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Influence of the environment on the morphology, optical and electrical characteristics of the PEDOT:PSS polymer

The paper presents the results of studying the influence of the environment on the surface structure, optical and electrical characteristics of the PEDOT:PSS film. The studies have been carried out in three different types of atmosphere under the same conditions of thermal annealing of the films. It has been established that the modification of the surface of a polymer film with ethanol and isopropanol in vacuum, in a nitrogen atmosphere, and in the air atmosphere leads to a change in the surface morphology and the optical electric transport properties of the polymer. Depending on the environment, when the PEDOT:PSS film is modified with a certain concentration of ethyl and isopropyl alcohols, the absorption spectra show a shift in the absorption maximum responsible for PEDOT to the short-wavelength region of the spectrum, as well as a decrease in the absorption peak of the part of the spectrum responsible for the absorption of the aromatic fragment PSS. It is identified that the structural features of the PEDOT:PSS surface morphology affect the electrical transport parameters of the films: R_h is the resistance of the PEDOT:PSS polymer film, R_{ext} is the charge carrier transfer resistance at the PEDOT:PSS/electrode interface, k_{eff} is the effective charge carrier extraction rate and τ_{eff} is the effective transit time of charge carriers. The optimal technological parameters for film production have been determined, at which the electrical transport properties of PEDOT:PSS polymer films are increased.

Keywords: PEDOT:PSS, isopropanol, ethanol, vacuum, nitrogen atmosphere, air atmosphere, surface morphology, optical spectroscopy, impedance spectroscopy.

Introduction

Currently, global manufacturers of electronic devices and components for solar energy pay special attention to elements based on organic semiconductor materials (OPV) [1–3]. The photoelectric characteristics of OPV devices are strongly influenced by the structural features and surface morphology of the organic material of the films they are made of [4, 5].

The most common organic semiconductor polymer used PEDOT:PSS as a hole transport layer (HTL) in OPV devices [6]. The electrical transport properties of PEDOT:PSS directly depend on the surface morphology, which, in turn, depends on the type of dopants, solvents, annealing temperature, and environment. Alcohols are suitable and effective additives in PEDOT:PSS due to their low cost, non-toxicity, and good polymer solubility in it [7, 8]. The addition of alcohol solvents to the PEDOT:PSS polymer leads to a significant increase in conductivity [9, 10]. In addition, due to low boiling points, alcohols are easily removed during heat treatment, and alcohol-treated PEDOT:PSS films are smooth, which makes them well-suited for use as an HTL layer in organic photoconverters [11].

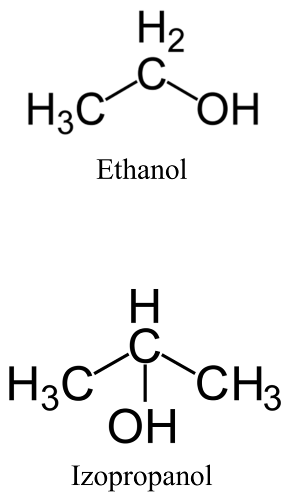
It should be noted that the heat treatment of PEDOT:PSS films leads to an increase in the crystallinity of the polymer and a change in the surface morphology [12–16]. At the same time, the combined influence of the environment and annealing of PEDOT:PSS films on the surface structure, optical and electrical characteristics of the PEDOT:PSS film have not been practically studied [17–20].

In this regard, in this paper, we carried out studies on the influence of the environment on the structural, optical, and electrical transport parameters of the films. To change the surface morphology, PEDOT:PSS films were obtained in a vacuum, nitrogen, and air atmosphere, with the addition of a certain concentration of alcohols. The obtained results were analyzed by comparing the surface morphology, optical and impedance spectra of PEDOT:PSS films.

Experimental

Films were obtained in three different environments: in vacuum, in nitrogen and air atmosphere. To change the surface morphology, the polymer with hole conductivity PEDOT:PSS was extended with a certain concentration of alcohol (ethyl, isopropyl) and placed in the test environment. A comparative analysis of the modified PEDOT:PSS film was carried out by comparing the structure of the surface morphology, optical and electrical transport properties, depending on the preparation environment.

Figure 1 shows the structural formulas of the compounds. The preparation of the substrates was carried out according to the procedure [21]. We used PEDOT:PSS (1%, Ossila Al4083), Isopropanol, Ethanol (pure 99.9% Sigma Aldrich). Before starting the experiments, the PEDOT:PSS solution was filtered through a 0.45-micrometer filter. PEDOT:PSS films were obtained on the surface of quartz glass by centrifugation (on a SPIN150i centrifuge manufactured by Semiconductor Production System) at a rotation speed of 5000 rpm. The choice of the concentration of alcohol solvents was determined based on the studies of the authors [22]. They proved that the optimal proportion of alcohol in the polymer is 50% by weight.



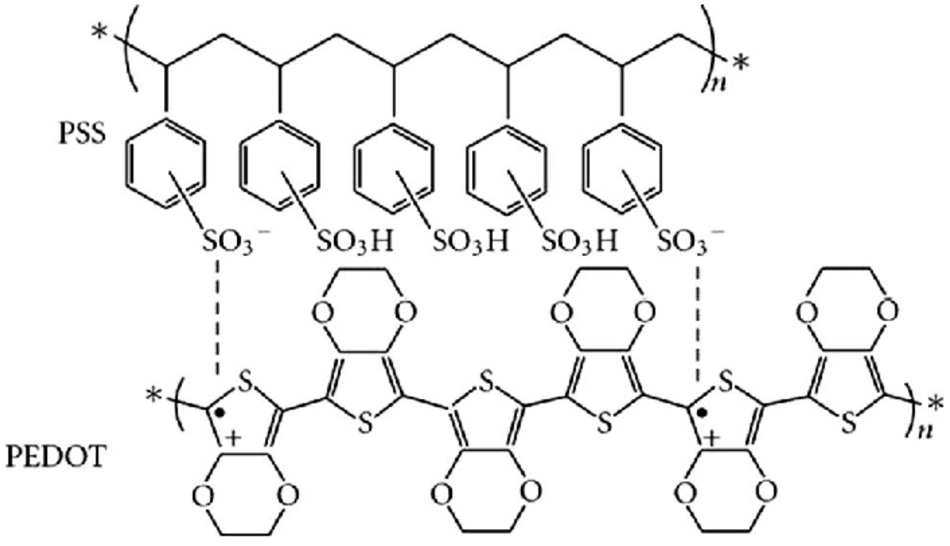


Figure 1. Chemical structure of Ethanol, Isopropanol, PEDOT and PSS

For experiments in a vacuum, the samples were placed in a vacuum furnace (YHCHEM, Shanghai Yuanhuai Industrial Co.) and annealed at 120°C for 10 minutes. For experiments in a nitrogen atmosphere, the samples were deposited and annealed at 120°C for 10 minutes in a specialized two-chamber inert atmosphere glove box (CY-VGB-6-II-LD, Shanghai Yuanhuai Industrial Co.). To carry out experiments in air, the samples were deposited at room temperature and annealed at 120°C for 10 minutes.

The surface topography of the samples was studied using an atomic force microscope (AFM) JSPM-5400 (JEOL, Japan). The AFM images were processed using a special modular program for analyzing scanning probe microscopy data (Win SPMII Data-Processing Software). Surface morphology, roughness of PEDOT:PSS thin films were analyzed from AFM images. The images of the surface of the PEDOT:PSS films were obtained in the mode of the semi-contact scanning method. The absorption spectra of the studied samples in the range of 200–1100 nm were recorded on an AvaSpec-ULS2048CL-EVO spectrometer (Avantes). The impedance spectra were measured using a P-45X potentiostat (Elins) with an additionally installed FRA-24M frequency analyzer module. Fitting and analysis of the spectrum parameters were carried out using the EIS-analyzer software package, according to the procedure [23].

Results and Discussion

Figure 2 illustrates images of the surface morphology of PEDOT:PSS films in a vacuum with different ratios of ethyl and isopropyl alcohols. Table 1 shows the roughness values of PEDOT:PSS films. Figure 2 shows that the PEDOT:PSS film without the addition of alcohols after thermal annealing has a rather pronounced relief. At the same time, the surface morphology has a pronounced heterogeneity; the surface roughness is 0.64 nm.

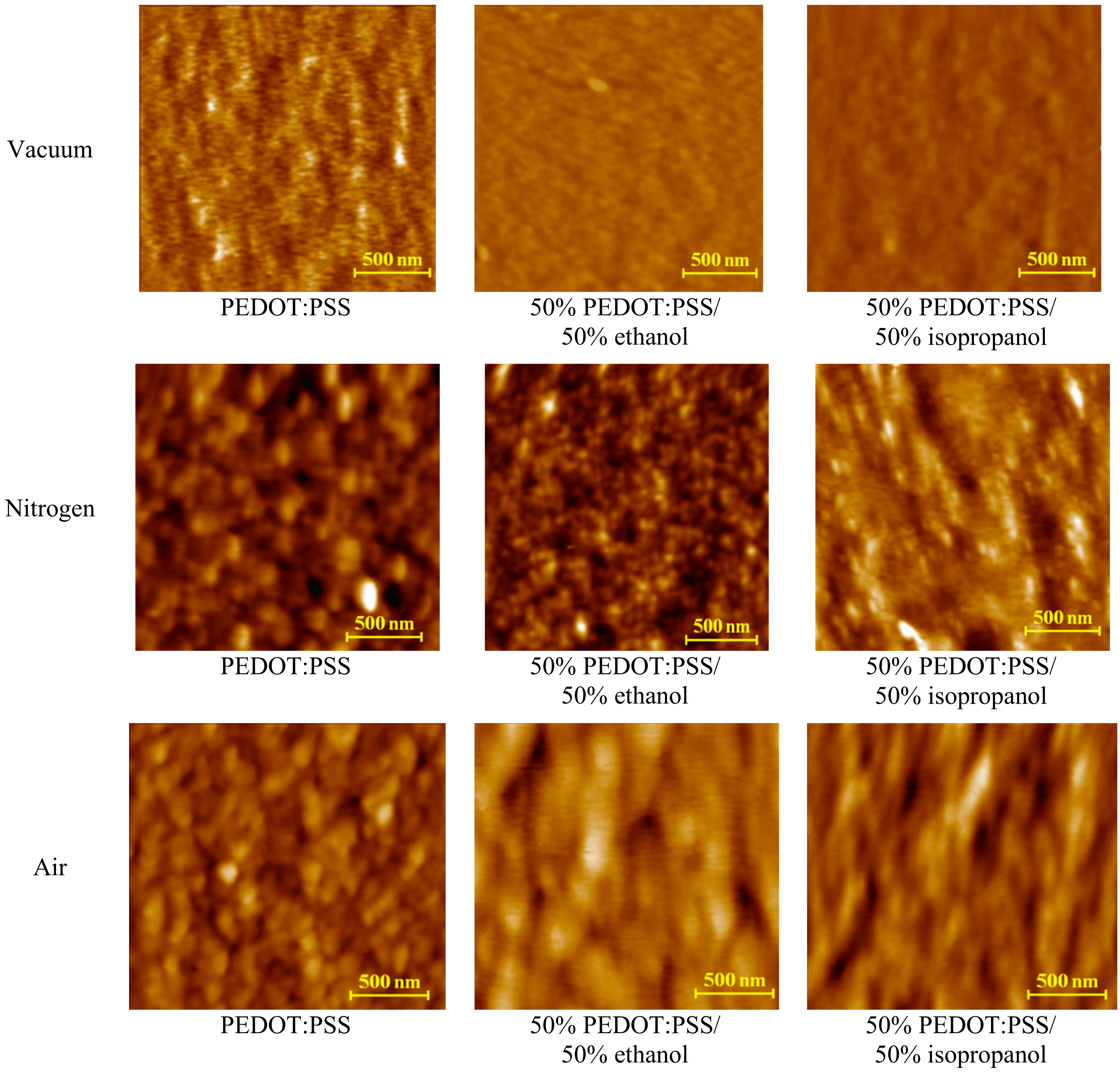


Figure 2. Surface morphology images of PEDOT:PSS films

In PEDOT:PSS film prepared in 50/50 ethyl alcohol, the surface roughness of PEDOT:PSS film is reduced to 0.45 nm. The addition of 50/50 isopropyl alcohol to the PEDOT:PSS film resulted in smoothing of the film surface with a roughness of 0.43 nm. Comparative analysis of changes in surface roughness showed that in the process of film preparation with the addition of ethyl alcohol, the surface roughness decreases by 1.4 times, and isopropyl alcohol – by 1.5 times.

Figure 2 also demonstrates images of the surface morphology of PEDOT:PSS films prepared in a nitrogen atmosphere after exposure to ethyl and isopropyl alcohol vapors in a ratio of 50/50%. The PEDOT:PSS film has an inhomogeneous surface structure with a roughness of 0.65 nm (Table 1).

When the PEDOT:PSS polymer film is kept in ethanol vapor in an inert atmosphere, the surface is smoothed. The film roughness decreased and amounted to 0.58 nm (Table 1). When keeping the film in vapors of isopropyl alcohol, the roughness of the PEDOT:PSS film was 0.43 nm. Thus, the obtained results indicate that the smallest film surface roughness is obtained upon annealing in isopropanol vapor.

To study the effect of the air atmosphere on the polymer surface morphology, the film was kept in vapors with a certain concentration of ethyl and isopropyl alcohols. It can be seen from Figure 2 that the PEDOT:PSS film has a grain structure. At the same time, against the background of a fine grain structure, large particles are observed; the surface roughness is 0.63 nm (Table 1).

After treatment with alcohol vapors for 10 minutes, the proportion of large particles decreases significantly, the roughness becomes 0.48 nm for ethyl alcohol and 0.45 nm for isopropyl alcohol. The addition of alcohol solvents to the film causes a smoothening of the film surface.

Table 1

Surface roughness of PEDOT:PSS films at different concentrations of alcohols in the volume during annealing in vacuum, nitrogen and air atmosphere

Sample	R_a, nm
Vacuum	
PEDOT:PSS	0.64
50% PEDOT:PSS/50% ethanol	0.45
50% PEDOT:PSS/50% isopropanol	0.43
Nitrogen	
PEDOT:PSS	0.65
50% PEDOT:PSS/50% ethanol	0.58
50% PEDOT:PSS/50% isopropanol	0.43
Air	
PEDOT:PSS	0.63
50% PEDOT:PSS/50% ethanol	0.48
50% PEDOT:PSS/50% isopropanol	0.45

Figure 3a shows the absorption spectra of PEDOT:PSS films prepared in a vacuum, annealed at T=120C° with 50% ethanol and isopropyl alcohol. It can be noted that the original PEDOT:PSS film has a maximum at a wavelength of λ_1 = 216 nm with a spectral half-width of 10.2 nm (Table 2). In the absorption spectra of all films, a shoulder λ_2 is observed with a maximum at 224 nm (Fig. 3a). The absorption bands with a maximum at 224 nm are associated with the absorption of the polymer PSS – poly(styrenesulfonate) [24].

When ethyl alcohol is added to the film during preparation, the positions of the maxima in the absorption spectra do not change, only a decrease in the optical density and a decrease in the half-width of the spectrum are observed. The value of the maximum at a wavelength of 216 nm decreased by 1.2 times, and at a wavelength of 224 nm – by 1.3 times.

A comparison of the shapes and positions of the absorption spectra maxima of films with isopropyl and ethyl alcohol showed no visible changes. The half-width of the absorption spectrum remained within the same range as for ethyl alcohol. The values of the optical density at the absorption maxima decrease. The value of the maximum at a wavelength of 216 nm decreased by 1.8 times, and at a wavelength of 224 nm – by 2.3 times.

Figure 3b presents the absorption spectra of PEDOT:PSS films prepared in a nitrogen atmosphere. Table 2 indicates the absorption spectra parameters. The absorption maximum of the original PEDOT:PSS film is 216 nm with a half-width of 9 nm. It can be seen from Figure 3b that the absorption spectra of the PEDOT:PSS films treated with alcohol vapors in an inert gas atmosphere show a change in shape. Thus, in addition to the short-wavelength narrow band, a rather broad long-wavelength band with a maximum of 230 nm is observed in the spectrum. Also, when the film is treated in alcohol vapors, the absorption spectrum of the final film shows a shift of the absorption maximum relative to the initial film to the short-wavelength region of the spectrum. Moreover, a shift is observed for the short-wavelength maximum, which is responsible for the PEDOT component, while the position of the long-wavelength maximum remains constant. The values of optical densities decrease at the absorption maximum. For the film treated with ethyl alcohol vapor, the optical density decreased to a value of 0.53, and for isopropyl alcohol – to 0.48 (Table 2). The half-width of the spectra does not change.

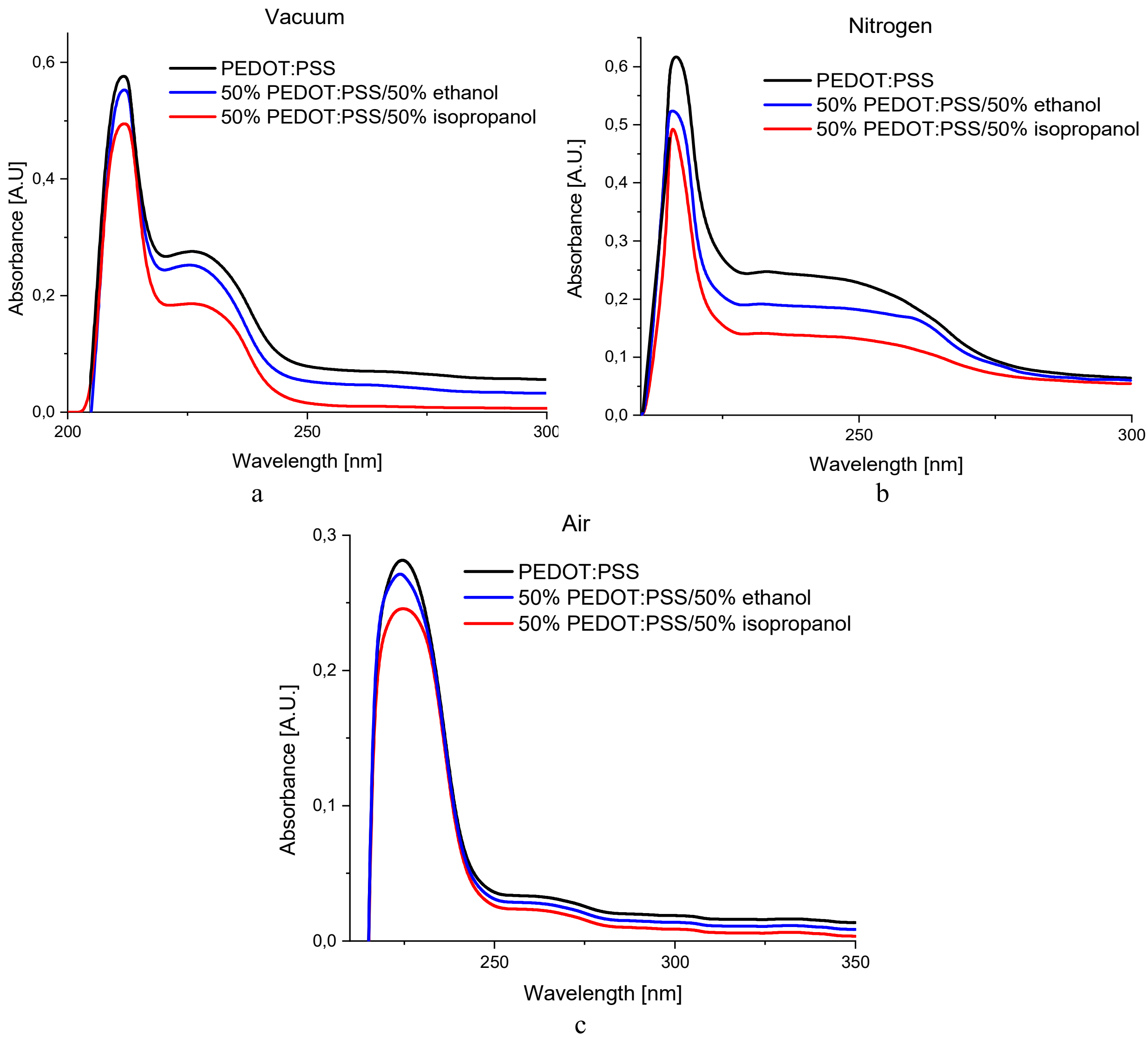


Figure 3. Absorption spectra of PEDOT:PSS films in vacuum (a), nitrogen atmosphere (b) and air atmosphere (c)

Figure 3c shows the absorption spectra of the original PEDOT:PSS film and PEDOT:PSS films treated in alcohol vapor prepared in air. It can be seen that the initial PEDOT:PSS film has a maximum at a wavelength of λ_1 = 224 nm with a spectral half-width of 28 nm (Figure 3c). In the absorption spectra of all films, a shoulder with a maximum of 260 nm is observed, which is associated with the absorption of the PSS aromatic fragment [24]. The position of the absorption maxima of the films obtained by preparing PEDOT:PSS solutions with alcohol solvents does not change, the half-width of the spectra increases (Table 2).

The value of the optical density at the absorption maximum does not undergo significant changes. Treatment with ethanol vapor leads to a change in the value of optical density at the maximum of short-wavelength absorption by 0.1, and the value of the long-wavelength shoulder practically does not change. When treated with isopropyl alcohol vapor, a similar picture is observed.

It should be noted that a comparative analysis of the change in the optical density values at the absorption maxima of the films shows that for isopropyl alcohol a greater decrease in absorption is observed than for ethyl alcohol.

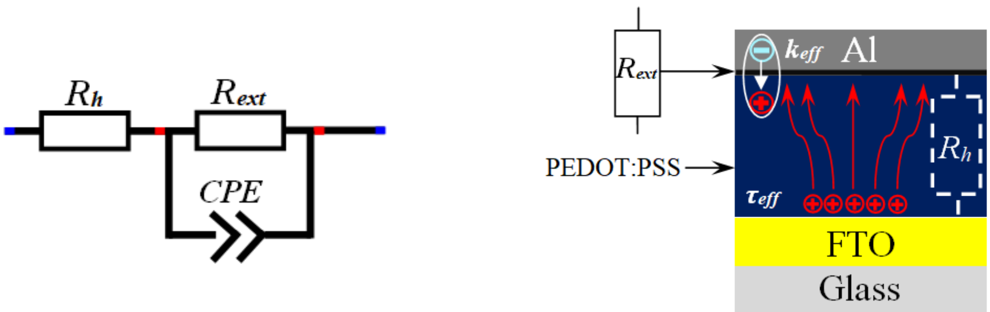
Table 2 lists the characteristics of the absorption spectra of PEDOT:PSS films in various types of atmosphere.

Table 2

Characteristics of absorption spectra of PEDOT:PSS films

Sample	Absorption Peaks		D_1	D_2	FWHM, nm
	λ_1, nm	λ_2, nm			
Vacuum					
PEDOT:PSS	216	224	0.58	0.28	10
50% PEDOT:PSS/50% ethanol	216	224	0.55	0.25	9.5
50% PEDOT:PSS/50% isopropanol	216	224	0.49	0.18	8.5
Nitrogen					
PEDOT:PSS	216	230	0.61	0.24	9
50% PEDOT:PSS/50% ethanol	215	230	0.53	0.19	9
50% PEDOT:PSS/50% isopropanol	214	230	0.48	0.14	9
Air					
PEDOT:PSS	224	260	0.28	0.03	28
50% PEDOT:PSS/50% ethanol	224	260	0.27	0.03	29
50% PEDOT:PSS/50% isopropanol	224	260	0.25	0.02	32

Next, we studied the effect of modification of the PEDOT:PSS structure on the transport of charge carriers in the cells of the FTO/PEDOT:PSS/Al structure using the method of impedance spectroscopy. The analysis of the impedance measurement results was carried out according to the diffusion-recombination model and the equivalent circuit shown in Figure 4a was used for the fitting, where CPE is a constant phase element, which is an equivalent component of an electrical circuit that simulates the behavior of a double layer but is an imperfect capacitor. The main electrical transport parameters were calculated from the spectra (Table 3), where: k_{eff} is the effective charge carrier extraction rate from PEDOT:PSS, τ_{eff} effective transit time through PEDOT:PSS, R_h is the resistance of the PEDOT:PSS film, R_{ext} is the resistance of charge carrier transfer at the PEDOT:PSS/electrode interface. Figure 4b designates the diagram of the movement of charges in the cell.



a b

Figure 4. Equivalent electrical circuit (a) and scheme of charges transport in the cell (b)

Figure 5 indicates the impedance spectra of PEDOT:PSS films in vacuum, nitrogen and air atmospheres. Table 3 shows the values of the electrical physical parameters of the films. As can be seen from the Table 3, the modification of PEDOT:PSS with organic solvents in various types of atmosphere affects the transport of charge carriers in PEDOT:PSS. Cells based on films obtained from solutions with organic solvents (ethanol, isopropanol) have better electrical transport properties (Table 3). In all types of atmosphere, the addition of ethanol reduces the resistance of the PEDOT:PSS (R_h) film and the resistance of the PEDOT:PSS/Al (R_{ext}) interface, which increases the efficiency of hole transport from FTO to Al through PEDOT:PSS. When using isopropyl alcohol, the decrease in R_h and R_{ext} is more significant: in a vacuum, R_h decreased by 2.6 times, while R_{ext} decreased by 3.9 times compared to the original PEDOT:PSS, in a nitrogen atmosphere, the film resistance decreased by 2 times, and the resistance the interface decreased by 2.4 times compared to PEDOT:PSS, and in air atmosphere, the resistances R_h and R_{ext} decreased by 2.3 and 3.1 times, respectively.

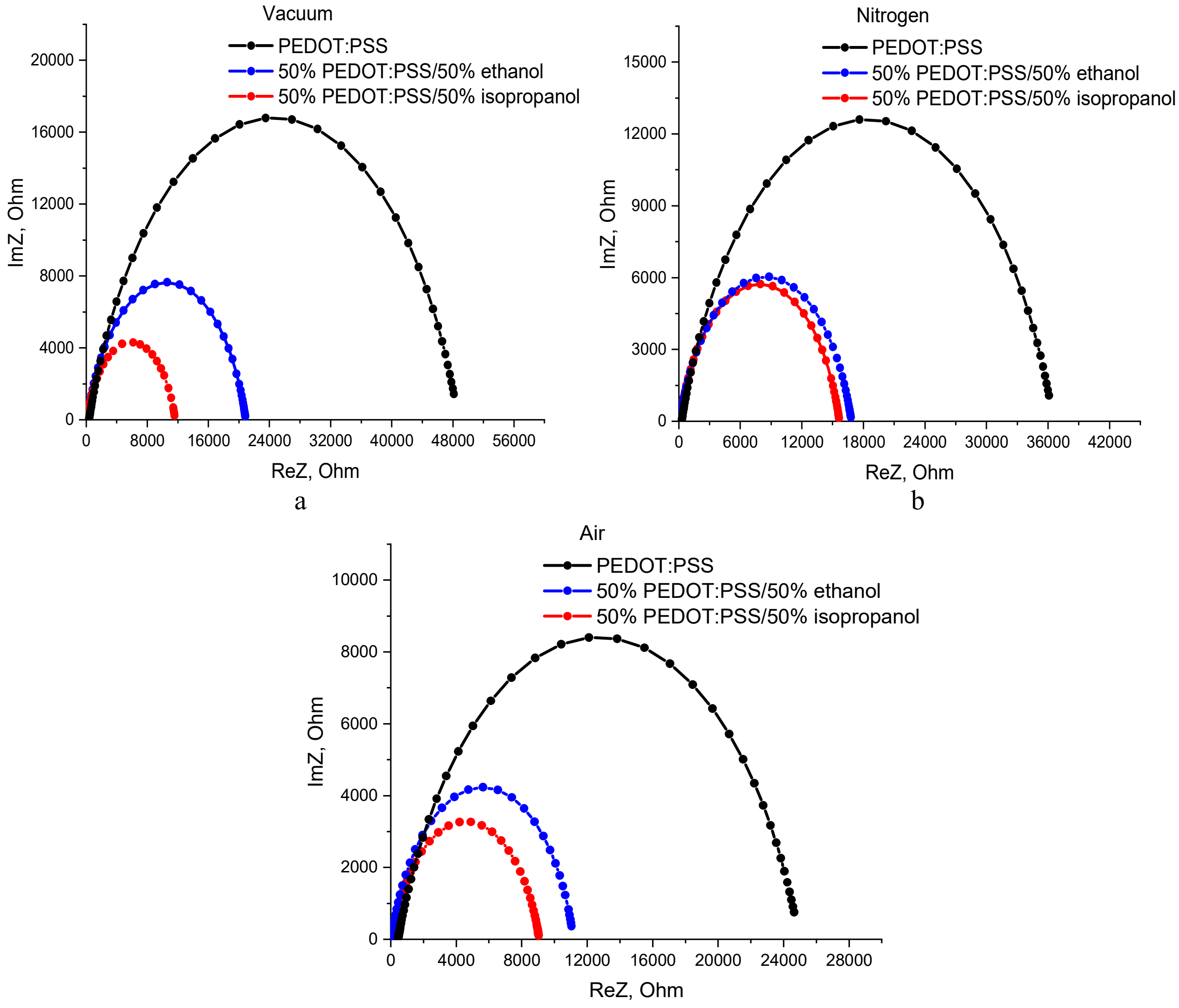


Figure 5. Impedance spectra of PEDOT:PSS films in vacuum (a), in nitrogen atmosphere (b) and in air atmosphere (c)

The values k_{eff} and τ_{eff} characterize the effective charge carrier extraction rate from PEDOT:PSS and the effective transit time through PEDOT:PSS. As can be seen from Table 3, the addition of ethyl and isopropyl alcohol to PEDOT:PSS has a noticeably positive dynamic in k_{eff} and τ_{eff}. The atmosphere in which the films are prepared also influences these parameters. When ethyl alcohol is added to the film, a positive dynamics is observed. However, the best results are shown by films prepared with the addition of isopropyl alcohol. The effective charge carrier extraction rate from PEDOT:PSS films obtained from a solution with isopropyl alcohol more than doubled, and the effective transit time of charge carriers decreased inversely. The highest value of τ_{eff} is observed in films prepared in the air atmosphere (Table 3). This means that the lifetime of charge carriers in films prepared in air is longer than in films prepared in a vacuum and a nitrogen atmosphere. Holes injected into PEDOT:PSS diffuse to the electrode, where they recombine with electrons. Fast transport of injected holes to the outer electrode is paramount since this reduces the probability of their reverse recombination. In our case, fast hole transport is provided by improving the structure of PEDOT:PSS after adding isopropyl alcohol to the initial solution, which leads to an improvement in the quality of the PEDOT:PSS/FTO interface [25, 26].

Table 3

The value of the electrical physical parameters of the films

Sample	R_h, Ω	R_{ext}, Ω	k_{eff}, s^{-1}	$τ_{eff}$, ms
Vacuum				
PEDOT:PSS	268.7	48745	157.5	6.4
50% PEDOT:PSS/50% ethanol	148.5	21054	259.4	3.9
50% PEDOT:PSS/50% isopropanol	104.7	12487	348.1	2.9
Nitrogen				
PEDOT:PSS	197.8	36748	74.8	13.4
50% PEDOT:PSS/50% ethanol	104.2	16874	110.8	9.1
50% PEDOT:PSS/50% isopropanol	98.5	15478	154.5	6.5
Air				
PEDOT:PSS	145.9	28876	48.5	20.6
50% PEDOT:PSS/50% ethanol	65.5	13564	53.7	18.6
50% PEDOT:PSS/50% isopropanol	63.7	9456	92,1	10.9

Conclusions

An analysis of the experiments showed that changing the film preparation environment and adding an alcohol solvent affects the surface structure of PEDOT:PSS films, which, in turn, affects the process of charge carrier transport. It has been established that the addition of alcohol to the PEDOT:PSS polymer in all types of studied atmospheres leads to a decrease in surface roughness. When the PEDOT:PSS surface is modified in different types of atmosphere, the absorption spectra show shifts in the maximum of the absorption spectra responsible for PEDOT in the short-wavelength region, as well as a decrease in the absorption of the PSS aromatic fragment. Changes in the structure and morphology of the PEDOT:PSS surface affects the electrical transport parameters of the films. It has been established that the surface of the PEDOT:PSS film modified in the volume of isopropyl alcohol and prepared in air atmosphere has the lowest resistance parameters R_h and R_{ext}, and the highest value of $τ_{eff}$, at which, due to the change in the structure of the PEDOT:PSS surface, the fastest transport of charge carriers is ensured.

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PEDOT: PSS полимерінің морфологиясына, оптикалық және электрофизикалық сипаттамаларына қоршаған ортаның әсері

Мақалада PEDOT: PSS пленкасының беттік құрылымына, оптикалық және электрофизикалық сипаттамаларына ортаның әсерін зерттеу нәтижелері берілген. Зерттеулер атмосфераның үш түрлі түрінде пленкаларды термиялық өңдеудің тең жағдайында жүргізілді. Вакуумда, азот ортасында және атмосферада этил және изопропил спирттерімен полимерлі пленканың бетін өзгерту беттік морфологияның, полимердің оптикалық электрлік қасиеттерінің өзгеруіне әкелетіні анықталды. PEDOT: PSS пленкасын модификациялау кезінде ортаға байланысты этил және изопропил спирттерінің белгілі бір концентрациясымен жұтылу спектрінде PEDOT жауап беретін жұтылу максимумының спектрдің қысқа толқындық аймағына ауысуы, сондай-ақ PSS хош иісті фрагменті жұтылуға жауап беретін спектрдің бір бөлігінің жұтылу шыңының төмендеуі байқалады. PEDOT: PSS беттік морфологиясының құрылымдық ерекшеліктері электрлік тасымалдау пленкасының параметрлеріне әсер етеді, мысалы: R_h - PEDOT: PSS полимерлі пленкасының кедергісі, R_{ext} - PEDOT: PSS / электрод интерфейсіндегі заряд тасымалдаушылардың тасымалдау кедергісі, k_{eff} - заряд тасымалдаушыларды алудың тиімді жылдамдығы және τ_{eff} - заряд тасымалдаушылардың тиімді ұшу уақыты. PEDOT: PSS полимерлі пленкалардың электрлік тасымалдау қасиеттері жоғарылайтын пленкаларды алудың оңтайлы технологиялық параметрлері анықталды.

Кілт сөздер: PEDOT: PSS, Izopropanol, Ethanol, вакуум, азот атмосферасы, ауа атмосферасы, беттік морфология, оптикалық спектроскопия, импеданс спектроскопиясы.

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Влияние среды на морфологию, оптические и электрофизические характеристики полимера PEDOT: PSS

В работе представлены результаты исследования влияния среды на структуру поверхности, оптические и электрофизические характеристики пленки PEDOT: PSS. Исследования проводились в трех разных типах атмосферы при равных условиях термического отжига пленок. Установлено, что модификация поверхности полимерной пленки этиловым и изопропиловым спиртами в вакууме, в среде азота и на атмосфере приводит к изменению морфологии поверхности, оптических электротранспортных свойств полимера. Показано, что, в зависимости от среды при модификации пленки PEDOT: PSS определенной концентрации этилового и изопропилового спиртов, в спектрах поглощения наблюдается сдвиг максимума поглощения, отвечающего за PEDOT, в коротковолновую область спектра, а также уменьшение пика поглощения части спектра, отвечающего за поглощение ароматического фрагмента PSS. Показано, что структурные особенности морфологии поверхности PEDOT: PSS оказывают влияние на электротранспортные параметры пленок, такие как R_h — сопротивление полимерной пленки PEDOT:PSS; R_{ext} — сопротивление переноса носителей заряда на границе раздела PEDOT: PSS/электрод; k_{eff} — эффективная скорость извлечения носителей заряда и τ_{eff} — эффективное время пролета носителей заряда. Определены оптимальные технологические параметры получения пленок, при которых повышаются электротранспортные свойства полимерных пленок PEDOT: PSS.

Ключевые слова: PEDOT:PSS, Izopropanol, Ethanol, вакуум, атмосфера азота, атмосфера воздуха, морфология поверхности, оптическая спектроскопия, импедансная спектроскопия.