

MAR05-2004-010166

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Mesoscopic transport in carbon nanotubes with boron and nitrogen substitutions

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This theoretical study is devoted to the electronic structure and (magneto)transport properties of carbon nanotubes containing boron or nitrogen substitutions. It addresses large devices with a mesoscopic approach, in order to tune the density of substitutional atoms and to take random multiple interference effects into account. The electronic properties are treated within a modified tight-binding model, with parameters adjusted on ab initio results, allowing to treat correctly charge transfer due to impurities. The transport properties were calculated using the Kubo formalism. The evolution of the generic transport properties (conduction regime, conductance, etc.) versus the density of substitutional atoms has been studied. The regime is found to be highly sensitive upon the energy and the density of dopants: following the cases, it may be quasi-ballistic, diffusive (here, the mean free paths follow usual scalings), or strongly localized. Finally, when a magnetic field is applied along the nanotube axis, an anomalous Aharonov-Bohm phenomenon in the conduction properties has been pointed out.