The Effect of Vacancy Defects on Electron Scattering in Carbon Nanotubes

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Abstract

There has been much interest in carbon nanotubes (CNTs) in recent years due to their unique physical properties. Their defect free ballistic transport makes them an ideal material for use in nanoelectronic devices [1]. However, due to their low dimensionality introduction of defects can result in dramatic changes in both chemical and physical properties [2]. Because of their quasi-one dimensional structure, charge carriers propagate primarily along the CNT axis and consequently scattering at defects cannot be avoided. A detailed understanding of CNT defects is therefore of critical importance for the wide spread adoption of CNTs in technological applications.

The most widely observed defects in CNTs are mono- and divacancies (defects with one or two atoms respectively missing at the defect site) [3] and consequently these defects are the focus of this work. We consider two configurations for the divacancy defect, the first consisting of an octagon bordered by two pentagons (585) and the second formed by three pentagons and three heptagons (777555). In particular, we consider large diameter CNTs (up to ~4.2 nm) in this work. We use density functional theory (DFT) as implemented by OpenMX [4] to calculate the formation energies for mono- (ΔE_{mono}) and divacancy ($\Delta E_{latdivac}$, $\Delta E_{vertdivac}$, ΔE_{777555}) defects in armchair (AC) and zig-zag (ZZ) CNTs and graphene. We then use TIMES [5] to calculate transport properties (without self-consistency) from DFT electronic structure calculations. Transport results are therefore subject to the same limitations as standard DFT calculations.

For AC and ZZ CNTs, $\Delta E_{latdivac} < \Delta E_{vertdivac} < 2\Delta E_{mono}$ (i.e. the formation of the lateral divacancy is least unfavourable) consistent with results previously reported for small diameter CNTs [6]. The formation energies for the 585 defects are smaller than for the 777555 defects for the ZZ CNTs studied, while ΔE_{777555} is smaller than the 585 defect formation energies for the (30,30) AC CNT confirming the estimation from an exploration based on continuum mechanics for this crossover made by Amorim *et al* [7]. Thus at larger diameters (and hence less curvature) 777555 defects are more easily formed than 585, as is the case in zero-curvature graphene.

In all cases, the introduction of a defect results in decreased transmission relative to the pristine CNT, with the greatest reduction occurring for the 777555 defect (Figure 1). Of particular significance is the drop in transmission to ~0.1G close the Fermi level for the (30,30)-CNT. This large scattering would necessarily have to be considered in applications involving large diameter CNTs, as it is in such case this defect becomes relatively more stable than the 585. We estimate the mean free path (λ) using the independent scattering approximation. As the CNT diameter increases, λ increases significantly for fixed defect concentration, this is attributed to the diminishing scattering resistance (which is proportional to the ratio of the defect scattering concentration to the CNT diameter).

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Figures

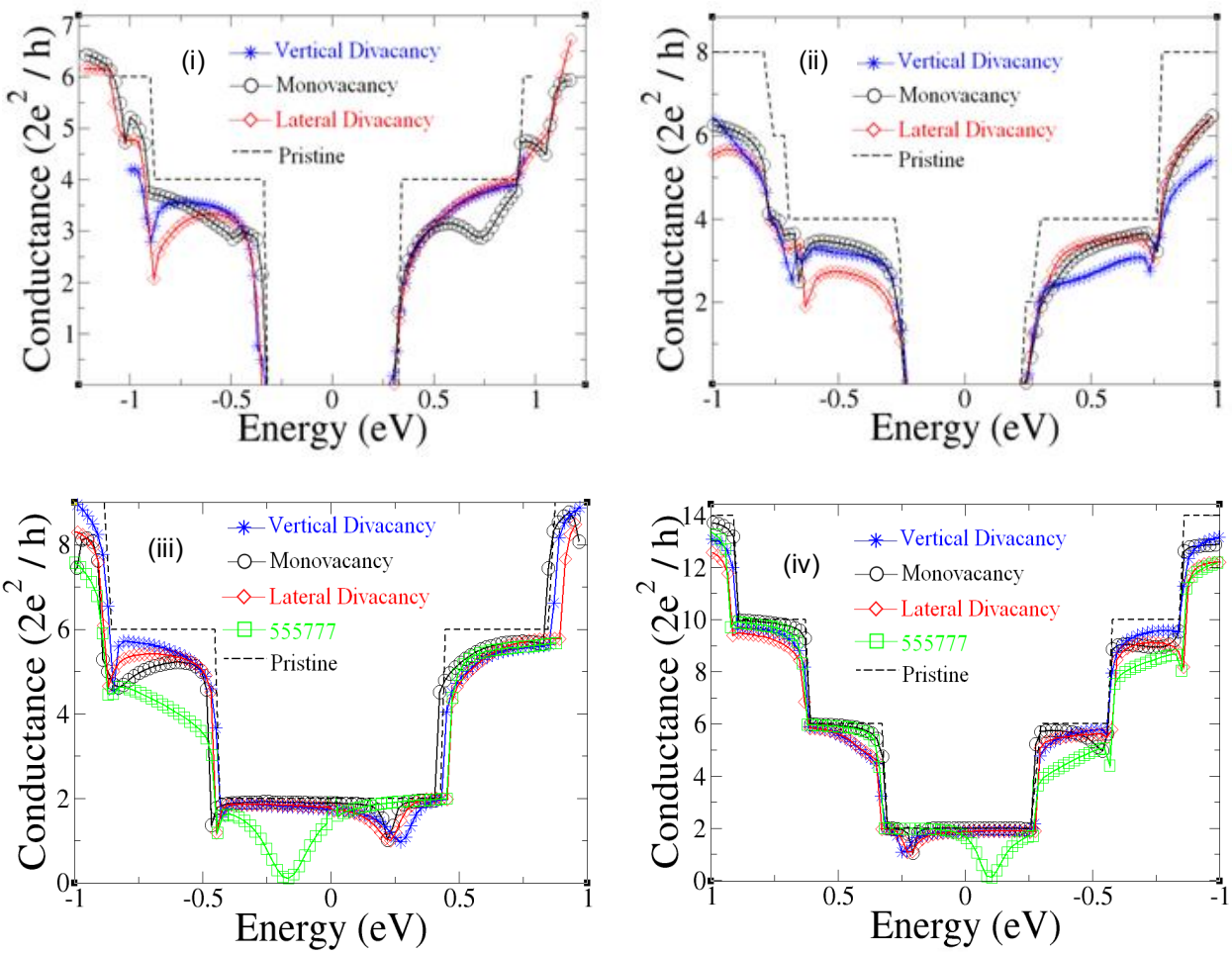

Figure 1. Conductance spectra for zigzag semiconducting tubes (graphs (i) and (ii) for (20, 0) and (30, 0) respectively) and armchair metallic tubes (graphs (iii) and (iv)for (20, 20) and (30, 30) respectively). Note the greater amount of scattering for the 555777 configuration of the divacancy defect.

Acknowledgments

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