

ELECTRONIC STRUCTURE OF AND PROPERTIES OF CARBON NANOTUBES

Nischenko M.M.^{*}, Lichtorovich S.P., Lisunova Y.O.

Institute of Metal Physics, National Academy of Science of Ukraine,
36 Vernadsky str, Kiev-142, 03142 Ukraine

^{*}E-mail: nish@imp.kiev.ua

Introduction

Carbon nanotubes (CNTs) being investigated because of their unique electric, emission and elastic properties [1]. CNTs are on ten times as stiffness as steel, six times as easy as copper. These molecules are characterized by gape zone (0-2eV). The width of gape zone depends on atomic structure of molecule: on its diameter, chiral vector and defects. For example, being appeared only one defect such as pair "pentagon-heptagon" (Stone-Wells defects) in single walled CNT the metal-semiconductor transition are formatted. One of the most striking features of CNTs is that it has anisotropic atomic structure, it can be regarded as a rolled-up graphite-sheet in the cylindrical form. The big distance d_{002} and weak Van-der-Waals (VDW) interaction between layers characterize multi-walled CNTs. CNTs are determined by technology of reception and its influence.

Results and discussions

Methods of electro-physical and electro-positron annihilations are sensitive to internal structure and defects of a structure. Multiwalled carbon nanotubes are investigated: helicoid and direct thin-walled, received electro-arc and matrix methods accordingly [2]. Straight CNT, as against helicoid, grow inside a cavity the nanopore in diameter of 40-60 nm. In result 10 cylindrical layers with internal diameter 30-50 nm are formed on the average. Spectra of angular distribution of the annihilation photons (ADAP), representing distribution of electrons on pulses are received.

It's shown, that the positrons are pushed out by field of positive nucleus in free volume-intervals between layers (VDW) or are grasped by the defects. It is established, that spectra of ADAP of multi-walled nanotubes are well approximated to two gaussoids.

According to the distribution of electrons on pulses are determined a degree of electron localization in the field of free volume and defects, probability of annihilations of electrons with positrons in defects, the sizes of inter-nuclear and inter-layer intervals. It defines electronic structure and electronic properties of the CNTs.

Results of calculation of ADAP spectra of carbon materials are listed in the table

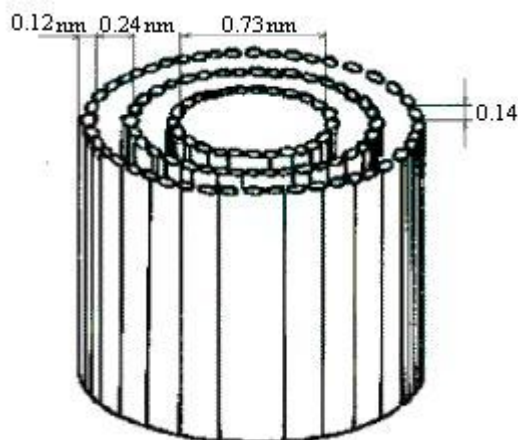
Sample	Radius of localization of π -electrons wave function between carbon layers, ($\pm 0,001$ nm)	Annihilating part of positron in defects, %
Standard: 1. Fullerenes (C_{60}) 2. Graphite	0,121 0,112	22 18
Nanotubes: 3. helical(arc method) CNTs 4. Thin-walled CNTs (matrix method)	0,109 0,116	10 2

In spectra of ADAP is absent a parabolic component. It responsible for annihilations with free electrons. For components of a pulse the condition satisfies: $p_r \gg p_z$ at which p electronic state located for all length of nanotubes, to a lesser degree - on a circle of radius R ($\ell=2\pi R$), and are located in a radial direction (r).

It means, that the electronic subsystem of nanotubes is not completely located as in metals, and forms two-dimensional (2D) electronic. The greatest radius of localization of wave function of p electrons in a direction of quantization of energy of electrons is observed for thin-walled nanotubes $L_r=0,116$ nm. The average distance according to the electronic and positron annihilations makes 0,355 nm, that on 0,020 nm more than inter-plane distance in graphite.

Radius of localization of wave function of electrons in the field of defect for thin-walled and continuous nanotubes practically equally ($r_{m2}=0,05$ nm), that specifies close characteristics of defects. However probability annihilation of positrons with electrons in the field of specified defects S differ: in nanotubes of the helicoid form- 10 %, and in direct thin-walled nanotubes - 2 %. Reduction of this size reduces dispersion of electrons on defects that is necessary for increase in electro-conductivity.

The model of CNT is constructed. According to this model the "cylindrical" quantum hole in width of 0,23 nm for π - electrons is formed between the carbon layers. It grasps positively charged particles: positrons, protons and cation.



Rolling-up graphite-sheet in the cylindrical form the internal pressure appear. It increases inter-layer distances and influence on physical properties of CNTs. Expression for an estimation the size of a gain Δr inter-layer distances d_{002} is received at growth the CNT inside a cavity in comparison with equilibrium value d_{002} for a case of growth of a skeleton on a spiral:

$$\Delta r = \sqrt{\frac{2d_{002} \cdot E}{N \cdot \kappa}}.$$

From here follows, that with reduction of diameter of nanotubes the number of atoms N in a chain decreases and the size Δr grows..Last causes increase in internal pressure.

For nanotubes with external radius 22 nm number of atoms in one-dimensional chain

$N \approx 2300$ and at $E_{cov} \approx 5$ eV a gain $\Delta r \approx 0,015$ nm that is close to the value received according to positron annihilation (0,020 nm). It is necessary to expect, that the insignificant increase d_{002} in the CNT and occurrence of internal pressure lead to reduction of a degree of overlapping of wave functions p the electrons poorly connected to the atoms, to change of parameters of electronic structure and reduction of electroconductivity, especially, for multilayered nanotubes of small diameter. We shall notice, that inter-layer distances and internal pressure for nanotubes, received matrix synthesis appears more than for nanotubes, received by an electroarc method.

It is shown, that a temperature courses of electroresistance of nondirectional the CNT and nanocomposits has semi-conductor character.

Conclusions

The electronic subsystem of thin-walled nanotubes is not completely located as in metals, and two-dimensional electronic gas is formed of the π -electrons described by higher mobility of electrons in comparison with a three-dimensional case.

The radius of localization of wave function of π -electrons in a radial direction in nanotubes, according to positron annihilations, is equal 0,116 nm, and width of a formed "cylindrical" quantum hole for π -electrons - 0,24 nm.

Reference

- 1.Shpak A.P., et al. Cluster's and nanostructured materials. (2001).
- 2.Brichka A.B. //Ukrainian Chem. Journal 2003; 69(8):67-70.