Simulation of Electromagnetic Properties in CNT and Graphene Based Nanostructures

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CNT and graphene nanostructures (e.g.,GNR) constitute the basis of high-speed nanoelectronics and nanosensors. Special attention is paid to fundamental properties of various CNT-Me, GNR-Me and CNT-graphene interconnects. The cluster approach based on the multiple scattering theory formalism as well as effective medium approximation can be used for nano-sized systems modeling including calculation of dispersion law, electronic density of states, conductivity,etc. The multiple scattering problems are solved for radial (quantum dots) and axial (nanowires,nanotubes) symmetry approaches. Technological interest to contacts of CNTs or GNRs with other conducting elements in a nanocircuit is a reason to estimate C-Me interconnect resistances depending on chirality effects in interconnects of single-wall and multi-wall CNTs, single-layer and multi-layer GNRs with the fitting metals for the predefined carbon system geometry. Simulations of electromagnetic properties of interconnects demand the calculations of interconnect impedances. Evaluation of interconnect capacitances and frequency properties (GHz&THz) have been performed. Temperature properties of CMT-Me and GNR-Me interconnects have been simulated too. Parametric calculations of CNT dc- and ac-conductivities for various chiralities (Kubo-Greenwood formula) provide important information for nanotechnology. The model of CNT growth with predefined chiralities in a magnetically managed CVD process using magnetically anisotropic FexPt1-x nanoparticles with various substitutional disorders has been developed. Special attention is paid to presence of dangling atomic bonds in interconnects that make them chemically, electrically and magnetically sensitive. Thus, interconnects can be considered as perspective nanosensor structures.

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Electronic and optical properties of silicon nanowires

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By means of first principles calculations the electronic and optical properties of -, -, - and -oriented silicon nanowires passivated by hydrogen have been investigated. Silicon nanowires with axes are found to possess the direct bend gap nature. In the case of - and -oriented silicon nanowires their band gap is characterized by quasidirect nature because the energy difference between the first direct and indirect transitions has turned out to be a few meV. Nevertheless, an expansion in the lattice parameter along the wire axis leads to the stabilization of the first direct transition. The indirect nature of the gap is revealed for silicon nanowires in growth orientation. Estimates of the dipole matrix elements of the first direct transition for - and -oriented silicon nanowires have shown sizable values if silicon dimmers are formed on {001} facets indicating these nanostructures to be a perspective material for manufacturing light emitting devices integrated in the common silicon technology.

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