CARRIER SPECTRA IN A SEMICONDUCTOR NANOTUBE WITH ADSORBED INCOMMENSURATE STRUCTURES

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Carbon nanotubes (CNTs) are nano materials with a small diameter of about 1 nm, length of about 1 µm and the mean free path of the charge carriers exceeds 10 µm [1] what is important for quantization [2]. Functionalization is new powerful method for tuning CNTs properties [3]. Theory of energy spectra tuning in the semiconductor (SC) CNTs as the result of functionalization by molecular films was developed in work [4].

The aim of this research is to develop theoretical approach to the CNTs spectra tuning as result of functionalization by thin molecular layer which forms misfit dislocations. We consider the effect of the interaction of the uncompensated charge of a carrier in a quantum nanowire with the neighboring medium, which has low mechanical rigidity and consists of molecules possessing an intrinsic electric-dipole moment. The incommensurate molecular structure is formed along the nanotube..

The selfconsistent system of equations is obtained similarly [4]. The system includes the time-independent Schrödinger equation for a charge carrier in a semiconductor carbone nanotube, nonlinear equation for incommensurate molecular structure, the material equations for interaction an extra carrier in a nanotube and molecular electric dipoles subsystem, the material equations for renormalizing of molecules-substrate interaction in the carrier presence. The periodic system of misfit dislocations of the adsorbed molecules creates a superlattice potential for a carrier inside a nanotube. These misfit dislocations may be of two kinds: with interstitial molecular row or with lack one. The periodic quantum barriers are relatively narrow and can form the superlattice carrier spectrum. In turnes, the carrier attracts the molecular layer what leads to the coherent regions widening and dislocation rearrangement. The periodic quantum wells rather can lead to a carrier localization. In semiconductor CNT the hole and electron spectra are symmetric. The layer of the intrinsic electric dipoles of the adsorbed molecules breaks this symmetry. This dipoles layer creates opposite conditions for a carrier localization or tunneling along dislocation superlattice in dependence on charge sign and dipole orientation.

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