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Ameliorating and Tuning the Microstructure and Optical Features of PMMA/PS/$SrTiO_3$ Solid State Nanocomposites For Flexible Optoelectronics Applications

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Poly-methylmethacrylate (PMMA)-polystyrene (PS) blend doped with strontium titanate ($SrTiO_3$) nanocomposites have been fabricated for optical and optoelectronics applications. The films (PMMA-PS/$SrTiO_3$) were produced using the casting process. The structure and optical features of PMMA-PS/$SrTiO_3$ nanostructures were examined, the structure characteristics of PMMA-PS/$SrTiO_3$ nanostructures included: FTIR and optical microscope. The optical characteristics were recorded at wavelengths (λ) ranging from 260 to 860 nm. The results revealed that when the $SrTiO_3$ NPs ratio reached 5 wt.%, absorbance (A) rose and transmission (T) decreased, making it suitable for a wide range of optical applications. When the $SrTiO_3$ NPs concentration reached 5 wt.%, the energy gap (E_g) of (PMMA-PS) reduced, making PMMA-PS/$SrTiO_3$ nanostructures important for optical and optoelectronics nanodevices. The optical constants(absorption coefficient, refractive index, extinction coefficient, real and imaginary dielectric constants, as well as optical conductivity)were rise with rising concentrations of $SrTiO_3$ NPs. The results revealed that the PMMA-PS/$SrTiO_3$films may be consideredas future nanocomposite to employ in numerous prospective optical and nanoelectronics applications.

Keywords: PMMA; optical constants; $SrTiO_3$; optoelectronics; PS; energy gap.

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Introduction

Polymer nanocomposites provide a viable alternative to traditional polymers and materials. Adding nanofillers to polymers can improve their thermal, mechanical, barrier, and flammable characteristics, making it a cost-effective and simple way to change their structure [1].Polymers and organic materials have gained popularity due to their unique properties. Develop lightweight, environmentally friendly, versatile, and cost-effective electrical gadgets. Polymer medium composites display distinct characters and include found ever-increasing applications [2,3]. Polymer nanocomposites are a new type of material that has nanoscale fillers with evenly distributed throughout the polymer matrix. Polymer nanocomposites not only improve mechanical qualities but also provide additional multifunctional properties (e.g., electrical and thermal) [4]. Nanomaterials have received a lot of interest from materials scientists, and their characteristics are determined not only by their composition, but also by their form and size distribution [5].Nanomaterials has been getting attention of concentrated research in recent years but still there is much scope of improvement as well as further investigations. Due to their outstanding mechanical and electrical properties [6]. Polystyrene (PS) has gained popularity due to its exceptional qualities, including high transparency, electrical insulation, high refractive index, and low water absorption.PS is a cost-effective commercial commodity plastic substance that is widely used in polymer production. Adding metal or semiconductor nanoparticles to PS increased its optical, magnetic, and mechanical capabilities. Metal nanoparticles have been shown to improve thermal conductivity and heat transfer in fluids. The use of noble metals in polystyrene for composite synthesis has potential applications in optoelectronics, catalysts, and chemical sensors [7]. Poly-methyl methacrylate, an electron donor, can be used to synthesize solid polymer substances. The ester group in the backbone chain resulted in an amorphous form. PMMA is a strong and transparent thermoplastic with a stable polar dimensional structure. Small organic molecules have smaller donor-acceptor surfaces with better crystallinity, preventing exciton dissociation and charge transfer. Polymer films with high molecular π-π stacking often have increased mobility for electric charge carriers [8]. PMMA has remarkable material qualities, including mechanical strength, hardness, stiffness, transparency, and insulation. PMMA is a high-impact, lightweight, and shatter-resistant organic optical material [9]. Perovskite-type oxides are exciting materials for condensed-matter research. Strontium titanate ($SrTiO_3$) is arguably the prototype member of this structural family, exhibiting a variety of unique features. This n-type semiconductor, with a band gap of approximately 3.2 eV, has been extensively studied for its exceptional physical properties (stability, wavelength response, and current-voltage), as well as its practical applications, including high static dielectric constant and good insulation [10].On the other hand, $SrTiO_3$ is a potential photocatalyst with excellent electrical and optical characteristics, thermal stability, photocorrosion resistance, and high catalytic efficiency [11]. This work aims to manufacture of PMMA/PS/$SrTiO_3$ nanostructures films to use in many optical and optoelectronics applications.

I. Experimental Part

Materials used in this study include poly-methylmethacrylate (PMMA), polystyrene (PS), and strontium titanate ($SrTiO_3$).The casting procedure was used to make the PMMA/PS blend and the $SrTiO_3$ doped PMMA/PS. The PMMA/PS blend film was created by dissolving 1 g of PMMA/PS blend with concentration in chloroform (30 ml) and mixing the polymer with a magnetic stirrer to obtain a more homogeneous solution.$SrTiO_3$ NPs were introduced to a PMMA/PS blend solution at ratios of 2.5% and 5% to form nanostructured films with varied concentrations of polymers (PMMA/PS) blend and ($SrTiO_3$) NPs. PMMA/PS/$SrTiO_3$ nanostructure films with a thickness of 100 μm were manufactured. Using an optical microscope, were studied the dispersion of $SrTiO_3$ NPs in the PMMA/PS blend. FTIR analysis for PMMA/PS/$SrTiO_3$ nanostructures films recorded by FTIR (Bruker company, type vertex -70) in wavenumber ranged 500 cm^{-1}-4000 cm^{-1}. The optical characteristics of PMMA/PS/$SrTiO_3$ nanostructured films were tested using a spectrophotometer (UV-18000A-Shimadzu) at wavelength range (260–860) nm. The absorption coefficient (α) is found by the equation [12,13]

$$\alpha = 2.303\ (A/l) \quad (1)$$

Wherever: A indicates absorbance and l signifies thickness. The extinction coefficient (k) is calculated using equation [14]:

$$k = \alpha\lambda/4\pi \quad (2)$$

λ denotes the wavelength of the incident photon. The refractive index (n) is defined by [15]:

$$n = \frac{1+\sqrt{R}}{1-\sqrt{R}} \quad (3)$$

Where R represents the reflectance. The die-electric constant portions for both real (ε_1) and imaginary (ε_2) are determined by [16]:

$$\mathcal{E}_1 = n^2 - k^2 \quad (4)$$

$$\mathcal{E}_2 = 2nk \quad (5)$$

The optical conductivity (σ_{op}) can be calculated as [17].

$$\sigma_{op}=\alpha nc / 4\pi \quad (6)$$

The energy gap is given by [18]:

$$\alpha h\upsilon=B(h\upsilon - E_g)^r \quad (7)$$

In this equation, B is the constant, hυ is photon energy, Eg is the energy gap, and r = 2 and 3 represent allowed and banned indirect transitions.

II. Results and Discussion

FTIR spectroscopy was performed on (PMMA-PS/$SrTiO_3$) nanocomposites. Figure (1) depicts the (FTIR) transmittance spectra of (PMMA-PS/$SrTiO_3$) nanocomposites with varying $SrTiO_3$ nanoparticle concentrations. The samples' FTIR spectra indicated interactions in nanocomposites.The peak at (2930.09, 2825.88) cm^{-1}i is allotted to C-H asymmetric stretching vibrations.The peak at roughly (1725.03) cm^{-1} caused by carbonyl stretch vibration C=O basically depicts PMMA interference.The peak at wave number (1419.65) cm^{-1} is caused by the polymer matrix's C-O groups.The bands at (1144.11) cm^{-1} is caused by the -CH2. The FTIR curves of $SrTiO_3$ complexes show distinct absorption peaks between (968.038 and 747.01) cm^{-1}, indicating the presence of $SrTiO_3$ nanoparticles. This Figure shows that the polymer blend has no interaction with the nanoparticle [19-23].

Figure 2 displays optical microscope pictures of (PMMA-PS/$SrTiO_3$) NCs collected at a magnification power of 10× for specimens with different $SrTiO_3$ nanoparticle concentrations. As the amount of Strontium titanate nanoparticles rises, a network develops in the main phase of the (PMMA-PS) mix following the addition of $SrTiO_3$NPs. This network has channels along which carriers will flow, leading in a change in material properties. [24-28].

Figure 3 depicts the absorbance of nanocomposites

($PMMA-PS/SrTiO_3$) as a function of incoming light wavelength. The nanocomposites have high absorbance for high photon energy. Adding $SrTiO_3$ to (PMMA-PS) blend increases absorbance intensity in the short wavelength region and shifts the absorption edge toward red wavelengths at all $SrTiO_3$ concentrations. Since ($SrTiO_3$) atoms absorb incoming light, the increase in absorbance with increasing filler concentration is comprehensible [29-35]. A little shift in the absorption edge toward the high-wavelength region indicates that the optical band gap has shrunk. This means that the samples are transparent, in addition to the absence of an absorption band in the visible region. [36]. PMMA-PS absorbance rose by approximately 28% when the $SrTiO_3$

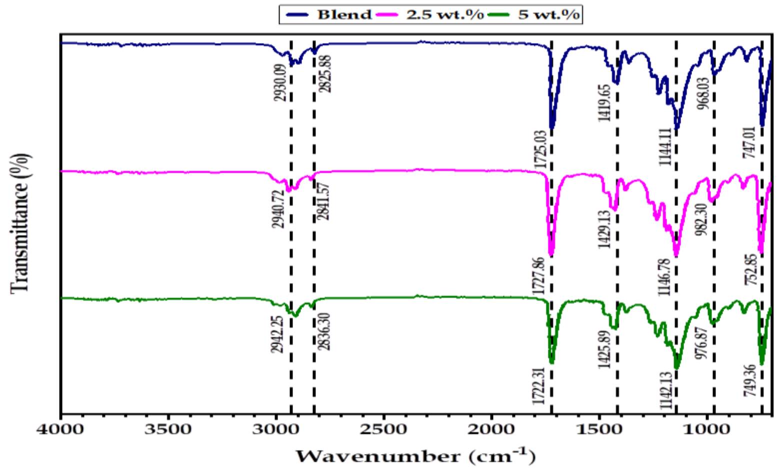

Fig. 1. FT-IR spectra ($PMMA-PS/SrTiO_3$) nanocomposites.

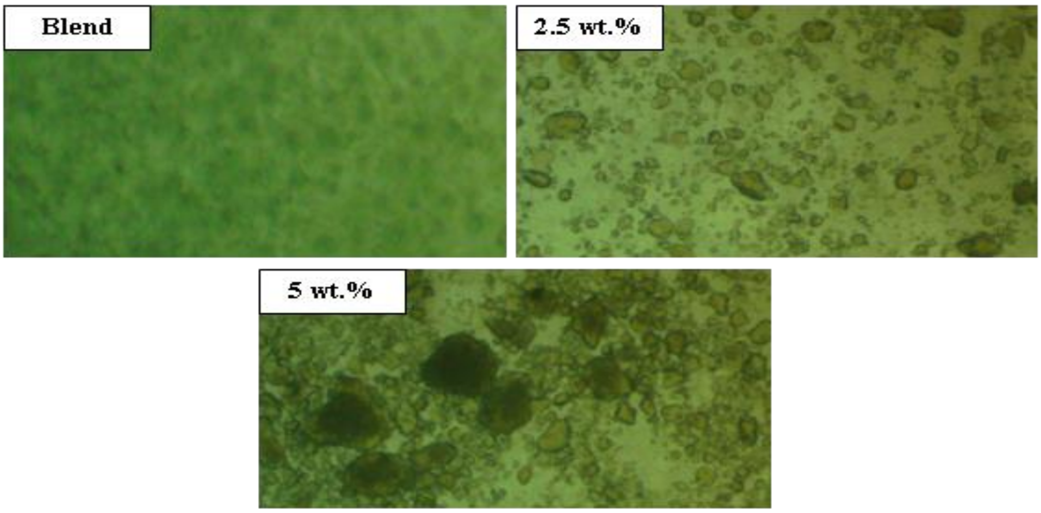

Fig. 2. Microscope images (X10) for ($PMMA-PS/SrTiO_3$) nanocomposites :
(A) for blend, (B) 2.5 wt.% $SrTiO_3$, (C) 5 wt.% $SrTiO_3$.

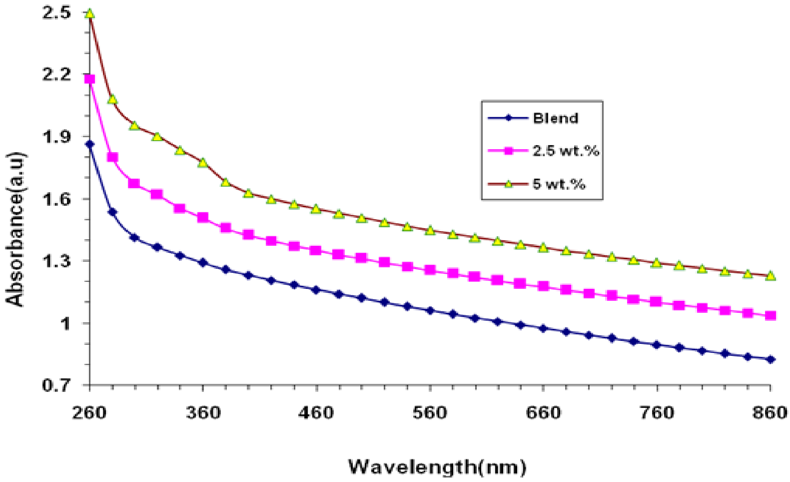

Fig. 3. Variation of absorbance for (PMM- PS/ $SrTiO_3$) nanocomposites with wavelength.

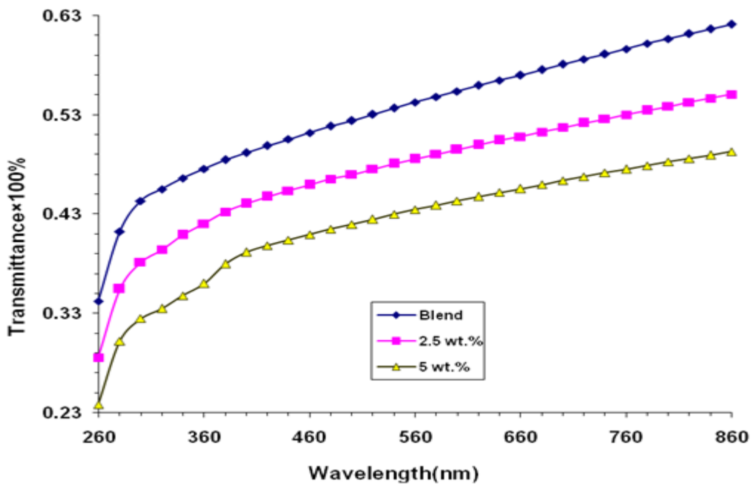

Fig. 4. Variation of transmittance for (PMMA-PS/$SrTiO_3$) nanocomposites with wavelength.

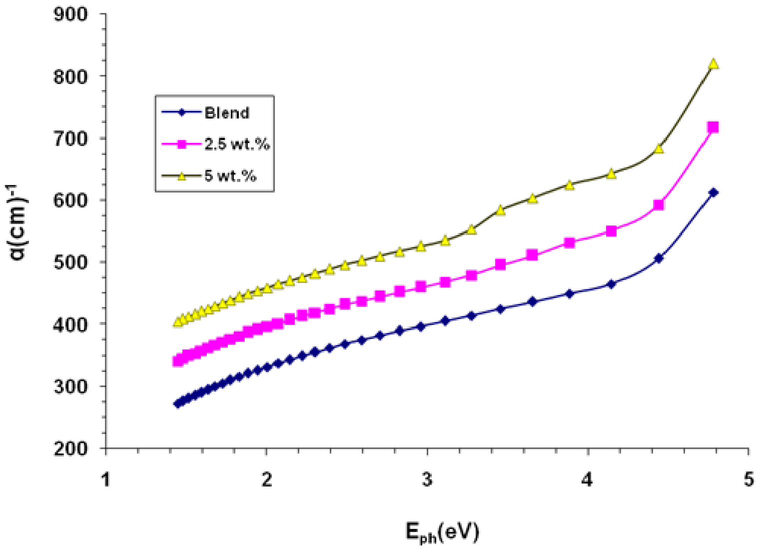

Fig. 5. Variation of absorbance coefficient (α) for (PMMA-PS/$SrTiO_3$) nanocomposites with photon energy.

concentration reached 5%.

Figure (4) depicts the transmittance spectra for (PMMA-PS/$SrTiO_3$) nanocomposites films with various Strontium titanate ($SrTiO_3$) NPs concentrations. Transmittance rises with wavelength and falls with concentration of Strontium titanate nanoparticles. Nanoparticles of strontium titanate absorb and scatter light from the PMMA-PS film. This occurs as a result of electrons in the outer orbits of the $SrTiO_3$ NPS absorbing electromagnetic energy from incident light and transitioning to higher energy levels. A portion of the incident light is absorbed by the substance and does not pass through it because the electrons that went to higher levels took up empty spaces in energy bands. [37-39].

Figure (5) depicts the variation in absorption coefficients with wavelength, which is consistent with the absorption measurements. At low energy, the absorption coefficient is lowest, suggesting that the photon's energy is inadequate to transfer an electron from the valence to the conduction band ($h\upsilon < Eg$). Absorption is stronger at higher energies, meaning that electrical changes are more frequent. As a result, the incoming photon has sufficient energy to transfer the electron from the valence band to the conduction band, thus crossing the forbidden energy gap. A high absorption coefficient ($\alpha > 10^4$ cm^{-1}) might indicate the kind of electron transmission. When the absorption coefficient is low ($\alpha < 10^4$ cm^{-1}), electrons travel indirectly while phonons maintain electronic momentum. As a result, the (PMMA-PS/$SrTiO_3$) nanocomposites exhibited an absorbance coefficient of less than 10^4 cm^{-1} at all concentrations. The absorption coefficient of nanocomposites increases as the concentration of Strontium titanate $SrTiO_3$ nanoparticles increases. This is ascribed to an increase in the number of charge carriers, resulting in an increase in absorbance and the absorption coefficient of the nanocomposite [40-42].

Figures (6) and (7) depict the energy gap values of (PMMA-PS/$SrTiO_3$) nanocomposites for permitted and prohibited indirect transitions. When r = 2, the optical energy gap of the allowed indirect transition is calculated; when r = 3, the optical energy gap of the forbidden indirect transition is found. As the concentration of Strontium titanate ($SrTiO_3$) nanoparticles rises, the optical energy gap values drop. This is responsible for the development of site levels in the forbidden optical energy gap. In this case, the transition occurs in two phases, with electrons traveling from the valence band to the local levels to the conduction band as the $SrTiO_3$ NPs loading rises [43-46]. Because nanocomposites are heterogeneous, an increase in $SrTiO_3$ nanoparticles produces electronic channels in the polymer, allowing electrons to pass from the valance band to the conduction band, explaining the decrease in optical energy gap. [47].

Figure (8) depicts the extinction coefficient of PMMA-PS/$SrTiO_3$ nanocomposites as a function of photon wavelength. The extinction coefficient relates to

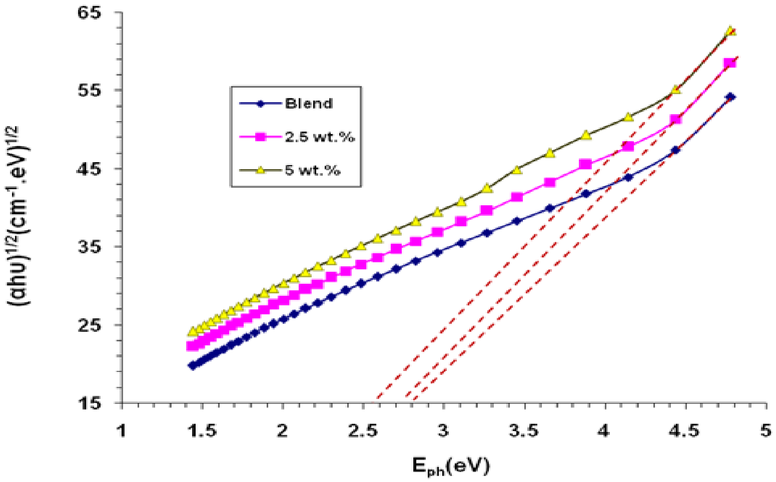

Fig. 6. Variation of $(\alpha h\nu)^{1/2}$ for (PMMA-PS/$SrTiO_3$) nanocomposites with Eph.

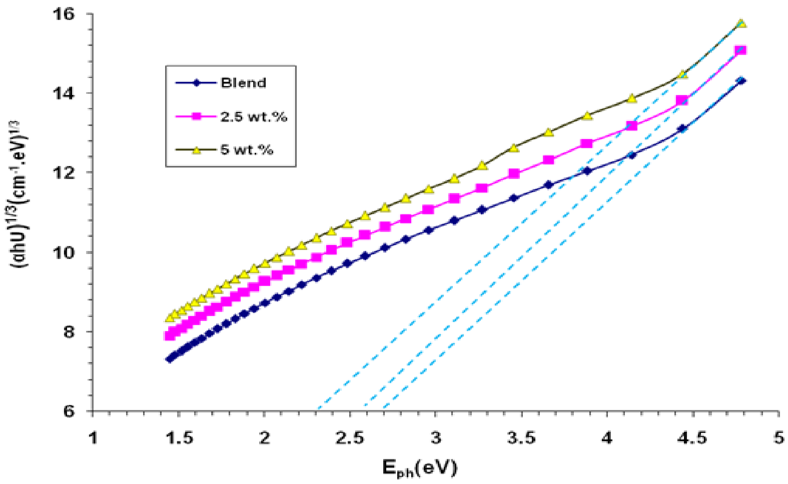

Fig. 7. Variation of $(\alpha h\upsilon)^{1/3}$ for (PMMA-PS/$SrTiO_3$) nanocomposites with Eph.

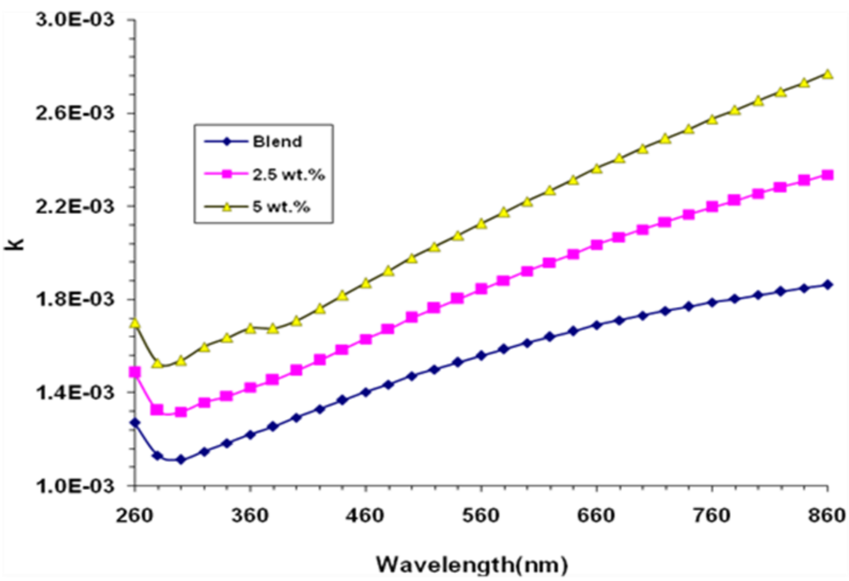

Fig. 8. Variation of extinction coefficient for (PMMA-PS/$SrTiO_3$) nanocomposites with wavelength.

When an electromagnetic wave passes through a material, the absorption loss, or the percentage of light lost due to scattering and absorption per unit distance of a penetration medium, is measured. As photon energy increases, the extinction coefficient decreases, suggesting an increase in the fraction of light lost due to scattering and absorption. Furthermore, the loss factor increases proportionally to photon energy. The photon was absorbed by the $SrTiO_3$ nanoparticles. [48,49]. Because of improved optical absorption and photon dispersion in the (PMMA-PS) polymer matrix, it was revealed that k has a lower value at low concentrations, owing to an increase in the absorption coefficient with larger doping percentages of added salt ions. Extinction coefficient is high at long wavelengths and big concentrations [50].

Figure (9) displays the change in refraction index with wavelength for (PMMA-PS/$SrTiO_3$). The refractive index of PMMA-PS/$SrTiO_3$nanocomposites decreases with increasing wavelength. The refractive index is mostly determined by reflectance. Increasing the concentration of $SrTiO_3$ leads to a rise in refractive index and reflectance, indicating an increase in density [51-53]. The refractive index is higher in the UV area due to poor transmittance, whereas it is lower in the visible and near IR regions due to high transmittance [54].

Figures (10) and (11) show the response of the real and imaginary components of the dielectric constant to wavelength for (PMMA-PS/$SrTiO_3$) nanocomposites. The concentration of Strontium titanate$SrTiO_3$ nanoparticles improves the real and imaginary components of the (PMMA-PS) blend's dielectric constant, as seen in the figures. The addition of $SrTiO_3$ NPs in the sample enhances electrical polarization, which raises the dielectric constant of the (PMMA-PS) mix and causes a fractional increase in charge within the polymers. The dielectric constant varies with wavelength. The refractive index impacts the real component of the dielectric constant [55]. The extinction coefficient influences the imaginary component of the dielectric constant, notably in visible and near-infrared wavelengths when the refractive index is largely constant and the extinction coefficient increases with wavelength [56].

Figure (12) depicts the correlation between optical conductivity and photon energy. Pure and doped samples behave differently. The optical conductivity increases at low photon energies and then decreases at higher photon energies; this behavior is comparable to the absorption coefficient, because the optical conductivity is reliant on the absorption coefficient [57]. Furthermore, the inclusion of Strontium titanatenanoparticles increased optical conductivity; this effect is attributed to the creation of localized levels in the energy gap, which caused an increase in $SrTiO_3$ NPS concentrations. The number of

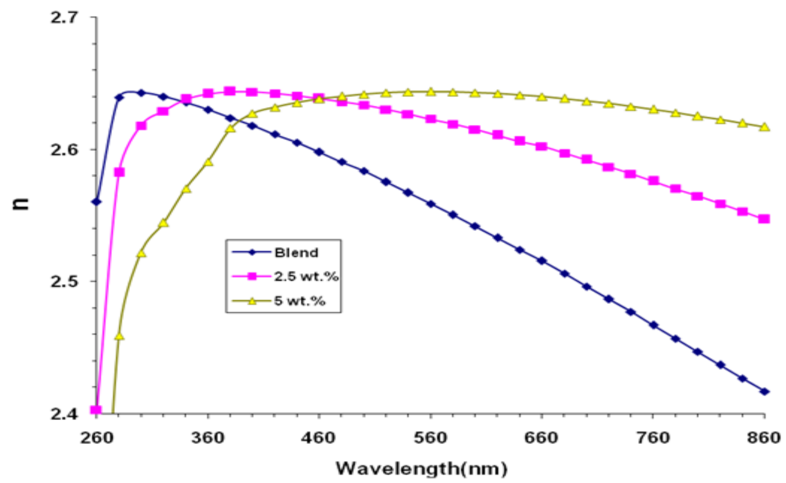

Fig.9. Variation of refractive index for (PMMA-PS/$SrTiO_3$) nanocomposites with wavelength.

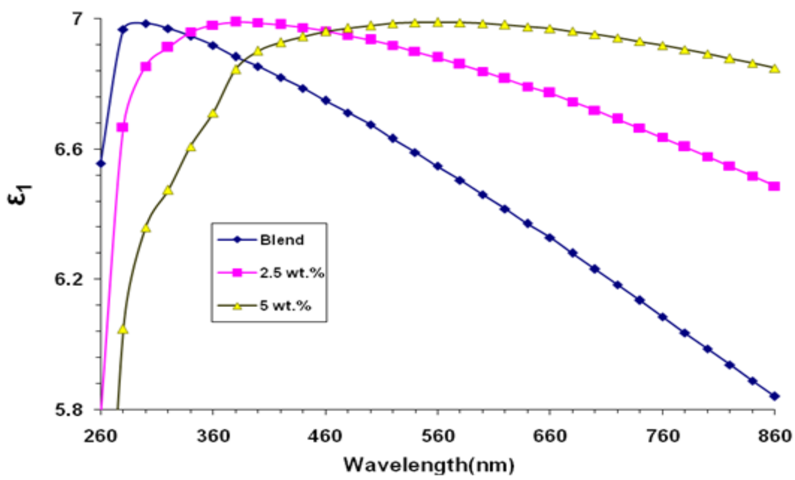

Fig. 10. Performance of real part of dielectric constant for (PMMA-PS/$SrTiO_3$) nanocomposites with wavelength.

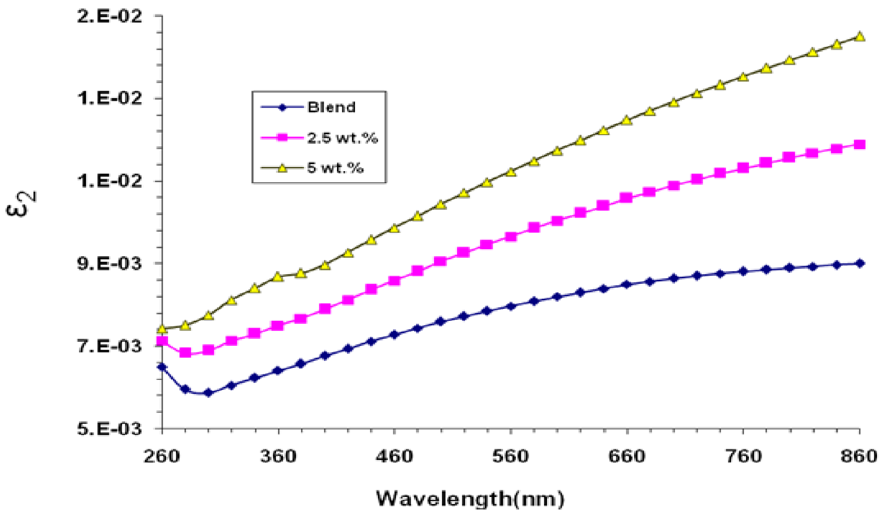

Fig. 11. Performance of imaginary part of dielectric constant for (PMMA-PS/$SrTiO_3$) nanocomposites with wavelength.

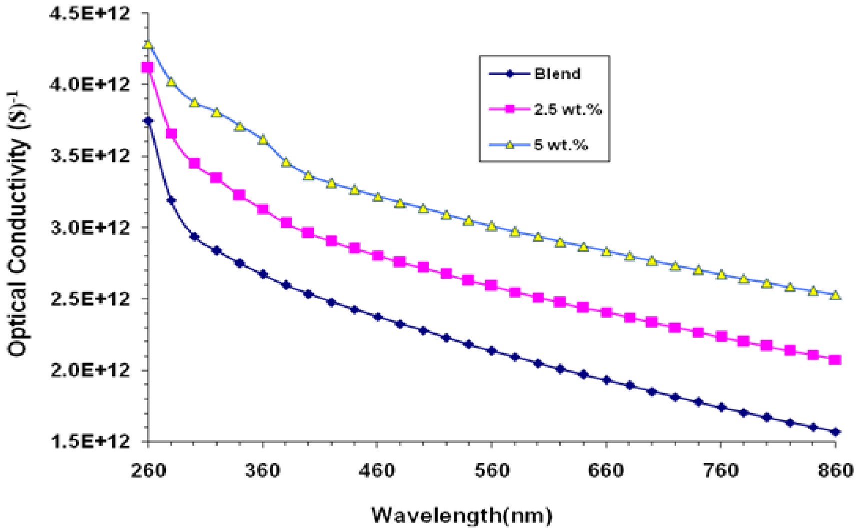

Fig. 12. Variation of optical conductivity for (PMMA-PS/$SrTiO_3$) nanocomposites with wavelength.

nanoparticles increases the density of localized states in the band structure [58].

Conclusion

This study contains the production of (PMMA-PS/$SrTiO_3$) nanostructures as potential nanomaterials for future applications in nanoelectronics and photonics domains such as photovoltaic cells, optical devices, sensors. The morphological and optical features of PMMA-PS/$SrTiO_3$ nanostructures were examined. The optical microscope pictures demonstrated a homogenous distribution of nanoparticles in the polymer mix and the emergence of network routes as the concentration of $SrTiO_3$ increased. The FTIR studies demonstrate vibration bands for the polymer blend before and after the addition of $SrTiO_3$ nanoparticles, suggesting the polymer blend (PMMA-PS) after addition may have produced chained networks of polymer nanocomposites, with their impacts in optical characteristics. The absorbance, absorption coefficient (α), extinction coefficient (k), refractive index (n), real and imaginary dielectric constants of (PMMAPS/$SrTiO_3$) nanocomposite increase with increasing the nanoparticles concentrations. The absorbance of PMMAPS increased about 28% when the $SrTiO_3$concentration reached 5%. The Transmittance and energy gap reduces with increasing concentration of the additive. The (PMMA-PS/$SrTiO_3$) nanocomposites show strong absorbance in the U.V region. These compounds can be employed in UV-shielding and optical applications. The results showed the $SrTiO_3$concentration of 5% have better optical properties to apply in many optoelectronics applications.

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Покращення і налаштування мікроструктури та оптичних властивостей твердотільних нанокомпозитів типу PMMA/PS/$SrTiO_3$ для оптоелектроніки

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На основі суміші поліметилметакрилату (PMMA) та полістиролу (PS) виготовлено нанокомпозити, леговані наночастинками стронцій титанату ($SrTiO_3$) для використання в оптичних та оптоелектронних пристроях. Структуру та оптичні характеристики наноструктур PMMA-PS/$SrTiO_3$ проаналізовано з використанням Фур'є-ІЧ спектроскопії (FTIR) та оптичної мікроскопії. Оптичні властивості реєструвалися в діапазоні довжин хвиль 260–860 нм. Результати показали, що при вмісті $SrTiO_3$ на рівні 5 мас.%, поглинання зростає, а пропускання зменшується, що робить матеріал придатним для широкого спектру оптичних застосувань. При цій концентрації також зменшується ширина забороненої зони (Eg), що робить наноструктури PMMA-PS/$SrTiO_3$ перспективними для оптичних та оптоелектронних нанопристроїв. Оптичні константи (коефіцієнт поглинання, показник заломлення, коефіцієнт екстинкції, дійсна та уявна частини діелектричної проникності, а також оптична провідність) покращувалися зі збільшенням концентрації наночастинок $SrTiO_3$. Отже, плівки PMMA-PS/$SrTiO_3$ можна розглядати як перспективні нанокомпозити для майбутніх оптичних та оптоелектронних пристроїв.

Ключові слова: PMMA; оптичні константи; $SrTiO_3$; оптоелектроніка; ширина забороненої зони.