Tight-binding calculations of electron scattering rates in semiconducting zigzag carbon nanotubes

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ISSN 1652-8948, Mid Sweden University Licentiate Thesis 55, ISBN 978-91-86694-15-9

ABSTRACT

The technological interest in a material depends very much on its electrical, magnetic, optical and/or mechanical properties. In carbon nanotubes the atoms form a cylindrical structure with a diameter of the order 1 nm, but the nanotubes can be up to several hundred micrometers in length. This makes carbon nanotubes a remarkable model for one-dimensional systems. A lot of efforts have been dedicated to manufacturing carbon nanotubes, which is expected to be the material for the next generation of devices. Despite all the attention that carbon nanotubes have received from the scientific community, only rather limited progress has been made in the theoretical understanding of their physical properties. In this work, we attempt to provide an understanding of the electron-phonon and electron-defect interactions in semiconducting zigzag carbon nanotubes using a tight-binding approach.

The electronic energy dispersion relations are calculated by applying the zone-folding technique to the dispersion relations of graphene. A fourth-nearest-neighbour force constant model has been applied to study the vibrational modes in the carbon nanotubes. Both the electron-phonon interaction and the electron-defect interaction are formulated within the tight-binding approximation, and analyzed in terms of their quantum mechanical scattering rates. Apart from the scattering rates, their components in terms of phonon absorption, phonon emission, backscattering and forward scattering have been determined and analyzed. The scattering rates for (5,0), (7,0), (10,0), (13,0) and (25,0) carbon nanotubes at room temperature and at 10K are presented and discussed. The phonon scattering rate is dependent on the lattice temperature in the interval 0-0.17 eV. We find that backscattering and phonon emission are dominant over forward scattering and phonon absorption in most of the energy interval. However, forward scattering and phonon absorption can be comparable to backscattering and phonon emission in limited energy intervals. The phonon modes associated with each peak in the electron-phonon scattering rates have been identified, and the similarities in the phonon scattering rates between different nanotubes are discussed.

The dependence of the defect scattering rate on the tube diameter is similar to that of the phonon scattering rate. Both the phonon and the defect scattering rates show strong dependence on the tube diameter (i.e., the scattering rate decreases as a function of the index of the nanotube). It is observed that the backscattering and forward scattering for electrons interacting with defects occur with same frequency at all energies, in sharp contrast to the situation for phonon scattering. It is demonstrated that the differences in the scattering rate between different tubes are mainly due to the differences in their band structures.

Keywords: Tight-binding, carbon nanotubes, electron-phonon scattering, backscattering, forward scattering