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”Monte Carlo simulation of electron transport in semiconducting zigzag carbon nanotubes”

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Abstract:

Since the advent of nanoscale material based electronic devices, there has been a considerable interest in exploring carbon nanotubes from fundamental science and technological perspectives. In carbon nanotubes, the atoms form a cylindrical structure with a diameter of the order 1nm. The length of the nanotubes can extend up to several hundred micrometers. Carbon nanotubes exhibit a variety of intriguing electronic properties such as semiconducting and metallic behaviour, due to the quantum confinement of the electrons in the circumferential direction. Much of the study dedicated to describe the behaviour of carbon nanotube-based devices assumes for simplicity the nanotube to be a ballistic material. However, in reality the phonon scattering mechanism exists also in nanotubes, of course, and can generally not be neglected, except in very short nanotubes. In this work, we focus attention on exploring the steady-state electron transport properties of semiconducting single-walled carbon nanotubes, including both phonon scattering and defect (vacancy) scattering, using the semi-classical bulk single electron Monte Carlo method.

The electron energy dispersion relations are obtained by applying the zone folding technique to the dispersion relations of graphene, which are calculated using the tight-binding description. The vibrational modes in the carbon nanotubes are studied using a fourth nearest-neighbour force constant model. Both the electron-phonon and the electron-defect interactions are formulated within the tight-binding framework, and their corresponding scattering rates are computed and analyzed. In particular, the dependence of the phonon scattering rate and the defect scattering rate on the diameter of the nanotube, on temperature and on electron energy is studied. It is shown that the differences observed in the scattering rate between different nanotubes mainly stem from the differences in their band structure.

A bulk single electron Monte Carlo simulator was developed to study the electron transport in semiconducting zigzag carbon nanotubes. As a first step, we included only electron-phonon scattering, neglecting all other possible scattering mechanisms. With this scattering mechanism, the steady-state drift velocity and the mobility for the nanotubes (8,0), (10,0), (11,0), (13,0) and (25,0) were calculated as functions of the electric-field strength and lattice temperature, and the results are presented and analyzed here. The dependence of the mobility on the lattice temperature can be clearly seen at low electric-field strengths. At such electric-field strengths, the scattering is almost entirely due to acoustic phonons, whereas at high electric-field strengths optical phonon emission processes dominate. It is shown that the saturation of the steady-state drift velocity at high electric-field strengths is due to the emission of high-energy optical phonons.

The results indicate the presence of Negative differential resistance for some of the nanotubes considered in this work. The discrepancy found in the literature concerning the physical reason for the appearance of negative differential resistance is clarified, and a new explanation is proposed. It is also observed that the backward scattering is dominant over the forward scattering at high electric-field strengths.

We then included also defect scattering, actually electron-vacancy scattering, for the nanotubes (10,0) and (13,0). The steady-state drift velocities for these nanotubes are calculated as functions of the density of vacancies, electric-field strength and the lattice temperature, using three different vacancy concentrations. The results indicate the presence of Negative differential resistance at very low concentration of defects, and how this feature may depend on the concentration of defects. The dependence of the steady-state drift velocity on the concentration of defect and the lattice temperature is discussed. The electron distribution functions for different temperatures and electric field strengths are also calculated and investigated for all the semiconducting nanotubes considered here. In particular, a steep barrier found in the electron distribution function is attributed to the emission of high energy optical phonons.

Keywords: Carbon nanotubes, Monte Carlo method, drift velocity, mobility, electron-phonon scattering, and electron-defect scattering.