Effect of the hydrogen atomic adsorption on the transport properties of single-walled carbon nanotubes

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Abstract

Currently, considerable interest is the generation of carbon nanostructures with specified characteristics. These structures may be applied in various fields of modern electronics, materials, chemistry and medicine [1, 2]. Transport properties of carbon nanotubes (CNTs) are one of the most important from the point of view for practical applications. Any solid surface coated with films of atoms or molecules adsorbed from the environment or left on the surface during the diffusion process under normal conditions [3]. Significant interest causes the study of the effect of atomic adsorption for different chemical elements and molecules on the electrical properties of carbon nanostructures.

The Anderson's Hamiltonian [4, 5] initially proposed for the description of the electronic states of impurity atoms in the metal alloys is often used in the theory of adsorption. This model has been successfully applied to study the adsorption of atoms on metal surfaces and semiconductors [6], the adsorption of hydrogen on the surface of graphene [7] and carbon nanotubes [8, 9]. We consider the hydrogen atomic adsorption influence for transport (conductive and diffusion) properties of "zigzag" single-walled carbon nanotubes in this paper. The interaction of hydrogen atoms, which adsorbed on the surface of carbon nanotubes is described within the framework of the periodic Anderson model. This model is well suited to describe the adsorption on the nanotubes surface, because the geometric configuration of the nanotubes determines their conductive properties. Transport coefficients (conductivity and electron diffusion coefficient) of CNT are calculated by solving the Boltzmann kinetic equation [10] in the relaxation time approximation. This technique has been successfully applied by authors for calculating the transport properties of ideal carbon nanotubes [11], graphene, bilayer graphene [12] and bilayer graphene nanoribbons [13].

State of the electrons in the crystal containing impurities in the π-electron approximation and in the nearest neighbor approximation is described in the periodic Anderson model by the effective Hamiltonian, having the following common form [5]:

$$H = \sum_{j,\Delta,\sigma} t_\Delta \left(c^+_{j\sigma} c_{j+\Delta\sigma} + c^+_{j+\Delta\sigma} c_{j\sigma} \right) + \sum_{l,\sigma} \varepsilon_{l\sigma} n^d_{l\sigma} + \sum_l U n^d_{l\uparrow} n^d_{l\downarrow} + \\ + \sum_{l,j,\sigma} \left(V_{lj} c^+_{j\sigma} d_{l\sigma} + V^*_{lj} d^+_{l\sigma} c_{j\sigma} \right), \quad (1)$$

where t_Δ is the electron hopping integral between the neighboring lattice sites of the crystal; *U* is the constant of the Coulomb repulsion of the impurity; $c_{j\sigma}$ and $c^+_{j\sigma}$ are the Fermi annihilation and creation operators of electrons in the crystal node *j* with spin σ; $d_{j\sigma}$ and $d^+_{j\sigma}$ are the Fermi annihilation and creation operators of electrons on the impurities *l* with spin *σ*; $n^d_{l\sigma}$ is the operator of the number of electrons on impurities *l* with spin *σ*; $\varepsilon_{l\sigma}$ is the energy of the electron by the impurity *l* with spin *σ*; V_{lj} is the matrix element of hybridization of impurity electron *l* and atom *j* of the crystal.

The band structure of single-walled carbon nanotubes with adsorbed hydrogen atoms obtained using the Fourier transform of the creation and destruction operators of electrons in the crystal, and the Green function method takes the form [8, 9].

The external electric field is applied along the x axis directed along the axis of the nanotube. Method of calculation of the transport coefficients of electrons in carbon nanotubes is described in the papers [11 - 13]. Longitudinal component of the current density has the form.

$$j(x) = \sigma(\mathbf{E})\mathbf{E} + D(\mathbf{E}) \frac{\nabla_x n}{n} \quad (2)$$

The formulas for the transport coefficients of single-walled carbon nanotubes there are electrical conductivity and electron diffusion coefficient obtained for the case of a homogeneous temperature distribution and the linear approximation in the gradient magnitude of the electron concentration.

The conductivity tends to a constant value with increasing amplitude of the external electric field. The desire of the nonlinear conductivity of carbon nanotubes to a constant value is due to the limited number

of charge carriers involved in the transport of electric current on the surface of the nanotubes. Fewer electrons are able to participate in the transfer of power with increasing amplitude of the electric field because other electrons already at lower values of the field by the conduction electrons become involved in the transfer of current. Adding one of the adsorbed hydrogen atom reduce the conductivity by a small amount (about $2*10^{-3}$ S/m). Electrical conductivity decreases with the adsorption of hydrogen atom because that one of the electrons which localized in the crystallite forms a chemical bond with the impurity atom this atom is not involved in the process of charge transfer along the carbon nanotube. The electrical conductivity dependences of the external electric field magnitude for carbon nanotubes by (10,0) type, containing different concentrations of adsorbed hydrogen atoms were analyzed numerically. Increasing the number of adsorbed atoms decreases the electrical conductivity of «zigzag» carbon nanotube proportional to the amount of localized adsorption bonds. If you add one hydrogen adatom the conductivity of (10.0) carbon nanotube is reduced by 0.06%, if you add 100 adatoms the conductivity is reduced by 0.55%, the addition of 300 adatoms - 1.66%, if you add 500 adatoms the conductivity is reduced by 2.62%.

Dependence between the electron diffusion coefficient of the single-walled carbon nanotubes with adsorbed hydrogen atoms and the electric field amplitude has a pronounced non-linear. Electron diffusion coefficient initially increases and then decreases to a steady value with increasing electric field. This phenomenon is common to all systems with periodic and limited electron dispersion laws [17]. Maximum value of the diffusion coefficient for semiconductor carbon nanotubes observed at the electric field strength of the order of $E \approx 4{,}8*10^{5}$ V/m. If we add one adsorbed hydrogen atom, the electron diffusion coefficient reduced by 0.05%. This behavior of the electron diffusion coefficient in an external electric field is observed for different hydrogen adatom concentrations for semiconductor carbon nanotubes with different diameters when 100 adsorbed atoms added. At present one needs the study of transport and conduction properties of semiconductor carbon nanotubes with adsorbed hydrogen atoms for determining the operating parameters of nanoelectronic devices and for the miniaturization of the modern element base of microelectronics, such as transistors, and for creating new devices based on the unique properties of carbon nanotubes.

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