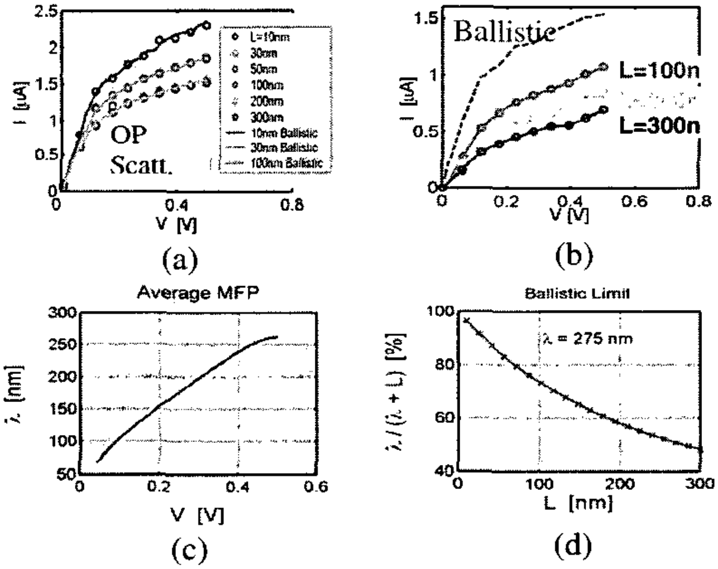

Figure 2: MC simulation of a semiconducting tube with Schottky contacts at the end and $t_{ins} + r_{cnt} = 2L$. (a) When only OPs are present, for nondegenerate systems, the predicted current (circles) is exactly equal to the ballistic limit (solid lines). (b) With APs, the predicted current is less than the ballistic limit. Part (c) shows the variation of the MFP with bias. Part (d) shows the variation of the ratio ($I / I_{ballistic}$) with length.

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