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## Features cells based on modifying carbon nanotubes.

*In this paper I reviewed the process of designing structures for the formation of integrated elements based on carbon nanotubes. I measured the response of such structures that are based on different types of nanotubes for toxic substances.*

*Key Words: spectroscopy, modification carbon nanotube, band gap, conductivity.*

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## Особливості елементів на основі модифікованих вуглецевих нанотрубок.

*У роботі я розглянув процес конструювання інтегральних структур для формування елементів на основі вуглецевих нанотрубок. Була виміряна реакція подібних структур, створених на основі різних типів нанотрубок для токсичних речовин.*

*Ключові слова: спектроскопія, модифікована вуглецева нанотрубка, заборонена зона, провідність.*

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Modification carbon nanotubes (MCNT) are unique carbon supramolecules show a remarkable electrical properties that could potentially find wide application in various fields of science and engineering applications. In general, the MCNT are rolled into a seamless cylinder graphene sheet plane (the plane of the hexagonally arranged carbon atoms) is illustrated in Fig 1 [1, 3].

MCNT properties can be used in various devices, such as integrated molecular electronics elements. These devices can be used in various functional applications: such as physical, chemical and biological sensors in security devices and control of the environment, health and clinical diagnostics, biotechnology for gene mapping and detection of drugs. In particular, MCNT taking into account environmental and political situation in the world today, detecting the presence of toxic substances in the environment is a prerequisite for both personal safety and the prevention of mass releases of hazardous substances. Thus, the need to develop improved prototypes of chemical sensors that provide early and rapid detection and prevention of dangerous situations for humans. [1, 3].

The distinctive characteristics of sensors MCNT are fast response, high sensitivity with a high signal transducer response, high selectivity, large dynamic range, reusable regeneration, the simultaneous detection and identification of maximum possible number of substances, low temperature operation, small size combined with ease of use. The achievement of these characteristics is a relatively time-consuming task for traditional touch application requires a trained work environment. For example, conventional electronic sensors provide advanced functionality at temperatures above 300°C, and the resistive response is not sufficient to provide the desired level of molecular detection. [1, 2].

In the manufacture of MCNT is the most common method of thermal spraying graphite electrodes in plasma arc. This is an intensive thermal evaporation of the anode to the cathode end surface to form a precipitate, which formed MCNT. The maximum number MCNT with a length of 40 microns formed when the plasma current is minimal, and its density is about 100 A/cm$^2$. They grow on a flat surface perpendicular to the cathode side of the building and self-assembled into bundles diameter 50 microns. Also has a MCNT capillary property. To open MCNT, it is necessary to remove the upper part - the cap. One way is to remove the MCNT annealing at a temperature of 8500°C for several hours in a stream of carbon dioxide. As a result of oxidation of about 10 % of MCNT are open. Another way to end the destruction of closed MCNT - excerpt
in concentrated nitric acid for 5 hours at 2500°C. As a result of this treatment, 80 % of the MCNT is open [1].

The presence of cylindrical cavity inside MCNT can implement various elements, including lawn metals. In all these cases should proceed with new material and yet experimentally studied properties.

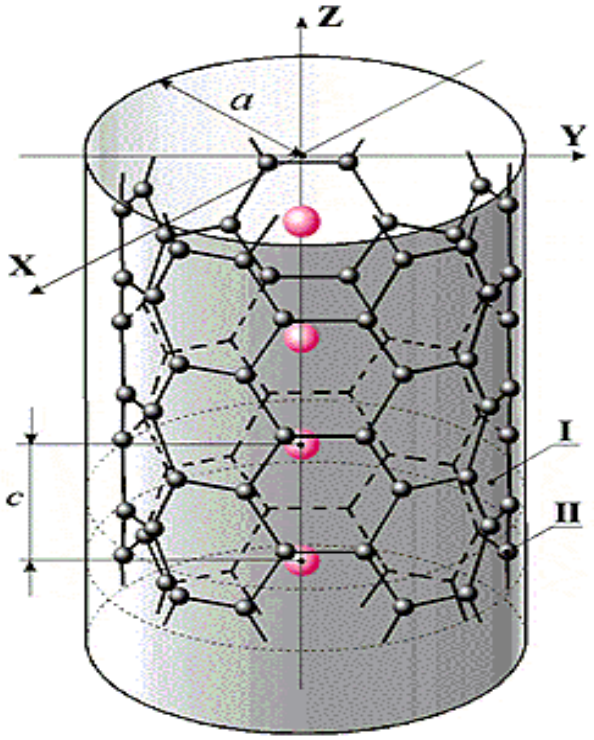


Fig. 1. Alloy metal carbon nanotube inside a cylindrical potential barrier (MCNT). I - constant area interatomic potential, II - Region atomic potential. [1].

For example, when converting electrical oscillations into mechanical vibrations necessary to excite the MCNT under an electric field to fix one of the two electrodes at an angle to the other electrode. When applying voltage to the electrodes and the tube is charged by the electrostatic attraction is diverted to the second electrode. When applying voltage to the electrodes and the tube is charged by the electrostatic attraction is diverted to the second electrode. If the electrodes apply a variable voltage, whose frequency coincides with the frequency of natural oscillations of MCNT, depending on its thickness and length, any mechanical vibrations of MCNT. Spectroscopic methods of determining the frequency of natural oscillations and attach it to the sample, we can determine the frequency of oscillation loaded MCNT. This frequency will be less than the free vibration frequency MCNT because of increased weight and stiffness remained unchanged [1, 2].

Calculations metallic MCNT require the development of new quantum chemical method (method associated linearized cylindrical waves). In this method made the assumption that the system is inserted into the impenetrable cylindrical potential barrier, where atom in a spherically symmetric potential *E* (practically coincides with atomic), and interatomic space constant (Fig. 1). Then the electronic spectrum of the system is determined by the free movement of electrons in the interatomic space and nuclear scattering centers [1].

MCNT with different indices (n, m) - are polymers of different structure, so they must have different electrical properties. Dependence of the electrical properties MCNT geometrical parameters were predicted on the basis of quantum-chemical calculations of the band structure. Introduction metals in MCNT leads to a sharp increase in conductivity as semiconductor MCNT due to the appearance in the bandgap electronic states of the metal and metal by increasing the density of states near the Fermi level. Introduction to these metals with the formation of structures of the type that is shown in Fig. 1 leads to the formation of the metal band structure of the system. Introduction metals in nanotubes leads to a sharp increase in conductivity. If one half of semiconductor MCNT filled with metal, and the other left intact, will again molecular heterojunction metal-semiconductor on which you can build nanodiodes and other elements that can operate over a wide temperature range. Stoichiometric control and p-electronic interactions in the calculation of the total energy of the modified MCNT showed that the joining of atoms on the outside MCNT profitable than domestic. In this case, the atoms must first join to the open ends of MCNT, and then align along of creating. In MCNT F - (n, n) and F - (n, 0) is quite long, so you can ignore the final effect of the latter type of mount would be a major. By adding metal to the outer surface of the varies mesh p - contacts, so – electrical and other physical properties. Therefore, all the MCNT F - (n, n) - semimetals in which the edge of the Brillouin zone and there is no gap, because all nanotubes (n, n) metal, half MCNT are molecular heterojunction metal-semimetal, regardless of their diameter. According to calculations, the crack gap in nanotube type F - (n, 0) vanishes if the (n + 1) three fold (Fig. 2). In other cases, modified tube - Semiconductor. As in the original, pure carbon nanotubes (n, 0), the Fermi surface is absent if n multiple of three, then the half-modified nanotubes (n, 0) will, depending on the diameter, to form heterojunction types. If (n - 1) three fold ($n = 3\ell + 1$, $\ell = 1, 2.$) It will heterojunction semiconductor-semiconductor, and gap width of the slit in the MCNT is approximately two times less than in the initial (Fig. 2). For other values of n heterojunction formed metal-semiconductor, but n, three f old, corresponding unmodified metal end of MCNT, and when $n = 3\ell + 2$ - modified. In Fig. 3 shows the

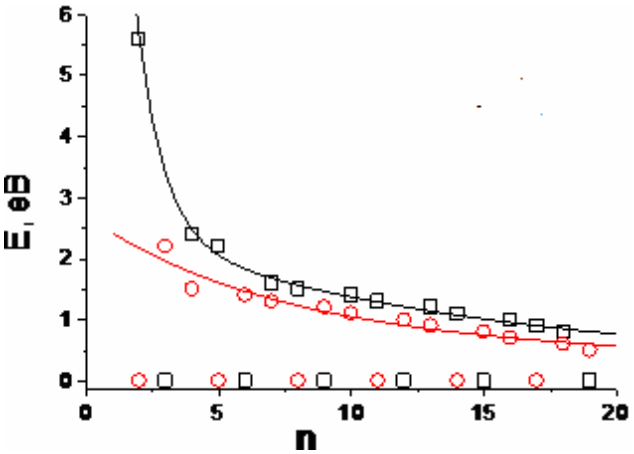


Fig. 2. The dependence of the energy gap for the initial and MCNT of type (n, 0) on the parameter of diameter n. □- with modification, ○ - without modification [1].

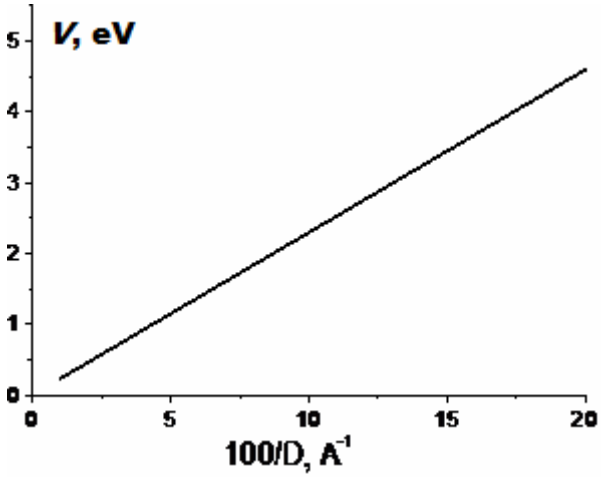


Fig. 3. The dependence of the band gap of the inverse MCNT diameter.

dependence of the width of the gap semiconductor nanotube diameter on their feedback, which shows that increasing the diameter of the tube gap decreases. To study the electronic structure MCNT used scanning tunneling microscopy (STM) using the local electron spectroscopy. Hence, the position of the probe was fixed MCNT and recorded the dependence of the tunneling current on the voltage *U*, applied between the tip and MCNT. I find thus conductance $G = I / U$ is directly related to the local density of electronic states, which is a measure of how close the energy levels are to each other.

MCNT are exceptionally durable material as stretching and bending. Moreover, under mechanical stress, which exceeds the critical, nanotubes do not "rush" and rebuilt [1, 3]. Due to the small size of the nanotubes was only directly measure their electrical resistivity four probe method (Fig. 5). On the polished surface of sapphire in a vacuum deposited gold stripes. Between them sprayed MCNT length 2÷3 mm. Then one of the selected measuring 4 MCNT deposited tungsten wire thickness of 50 nm. Each tungsten wires had contact with one of the gold bars. The distance between the contacts to the MCNT ranged from 0,1 to 0,6 microns. The results of direct measurements showed that the resistivity of MCNT can vary considerable range - from $5{,}1*10^{-6}$ to 0,8 Ohm/cm. Minimum order of magnitude lower resistance than graphite. Most of the MCNT has metallic conductivity and smaller shows properties of the semiconductor band gap from 0,1 to 0,3 eV. Features of the charge transfer in MCNT significantly different from those of the conventional conductors and probably due to one-dimensional character of the charge transfer [1, 3].

Creating semiconductor heterostructures, ie structures of metal / semiconductor junction or two different semiconductors can be used in nanoelectronics. During nanotube growth it creates structural defects (replacement of a carbon hexagons and pentagons heptagon (see Fig. 1, 4). Then one part MCNT is metallic and the other - a semiconductor. In Fig. 5 and Fig. 6 STM measurements show - spectroscopy as depending normalized differential conductance (dI/dV)/(I/V) of applied between MCNT and the probe voltage V. To the left of the spectrum (dI/dV) / (I/V) = 1 in a wide range of V, which means the performance of Ohm's law. With energy gap in the story. It is located in the energy region corresponding to small increments of power. Width of the field voltage is a measure of the value gap. For semiconductor indications on the left graph, it is 0,7 eV.

With a large voltage V observed sharp peaks in the density of states characterizing the low

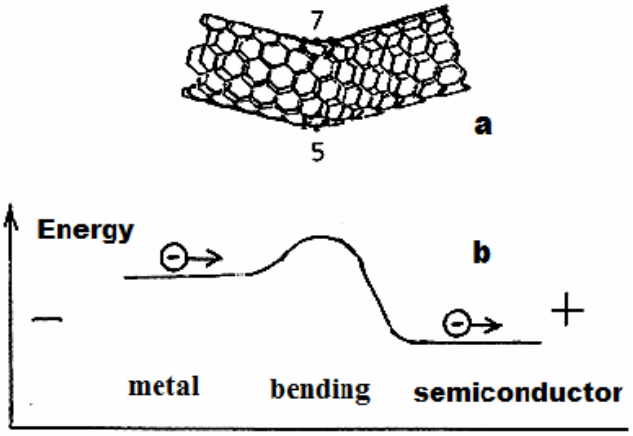


Fig. 4. Effect of pentagon-heptagon defect on the nanotube geometry (a) and the energy of moving electrons (b) [2].

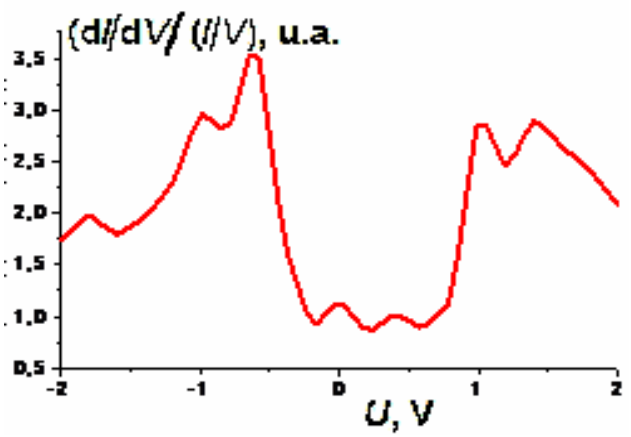


Fig. 5. The results of STM spectroscopy as depending normalized differential conductance (d$I$ / d$V$) / ($I$ / $V$) of applied between the tube and the probe voltage $V$ for a metal MCNT.

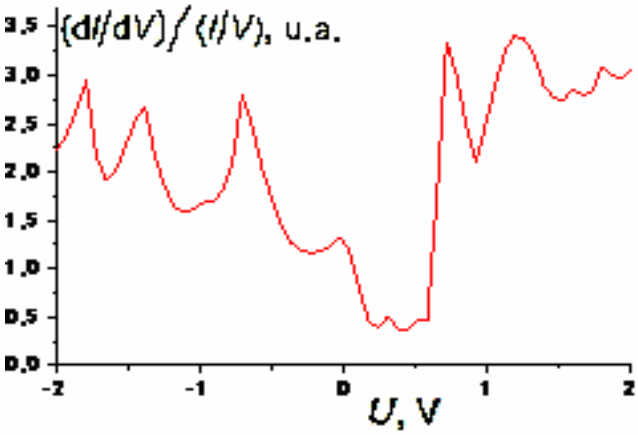


Fig. 6. The results of STM spectroscopy as depending normalized differential conductance (d$I$/d$V$) / (I/V) of applied between the tube and the probe voltage $V$ for a semiconductors MCNT.

conductivity material dimension. Spears appeared on the bottom shelf and set subzones. If electrons in quantum theory can be regarded as a wave. then the wavelength of the electron does not fit an integer times the circumference tube is interfering with itself with dissipation, so that allowed only those wavelengths of electrons that fit an integer number of times around the perimeter MCNT. This greatly limits the number of states eligible for conductivity around the cylinder. The dominant conduction direction is the direction along the tube, which makes functional MCNT -dimensional quantum wire. Electronic states MCNT do not form a continuous broad energy band, and split into one-dimensional subband (see Fig. 5). Such states can be modeled quantum well as well with a depth equal to the length MCNT [1].

Transport of electrons on single-walled MCNT is determined by the quantum size effect. For metal nanotube, which lies between two metal electrodes can be seen especially in the form of steps to bios characteristic (see Fig. 6). Steps appear at a voltage that depends on the voltage applied to the third electrode electrostatically associated with the nanotubes. It resembles the construction of FET on MCNT. Steps to CVC is the result of electron and resonant tunneling through individual molecular orbitals. Electronic transfer is blocked at low voltages. With the gradual increase of the gate voltage, electrons alone can penetrate MCNT.

Electron transfer in the tube occurs through tunneling between discrete electronic states. Changing the current at each step (see Fig. 5, 6) associated with the addition of one molecular orbital. This means that the electrons in MCNT is highly localized, and located at a distance along the tube. The usual presence of a defect in the system is one-dimensional localization of electrons, but a defect in MCNT does not lead to localization, because its effect is averaged around the perimeter of the tube. This is due to toroidal shape of the wave function. In the metallic state conductivity of MCNT is very high, MCNT can pass very large currents without significant heating. One reason for the high conductivity MCNT is very small defects that cause electron scattering and thus a very low resistance.

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