World Journal of Advanced Research and Reviews
eISSN: 2581-9615 CODEN (USA): WJARAI
Cross Ref DOI: 10.30574/wjarr
Journal homepage: https://wjarr.com/

(RESEARCH ARTICLE)

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Exploration the effect of doping ($BaTiO_3$) on optical properties of Polymer (PVP)

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World Journal of Advanced Research and Reviews, 2023, 19(03), 954–963

Publication history: Received on 03 August 2023; revised on 11 September 2023; accepted on 13 September 2023

Article DOI: https://doi.org/10.30574/wjarr.2023.19.3.1845

Abstract

In this paper, composites of polyvinyl pyrrolidone (PVP) reinforced with different Barium Titanate ($BaTiO_3$) loadings (0, 2,4, and 6) wt. % were obtained via the solution casting method. The optical properties have been investigated. The increase in $BaTiO_3$ nanoparticles ratio in the PVP lead to increase in absorbance and decrease in transmittance. The (PVP/ $BaTiO_3$) nanocomposite exhibited a reduction in energy gap from 3.68 eV for pure PVP to 3.5 eV for allowed indirect transition and from 3.63 eV to 3.48 eV for forbidden indirect transition, upon the incorporation of ($BaTiO_3$) nanoparticles at a concentration of 6 wt.%. The weight percentages of $BaTiO_3$ nanoparticles exhibit a positive correlation with their absorbing factor, extinction factor, index of refraction, real and imaginary components of dielectric constants, and optical conductivity. The results confirm that (PVP/ $BaTiO_3$) films nanocomposites have excellent optical properties, which may encourage the application of these composites in different optoelectronic utilization.

Keyword: PVP: $BaTiO_3$ NPs: Optical properties: Optoelectronic devices

1. Introduction

The utilization of polymer nanocomposites has garnered significant interest in the academic community due to their exceptional efficacy and multifaceted attributes, which are achieved by incorporating a small quantity of nanoparticles within the polymeric matrix. The utilization of nano-scale fillers in polymer nanocomposites has been observed to result in notable property enhancement, even at lower loadings when compared to conventional polymer composites [1]. The host material and nano-filler chosen for nanocomposites affect their use and device efficacy [2]. The chemical and physical characteristics of inorganic nanoparticles (NPs) and their electrostatic interactions with polymeric chains affect molecular structure microstructure [3]. Nanocomposite materials can be regulated by changing the concentration of their constituent components in the polymeric matrix composition [4,5]. The composites substances have been broadly utilized in the a variety of fields such as sensors, aerospace, optical, electronics appliances..etc. However, these appliances fields ceaselessly command further characters and uses. Nanocomposites of organic& inorganic maters could possess advantages of together organic polymers and inorganic substances, thus have numerous appliances [6-10]. The compound Polyvinyl Pyrrolidone (PVP) was first utilized during World War II by German scientists as a substitute for blood plasma [11]. A water-soluble polymer is characterized by its notable capacity to form loose addition compounds with a diverse array of substances, rendering it a highly valuable property. Polyvinylpyrrolidone (PVP) is a hydrophilic and biocompatible material that has been utilized by the pharmaceutical industry. Moreover, it possesses notable potential in the field of wound healing [12]. From a commercial perspective, PVP possesses significant advantages in terms of its relative ease and low cost of utilization [13]. Barium Titanate (BaTiO3) is a viable material for the production of thin films. Barium titanate (BaTiO3) possesses noteworthy characteristics that have been utilized for six decades. It is chemically and mechanically highly stable, demonstrating ferroelectric properties above ambient temperature. BaTiO3 has a Curie temperature of 120°C [14], a high dielectric constant [10] of at least 1500 at room temperature, a low dielectric loss [11], and an exceptionally large band gap energy [15]. Barium titanate finds utility in

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various applications, including capacitors [16], high-density multilayer ceramic capacitors [17], Ferroelectric Random Access Memory (FRAM), Dynamic Random Access Memory (DRAM). Its piezoelectric properties make it suitable for microactuators and sensors, while its polarizability characteristics enable its use in Nonvolatile Ferroelectric Random Access Memories (NvFeRAMs) [18]. The utilization of BaTiO3 as a material for solar cells has been seen due to its characteristic energy gap of around ± 3 eV and a conductivity of 105 S/cm. This property of having a tiny band gap has been shown to boost the photovoltaic effect of ferroelectrics, as reported in reference [19]. The aim of this research is to examine the changes in the optical properties of a pristine polyvinylpyrrolidone (PVP) when various amounts of Barium Titanate (BaTiO3) are included.

2. Materials and Method

The pure polymer was dissolved of 1 g of polyvinyl pyrrolidone (PVP) polymer was in 50 mL of distilled water and using a magnetic stirrer for half an hour and temperature 50^{o}C after which it would completely dissolve and become a homogeneous mixture. The investigate of nanocomposite by adding of the $BaTiO_3$ NPs to solution (PVP) with content 2, 4 and 6 wt. %. Then it is casting method was used and left to dry for 72 hours. The optical characteristics of (PVP/$BaTiO_3$) nanocomposite were tested using spectrophotometer (UV-18000A-Shimadzu).

The absorption coefficient (α) is calculated by [20]

$$\alpha = 2.303\ (A/d) \qquad (1)$$

Where the A is the absorbance&d is the thickness of sample. The energy gap is given by[20]

$$(\alpha h\upsilon)^{1/m} = C(h\upsilon - Eg) \qquad (2)$$

wherever C is constant, hυ is the photon energy, Eg is the energy gap, m = 2 and 3 to allowed and forbidden indirect transitions.

The extinction coefficient (k) is determined by[21]

$$k = \alpha\lambda/4\pi \qquad (3)$$

wherever λ is the wavelength. The refractive index (n) is defined by [22]

$$n = (1+\sqrt{R}) / (1-\sqrt{R}) \qquad (4)$$

wherever R is the reflectance. The dielectric constant parts: real (ε_1), and imaginary (ε_2) are given by[23]:

$$\varepsilon_1 = n^2 - k^2 \qquad (5)$$

$$\varepsilon_2 = 2nk \qquad (6)$$

The optical conductivity (σ_{op}) is defined by[23]:

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

3. Result and discussion

Figure 1 illustrates the absorption properties of both pure polyvinylpyrrolidone (PVP) and a nanocomposite consisting of PVP and barium titanate nanoparticles ($BaTiO_3$) at different weight percentages (2, 4, and 6 wt.%). The measurements were conducted within the wavelength range of 300-1100 nm. The data shown in this figure demonstrates that all of the samples display increased absorption values within the ultraviolet (UV) spectrum. The electrons originating from the donor were induced to undergo a transition from a state of lower energy to a state of higher energy. Moreover, the results revealed a noteworthy level of photon absorption by the specimens in the ultraviolet range. As a result, the photons exhibited sufficient energy to stimulate the excitation of atoms, specifically when the wavelength was 300 nm. The analysis includes a chart that illustrates the influence of BaTiO3 nanoparticles and load ratio on absorbance. In this study, it was observed that the absorbance of the system exhibited a direct correlation with the PVP/$BaTiO_3$ NPs ratio as the load ratio was varied from 2 wt.% to 6 wt.%. Additionally, a negative relationship between absorbance and wavelength was observed. The observed rise in absorbance could perhaps be attributed to an increase in the density of charged carriers. The observed phenomena may be explained by the limited ability of collapsed photons to participate in atomic interactions, perhaps due to their low energy levels and the propagation of photons at longer wavelengths [24-28].

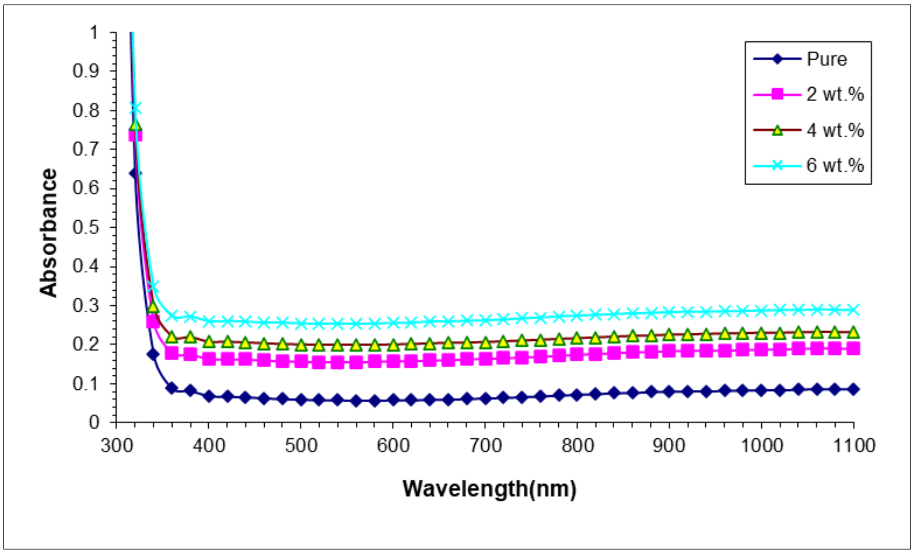

Figure 1 Absorbance spectra of PVP/ $BaTiO_3$nanocomposites

The figure (2) displays the transmission characteristics of the PVP/$BaTiO_3$ nanocomposite with varying ratios of $BaTiO_3$ loading. The transmittance of the material depicted in the figure decreases as the ratio of $BaTiO_3$ increases. This can be attributed to the agglomeration of nanoparticles, which results in an increase in surface roughness. Consequently, there is an increase in the scattering of light due to the enhanced surface fragmentation. However, the transmittance experiences a significant decline as the weight percentage of $BaTiO_3$ further increases. This characteristic, which was induced by the absorption and despite the potential financial implications, the nanocomposite films exhibit reduced transmission of UV wavelengths, rendering them viable for application in the field of pharmaceutical packaging. [29].

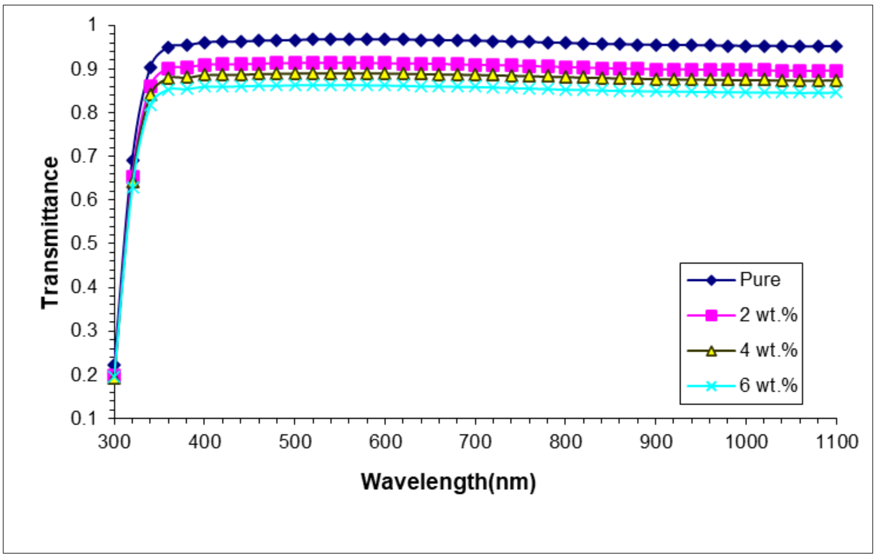

Figure 2 Transmittance spectra of PVP/ $BaTiO_3$nanocomposites

Figure 3 illustrates the absorbance coefficient of pure polyvinylpyrrolidone (PVP) and a nanocomposite of PVP and barium titanate ($BaTiO_3$) with varying ratios of $BaTiO_3$ loading. According to the data presented in the figure, it can be observed that the absorption coefficient for all samples exhibits an increase in ratios with an increase in NPs. This suggests that there is an augmentation in the carrier of charge within the nanocomposites. The absorption coefficients of all prepared samples exhibit low values at low energies, indicating a limited likelihood of electron transfer. However, these coefficients increase as the incident photon's energy rises, indicating a higher probability of electron transfer. This implies that the incident photons possess sufficient energy to interact effectively with the atoms. The observed α values of the produced films, which are below 104 cm^{-1}, suggest a high probability of indirect electronic transitions occurring. These results are in agreement with. [30].

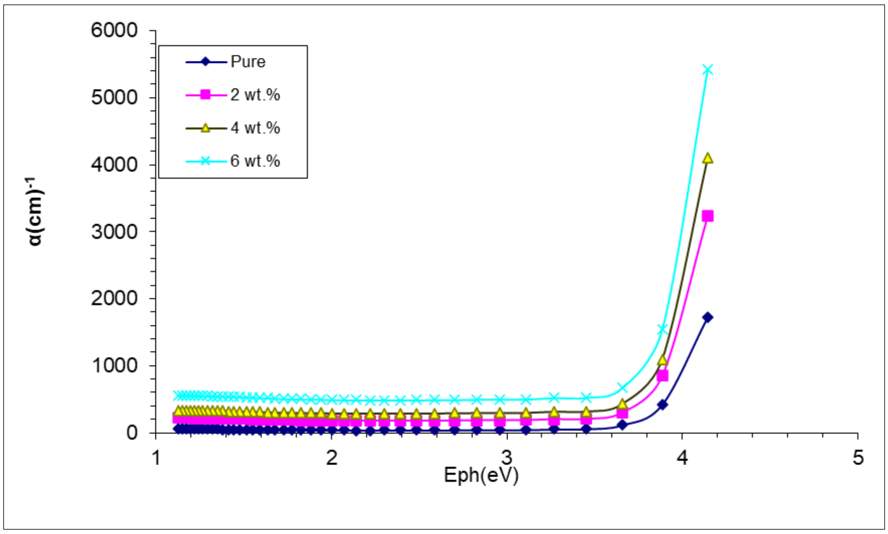

Figure 3 Absorption coefficient of PVP/ $BaTiO_3$ nanocomposites

Figures 4 and 5 illustrate the indirect band gap of both pure PVP and PVP/ $BaTiO_3$nanocomposite. Utilizing the intercept of the extrapolated linear segment. A linear segment was constructed from the upper region of the depicted curve in figures (4 and 5) for the purpose of analyzing the energy differential. The figure illustrates a notable decrease in the energy gap as the concentration of NPs increases, as evidenced by the data presented in Table 1. The permitted band gap of PVP/ $BaTiO_3$nanocomposites has been observed to decrease from 3.68 eV in PVP polymers to 3.5 eV. The observed forbidden band gap underwent a decrease in magnitude, shifting from 3.63 eV for PVP to 3.48 eV for the PVP/ $BaTiO_3$ nanocomposites, due to the manipulation of the polymer ratio and an increase in load ratio from 0 to 6 wt.%. The observed phenomenon can be attributed to the variations in localized levels of the parity and delivery packages. In this specific scenario, the electron experiences a transition from the parity state to the positional states, subsequently advancing towards the two stages. The positioning of connectivity package levels is congruent with findings from other scholarly investigations [31,32].

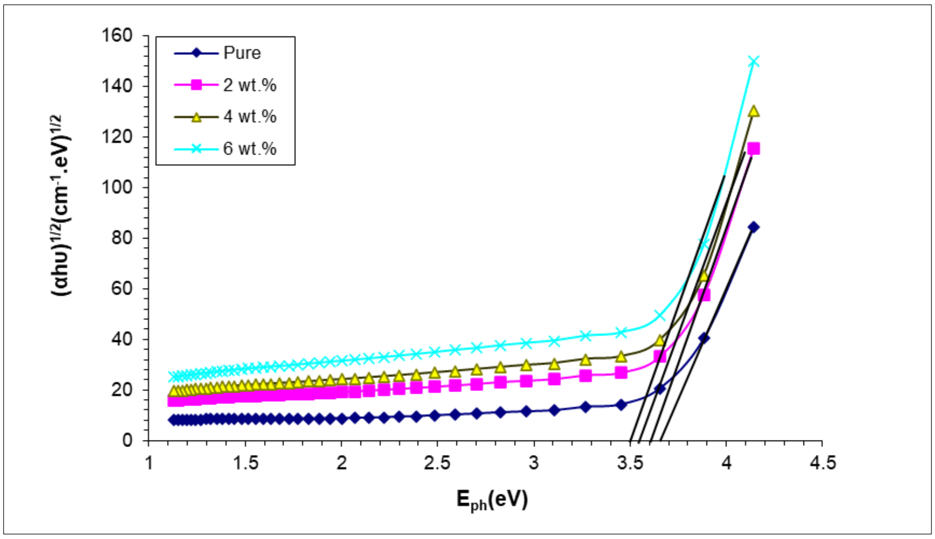

Figure 4 Relation between $(\alpha h\nu)^{1/2}$ versus $(h\nu)$ for pure PVP and PVP/ $BaTiO_3$nanocomposites

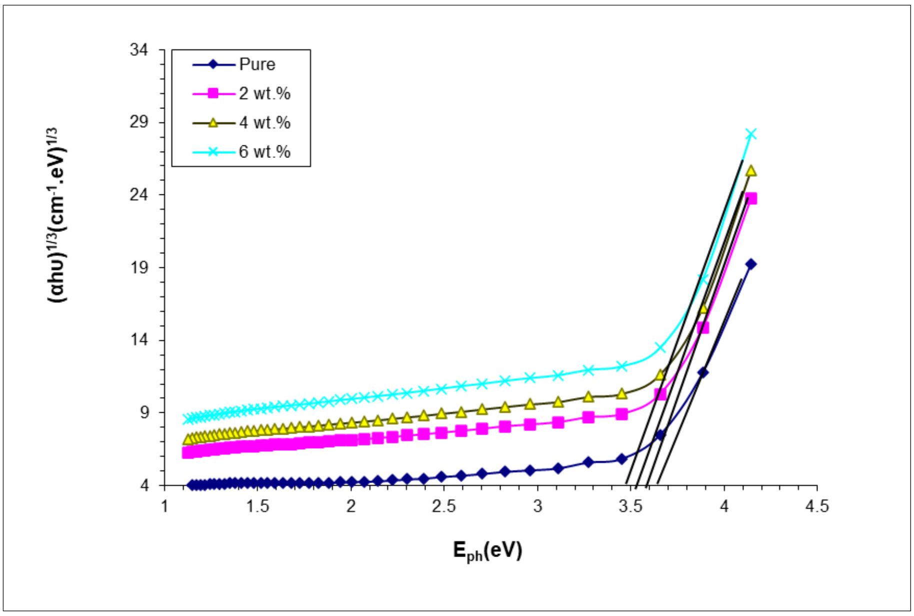

Figure 5 Relation between $(\alpha h\nu)^{1/3}$ versus $(h\nu)$ for pure PVP and PVP/ $BaTiO_3$nanocomposites

Table 1 Values of the energy gap for the permitted and prohibited indirect transition of PVP/ $BaTiO_3$nanocomposites

$BaTiO_3$ NPs wt% content	**E_g allowed indirect (eV)**	**E_g forbidden indirect (eV)**
0	3.68	3.63
2	3.6	3.58
4	3.55	3.53
6	3.5	3.48

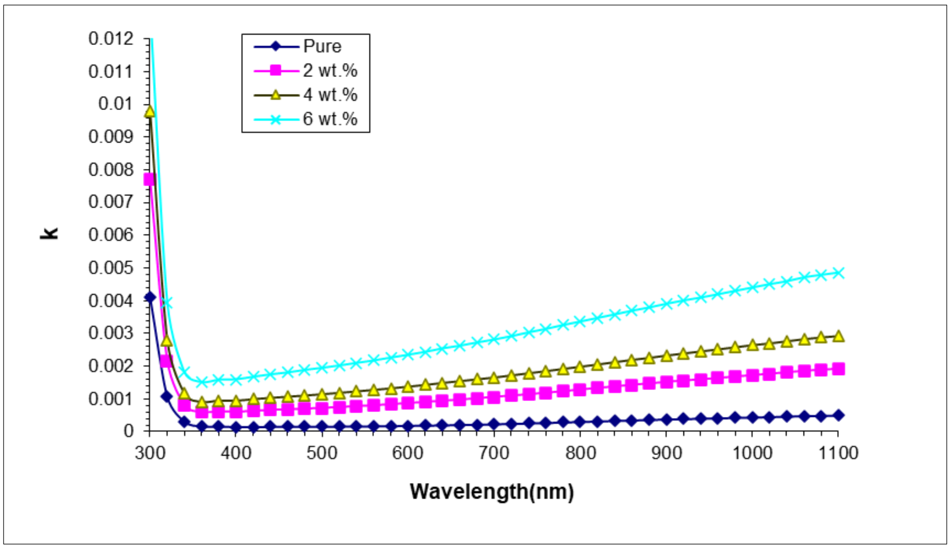

Figure 6 Extinction coefficient ofPVP/ $BaTiO_3$nanocomposites

Figure 6 illustrates the extinction coefficient (k) of PVP/$BaTiO_3$ nanocomposites. According to the data presented in Figure 6, it can be observed that the extinction coefficient of PVP/$BaTiO_3$ nanocomposites exhibits an increasing trend as the wavelength increases. This behavior can be due to the corresponding increase in photon energy. The relationship between the concentration ratio of $BaTiO_3$ nanoparticles and the extinction coefficient of nanocomposites is clearly observable. This phenomenon can be attributed to an augmentation in the absorption of incident light [33].

Figure 7 depicts the index of refraction (n) of PVP/$BaTiO_3$ nanocomposites. According to Figure 7, the index of refraction for PVP/BaTiO3 nanocomposites exhibits a notable peak at lower energies (namely, 300 nm), followed by a reduction at higher energies. In the visible and near-infrared (NIR) range, the index of refraction remains constant. Additionally, it has been observed that the refractive index increases when the concentration ratio of $BaTiO_3$ nanoparticles (NPs) grows. This phenomenon might be attributed to the corresponding increase in nanocomposite density [34].

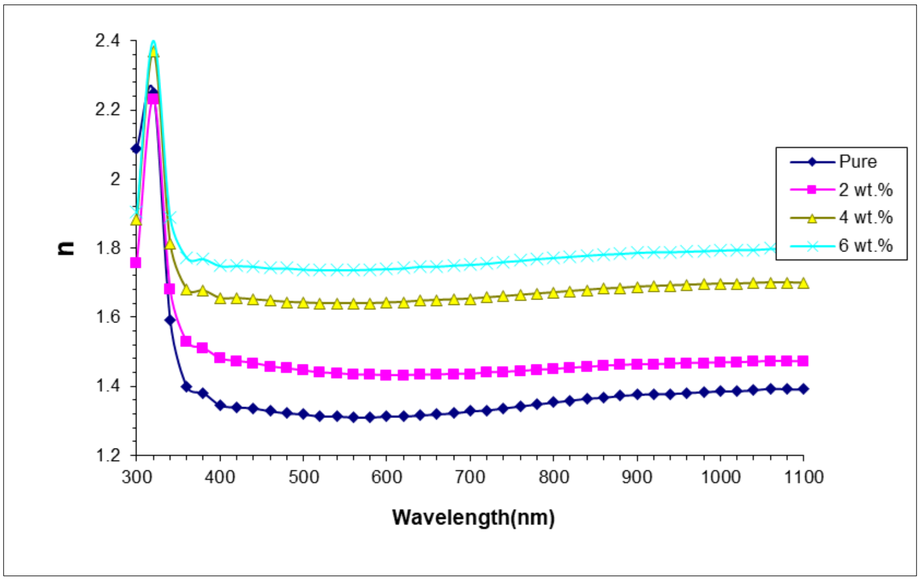

Figure 7 Refractive index of PVP/ $BaTiO_3$nanocomposites

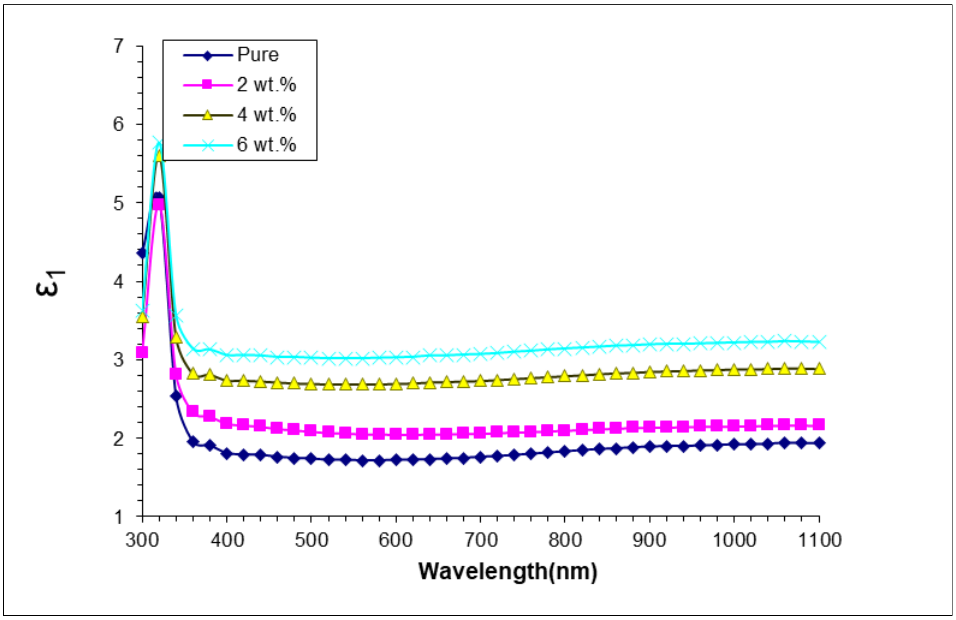

Figure 8 Real dielectric constant of PVP/ $BaTiO_3$nanocomposites

Figures 8 and 9 depict the fluctuations seen in the real component (Ɛ1) and imaginary component (Ɛ2) of the dielectric constant for both pure polyvinylpyrrolidone (PVP) and a nanocomposite of PVP and barium titanate ($BaTiO_3$), with varying ratios of $BaTiO_3$ nanoparticles (NPs). The provided figures indicate that the dielectric constant of pure PVP polymer has elevated values for both the real and imaginary components at shorter wavelengths, then diminishing as the wavelength increases. There is a discernible increase in both real and imaginary values observed at low frequency wavelengths, which is then followed by a notable drop in higher energy across all nanocomposite films. The observed resemblance can be elucidated by the reliance of the real dielectric constant on the magnitudes of (n) to a larger extent compared to the magnitude of (k), given that the latter magnitudes are considerably less than the refractive index, particularly when squared. [35,36].

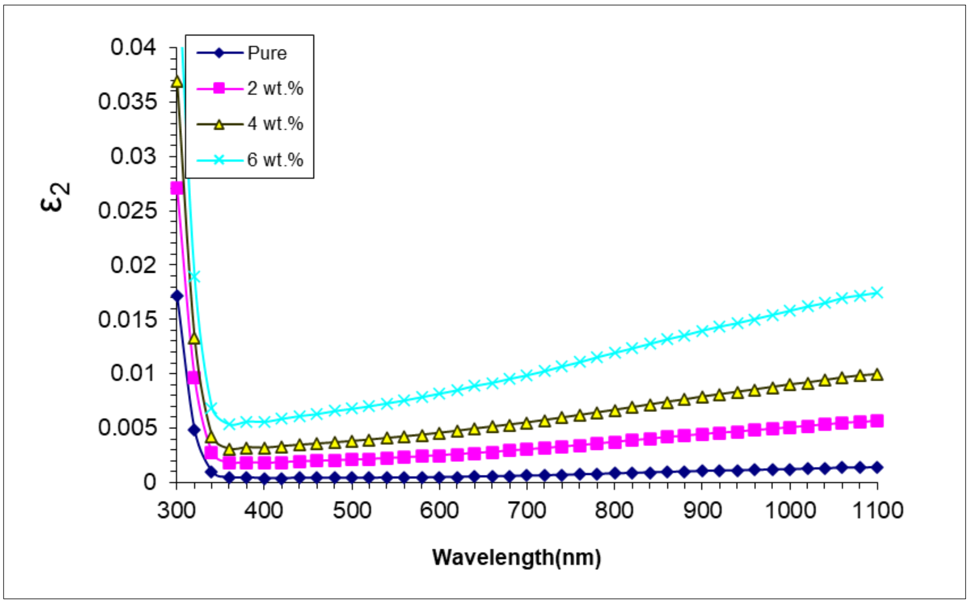

Figure 9 Imaginary dielectric constant of PVP/ $BaTiO_3$nanocomposites

Figure 10 displays the optical conductivity of both pure PVP polymer and the PVP/$BaTiO_3$ nanocomposite, with varying ratios of $BaTiO_3$ NPs. The optical conductivity of pure PVP polymer has a high value at shorter wavelengths, followed by a reduction at longer wavelengths. This behavior can be explained to the concurrent increase in the absorption coefficient. The relationship between the concentration of $BaTiO_3$ nanoparticles and the observed optical conductivity is found to be directly proportional. The observed phenomena can be ascribed to the rise in the absorption coefficient. [37].

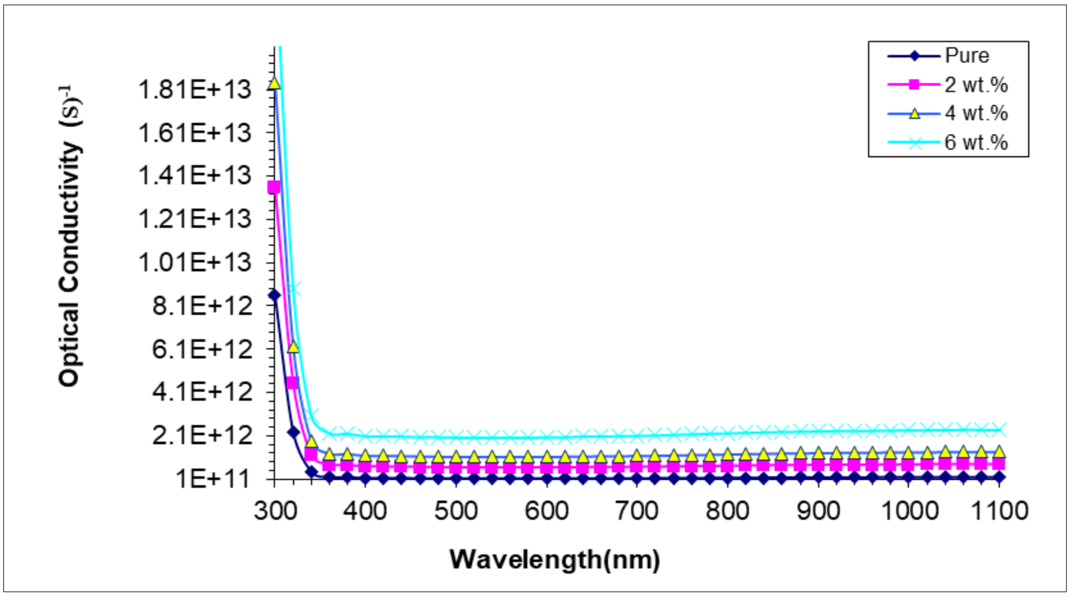

Figure 10 Optical conductivity of PVP/ $BaTiO_3$nanocomposites

4. Conclusion

The present research provides an overview of a successful casting methodology employed in the fabrication of PVP/ $BaTiO_3$nanocomposites. The findings suggest a positive correlation between the concentration of ($BaTiO_3$) NPs and the absorbance of (PVP/ $BaTiO_3$) nanocomposite, which is accompanied by a reduction in transmittance. The incorporation of ($BaTiO_3$) NPs at a concentration of 6 wt.% in the (PVP/ $BaTiO_3$) nanocomposites resulted in a reduction of their energy gap. Specifically, the energy gap decreased from 3.68 eV, as observed in pure PVP, to 3.5 eV for allowed indirect transition and from 3.63 eV to 3.48 eV for forbidden indirect transition. There exists a direct relationship between the weight percentages of $BaTiO_3$NPs and various optical properties such as absorption coefficient, extinction coefficient, refractive index, real and imaginary components of dielectric constants, and optical conductivity. Enhancements in the optical properties of (PVP/ $BaTiO_3$) nanocomposite samples can lead to the optimization of diverse optical parameters, including filters, switches, and optical coatings. The feasibility of incorporating nanocomposites with a low concentration of $BaTiO_3$NPs in optoelectronic applications is attributed to the enhancement of their optical properties.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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