Modeling of field emission from nano-carbons

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Nano-carbon materials show remarkable field emission characteristics specifically low-field emission and high current densities. This makes them very attractive as cold cathodes for vacuum microelectronic devices [1, 2]. The field emission characteristics depend on topology of the cathode surface and material properties. While shape and aspect ratio is the most important parameters of an individual emission site, their density determines threshold field and emission current for whole cathode. The highest emission currents are available with optimization of distance between the emission sites having certain geometry.

We report here computer modeling and experimental study of carbon cathodes made of carbon nanotubes [1] and plate-like graphite nanocrystallites [2]. To simulate the infinite arrays of emitters the 3D Laplace problem with periodic boundary conditions was solved. The emission current density was calculated by Fowler-Nordheim equation. We assumed the nano-carbon film as a flat array of cylinders (nanotubes) and planes (nanoflakes) with perpendicular orientation to the substrate. The height and width of emitters were 1?m and 10nm respectively. By varying distance between emitters we found the dependencies of field enhancement factor ? and current densities. As a result we obtained optimum distances between emitters 2?m and 5?m for cylinders and planes respectively. These results were verified experimentally.

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Nanorelay based on multi-walled nanotubes

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Considerable progress has been achieved in nanotechnology techniques in the field of production of nanoelectromechanical systems (NEMS). Remarkable properties of carbon nanotubes, like free relative sliding and rotation of the walls and metallic conductivity, allow to use the walls of nanotubes as movable elements and elements of electric circuit in NEMS [1, 2].

We propose new schematics of electromechanical nanorelay based on the relative motion of the walls with the electrodes made of carbon nanotubes. The two-terminal and three-terminal nanorelays (with the third control electrode) are considered. The operation of the nanorelay is based on the following principles. When the voltage is applied, the electrostatic force pulls out the inner wall of a double-walled nanotube (the first electrode), which subsequently gets attracted to the second electrode by the Van der Waals force (position 'on'). When the voltage is off, the inner wall retracts back into the outer wall by capillary force (position 'off').

The balance of forces, which determines the operation of nanorelay is analyzed. The density functional AIMPRO supercell code within the local density approximation has been used to calculate the interaction between the walls of the first electrode (the details of calculations can be found in [3,4]). The structure of the caps of the nanotubes used as the electrodes of nanorelay has been obtained using Q-Chem 2.1 quantum chemistry package. The Lennard-Jones potential has been used for computing the van der Waals interaction between the electrodes of nanorelay. It is shown that the proposed nanorelays can be used as memory cells of external or on-line storage depending on the atomic structure and the length of the electrodes. The dependence of the lifetime of a memory cell of external storage on its size is calculated. For the memory cell of on-line storage, the voltage of the switching between position "off" and "on" estimated to be about 6V, the voltage needed to hold the nanorelay in position "on" is about 4.8V. The operation frequency of the proposed memory cells is estimated to be about 100 GHz.

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Nonlinear interlayer transport in the aligned carbone nanotube films and graphite

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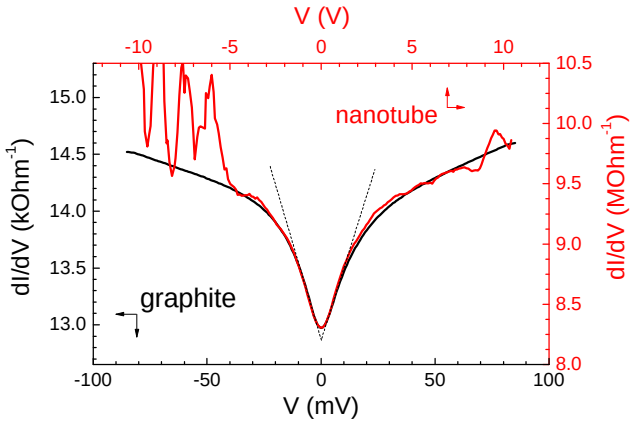
That is widely accepted now that in many classes of layered highly anysotropic materials as high temperature superconductors, manganites, charge density wave materials electron transport across the layers occurs via interlayer tunneling. That gave rise to interlayer tunneling spectroscopy of these materials [1]. Another class of highly anysotropic carbon based materials as graphite and nanotubes has not yet been studied by this technique.

In present studies we investigated interlayer transport on mesa-type graphite structures and aligned carbon nanotube films. In this way we compare interlayer transport between flat and curved elementary carbon layers. The mesa-type structures have been fabricated by double-sided focused ion beam technique [2] on thin single crystals of natural graphite. They have 1μ x 1μ lateral sizes and contain few tens of elementary carbon layers. The dense nanotube films with nanotube axis oriented perpendicular to the substrate have been grown by electron beam evaporation technique [3].

We found that interlayer tunneling is essentially non-linear and has universal dependence for both type of objects. That points out to its fundamental origin related with tunneling density of states. The initial linear growth of DOS is observed on graphite up to 10 mV with the following gradual saturation. The linear density of states has been recently reported on graphite from ARPES experiments [4] as being originated from the presence of Dirac fermions.



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Electromagnetic solitons in carbon nanotube ropes

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Modern technologies impose ever greater requirements upon research and development, especially in the field of nanoscale phenomena. This is due to progress in computer engineering, where the smaller size of electronic devices increases their response and reduces consumed energy. The unique properties of carbon nanotubes (CNT) led to their extensive studies and applications within the framework of nonlinear optics. A major and most promising approach in this field is to study the propagation of ultrashort light pulses (optical solitons) in CNT [1]. Major aim of modern optics is the development of all-optical devices in which light can be controlled with light. A result of this is rapidly expanding research into optical effects related to the interaction of electromagnetic solitons. Interest in this research is stimulated both by successful experiments, which led to multidimensional optical solitons (stable localized light structures), and new materials, which are promising for developing all-optical devices.

When constructing the model of the propagation of an ultrashort optical pulse in nanotube ropes, we shall describe the electromagnetic field of a pulse in the classical way, based on the Maxwell equations. Taking into account the dielectric and magnetic properties of CNT, the Maxwell equations and the classical Boltzmann kinetic equation in the approximation of relaxation time can be written as follows:

$$\frac{\partial^2 \vec{A}}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} + \frac{4\pi}{c}\vec{j} = 0\,,\ \frac{\partial f}{\partial t} - \frac{q}{c}\frac{\partial A_z}{\partial t}\frac{\partial f}{\partial p_z} = \frac{F_0 - f}{\tau}\,,$$

where the quasipulse **p** is given as (p_z, s), s = 1, 2, ..., m, z – (m, 0) CNT axis, x – orthogonal to z axis, **A** = (0, 0, A_z(x, t)) - vector potential, f = f(p_z, s, t) - distribution function.

An efficient equation for the dynamics of an electric field in a CNT ropes was obtained; the equation has a form similar to the double sine-Gordon equation. The equations studied were solved numerically using the cross-type finite difference scheme. Temporal and coordinate steps were determined from the standard conditions of stability.

A pulse entering the CNT rope at a larger group current velocity was found to induce a larger current. The total current flowing through the system of nanotubes is determined both by the "area" of the electromagnetic pulse and the relaxation time of the electron distribution function to an equilibrium value.

When passing the CNT system, an electromagnetic pulse is divided into two, the smaller pulse having the value determined by the initial group velocity of the pulse. This behavior is related to the presence of an analog of the theorem of areas in systems described by the double sine-Gordon equation.

A current pulse is generated with a delay with respect to the initiating electromagnetic-field pulse; this is due to the description of the electron dynamics within the framework of the classical Boltzmann kinetic equation in a relaxation-time approximation.

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Current domains in carbon nanotube ropes

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The unique properties of carbon nanotubes (CNT) led to their extensive studies and applications within the framework of nonlinear optics. A major and most promising approach in this field is to study the propagation of ultrashort light pulses (optical solitons) in CNT [1]. Major aim of modern optics is the development of all-optical devices in which light can be controlled with light. A result of this is rapidly expanding research into optical effects related to the interaction of electromagnetic solitons. Interest in this research is stimulated both by successful experiments, which led to multidimensional optical solitons (stable localized light structures), and new materials, which are promising for developing all-optical devices.

The dynamics of periodic electromagnetic pulse in CNT has been described in the classical way, based on the Maxwell equations. Taking into account the dielectric and magnetic properties of CNT, the Maxwell equations and the classical Boltzmann kinetic equation in the approximation of relaxation time can be written as follows:

$$\frac{\partial^2 A_z}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 A_z}{\partial t^2} + \frac{q}{\pi\hbar\tau}\sum_m c_m \sin\left(\frac{maq}{c}A_z(t)\right) = 0\,,\ \frac{\partial f}{\partial t} - \frac{q}{c}\frac{\partial A_z}{\partial t}\frac{\partial f}{\partial p_z} = \frac{F_0 - f}{\tau},$$

$$c_m = \sum_s a_{ms} b_{ms}\,,\ b_{ms} = \int_{-q_0}^{q_0} dp_z \cos(map_z) F_0(\vec{p})\,.$$

where the quasipulse **p** is given as (p_z, s), s = 1, 2, ..., m, z – (m, 0) CNT axis, x – orthogonal to z axis, **A** = (0, 0, A_z(x, t)) - vector potential, f = f(p_z, s, t) - distribution function.

An efficient equation for the dynamics of periodic electromagnetic pulse in a CNT ropes was obtained; the equation has a form similar to the double sine-Gordon equation. The equations studied were solved numerically using the cross-type finite difference scheme. Temporal and coordinate steps were determined from the standard conditions of stability.

A pulse entering the CNT rope at a larger group current velocity was found to induce a larger current. A current pulse is generated with a delay with respect to the initiating electromagnetic-field pulse; this is due to the description of the electron dynamics within the framework of the classical Boltzmann kinetic equation in a relaxation-time approximation.

Periodic electromagnetic pulses in carbon nanotubes ropes passes in a course of the evolution of a stage similar to behavior of brizers of the sine-Gordon equation.

When periodic electromagnetic pulses moving the areas with various meaning of current amplitude in them are formed, this can be interpreted as domains of a current.

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Anti ferromagnetic solitons in carbon nanotubes

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The decade researches have shown that carbon nanotubes have unique properties and number of other properties causing unlimited opportunities of their applications, for example in microelectronics. The especial interest, as well as followed, to expect cause nonlinear properties of carbon nanotubes (CNT). In given paper it is supposed to concentrate attention on nonlinear magnetic properties of CNT caused by strong electron interaction described by Hubbard's Hamiltonian.

Hamiltonian of ?-electron system of (m, 0) CNT has been taken in a traditional term offered Hubbard:

$$H = -\sum_{jÄσ} t(a^{+}_{j+Äó} a_{jó} + a^{+}_{jó} a_{j+Äó}) + ì \sum_{Ä} a^{+}_{jó} a_{jó} + U \sum_{j} a^{+}_{jó} a_{jó} a^{+}_{j+ó} a_{j-ó} \quad ,$$

where a^{+}_{js}, a_{js} - an electron appearance and annihilation operators on j point (j = {i, k}) with ? spin, t – transfer integral, U – Coulomb electron energy; ? – chemical potential. After transformations

$$a^{+}_{jσ} a_{jσ} = 1/2 - S^{z}_{j} \exp(iπ(1/2 + σ)), \qquad S^{-}_{j} = a^{+}_{jσ} a_{j-σ}, \qquad S^{+}_{j} = a^{+}_{j-σ} a_{jσ}$$

effective anti-ferromagnetic Heisenberg's Hamiltonian has been obtained:

$$H_{eff} = 2\frac{t^2}{U} \sum_{jΔ} \vec{S}_j \vec{S}_{j+Δ},$$

where S^{z}_{j} describes electron magnetic moments localized on j point. Spin components can be represented as

$$S^{\pm}_{j} = 1/2 \sin\theta_j \exp(\pm i\varphi_j), \qquad S^{z}_{j} = 1/2 \cos\theta_j.$$

Applying Lagrange's formalism the motion equation for parameters q_j, j_j have been obtained as follow:

$$\frac{\partial^2 q}{\partial t^2} = c^2 \left\{ \frac{\partial^2 q}{\partial x^2} - \frac{1}{2} \sin 2q \left\{ (\frac{\partial j}{\partial x})^2 - (\frac{1}{c} \frac{\partial j}{\partial t})^2 \right\} \right\}.$$

$$\frac{\partial}{\partial t}(\sin^2 q \frac{\partial j}{\partial t}) = c^2 \frac{\partial}{\partial x}(\sin^2 q \frac{\partial j}{\partial x})$$

Classic soliton solutions of nonlinear equation system are follow:

$$j = w(t - vx/c^2)/g$$

$$q = 2arctg \exp(w(x - vt/gc),$$

where v - soliton velocity, $g = (1 - v^2/c^2)^{1/2}$, $c = \frac{6\sqrt{2} m t^2 a}{U}$, a – C-C bond length.

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Electron emission from metal cathodes modified by carbon nanostructures

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Many electrovacuum and gas-discharge devices and mechanisms are based on the action of electron emission. Work function is the property that reflects atomic bonding force of materials and to a great extent is determined by the state of its surface. In the presence of electronegative admixtures (O, N etc.) as well as oxides and oxynitrides on crystallites surface, work function increase and emission properties of a material are deteriorated. Therefore creation of the barrier layer on the surface of materials is important for preventing adsorption of electronegative admixtures.

The usage of nanostructured materials as cathodes can provide the work function declining. However, as it is generally known, nanostructured materials and coverings on their basis are non-equilibrium and at high temperatures, as a rule, are damaged [1].

To achieve the maximum possible working temperatures of cathode declining and effective work function of electron diminishing, the backs acceptor-type properties were used. Emission properties of dispersible $LaNi_5$ with carbon-carbonic nanostructured film ($LaNi_5$/CNS) on the surface at heating by both the impulsive laser radiation in short-distance infrared-diapason and by continuous radiation containing in light-spectrum ultraviolet component, are studied. It is assumed that a nanostructured carbon layer will be a barrier to electronegative admixtures, such as O, N etc. that heighten the value of work function.

The data are compared with the metals Molybdenum of (100) crystal face (Mo) and Niobium (Nb). For $LaNi_5$/CNS it is $2 \cdot 10^3$ W/cm^2, and for Mo (100) - $80 \cdot 10^3$ W/cm^2. The temperature of at which electron emission irradiated by light radiation from nanoparticles $LaNi_5$/CNS and polycrystalline Nb began observed are in the range 340–370K and 770–870K respectively.

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Quantum-mechanical model of atomic hydrogen adsorption on carbon nanotube surface

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High adsorption properties of carbon nanotubes [1] attract a great interest to use as gas accumulators, for example, hydrogen. We have studied the energy characteristics of atomic hydrogen adsorption processes on single wall carbon nanotube (SWNT) surface.

Atom Í and single wall carbon nanotube have been considered as quantum system, and Schroedinger's equation in cylindrical coordinates for a finding of wave function of system has been solved. As potential of interaction the modeling potential as superposition of a potential hole and a barrier was chosen (proceeding from the empirical data):

$$U(r)=\begin{cases}\infty, & 0\le r\le R;\\ -U_{ads}, & R<r<a;\\ U_a, & a\le r\le b;\\ 0, & r>b.\end{cases} \qquad (1)$$

where R – radius of a tube, U_{ads} - energy of Ñ-H chemical binding, U_a – activation energy which is necessary for overcoming to atom Í for formation of chemical connection, a and b – character widths of energy bottom and barrier accordingly. Parameters U_{ads}, U_a, *a* and *b* have been calculated from quantum-chemical semi-empirical MNDO and PM3 schemes within the framework of molecular cluster method [2].

The solution of Schroedinger's equation has been expressed by Bessel's functions. Possibility current densities have been calculated and coefficients of reflection and transformation through the potential barrier have been found. These characteristics will allow analyzing process of atom Í adsorption analytically and finding opportunity interesting quantum effects.

This work is supported by Russian Foundation of Basic Researches (grant 1 07-03-96604).

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Electromechanical nanothermometer based on carbon nanotubes

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With considerable progress in nanotechnology techniques, a number of feasible designs of nanoelectromechanical systems (NEMS) have recently evolved, in which the elements of electric circuits represent nanoobjects of progressively smaller scale reaching the size of a molecule. The operation of some NEMS is based on changes in electronic structure and conductivity of a system due to the change in the relative position of its components at subnanometer scale [1, 2].

A new concept of an electromechanical nanothermometer based on the interaction and relative motion of the components of a nanosystem is proposed. Temperature measurements are carried out through the measurements of the conductivity of the components assuming that the total conductivity of a system depends significantly on the temperature due to the thermal relative vibrations of the components. A model implementation of the nanothermometer based on double-walled carbon nanotubes (DWNTs) with armchair walls is suggested. Possible schematics of the nanothermometer are considered. The dependence of the interwall interaction energy on the relative displacement of the walls is computed *ab initio* using density functional theory (the details of calculations can be found in [3, 4]). Conductivity of the DWNTs is calculated within the Huckel-Hubbard model. The nanothermometer can be used for accurate temperature measurements in the temperature range of 100-300K. The minimal size of nanotermometers based on different DWNTs, which can be used in either pulse or stationary operation modes is estimated. It is shown that the nanothermometer can be used in localized regions with dimensions of several hundred nanometers.

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MNDO-based investigation of capillary effect during penetration of elemental hydrogen into single-wall carbon nanotubes

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From the very first steps of investigation some unique sorption properties of carbon nanotubes were figured out, including those properties, which are determined by capillary effects. At that, the graphite shell protects stored substance from external influences of different nature. Today, intensive research work is carried out to develop tubulene-based devices for storage of gaseous hydrogen. In [1] a process of filling of carbon nanotubes with elemental hydrogen is investigated. It is necessary to study capillary penetration of molecular hydrogen into nanotube cavity.

Some (n,0) nanotubes and (n,n) nanotubes, containing 6, 8 hexagons along the perimeter with cylindrical symmetry were examined to determine possible regularities in penetration of molecular hydrogen into single-wall carbon nanotubes. Hydrogen molecule Í $_2$ penetrated into a nanotube, going through the center of a nanotube butt-end hole. The "Í $_2$–nanotube" complex geometry was optimized during MNDO-based calculations.

Semi-empirical research has shown, that Í $_2$ doesn't penetrate into (6,0) and (8,0) tubulenes, so we can assume that molecule energy is not enough to overcome the arising potential barrier. As the diameter grows, the process of hydrogen molecule penetration into nanotube cavity becomes of typical non-barrier nature, moreover the forming structure is stable.

As Í $_2$ penetrates into open (6,6) and (8,8) tubulenes, the process of intense capillary suction of hydrogen takes place. The very same process appears during intercalation with hydrogen of (6,6) and (8,8) nanotubes with border modifications (with functional groups).

It is interesting to mention, that modification of nanotube bordering area with functinal groups (such as oxygen atoms, hydroxyl groups and amides) makes hydrogen molecule able to penetrate nanotubes with minor diameters (6,0) and (8,0), thus overcoming potential barrier of 2.5 eV. It is obvious and can be explained through occurrence of additional forces of electrostatic interaction, appearing due to the presence of bordering functional groups, which provide positive bordering effect.

On every step of Í $_2$ hydrogen molecule penetration into nanotube cavity, main hydrogen molecule geometric parameters have been studied: molecule orientation to long axis of a nanotube has been determined. It has been also determined that no H_2 molecule bond breakage happens and a long axis capillary penetration of H_2 takes place.

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Electron transport in crossed nanotubes

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The theoretical interest to the electron transport in crossed carbon nanotubes is stipulated by recent experimental studies of these structures [1, 2]. The purpose of the present paper is a theoretical investigation of the electron transport in crossed semiconductor carbon nanotubes with a point contact between them. To describe the electron states in the tubes we use Hamiltonians H_1 and H_2 of a free electron confined on the cylindrical surface. The contact between the cylinders is described in the framework of the zero-range potential theory. Solving the Schrodinger equation, we have obtained transmission coefficients for the electron and then using the Landauer formula we have found an evident form for the conductance G_{11} of the first tube as a function of the Fermi energy m

$$G_{11}(m) = G_0 \left\{ N(m) - \frac{(\mathrm{Im}\, Q_1)^2 \, |Q_2|^2}{|Q_1 Q_2 - a^2|^2} - 2\frac{a^2 \,\mathrm{Im}\, Q_1 \,\mathrm{Im}\, Q_2}{|Q_1 Q_2 - a^2|^2} \right\}. \qquad (1)$$

Here G_0 is the conductance quantum, $N(m)$ is the number of occupied electron states in the first tube, $Q_j(m)$ (j=1,2) is the renormalized Green function of the Hamiltonian H_j, and a is a dimensionless parameter determining the coupling between wave functions in different tubes. The evident form of the function $Q_j(m)$ can be found in [3].

If the contact between the cylinders is absent ($a = 0$) then equation (1) contains the first term only and the dependence $G_{11}(m)$ is step-like. The second term in equation (1) is responsible for the back-scattering on the contact point and the last term is stipulated by the transmission of electrons from the first cylinder to the second one. The dependence $G_{11}(m)$ has a number of sharp dips stipulated by the resonance scattering on contact. The maximal depth of the dip does not exceed G_0. If diameters of the tubes are different then asymmetric resonances appear in the conductance. The resonances are stipulated by van Hove singularity in the electronic density of states. It should be noted that similar asymmetric resonances have been observed experimentally [1] in the conductance of crossed nanotubes. The conductance $G_{21}(m)$ between the tubes is proportional to the last term in equation (1). The maximal value of the conductance $G_{21}(m)$ does not exceed a unit of conductance quantum. We relate this result to the limited transparency of the point contact.

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Properties of iron nanowires encased in multiwalled carbon nanotubes

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The Fe-filled multiwalled carbon nanotubes with diameter of 100 nm and length of 30 mkm are studied using XRD, TEM, ferromagnetic and methods of magnetic resonances (ferromagnetic (FMR) and electron paramagnetic (EPR) resonance). Nanotubes are grown at Si/SiO_2 substrate (see details in [1]).

The iron within the nanotubes is found to be in three phases: the austenite gamma-Fe is located at the top of the nanotubes, while the ferrite alpha-Fe?and cementite theta-Fe3C is found close to the substrate.

Two FMR signals are obtained in the spectrum of the nanowires: one comes from the ferromagnetic α-iron, the second, more intensive and broadened, belongs to cementite. Both signals reveal uniaxial anisotropy with the anisotropy field 1.033 Ò for the α-Fe clusters and 0.7 Ò for the Fe_3C precipitates. Because of the nanoscale thickness, both values are larger than those for the bulk samples. The angle dependence of the resonance field for the FMR signal from the α-iron shows that its nanocrystal particles are elongated along the tube axis, which is consistent with TEM data.

The magnetization decreases linearly with decreasing temperature. Two hypothetical explanations are proposed: (i) an increase of the hydrostatic pressure due to the carbon shell because of its higher thermal coefficient of expansion as compared to other phases constituting the nanotube; (ii) the antiferromagnetic dipole-dipole interaction of the parallel α-iron nanowires.

As the ferromagnetism disappeared, two paramagnetic signals are observed below 100 K. Based on the character of the temperature dependence of their integral intensities, the conclusion is made that the first one with $g_1 = 2.029 \pm 5 \cdot 10^{-4}$ and the line-width $\Delta H_1 = 14 \pm 0.5$ Î å is related to localized paramagnetic centres, whereas the second one with $g_2 = 1.979 \pm 5 \cdot 10^{-4}$ and the line-width $\Delta H_2 = 8 \pm 0.5$ Î å belongs to the conduction electrons.

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The current-voltage characteristic of carbon nanotubes in non-linear model

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The decade researches have shown that carbon nanotubes (CNTs) [1] have unique conductivity properties and number of other properties causing unlimited opportunities of their applications, for example in microelectronics. In this work the theoretical calculation of current-voltage characteristic of the carbon nanotubes are represented with the Coulomb's repulsion of electrons.

Electronic states are described by the model Hubbard's Hamiltonian:

$$H = U\sum_k a_k^+ a_k a_{k-1}^+ a_{k-1} - \sum_k t_\Delta (a_{k+1}^+ a_k + a_k^+ a_{k+1}) + m\sum_i a_k^+ a_k \ ,$$

where U – Coulomb's repulsion electron energy, t_Δ - jumping integral (resonance integral), ? – chemical potential, the $a_k^+(t)$ and $a_k(t)$ - Fermi operators of creation and annihilation of an electron on k point (k – space and spin index) in the Heisenberg representation. The summation is over the nearest neighbour cells of the one-dimensional chain of period a_0.

The basic Heisenberg's equations for the $a_f(t)$ operator are following:

$$i\hbar \dot{a}_f(t) = \lfloor a_f(t), \quad \rfloor .$$

The method clearly described in [2] has been used for solution of the infinite system of non-linear equations. After simple transformations the Schrodinger's equation with cubic non-linearity has been obtained:

$$i\hbar \dot{j}(x,t) = a\, j(x,t) - b\, j_{xx}(x,t) - c\,|\, j(x,t)|^2\ j(x,t) .$$

This equation has a soliton solution which allowed creating the single-particle wave function for CNTs electrons. The current-voltage characteristic of CNTs has been calculated by the single-electron wave function.

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