Journal of Nano- and Electronic Physics
Vol. **8** No 3, 03047(3pp) (2016)

Журнал нано- та електронної фізики
Том **8** № 3, 03047(3cc) (2016)

Short Communication

The Mechanism of Interaction of Esters of Methacrylic Acid with Carbon Nanotubes to Create a New Polymer Composite Material

I.V. Zaporotskova, L.S. Elbakyan

Volgograd State University, 100, University prosp., 400062 Volgograd, Russia

(Received 04 May 2016; published online 03 October 2016)

In this work is considered the possibility of creating new polymeric composite materials based on complex esters of methacrylic acid by reinforcing them with carbon nanotubes. Theoretical calculations are done: interaction of the main components of the polymeric material with a single-layer carbon nanotubes. The presence of good connection of polymer matrix with reinforcing nanotubes is proved. The influence of carbon nanotubes on the conductivity of the considered composite polymer materials is studied. The calculations are performed using DFT method within the model of molecular cluster.

Keywords: Carbon nanotube, Polymer composites, Doping, Polymetilmetacrilate, Adsorption, Conductivity.

DOI: 10.21272/jnep.8(3).03047 PACS number: 81.07._b

1. INTRODUCTION

In recent years the use of materials on the basis of methylmethacrylate (MMA) is growing actively. Due to the unique properties the systems based on MMA have found application in almost all industries, including aviation, engineering and automotive. Within the sphere of application are also included, light, food and pharmaceutical industries and construction.

Great expectations in the field of new materials are associated with the use of carbon nanotubes (CNTS) [1]. High surface activity of the nanotubes determines the possibility of creation of composite structures of various types, with various properties [2]. Due to its electrical and thermal conductivity, and high chemical, thermal and mechanical stability of CNTS are considered as one of the most promising objects for nanoelectronics [3]. Using CNTS as reinforcing additives, you can achieve a significant improvement in many characteristics of polymeric materials. Mechanical and electronic properties of the matrix are changed.

2. DESCRIPTION OF THE OBJECT AND METHODS OF STUDY

In this work, the processes of interaction of single-layer carbon nanotubes with individual components of the methacrylate are studied, the main electron-energy characteristics of the process and geometrical features of interacting systems are determined. The influence of adsorbed components of MMA on the conductive properties of the polymer composite system is discussed. The calculations are performed using DFT method within the model of molecular cluster.

The DFT-calculations of the process of interaction of molecules of methacrylic acid, methyl methacrylate with the surface of the single-layer carbon nanotubes were done to determine the feasibility of realization of the adsorption mechanism of interaction of polymeric materials on the bases of esters of methacrylic acid with carbon nanotubes resulting the creation of a new composite polymer. The CNT differs in diameters and chirality. The calculations were performed using the software package Gaussian [5].

3. DESCRIPTION AND ANALYSIS OF THE RESULTS

The molecular cluster of the nanotube depending of the type contained from 96 to 334 carbon atoms and dangling bonds at the boundary of the confined hydrogen pseudoatoms. The process of interaction for each molecule was modeled by incremental method (in increments of 0,1 Å) along the direction perpendicular to a C atom located in the centre of the cluster to the external surface of the nanotube. The choice of the place of adsorption at the center of molecular cluster avoids edge effects influence on the process of pseudoatoms. The geometrical parameters of the system were optimized at each step. In the structure of the molecules of the components were the most active centers that are able to provide a stable connection of the molecules with the surface of the CNTs. So for molecules were investigated following active centers: a) center 1 – atom oxygen molecules; b) center 2 – carbon atom of the molecule of methyl methacrylate by radical substitution of the hydrogen atom (Fig. 1)

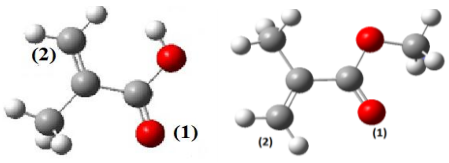

Fig. 1 – Molecules of methacrylic acid and matyl metacrilate with possible active centers 1 and 2

Table 1 presents the basic characteristics of the process of interaction of considered types of CNTS with molecules of methyl methacrylate and methacrylic acid wich are obtained in the result of colculations. Analysis of the results showed that the maximum

 © 2016 Sumy State University

Table 1 – The basic characteristics of the process of interaction of considered types of CNTS with molecules of methyl methacrylate and methacrylic acid for two variants of interaction with active centers of 1 and 2 molecules: r – the distance of adsorption, E_{ad} – the energy of adsorption

Types of nanotubes		The interacting molecules							
		Methacrylic acid				Methyl methacrylate			
		active centers of 1		active centers of 2		active centers of 1		active centers of 2	
		r, Å	E_{ad}, eV	r, Å	E_{ad}, eV	r, Å	E_{ad}, eV	r, Å	E_{ad}, Ev
Achiral	(5,5)	2,9	– 0,06	–	–	–	–	–	–
	(6,6)	3,0	– 0,02	–	–	2,9	– 0,12	–	–
	(8,8)	2,9	0,22	2,7	– 0,19	3,0	– 0, 15	2,7	– 0,13
	(6,0)	2,9	– 0,03	–	–	2,9	– 0,28	–	–
	(9,0)	2,9	– 3,50	2,5	– 2,76	3,0	– 1,58	2,6	– 2,73
	(12,0)	2,8	– 0,03	2,7	– 1,68	2,9	– 0,15	2,5	– 0,93
Chiral	(7,1)	2,9	– 0,03	2,8	– 0,18	2,9	– 3,06	2,7	– 0,13
	(8,4)	2,9	– 0,12	–	–	2,9	– 2,43	2,9	– 0,44
	(10,5)	2,9	– 3,03	2,8	– 2,72	3,0	– 3,05	2,5	– 0,40

adsorption activity is observed for the achiral nanotubes of (9,0) type and chiral CNT of (7,1), (8,4) and (10,5) types for. Which the values of adsorption energy, were the largest of all calculated.

Later were performed DFT-calculations of the process of interaction of single-layer nanotubes with polymer compound by PMMA [-CH2C(CH3)(COOCH3)-]n which include 3 structural units – molecules MMA. Nanotubes with a maximum sorption activity in respect of a molecule of methyl methacrylate were selected for research namely CNT types of (7,1), (9,0), (10,5) and (8,4). The interaction with active center 1 - atom oxygen molecules was examined the efficiency of which is due to the presence of double bonds. The process was simulated by approach of the PMMA to the center of the selected CNT. Inter-current model system PMMA+CNT presented in Fig. 2. The main results of the interaction of PMMA and CNT type (9,0), (7,1), (8,4) and (10,5) are presented in Table 2.

As a result of the research were built with single-electron spectra systems "PMMA+CNT" (Fig. 3-5), the analysis of which allowed to determine the values of the band gap ΔEg of the obtained composites, are shown in table 3. Found that the band gap of the obtained systems is comparable to the band gap of individual nanotubes, i.e. the presence of PMMA, which consists of three structural units, does not change the conduc-tivity type of system.

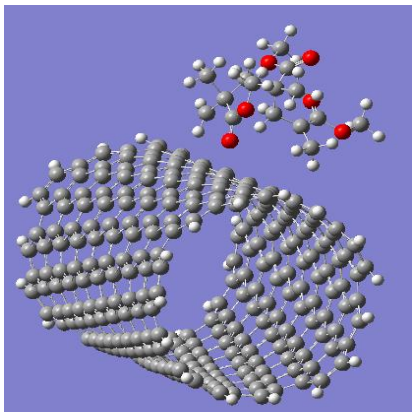

Fig. 2 – The interaction of the CNT type of (10, 5) with PMMA

Table 2 – The basic characteristics of the process of interaction of considered types of CNTS with polymethyl methacrylate: r – the distance of adsorption, E_{ad} – the energy of adsorption

Types of nanotubes	polymethyl methacrylate	
	r, Å	E_{ad}, eV
(7,1)	2,9	– 0,144
(9,0)	2,9	– 0,310
(10,5)	2,9	– 0,284
(8,4)	3,2	– 0,142

Table 3 – Value of bandgap for system CNT + PMMA

Type of tubes	value of bandgap	
	CNT	CNT +PMMA
(9,0)	0,25	2,78
(10,5)	0,62	0,54
(7,1)	0,102	0,102
(8,4)	0,27	0,27

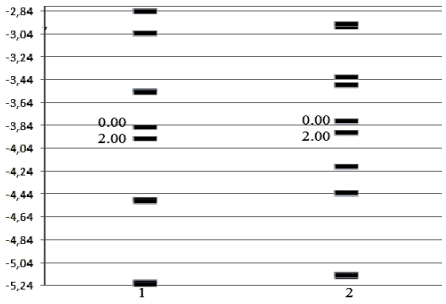

Fig. 3 – Spectra of one-electron states: 1 – CNT type of (7,1), 2 – PMMA + CNT type of (7,1)

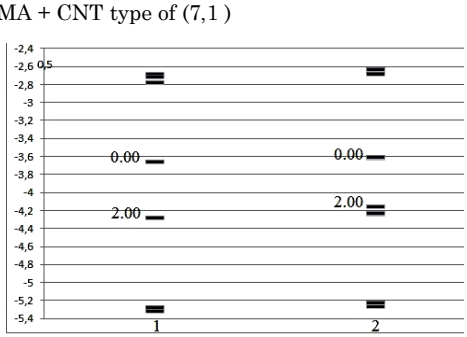

Fig. 4 – Spectra of one-electron states: 1 – CNT type of (10,5), 2 – PMMA + CNT type of (10,5)

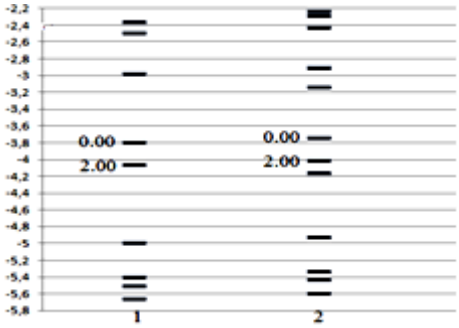

Fig. 4 – Spectra of one-electron states: 1 – CNT type of (8,4), 2 – PMMA + CNT type of (8,4)

4. CONCLUSIONS

The performed studies have proved the possibility of creation of high-strength plastic nanocomposites on the basis of polymethyl metacrylate doped with CNT, the adsorption of pmma on the surface of the cnts. The obtained nanosystems will save conductivity inherent in pure nanotubes, as illustrated by almost the same adsorption values of the band gap. Polymer composite system can be effectively used in many industrial fields, including, micro - and nanoelectronics as a system with stable conductivity.

REFERENCES

1. I.V. Zaporotskova, *Carbon and non-carbon composite nanomaterials and structures on their basis: structure and electronic properties* (Volgograd: Volsu: 2009).
2. I.V. Zaporotskova, L.V. Kogitov, V.V. Kozlov, *Vestnik of Volgograd state University. Series 10: Innovative activity* No 4, 63 (2009-2010).
3. A.V. Eletskii, *Succes Phys. Sci.* **179** No 3, 225 (2009).
4. A.V. Eletskii, V.Y. Zitserman, G.A. Kobzev, *Thermophysics of High Temperatures* **53** No 1, 117 (2015).
5. E. Butirskaya, *Computational chemistry. Basic theory and working with programs of Gaussian and GaussView* (Solon-Press: 2011).