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The effect of conductive polymer on the Structural and Surface Morphology Analysis of NiPcTs:PEDOT:PSS Blend

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ABSTRACT

The thin films of Ni-Phthalocyanine Tetrasulfonic acid tetrasodium salt and poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (NiPcTs:PEDOT:PSS) blend with different (PEDOT:PSS) concentrations (0.5 ,1, 2) on glass substrates were prepared by spin coating at thickness (100 nm). The structure and surface morphology of films were studied using X-ray diffraction , atomic force microscope (AFM),Scanning Electron Microscope (SEM),and showed that there was a change and enhance in the crystallinity. Analysis of X-rays diffraction patterns of NiPc in powder form structure is polycrystalline and display a strong reflection at (100) orientation. Another peak distinguished in the XRD pattern of as-deposited which represents a reflection at (102) orientation and grain size increased with increasing (PEDOT:PSS) ,This result was supported by AFM measurements, which exhibited a larger grain size. While (SEM)is observed that the shapes of grain is fiber to nanofiber with increasing PEDOT:PSS concentration.

1. Introduction

Organic semiconductors are a wonderful class of materials, with a wide range of properties [1,2]. Typical deposition techniques for organics are readily available or not very difficult to implement (spin-coating, drop-casting, direct printing via stamps or ink-jets). Their compatibility with light-weight, mechanically flexible plastic substrates, makes them possible candidates for future electronic devices. The design of the molecular structures can be engineered to enhance particular properties (solubility in different solvents, color of light emission, crystal packing). In particular, addition of polar groups in polymers (e.g. polyvinylidene fluoride and its copolymers with trifluoroethylene and tetrafluoroethylene) leads to rich systems for investigation of ferroelectricity [3]. Phthalocyanine is an organic semiconductor widely used for sensor applications and transistor fabrication, which has excellent stability against heat, light, moisture and oxygen[4]. The physical properties are controlled by traps, which are associated with dislocations, imperfections, grain boundaries and surface topology of film [5]. Nickel phthalocyanine is an organic semiconductor that contains alternate single and double bonds. As Fig.1 shows, small-molecule or monomer-based organics have a well defined molecular.

Weight and the simplest structure. Polymers are composed of long chains of molecules, consisting of an indeterminate number of repeating monomers. The diffract grams obtained are analyzed to study the structure and crystalline of films. Scanning electron microscopy (SEM) is one of the powerful tools for the investigation of surface topography and micro structural features [6, 7].

The nature of bonding in organic semiconductors is fundamentally different from their inorganic counterparts.

Organic molecular crystals are van-der-Waals-bonded solids implying a considerably weaker intermolecular bonding as compared to covalently bonded semiconductors like Si or GaAs. The consequences are seen in mechanical and thermodynamic properties such as reduced hardness or lower melting point, but even more importantly in a much weaker delocalization of electronic wave functions amongst neighboring molecules, which has direct implications for optical properties and charge carrier transport. The situation in polymers is somewhat different since the morphology of polymer chains can lead to improved mechanical properties. Nevertheless, the electronic interaction between adjacent chains is usually also quite weak in this class of materials [8].

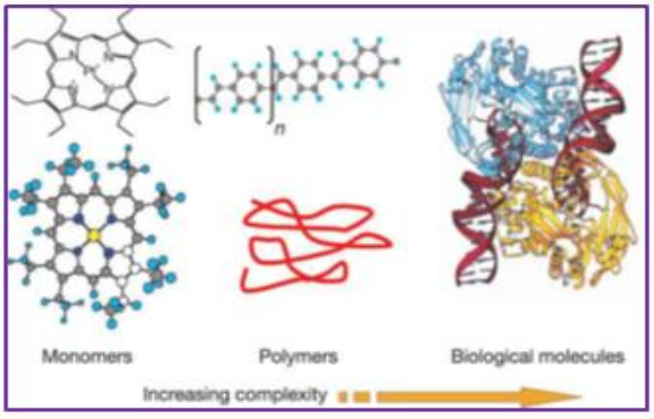

Fig 1. Different types of organic materials in order of increasing complexity[6].

2. Experimental

The p-type organic semiconductors NiPcTs and PEDOT:PSS were obtained from Sigma-Aldrich without more purification. Fig.2shows the structure of the NiPcTs andPEDOT:PSSmolecules .

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NiPcTs weighing and dissolving 65 mg/ml of deionized water and putting it on magnetic stirrer for 30 min and then shaking vigorously to help the material to be dissolved. the solution was filtered using (0.45, 0.2)µm filter to remove any contaminant or un dissolved material and get homogenous solution so the solution of PEDOT:PSS was filtered using (0.2) µm filter .Thin films blend (NiPcTs:PEDOT:PSS)with different (PEDOT:PSS) concentrations (0.5 ,1and 2) are prepared and putting it on magnetic stirrer for 30 min to mixing . After the preparation of organic material solution, it was put into a micro syringe and then drops on the substrate and left the substrate for two hours before spin coating. The spin rates was (1500) rpm for 1.5 mint, the thicknesses obtained is 100 nm, Fig.(3). After deposition the substrate was dried out at room temperature then annealed at (100)ºC. All the samples prepared by using Laurell WS-650Mz-23NPP Spin coater.

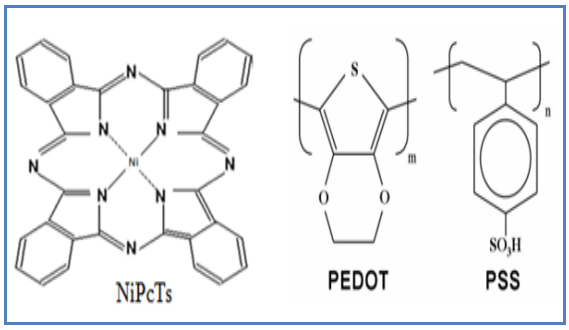

Fig 2. Molecular structure of the NiPcTs and PEDOT:PSS molecules.

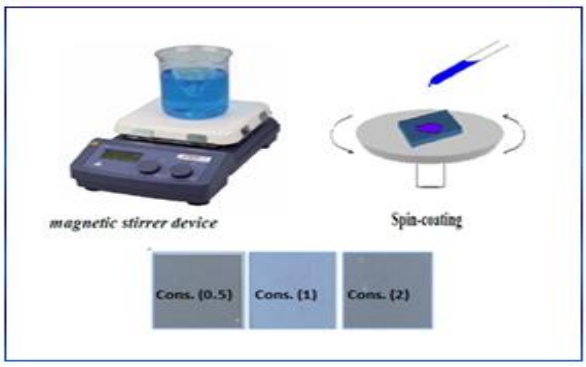

Fig 3. Preparation of NiPcTs:PEDOT:PSS Blend thin Films.

The X-ray diffraction, AFM and SEM of film deposited on glass substrate annealing are studied, the samples NiPcTS:PEDOT : PSS to an area of 0.5 to a temperature T_a (100)ºCfor 1 hour .The X-ray diffraction is recorded by "SHIMADZU" XRD-6000 X-ray diffract meter (cukα radiation λ=0.154 nm) in 2θ range from 2º-60º. The distanced d_{hkl} for different planes and average crystallitesize are measured using equ.1,2 .

$n\lambda=2d\sin\theta$ (1)

λ:wavelength of incident X-ray in angstrom 1.54 Aº, d:interplanar spacing of crystal in angstrom.

θ:angle between the incident rays and surface of the crystal in degree, n=1,2,3…..

Crystallite size=0.94 λ/FWHM. COSθ (2)

Surface morphological measurements for NiPcTs:PEDOT:PSS Blend thin Films with annealing temperature(100)ºC and different concentration of PEDOT:PSS were tested by using CSPM AA3000. AFM micrographs can provide information about 2D, 3D images for all studied samples, roughness and grain size.

SEM is used to examine the morphology of the formed blend.

The morphology and structures of the films are very important to determine the properties of the NiPcTs/PEDOT:PSS nanofiber size, structure and the shape using VEGA3 TESCAN, where high-resolution images of the surface of a sample is acquired. The microscope works by the same principle as an optical microscope, but instead of photons it measures the electrons scattered from the sample. Because electrons can be accelerated by an electric potential, the wavelength can be made shorter than the one of photons.This makes the SEM capable of magnifying images up to 200.000 times. At the same time it is possible to achieve high resolution pictures of the surface, making the instrument very useful in determining the size distribution of nanoparticles .

3. Results and Discussion

The X-ray diffraction of the NiPc powder used as the source material for sublimation The peaks are identified using the standard JCPDS File No. 11-0744 data. The Full Width at Half Maximum (FWHM), d-spacing and grain size were calculated as listed in table (1). The structure of NiPcTs powder was determined which gives a polycrystalline structure, monoclinic phase .The spectrum of the NiPcTs powder has shown sharp peaks at reflection surfaces (100),(102),(002),(204),(111) and (214).The peaks simulated by XPowder program to calculate the experimental values of FWHM and grain sizes of NiPcTs powder as shown in Fig. (4).Fig.5shows the X-ray diffraction patterns of deposit NiPcTS:PEDOT:PSS blend thin films on glass substrates with different (PEDOT:PSS) concentrations also shows Polymorphism structure and the simulations of tow peaks appear (100),(102) refers to NiPcTS While amorphous due to PEDOT:PSS, and the peak (102) disappeared in XRD pattern of in concentration (2) .Table (2) represents the XRD parameters which are obtained from this measurement for as-deposited NiPcTS:PEDOT:PSS thin film and show the grain size is increased with increasing (PEDOT:PSS) concentrations.

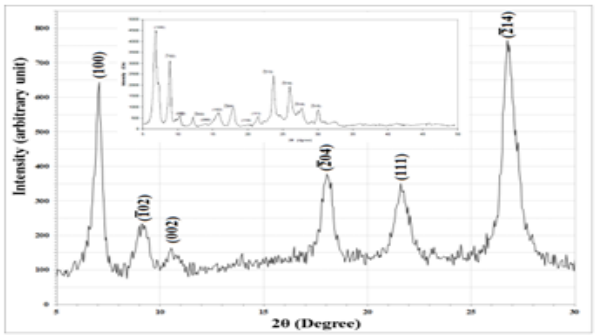

Fig 4. X-ray diffraction patterns of pure NiPcTs powders compared with NiPc powder.

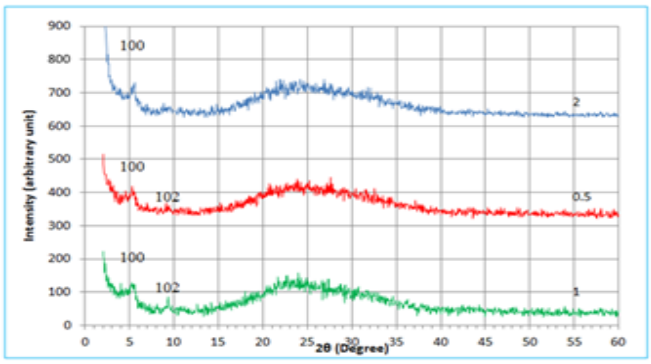

Fig 5. X-ray diffraction patterns of deposit NiPcTS:PEDOT:PSS blend thin films on glass substrates with different (PEDOT:PSS) concentrations.

Table 1. Structural parameters viz. inter-planar spacing and crystalline size of pure NiPcTs powder.

2θ(Deg.)	FWH(Deg.)	d_{hkl}Exp. Å)	G.S(nm)	d_{hkl} Std(Å)	phase	hkl
7.03	0.38	12.55	21.0	12.5	NiPc	(100)
9.14	0.66	9.66	12.1	9.79	NiPc	$(\bar{1}02)$
10.57	0.75	8.36	10.6	8.45	NiPc	(002)
18.05	0.58	4.91	13.9	4.91	NiPc	$(\bar{2}04)$
21.65	0.78	4.10	10.4	4.10	NiPc	(111)
26.81	0.67	3.32	12.2	3.39	NiPc	$(\bar{2}14)$

Table 2. structural parameters viz. inter-planar spacing and crystalline size of NiPcTs:PEDOT:PSS blend thin films.

Concentrations of PEDOT:PSS	2θ Deg.	FWHM Deg.	d_{hkl} Exp. Å	G.S nm	d_{hkl}Std. of NiPc Å	hkl
0.5	7.27	0.850	12.14	9.4	12.5	(100)
1	7.3	0.64	12.09	12.4	12.5	(100)
2	7.4	0.55	11.93	14.5	12.5	(100)

The morphology and roughness of the thin films were examined by atomic force microscopy in order to provide a large surface inspection of the micro-structural arrays, The observation of the surface morphology of the (NiPcTs:PEDOT:PSS) blend spin coated at room temperature at different (PEDOT:PSS) concentrations and treated thin films was determined by Atomic Force Microscopy (AFM) images as shown in Fig.(6)(7)(8). The AFM parameters such as average diameter ,average roughness and peak-peak for samples shown in table (3). It is found that the grains diameter increase with increasing PEDOT:PSS concentration, the smallest grains diameter indicated at conc.0.5,but the Roughness decreased. This result was supported by XRD measurements, which exhibited a smaller grain size. Scanning Electron Microscope (SEM) of the film prepared by Spin coating on glass substrate at annealing temperature 100ºC It is observed that the shapes of grain is fiber or nano fiber with increasing PEDOT:PSS concentration as shown in Fig. (9).

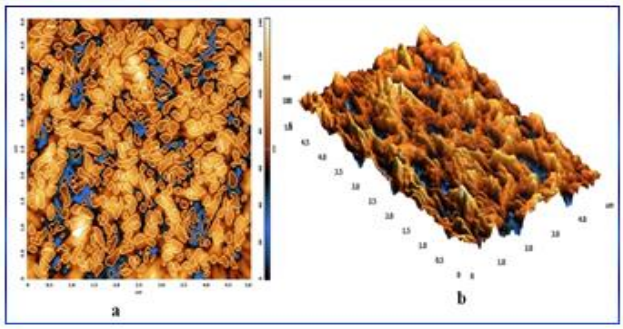

Fig 6. a&b is a 2D& 3D AFM images of(NiPcTs:PEDOT:PSS) blend thin films at PEDOT:PSS concentrations (0.5) .

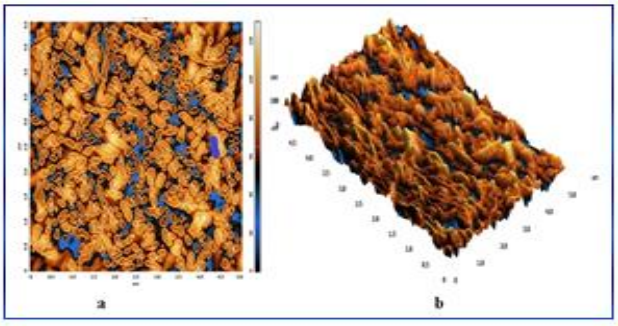

Fig 7. a&b is a 2D& 3D AFM images of(NiPcTs:PEDOT:PSS) blend thin films at PEDOT:PSS concentrations (1).

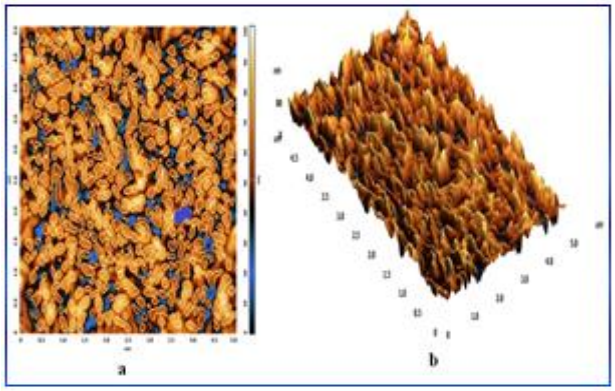

Fig 8. a&b is a 2D& 3D AFM images of(NiPcTs:PEDOT:PSS) blend thin films at PEDOT:PSS concentrations (2).

Table 3. Grain size, Roughness average and peak to peak (nm) of deposited (NiPcTs:PEDOT:PSS) blend thin films with different (PEDOT:PSS) concentrations.

PEDOT:PSS Concentration	Grain Size (nm)	Avg. Roughness (nm)	Peak-Peak (nm)
0.5	128	15.655	140.255
1	131	13.603	129.726
2	140	11.153	101.636

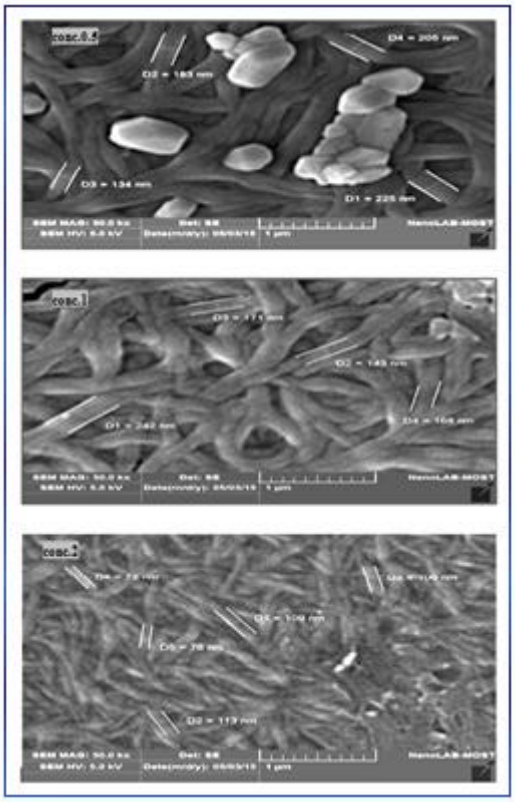

Fig 9. Scanning Electron Microscope (SEM) of (NiPcTs:PEDOT:PSS)lend thin films at different PEDOT:PSSconcentrations.

4. Conclusions

The XRD patterns show that the structure is polycrystalline and display a strong reflection at (100) orientation. Another peak distinguished in the XRD pattern of as-deposited which represents a reflection at (102) orientation, while this peak disappeared in concentration(2) FWHM decreased with increasing (PEDOT:PSS) concentrations while grain size increased . The AFM measurement observed that the grains diameter increase with increasing BEDOT:PSS concentration, the smallest grains diameter indicated at concentration (0.5),but the Roughness decreased.

This result was supported by XRD measurements, which exhibited a smaller grain size. The SEM measurement observed that the shapes of grain is fiber to nanofiber with increasing PEDOT:PSS concentration.

5. References

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