Obtaining and investigation of C_{60} <A_2B_6> semiconductor compounds with a view to create effective solar cells

M A Elistratova[1,2], I B Zakharova[1] and N M Romanov[1,2]

[1] St. Petersburg State Polytechnical University, 29 Polytechnicheskaya Street, St. Petersburg 195251, Russia
[2]Lappeenranta University of Technology, 34 Skinnarilankatu, Lappeenranta, 53850, Finland

E-mail: elistratovamari@yandex.ru

Abstract. Reproducible vacuum method of thin fullerene films production with Cd<Te> impurity on Si, glass and mica surfaces are developed. Thin composite films were obtained by Knudsen cell method. Initial studies of condensation and surface morphology of the films are investigated SEM methods. Optical spectroscopy was used to confirm the obtained results. Results showed the presence of an additional peak associated with the formation of C_{60}-CdTe molecular complexes. SEM results confirm absence of phase separation.

Introduction

Over the last couple decades carbon becomes one of the most studied chemical element. Discoveries and developments related with carbon allows to create new nanomaterials which will move forward science and industry. The practical scope of this research is wide - machinery, electronics, chemical industry, biology, medicine. This enables the carbon to be found as a strategic material of the future, which is confirmed by Nobel Prize in chemistry and physics, awarded for the discovery of new carbon forms, including fullerenes. Fullerenes and their chemical forms are promising materials for use in semiconductor technology and nanoelectronics [1]. The effect of fullerenes nonlinear transparency opens up the possibility of their using as of the laser radiation optical limiters intensity in the visible and near infrared ranges. The high light absorption efficiency and charge separation in conducting composites polymers and fullerene allows to predict the creation of photodiodes, transistors, solar cells and other opto-electrical devices on their basis [1, 2]. Composite materials based on fullerene with <A_2B_6> donor group find applications in the field of telecommunications and computer technology and optoelectronic devices. They form a new class of materials, which have easier manufacturing and low cost. Structures based on C_{60}<A_2B_6> also are of interest as a material for the efficient solar cells creation [3]. Studies show the presence of the photoexcited carriers transport from impurity molecules to the C_{60} molecule [4, 5]. This effect leads to photovoltaic effect appearance in these structures. CdTe was selected as impurity because of its low sublimation temperature, thus providing a much simpler samples obtaining method. This paper presents the results obtained from photoluminescence investigations and from composition analysis results of such samples.


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Obtaining method

The essence of a deposition thin films process implies that materials are heated by the special temperature. At this temperature atomic and molecular kinetic energy become enough to separate atoms and molecules from the bulk material surface to surround space. It becomes at such heating temperature when own material vapor pressure exceed, by several order, residual gas pressure. The atomic stream propagates linearly in this case. Evaporated atoms and molecules have a collisions with the surface and then condense on it. Fullerene and A_2B_6 materials transferred into vapor without liquid phase. Thus evaporation is carried out in short way: the solid phase – the liquid phase. It is called sublimation. Follow conditions was provided at a residual preasure of 10^{-6} Pa. This vacuum was easily achieved by mechanical foreline and high vacuum diffusion pumps. The substrate temperature has a great impact on films structure and also on its electrophysical and optical propirties. In this work substrates were kept at room temperature during the process. Sputtering on a cold substrate lead to amorphous and polycrystalline structure formation and possibly alignment of randomly distributed semiconductor clusters or molecular. The main advantage of this method is sterility of process. It allows to propagate high films quality without any contamination and what is more important without oxygen subject.

Thin fullerene films doped with CdTe were prepared by co-deposition technique from Knudsen cell. Open source evaporating allows to obtain composite films on various substrate. Powder of clear C_{60} and C_{60} with adding of 50 wt.% CdTe impurities was evaporated at 500-650 °C on Si, glass with ITO, KBr and mica substrate. Silicone substrates were cleaned by isopropyl alcohol. The cell was made from wolfram and surrounded by the wolfram capsule. The out part is connected to 0-1.5 V. To provide uniformal mixture distribution evaporator was slowly heated during 10 min. It promotes better oxygen adhesion which penetrate into fullerene. Films thickness was 200-500 nm. In comparison with the initial charge it can lead to a significant changing of a film composition. Obtaining a large area film possibility is an advantage of the Knudsen cell.

Experimental research of the samples

A scanning electron microscope Jeol JSM-6390 was used to study the surfaces' morphology. It worked with resolution of 3 nm. The films' composition in the selected area was measured by energy dispersive micro-analysis console "Oxford INCA Energy" with the utmost sensitivity 0.1wt%. Studies have shown a high homogeneity of the impurity distribution and the absence of the mosaic structure of the composite films. Photoluminescence spectra were measured by using automated installation based on Horiba Jobin Yvon monochromator. It is composed of FHR 640 monochromator with a grating of 1200 mm-1 and the Symphony II (1024 * 256) Cryogenic Open - Electrode CCD detector. . Excitation of photoluminescence were produced by continuous semiconductor laser with 408 nm wavelength. Filter was installed before the slit of the monochromator to avoid scattering lazer radiation falling into the monochromator. CCD chamber was maintained at the temperature of 77 K [7].

Photoluminescence spectra investigation

Obtained at 300 K photoluminescence (PL) spectra are shown at fig. 1. Pristine fullerene films has wide PL peak with 725 nm maximum. The large peak wide explained by two fullerene peaks contribution - at 720 nm and its vibration recurrence at 830 nm. CdTe adding leads to extra peaks appearing at the wavelength of 630 nm. The extra peak intensive increases with amount of impurity. This wavelength according to the energy of singlet-singlet transition in C_{60} energy structure. Such transition is forbidden for an isolated fullerene molecule for the reason of symmetry, but if CdTe forms a molecular complex with C_{60} symmetry of the cluster is reduced (from T_h to C_s). According to the results of quantum chemical calculations, in case of optimization geometry CdTe molecular is located on 6-6 bond of fullerene. However C_{60} molecules and C_{60} complexes interaction is limited. Limitation is going from standing in crystal lattice. C_{60} toluene solution PL spectra presented a big additional peak at 650 nm and a small degree at 600 nm. These values correspond to S_1-S_0 and S_2-S_0 fullerene transitions. It is possible because molecules in liquid phase are solvated by toluene and

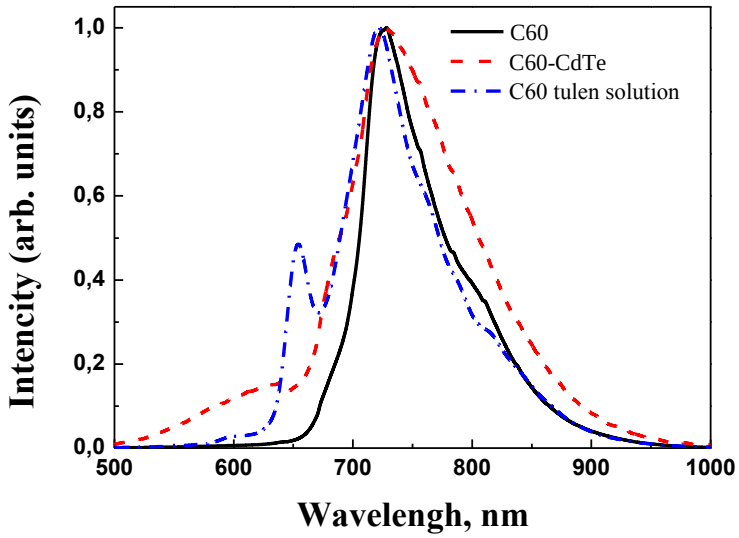

Figure 1. Photoluminescence spectra obtained at 300 K. Pure C_{60} spectrum is showed by solid line. C_{60} with 50% CdTe is showed by dash line. PL spectra of C_{60} toluene solution is showed by dash-dot line.

interact with each other, the degree of symmetry distortion increases and S_1-S_0 and S_2-S_0 transitions became permitted.

Scanning electron microscopy analysis

Figure 2 presents surface topography of C_{60}-CdTe sample contain 50% of impurity obtained by SEM. At most surface is clear without inhomogeneities (spectra 2 and 4). It may contains microcrystalline structure (spectra 1 and 3). X-ray analysis display that these microcrystals are from C_{60}-CdTe mixture and do not contain CdTe nanoparticle.

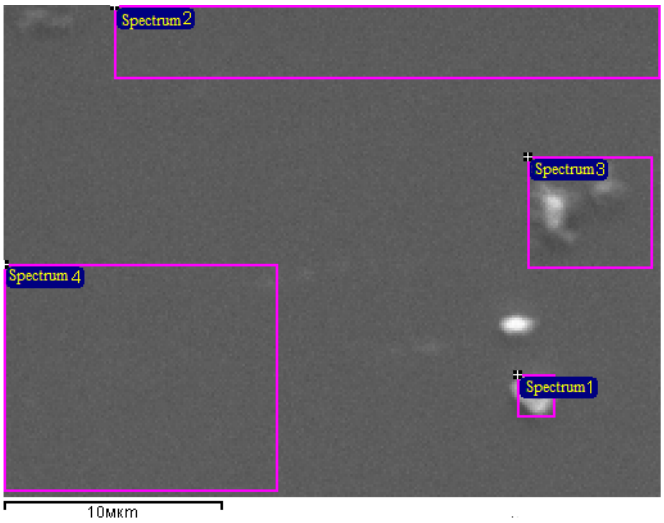

Figure 2. SEM image of C_{60}-CdTe (with 50% of CdTe) sample.

Chemical compositions spectra were measured by energy dispersive consoles (table 1). All spectra contain as C_{60} as CdTe. Points (2, 4) selected on a smooth homogeneous surface show sufficiently good uniformity of composition with an average content value of Cd – 2.37, Te – 5.53%. At opposite to atomic masses of Cd and Te, it mean that CdTe included in film in molecular form. Quantum-chemical calculations verified this fact [8].

Silicon appears in the spectra because the absorption of electrons and output of x-ray radiation is possible from the substrate when the film has thin thickness (about 500 nm). Oxygen also presents in spectra, because fullerene is susceptible of oxygen and water vapor. In comparison with the initial charge, which was 50% to 50%, it is noticed that amount of impurities became lower. Open source method production leads to significant depletion of the impurity in films.

Table 1. X-ray analysis result for sample contain 50% of CdTe impurities.

Spectrum	C	Si	Cd	Te	O	Total
Spectrum 1	14.32	17.84	2.35	5.34	60.15	100.0
Spectrum 2	15.47	15.69	2.33	5.68	60.83	100.0
Spectrum 3	16.39	14.06	2.33	5.53	61.57	100.0
Spectrum 4	15.43	15.73	2.48	5.59	60.77	100.0

Conclusions

It is shown that open source evaporating methods lead to a molecular dispersion of impurities in the amorphous films. X-ray composition analysis results displayed significantly depletion of impurity in film in comparison with the initial charge. It determined impurities intercalation way in fullerene matrix. Films compound analysis also showed that CdTe is in molecular form and generate molecular complexes with C_{60}. Photoluminescence spectra were measured for obtained samples. Additional peaks appeared. They related with singlet-singlet (S_1-S_0, S_2-S_0) transition of fullerene, which is forbidden for isolated molecule. C_{60}-CdTe complexes formation remove the symmetry prohibition. This removing also appears in solution for the reason of toluene solvating and interaction between molecules. These results well agree with SEM analysis and quantum-chemical calculations.

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