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تحسين الخصائص البصرية والتركيبية للمتراكب (UHMWPEO/ CuNPs/AgNPs) بواسطة جسيمات السيليكا النانوية

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ABSTRACT

<u>Background</u>: In this work, the optical and structural properties of an composite were studied, the optical properties were studied by the UV-Visible spectrophotometer technique, and the structural properties were studied by the X-ray diffraction technique.

<u>Materials and Methods</u>: Different amounts of silica nanoparticles (SiO₂ NPs) were loaded onto a composite consisting of ultra-high molecular weight polyethylene oxide (UHMWPEO), copper nanoparticles (Cu NPs), and silver nanoparticles (Ag NPs), and silica was added in different amounts (0.05, 0.07 and 0.09) wt%. This work was carried out using the traditional casting method.

<u>Results:</u> The results showed a good improvement in the optical and structural properties of the composite when it was loaded with silica nanoparticles.

<u>Conclusion</u>: In this study, we have successfully prepared and examined nanocomposite films with outside and inside SiO₂ with a thickness of (75-85) µm. The optical properties improve by decreasing the energy gap from (3.95) eV to (3.78) eV. As for the structural properties, where X-ray diffraction tests showed an increase in the crystalline size of the composite films, it was found that the crystalline size increased from (32.1) nm to (33.7) nm. Silica nanoparticles affect the growth of the crystalline structure of the composite.

Keywords: Casting method, Nanocomposite, Optical properties, UHMWPEO.



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INTRODUCTION

Creating materials with improved mechanical and physical qualities that are not present in each of its constituent pieces independently is the main goal of developing composite materials. Due to the urgent need for these unique and remote qualities in the original restrictions, their high potential for mutation and excellence in these properties has driven our world into a relentless race to construct these compositions[1,2].

The majority of polymers are relatively new to the creation of inexpensive goods with simple functionality. However, some industrially used materials have to be replaced with others because of the quick growth of technology. As a result, polymers have replaced iron and aluminum in a number of high-temperature and high-stress applications [3,4]. Polymer composites are unparalleled in their capacity to produce materials with properties such as high flexibility, low cost, and low temperature manufacture [5,6]. You can classify the polymers as either industrial or natural. Natural polymers include proteins, cellulose, starches, and rubber, for instance, poly(vinyl chloride), polypropylene, nylons, polyethylene, polyvinyl alcohol, polyacrylamide, polyesters, and polycarbonate are a few examples of synthetic polymers [7-8].

The diminutive word "nano" has gained a lot of popularity recently and has the power to upend society. Nanotechnology is one of the most significant areas of science today because it incorporates information from the disciplines of physics, chemistry, biology, medicine, informatics, and engineering. It is a new field of technology that has great potential to provide important discoveries with useful applications. Nanotechnology techniques and tools can be used to design and control new nano and biomaterials as well as nano devices [9,10].

The main objective of the current study is to examine the synergistic effects of silica nanoparticles on the optical properties of a composite consisting of UHMWPEO, Cu NPs, and Ag NPs. Remember that many electronic components need to be changed in order to handle various concerns with optoelectronic devices. Our globe has seen a surge in industrialization, particularly with regard to electronics. The objective of this study is to produce fresh movies that can be utilized for these functions.

MATERIALS AND METHODS

The polyethylene oxide (PEO) used had a molecular weight of 3x106 g/mol. It was highly pure (99.99%), and was available in a white granular form that was soluble in distilled water. Produced by a trading company, Central Drug Houses (CDH). The particle size (30 nm), specific surface area (15 m2/g), volume density (0.2 g/cm3), density (8.9 g/cm3), crystal shape (spherical), were the standards for copper nanoparticles used. In this experiment (brown). With an average particle size of 20 to 30 nm and high purity (99.95%), silver nanoparticles (Ag NPs) powder was produced by Sky Spring Nano Materials, lincoln national corp Lnc. A powder form of silica nanoparticles with a diameter of 20–30 nm, a purity of 99.8%, and a spherical shape were presented.

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The material preparation process was done by mixing the ingredients with a rotating device at room temperature (30 ± 5) °C for two hours until complete homogeneity. Using the casting method, the process was poured into a Petri dish with a diameter of 9 cm and the solution was left for 10 days to dry completely to obtain the appropriate films.

The addition process was carried out in stages because the concentrations of the base remained consistent while those of the (SiO_2) silica nanoparticles fluctuated over time. Below, in Table (1), are the pertinent concentrations.

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	Loadings		
PEO	Cu NPs	Ag NPs	SiO ₂ NPs
0.96	0.03	0.01	0.00
0.91	0.03	0.01	0.05
0.89	0.03	0.01	0.07
0.87	0.03	0.01	0.09

Table (1): Weight percentages for (PEO/Cu NPs/Ag NPS) composite and (SiO₂) NPs.

RESULTS AND DISCUSSION

The energy gap(E_g):

This equation is used to illustrate the energy gap and characterize transitions [11].

 $ahv = \mathbf{B} \left(hv - E_g\right) \tag{1}$

Where hv refers to photon energy, B constant and E_g the energy gap.

The creation of local levels in the forbidden energy gap is the reason why the energy gap values decrease as the weight percentage of nanoparticles increases [12]. In this case, the transition occurs in two stages, with the electron moving from the valence band to the local levels to the conduction band as a result of the increased weight percentage of nanoparticles. As demonstrated in figure (1) and table (2), the energy gap shrank with increasing nanoparticle concentration, which is consistent with previous study [13]. This is because the density of the spot state increased with increasing nanoparticle concentration.



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Table (2): Energy gab value of (PEO/Cu/Ag-SiO₂)

Sample	Direct Eg(eV)		
PEO/Cu/Ag	3.91		
PEO/Cu/Ag+0.05 SiO ₂	3.89		
PEO/Cu/Ag+0.07 SiO ₂	3.77		
PEO/Cu/Ag+0.09 SiO ₂	3.72		

Real and imaginary dielectric coefficient:

The dielectric constant expresses a polarization ability of the material , whose expression [14] is computed using the following equation:

$$\mathcal{E} = \mathcal{E}_1 - \mathbf{i}\mathcal{E}_2 \tag{2}$$

$$\mathcal{E} = \mathbf{N}^2 \tag{3}$$

$$(\mathbf{n} - \mathbf{i}\mathbf{k}_0)^2 = \mathbf{\xi}_1 - \mathbf{i}\mathbf{\xi}_2 \tag{4}$$

$$\mathcal{E} = (n^2 - k_0^2) - i(2nk_0)$$
 (5)

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The dielectric coefficient (ε) can be determined using the refractive index (n), join complex dielectric coefficient (ϵ) with complex refractive index (N).

Real and hypothetical complex dielectric coefficient can be stated as in the following equation from equations (6) and (7):

The relationship between the real and imaginary dielectric constants in nanocomposites (PEO/Cu/Ag-SiO₂) is shown in Figure (2). The figures demonstrate that when SiO₂ concentration grew, the r and I increased, the relationship between real and imaginary dielectric constants in nanocomposites (UHMWPEO/Cu/Ag-SiO²) is illustrated in Figure (2). The figures show that when the SiO2 concentration increased, new levels were formed by the nanoparticles.



Figure (2): The real part and imaginary part of (PEO/Cu/Ag-SiO₂).

X-ray Diffraction (XRD):

To find out the crystal structure of (PEO/Cu NPs/Ag NPs) film and their growth nature by Xray diffraction (XRD) study. Where the study was carried out in multiple stages before and after adding silica (SiO_2) to the matrix.

The X-ray diffraction patterns of the (PEO/Cu NPs/Ag NPs) superimposed film are shown in Figure (3), and it was found that the film of the superimposed has a semi crystalline nature and grows in a rhombohedra crystalline structure. It was observed that the main peaks appeared at 2Θ = $11.6^{\circ}, 18.5^{\circ}$ and 24.04° correlated to PEO polymer and belonged to (012),(110) and (021) respectively. The observed diffraction patterns are in good agreement with the standard PEO with code number (01-079-0988). The peaks appeared at $2\Theta = 38.07^{\circ}$ agreed with (Ag), and another peaks at $2\Theta = 43.22^{\circ}$ and 50.33° represent (Cu) and this corresponds with [15] (d values) سامعة بسابلل للعلوم الصدرفة والتطبيقية مجلبة جسامعة بسابل للعلوم الصدرفية والتظ

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calculated using Bragg's law equation (2-3) reveal that the absorbed d values are well matched to standard d values and are in good agreement with them, as shown in Table (3).



Fig. (3):X- ray diffraction pattern of (PEO/Cu NPs/Ag NPs) nanocomposite.

Grain Size	FWHM	(hkl)	20	Sample
nm	(degree)		degree	
42.8	0.197	021	11.60	PEO
26.0	0.389	110	18.50	PEO
29.9	0.352	012	24.04	PEO
21.3	0.393	111	38.07	Ag
43.4	0.196	111	43.22	Cu
29.7	0.295	200	50.33	Cu
Av=32.1				

Table (3):	Obtained	results fron	ı the	XRD for	· (PEO/Cu	ı NPs/Ag	(NPs) (composite.
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Figure (4) and table(4) shows the X-ray diffraction pattern of the (PEO/Cu NPs/Ag NPs) composite film doped in 0.05 wt.% silica (SiO₂). It was observed that the main peaks appeared at $2\Theta = 12.24^{\circ}$, 18.56° and 21.34° correlated to PEO polymer and belong to (110), (021) and (300). And the other peaks represent (Ag) by $2\Theta = 38.13^{\circ}$, and (Cu) by $2\Theta = 43.03^{\circ}$ and 50.44° respectively, and this is identical to (JCPDS Card No. 00 - 032 - 0346) for (PEO/Cu NPs/Ag NPs/SiO₂) [17]. Due to the amorphous stretcher of silica and the small amount of it in this

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composite, therefore the silica did not appear any peak in structure and all silica peaks were hidden. The results showed that the overlay is semi crystalline in nature and grows into a rhombohedra crystal linty.



Fig. (4):X- ray diffraction pattern of (PEO/Cu NPs/Ag NPs) composite with (0.05) wt.% SiO_2 $\ .$

Table (4): Obtained results from the XRD for	or (PEO/Cu NPs/Ag NPs)	composite with	(0.05) wt.%
	SiO ₂ .		

Sample	20	(hkl)	FWHM	Grain Size
	degree		(degree)	nm
PEO	12.24	110	0.483	16.8
PEO	18.56	021	0.239	34.8
PEO	21.34	300	0.189	44.7
Ag	38.13	111	0.393	40.4
Cu	43.03	111	0.243	36.3
Cu	50.44	200	0.300	29.2
				Av=33.7

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Figure(5) and table(5) show the X-ray diffraction pattern of (PEO/Cu NPs/AgNPs) composite film doped in 0.07 wt.% silica (SiO₂), mainly appeared for polymer $2\Theta = 12.26^{\circ}$, $2\Theta = 18.23^{\circ}$ and $(2\Theta = 24.05^{\circ})$, with miller indices (110), (021) and (300) respectively. And other peaks represent (Ag) $2\Theta = 36.13^{\circ}$ and (Cu) $2\Theta = 43.42^{\circ}$ and $2\Theta = 50.49^{\circ}$. These values were compared with cards (JCPDS Card No. 01 - 079- 0988) for (PEO/Cu NPs/Ag NPs/SiO₂) and reconciled for small differences. This may be due to the improvement and increase in granular size. The increase in grain size of the film (PEO/Cu NPs/Ag NPs/SiO₂). The results show that the superposition is semi crystalline in nature and grows into a rhombohedra crystal.[18,19]



Fig. (5):X- ray diffraction pattern of (PEO/Cu NPs/Ag NPs) composite with (0.07) wt.% SiO₂ .

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Sample	2 0 degree	(hkl)	FWHM (degree)	Grain Size nm		
PEO	12.26	110	0.590	13.7		
PEO	18.23	021	0.237	35.1		
PEO	24.05	012	0.152	56.4		
Ag	36.13	111	0.295	28.3		
Cu	43.42	111	0.225	43.4		
Cu	50.49	112	0.360	22.4		
				Av=33.2		

The crystal linty size was increased after loading which means that the silica was effectively growth in the matrix. There is no any new peaks append after adding the silica due to small amounts of it which was incorporated to the matrix but some matrix peaks were effected after adding and same peaks were decreased other hidden and broad.

Figure(6) and Table(6) show the X-ray diffraction pattern of the (PEO/ Cu NPs /Ag NPs) composite film doped in (0.09) wt.% silica (SiO₂),), mainly appeared for polymer $2\Theta = 12.24^{\circ}$, $2\Theta = 18.20^{\circ}$ and $2\Theta = 24.04^{\circ}$, with miller indices (110), (021) and (012) respectively. And other peaks represent (Ag) $2\Theta = 36.21^{\circ}$ and (Cu) $2\Theta = 43.03^{\circ}$ and $2\Theta = 50.36^{\circ}$. These values were compared with cards (JCPDS Card No. 00 - 032- 0346) for (PEO/Cu NPs/Ag NPs/SiO₂) and reconciled for small differences. This may be due to the improvement and increase in granule size. The increase in grain size of the film (PEO/Cu NPs/Ag NPs/SiO₂) indicates that the result is approximately close to [20].

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Figure (6):X- ray diffraction pattern of (PEO/Cu NPs/Ag NPs) composite with (0.09) wt.% SiO₂.

Table (6): Obtained results from the XRD for (PEO/Cu NPs/Ag NPs) composite with (0.09) wt.% SiO_2 .

Sample	20	(hkl)	FWHM	Grain Size
	degree		(degree)	nm
PEO	12.24	110	0.197	42.3
PEO	18.20	021	0.246	33.8
PEO	24.04	012	0.243	34.6
Ag	36.21	111	0.393	21.2
Cu	43.03	111	0.197	45.2
Cu	50.36	200	0.246	22.9
				Av=33.3

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CONCLUSION

In the study, we successfully prepared and investigated nano composite films with out and within SiO_2 in the thicknesses about (75-85) µm. The study indicates that the optical properties were studied by doping with silica nanoparticles (SiO₂). Doping is a process in which a small amount of one substance is added to another to modify its properties. According to the study, it was observed that most of the optical properties of the film increase with the increase in the percentage of doping with silica nanoparticles, except for the transmittance and energy gap, which decreases from (3.95) eV without silica to (3. 78) eV with a concentration of (0.09)wt% of SiO₂, this indicates that the presence of silica nanoparticles led to an improvement in the above-mentioned optical properties of the resulting films.

. X-ray diffraction assays showed an increase in grain size in the PEO/Cu/Ag composite films with the addition of silica nanoparticles, and this indicates that the nanoparticles affect the growth of the crystal structure of the composite. Overall, X-ray diffraction examination can provide valuable insights into the crystal structure of materials and how it may be affected by the addition of nanoparticles. The increase in particle size started from (32.1)nm without silica and increased with increasing SiO₂ weight ratios to (33.7)nm with a concentration of (0.05)wt% of SiO₂ observed in the PEO/Cu/Ag composite films with the addition of silica nanoparticles.

The outcomes films ,make these nanocomposites suitable for using in the optoelectronic devices, photo detectors, solar cells, UV-detectors and etc.

Conflict of interests.

There are non-conflicts of interest.

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الخلاصة

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<mark>الخلفية:</mark> في هذا العمل تمت دراسة الخواص البصرية والتركيبية للمتراكب حيث تمت دراسة الخواص البصرية بواسطة مطياف الاشعة المرئية والفوق البنفسجية ودراسة الخصائص التركيبية بواسطة حيود الأشعة السينية.

المواد والطرق: تم تحميل كميات مختلفة من جسيمات السيليكا النانوية (SiO₂ NPs) على متراكب يتكون من أكسيد البولي إيثيلين عالي الوزن الجزيئي (UHMWPEO) وجسيمات النحاس النانوية (Cu NPs) وجسيمات الفضة النانوية (Ag NPs)، وأضيف السيليكا بكميات وزنية مختلفة (0.00، 0.07و (0.09) تم تنفيذ هذا العمل بطريقة الصب التقليدية.

النتائج: أظهرت النتائج تحسنًا جيدًا في الخصائص البصرية والتركيبية للمتراكب عندما تم تحميله بجسيمات السيليكا النانوية.

الإستنتاج: في هذه الدراسة، نجحنا في تحضير وفحص أغشية المتراكب النانوي مع وبدون حسيمات السيليكا بسمك (75-88) ميكرومتر. تحسنت الخواص الضوئية بتقليل فجوة الطاقة من (3.95) الكترون فولت إلى (3.78) الكترون فولت. أما بالنسبة للخصائص التركيبية ، حيث أظهرت اختبارات حيود الأشعة السينية زيادة في الحجم البلوري للأغشية المركبة ، فقد وجد أن الحجم البلوري زاد من (32-1) نانومتر إلى (3.37) نانومتر . تؤثر جزيئات السيليكا النانوية على نمو التركيب البلوري للمكتب المركبة ، فقد وجد أن الحجم البلوري زاد من (32-88) التركيبية ، حيث أظهرت اختبارات حيود الأشعة السينية السابيكا النانوية على نمو التركيب البلوري للمركبة ، فقد وجد أن الحجم البلوري زاد من (32-1)

الكلمات المفتاحية: طريقة الصب, متراكب نانوي, خواص بصرية, بولي اثلين اوكسايد عالي الوزن الجزئي