ANNOTATION

dissertation research for a degree
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ZAVGORODNY ALEXEY VLADIMIROVICH

Photovoltaic processes in composite nanostructured films of semiconductor polymer–phthalocyanine

Relevance of the topic. Photoconductive organic materials currently used in photovoltaic systems are extremely diverse in chemical nature. The goal of numerous studies in this promising scientific direction is to create ordered molecular assemblies based on aromatic and heteroaromatic compounds with electron-donor and electron-acceptor properties, capable of forming charge transfer complexes that intensively absorb radiation in the ultraviolet, visible and infrared ranges of the spectrum. They are the basis of materials for molecular electronics, photoelectric converters with sufficiently high electrophysical and optical characteristics and long service life.

The development of polymer nanocomposite solar cells is one of the ways to improve the efficiency of converting solar energy into electrical energy. In such films, the doping of the polymer matrix with nanosized organic materials makes it possible to create a hybrid layer in which the conductivity of the polymer material will be combined with the high optical and electrical properties of organic nanostructures. It should be noted that the advantage of these composite materials is the simplified solar cell manufacturing process.

One of the promising classes of macroheterocyclic compounds are metal phthalocyanines, which have high mobility of charge carriers, efficiency of conversion of light energy, catalytic activity, are chemically and thermally stable, most of them easily form ordered thin films. It is also worth noting that metal phthalocyanines, when doped, have a strong effect on the degree of crystallinity of the polymer film. They are widely used as promising materials for composite photovoltaic converters.

The formation of separate phases of the donor and acceptor components of the active layer, as well as the mutual ordering of these phases, has a strong effect on the efficiency of organic photoconverters. It is generally accepted that the optimal domain size is close to the mean free path of excitons in a given material. With a smaller domain size, the efficiency of charge separation may even increase, but the transport of charges to the electrodes will be more difficult. The tendency to aggregation, the formation of polycrystalline domains of the donor-acceptor system are characterized by undesirable granularity and non-optimal crystalline ordering. These factors affect

the performance of film photoconverters, such as the efficiency of electron transport of charge carriers and the efficiency.

Thus, the study of the influence of the structural features of donor-acceptor systems in nanocomposite solar cells is of both fundamental and practical interest. First, the study of the optical and electrophysical properties of nanostructures will make it possible to evaluate the effect (defectiveness, change in the degree of crystallization, change in optical properties, etc.) on the active polymer layer upon doping. Secondly, they will optimize the electric transport and photovoltaic performance of nanocomposite solar cells.

The **aim of the dissertation** research is to study the influence of the structural features of donor-acceptor systems on the efficiency of generation and transport of charge carriers in nanocomposite polymer solar cells.

To achieve this goal in the process of performing the work, the **following tasks** were solved:

- obtaining solid films of phthalocyanines by vacuum thermal spraying;
- synthesis of phthalocyanine nanoribbons and its metal complexes by the method of physical gradient-temperature vapor deposition;
- study of the influence of the size effect on the generation and transport of charge carriers of phthalocyanines;
- obtaining nanocomposite solar cells based on fullerene P3HT: PCBM and fullerene-free derivatives PTB7-Th: ITIC, doped with nanoribbons;
- investigation of the processes of transport and recombination of charge carriers in polymer solar cells doped with nanoribbons;
- study of the effect of the effect of an external magnetic field on the short circuit current of organic and nanocomposite polymer solar cells.

The **objects of study** were solid films and nanowires of phthalocyanine and its metal complexes. Nanocomposite polymer solar cells P3HT:PCBM and PTB7-Th: ITIC doped with nanowires.

Research methods. Experimental studies were carried out by methods of optical spectroscopy, atomic force microscopy, voltammetry, impedance spectroscopy and X-ray diffraction.

Scientific novelty includes the following:

1. The technological conditions for the production of phthalocyanine nanowires by the method of physical gradient-temperature vapor deposition have been determined. A relationship is established between the observed absorption spectra of solid films and phthalocyanine nanowires.

2. The influence of the size effect on the efficiency of generation and transport of charge carriers in phthalocyanines is shown for the first time.

3. It was established for the first time that modulation by an external magnetic field reduces the probability of the formation of bipolarons, and with a decrease in the

dimension of the system due to the high probability of collision of polarons, the effect of "spin blocking" is more pronounced when modulated by an external magnetic field.

4. The role of phthalocyanine nanowires on the efficiency of generation and transport of charge carriers in a composite cell based on fullerene (P3HT:PCBM) and fullerene-free (PTB7-Th:ITIC) acceptors has been determined for the first time.

5. The influence of the magnetic field on the photocurrent in composite fullerene and fullerene-free cells has been investigated. It was found that modulation by a magnetic field blocks the charge transport channels "donor-Pedot:PSS" and "donor-NWsMPc-Pedot:PSS" of a polymer solar cell.

Provisions for Defense:

1. Size restrictions affect the efficiency of generation and transport of charge carriers in phthalocyanines.

2. The introduction of phthalocyanine nanowires into the photoactive layer enhances the degree of crystallization of the film, enhances the absorption of light and the injection of holes on the SC electrode.

3. When modulating the short-circuit current of MPc nanowires by an external magnetic field, the effect of “spin blocking” is more pronounced. The observed negative magnetic effect in polymer nanocomposite SCs is associated with the blocking of the “donor-Pedot:PSS” and “donor-NWs-Pedot:PSS” hole transport channels.

Personal contribution of the dissertation candidate. The author has performed work on obtaining phthalocyanine nanostructures and designing nanocomposite solar cells. Optical and X-ray phase measurements were carried out. The morphology of the surface of the obtained nanostructures and films was investigated using an atomic force microscope. The impedance spectra, I – V characteristics, and quantum efficiency of solar cells have been measured. Computer processing of the experimental measurement results has been carried out. The analysis of the results obtained and the conclusions of the work as a whole, as well as the preparation and writing of articles were carried out jointly with scientific consultants.

Communication of work with research programs. The dissertation was carried out in accordance with the plans of research work on the Programs of fundamental research coordinated by the Ministry of Education and Science of the Republic of Kazakhstan: "Development of a solar energy photoconverter based on semiconductor polymer and metal-phthalocyanines" (No. 544-F-19, 2019), "Development of a solar energy photoconverter based on organic semiconductor nanocomposites" (IRN AP08856176, 2020).

The structure and scope of the thesis. The structure of the dissertation work is determined by the tasks and consists of an introduction, 4 sections, a conclusion, a bibliography and an appendix. It is presented on 109 pages of typewritten text, illustrated with 55 figures, 12 tables, contains a list of used literature of 210 titles.

Scientific and practical significance of the work:

The optimal parameters of the organic photoconverter (structural features, production technology), which provide a high efficiency and quantum efficiency, have been determined. The development of composite solar cells has the prospect for the creation of light, technological and cheap in mass production of autonomous power supplies for a wide range of electronic devices and devices.

Approbation of work and publication. The main results of the work were reported and discussed at conferences: VIII International Conference on Photonics and Information Optics (NRNU MEPhI, 2019); 18th IUPAC International Symposium on Macromolecular-Metal Complexes (Russia, Moscow, June 10-13, 2019); Materials of the 11th International Scientific Conference “Chaos and Structures in Nonlinear Systems. Theory and Experiment "(Karaganda, 2019); IX International Conference on Photonics and Information Optics: (NRNU MEPhI, 2020); Proceedings of the international scientific-practical conference "Auezov readings - 18: the spiritual heritage of the great Abai" to the 175th anniversary of Abai Kunanbayev (Shymkent, 2020); Materials of the international scientific-practical conference "Al-Farabi in the modern Kazakhstan context" dedicated to the 1150th anniversary of Abu Nasr al-Farabi (Karaganda, 2020).

Publications. 15 scientific papers have been published on the topic of the dissertation, including 4 papers in journals indexed in the Clarivate Analytics databases, 1 work in Scopus, and in 4 editions recommended by the CCSES RK.