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Influence of Bi_2O_3 Nanofiller on the Optical Behavior of PVP-Based Nanocomposites

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Abstract

In this study, nanocomposite films based on polyvinylpyrrolidone (PVP) reinforced with bismuth oxide (Bi_2O_3) nanoparticles were successfully fabricated using the solution casting method, with filler loadings of 1.7, 3.4, and 5.1 wt.%. The optical properties of the prepared films were systematically examined. The results indicate that increasing the concentration of Bi_2O_3 nanoparticles leads to a significant increase in absorbance, attended by a corresponding decrease in optical transmittance. Furthermore, the combination of Bi_2O_3 nanoparticles significantly influences the optical band gap of the nanocomposite films. The energy gap was found to decrease from 4.8 eV for pure PVP to 3.65 eV for allowable indirect transitions, and from 4.58 eV to 3.0 eV for prohibited indirect transitions at a nanoparticle loading of 5.1 wt.%. This reduction in band gap is attributed to the formation of localized states within the polymer matrix due to nanoparticle inclusion.

In addition, an increase in Bi_2O_3 content resulted in enhanced optical parameters, including the absorption coefficient, extinction coefficient, refractive index, as well as the real and imaginary parts of the dielectric constant, and optical conductivity. These findings demonstrate that PVP/Bi_2O_3 nanocomposite films exhibit improved optical performance, highlighting their strong potential for use in advanced optical and nanoscale optoelectronic applications

Keyword: PVP, Bi_2O_3 NPs, Optical properties, Optoelectronic nanodevices

1- Introduction

Polymer nanocomposites as a novel class of advanced materials that can exhibit more functionality depending on the fraction level of the nanoscale fillers added into the polymer matrix have become an area of great interest within recent years. The addition of nanoparticles into polymers gives rise to considerable enhancement of optical, electrical and mechanical properties (in some cases at very low filler concentrations compared with composite materials) **[1].** Among many kinds of polymers, polyvinylpyrrolidone (PVP) has emerged as a new promising host material due to its superior physicochemical properties and broad range of applications.

polyvinylpyrrolidone (PVP), ubiquitous in the pharmaceutical and biomedical field, is a highly biocompatible and safe polymer that was initially developed as an artificial blood plasma substitute for World War II **[2].** It is a non-toxic and water soluble hydrophilic polymer which has the capacity to bind most organic and inorganic matter **[3].** This exceptional property is due to polar functional groups existing in the molecular structure of chitosan, which can interact with nanoparticles through hydrogen bond and electrostatic interaction **[4].** Therefore, the PVP has been extensively applied in drug formulations and for biomedicial such as drugs delivery system, wound stain **[5].**

Besides its biomedical relevance, PVP is of scientific interest as a material and shows several Centre de Nouveaux Matériaux, such as film-forming property chemical unerring and relative ease processing **[6].** Due to all above mentioned properties, it is an ideal matrix for the development of nanocomposites devoted to high tech applications. Since the structural and functional properties of materials can be largely altered by incorporating inorganic nanoparticles in a PVP **[7],** this allows the construction of new materials with desired properties,

Inorganic bismuth oxide (Bi_2O_3) is an important but little-developed material due to its unique electrical, optical and catalytic properties. It is present in many polymorphic formations with the a-phase being the most stable at ambient temperature [8]. Considering its unusually high refractive index, wide band gap and great dielectric property Bi_2O_3 has recently been proposed as a fantastic optoelectronic and electronic device [9]. Moreover, bismuths being high-Z materials are already known for their strong photon absorption that might be crucial in radiation-shielding and photonic applications similar to other metal oxides scale **[10].**

One important instance among those is the interaction of Bi_2O_3 nanoparticles with PVP matrix that plays a critical role in determining final properties of the nanocomposite. These interactions control the spatial distribution of nanoparticles, affect the composite microstructure and thus its optical and electrical properties **[11].** The concentration of Bio3 inside polymer matrix can be controlled to modify the properties of material according to applications **[12, 13].**

Accordingly, in the present study, the dependencies of optical and electrical properties of a certain concentration of Bi_2O_3 nanoparticles incorporated into PVP with a focus on its effect are studied. This work aims to investigate the opportunity that PVP/Bi_2O_3 nanocomposites offer for future advanced optoelectronic applications, where material performance can be engineered on a nanoscale.

2- **Materials and Method**

A polymer solution was prepared by dissolving 1 g of polyvinylpyrrolidone (PVP) in 50 mL of distilled water under continuous stirring using a magnetic stirrer at 70 °C for 30 minutes, until a clear and homogeneous solution was obtained. Subsequently, Bi_2O_3 nanoparticles were incorporated into the PVP solution at different weight fractions of 1.7, 3.4, and 5.1 wt.% to fabricate the nanocomposite films. The resulting mixtures were cast into plastic Petri dishes and allowed to dry at room temperature for 72 hours to obtain solid films.

The absorbance (A) is defined as the ratio of the intensity of absorbed light (I.) to the intensity of incident light (lo.), and it can be expressed using the following relation **[14]:**

$$A= Ia/lo \quad (1)$$

The transmittance (T) given by the relation **[14]**

$$T=10^{-A} \quad (2)$$

Where the A is the absorbance. The absorption coefficient (α) is calculated by [15]

$$\alpha= 2.303\ (A/d) \quad (3)$$

where d is the thickness of sample. The energy gap is given by **[15]**

$$(\alpha h\upsilon)^{1/m}= C(h\upsilon - Eg) \quad (4)$$

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

The extinction coefficient (k) is determined by **[15]**

$$k = \alpha\lambda/4\pi \quad (5)$$

The index of refraction (n) is definite by **[16]**

$$n = (1+\sqrt{R}) / (1-\sqrt{R}) \quad (6)$$

wherever R is the reflectance. The dielectric constant parts: real (ε_1), and imaginary (ε_2) are given by **[17]:**

$$\varepsilon_1= n^2 - k^2 \quad (7)$$

$$\varepsilon_2=2nk \quad (8)$$

The optical conductivity (σ_{op}) is definite by **[17]:**

$$\sigma_{op} = \alpha nc/4\pi \quad (9)$$

3. Result and discussion

The absorbance and transmittance spectra of the pure PVP blend and the PVP/Bi_2O_3 nanocomposites with different Bi_2O_3 nanoparticle concentrations (1.7, 3.4, and 5.1 wt.%) are presented in Figure 1 over the range of 200–1100 nm. All samples exhibit strong absorbance in the UV region, which is attributed to the excitation of electrons from lower to higher energy states under high-energy photon irradiation.

This is accompanied by a decrease in transmittance, thereby supporting the previously derived inverse correlation between absorbance and transmittance. There is a significant absorption peak at ~ 220 nm suggesting that the incident photons should have enough energy to stimulate the electronic properties of our material system. Thus, the distinctive UV absorbing properties quartered with transmission-linked low-stuff of such nanocomposites from an optoelectronics viewpoint divulge the above-discussed nanocomposite material options can also be useful for high energy radiation blocking or sensing-based applications similar/analogous to UV photodetectors and optical filtering devices.

Besides, the results demonstrate a specific Bi_2O_3 nanoparticle content dependence. When the loading ratio of HLA from 2 wt. % to 6 wt. The absorbance increased and transmittance decreased significantly at same concentration. This phenomenon can be easily attributed to both enhancement in photon-material interaction and additional localized state developed inside the polymer matrix associated with insertion of the nanoparticles. The IAs act as charge generation boosters to convert carrier lifetime from localized charge sources into spatially separated device performance benefits.

But, in the longer wavelength region absorbance is decreasing and transmittance increasing (figure (2)) due to the low photon energy which is no more enough to excite electrons effectively. The wavelength dependence of this optical behaviour enhances the attractiveness of PVP/Bi_2O_3 nanocomposites, for selective spectral applications. The complementary response of the UV absorbance and transmittance along with ability to easily modulate optical properties through nanoparticle loading validate their suitability for advanced optoelectronic applications. Our previous values were therefore consistent with our findings **[18, 19].**

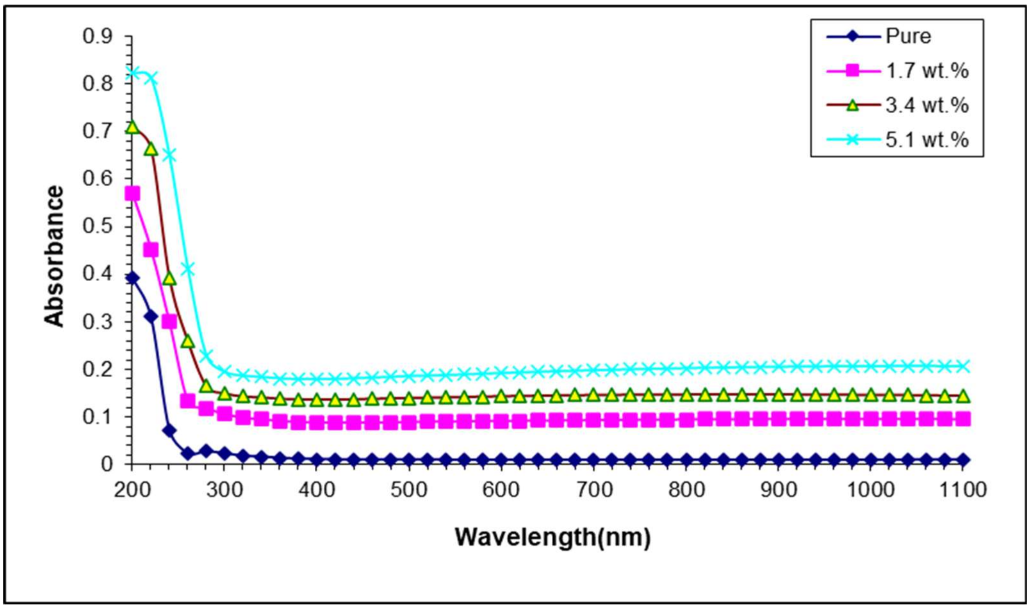

Figure (1) Absorbance spectra of PVP/Bi_2O_3 nanocomposites

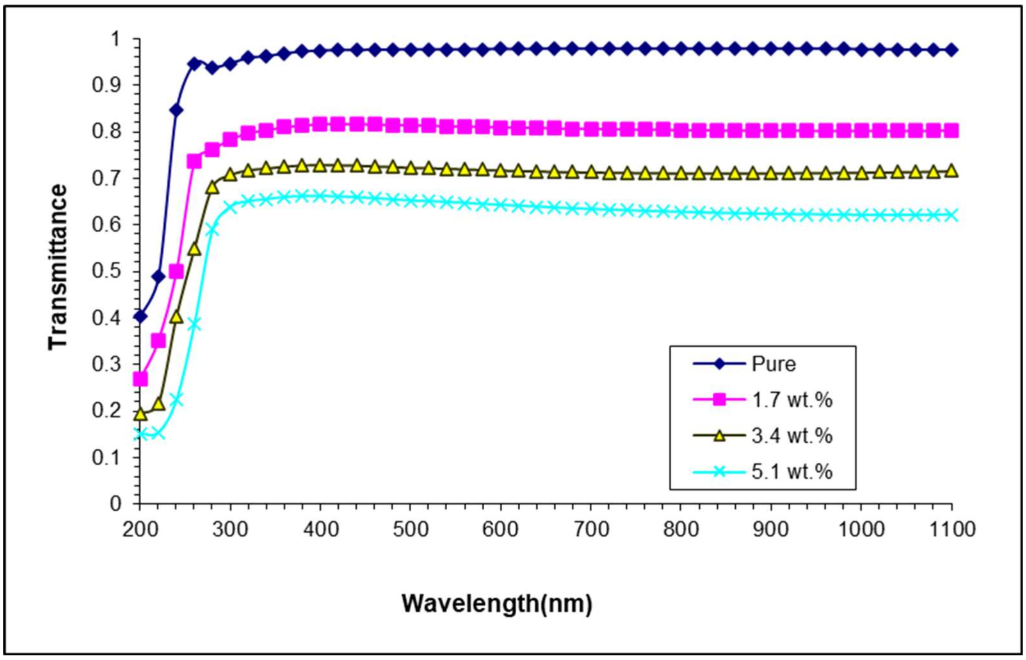

Figure (2) Transmittance spectra of PVP/Bi_2O_3 nanocomposites

In order to determine the absorption coefficient (a), Equation(3) was used. The changes of absorption coefficients for pure PVP and PVP/ Bi_2O_3 nanocomposite films at different Bi_2O_3 nanoparticle loadings are shown in figure (3). A progressive increase of absorption coefficient as Bi_2O_3 content increases is clearly observed. This can be ascribed to the increase in charge carrier density in nanocomposite owning to Bi_2O_3 nanoparticles.

At the lower photon energies, all samples have small absorption coefficient values due to a very low probability of electronic transitions, since there is not enough energy from the photon . However, the absorption coefficient increases greatly with increasing incident photon energy. With this in mind, we note that the probability of exciting an electron increases with increasing energy of the photon because the energy is sufficient to promote electrons to higher states within their material.

Moreover, the computed absorption coefficient data of all prepared films obtain less than 104 cm^1 due to indirect electronic transitions dominating in these nanocomposites. This behaviour is characteristic of polymer systems wherein phonon-assisted transitions dominate the optical absorption process. In general, this evidences the incorporation of Bi_2O3 nanoparticles is a successful way to modify the acutal optical response of PVP matrix and it becomes a promising candidate for optoelectronic applications. These results are in fair agreement with the previous reported studies **[19].**

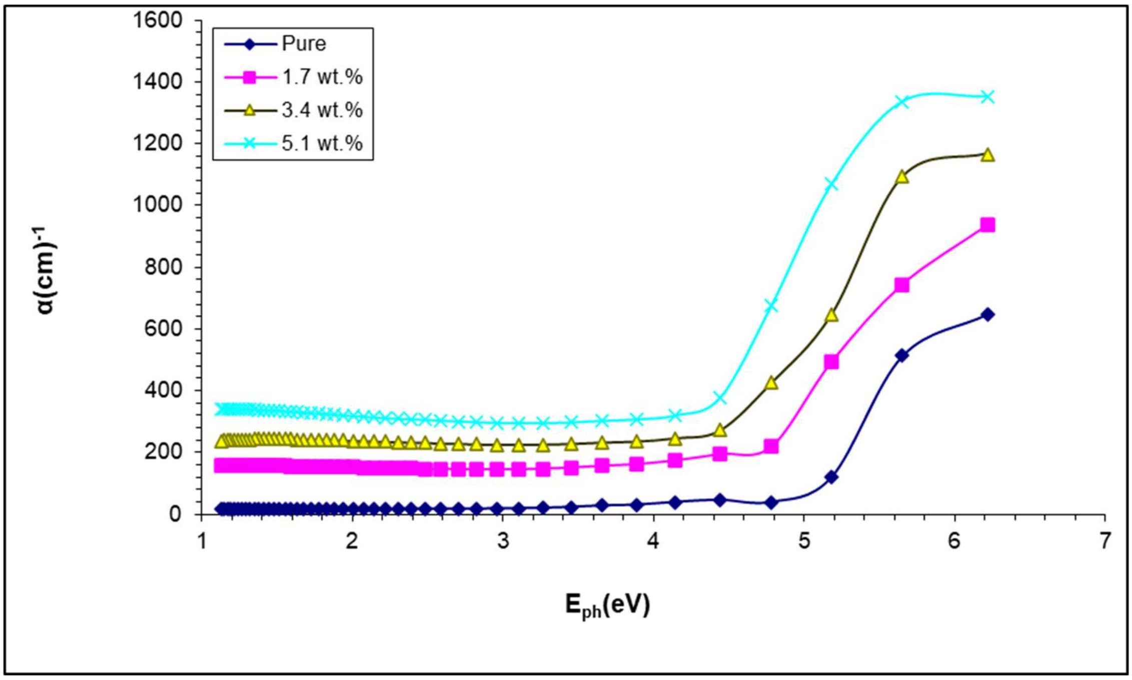

Figure (4) Absorption coefficient of PVP/Bi_2O_3 nanocomposites

The indirect optical band gap for allowed and forbidden transitions was calculated applying Equation (4). The variation of the indirect band gap for pure PVP and PVP/Bi_2O_3 nanocomposite films with varying concentrations of biomolecules into polymer matrix are given in Figs. 4 and 5, respectively. The band gap values were extracted by extrapolating the linear region of the plots in the high absorption regime to intercept with energy axis.

The findings established an unambiguous lowering of the optical band gap with increasing Bi_2O_3 nanoparticle loading that is highlighted in Table 1. In particular, the allowed indirect band gap varies from 4.8 eV of pure PVP to 3.65 at a Bi_2O_3 loading of 5.1 wt. % from 4.58 eV to 3.0 eV with the increase of nanoparticle concentration in indirect band gap. The band gap was reduced because localized energy states are generated in the polymer matrix alongside the interaction between PVP chains with Bi_2O_3 nanoparticles.

These localized states act as intermediate energy levels, facilitating electron transitions at relatively low photon energies which lead to effective reduction of the band gap. In terms of optoelectronic applications, this behavior is particularly important as it reflects the enhancement of a materials ability to absorb photons and generate charge carriers more efficiently. Due to the tunability of band gap with nanoparticle incorporation, PVP/Bi_2O_3 nanocomposites have great potential for photodetectors and optical sensors and in other nanoscale optoelectronic devices.

Overall, the trend observed is in agreement with already established studies revealing that building polymer composites by doping of inorganic nanoparticles lead to narrowing of band gap due to defect states and enhanced electronic interactions **[20].**

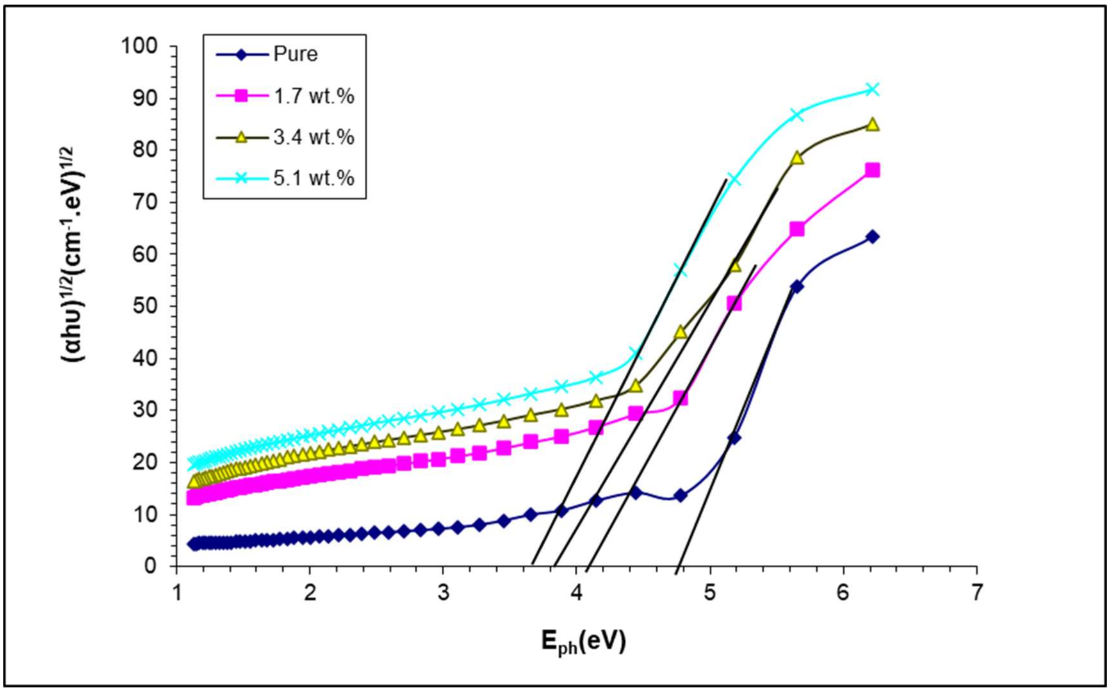

Figure (4) Relation between $(\alpha h\nu)^{1/2}$ versus $(h\nu)$ for PVP/Bi_2O_3 nanocomposites

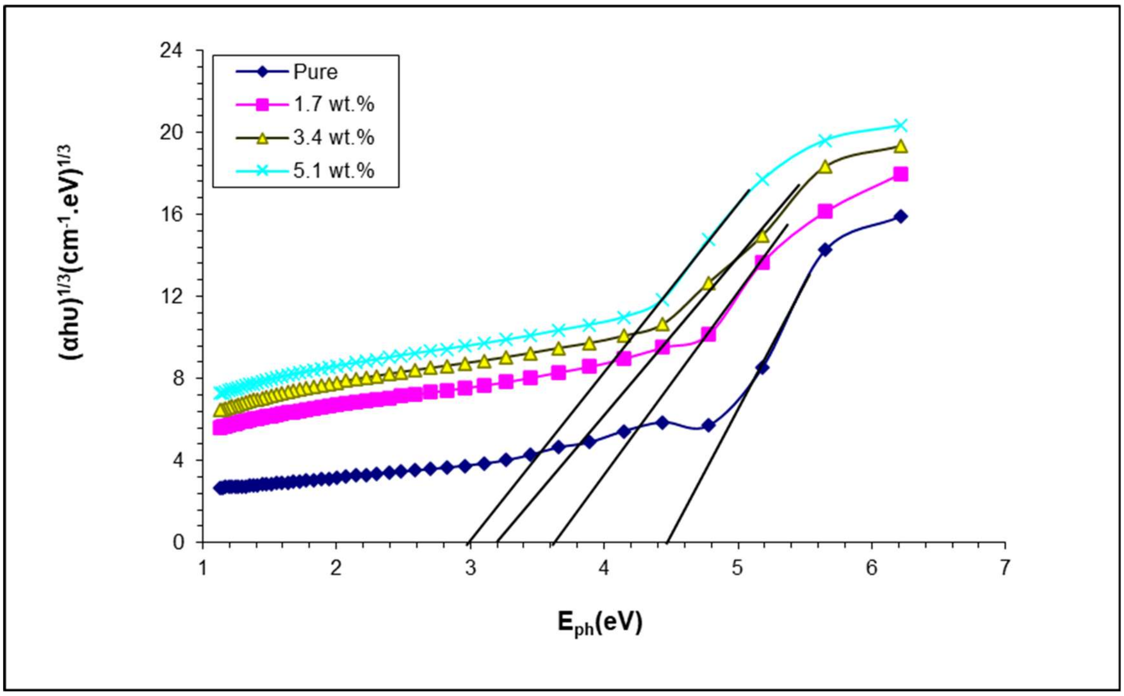

Figure (5) $(\alpha h\nu)^{1/3}$ versus $(h\nu)$ for PVP/Bi_2O_3 nanocomposites

Table (1) Values of the gap of energy for the allowable and banned indirect transition of PVP/Bi_2O_3 films

Bi_2O_3 NPs wt.% content	E_g allowable indirect (eV)	E_g prohibited indirect (eV)
0	**4.8**	**4.58**
1.7	**4.1**	**3.6**
3.4	**3.81**	**3.2**
5.1	**3.65**	**3**

Using relation (5), the extinction coefficient k of PVP/Bi_2O_3 nanocomposites was established. As shown in Figure (7), the extinction coefficient increases gradually with wavelength, and this can be related to the change of photon energy. In addition, there is a noticeable rise of the extinction coefficient when the incorporated content of Bi2O3 nanoparticles in PVP matrix increases. This trend is mainly due to the increased absorption of visible light may be because of increase in concentration of Bi_2O_3 nanoparticles **[21].**

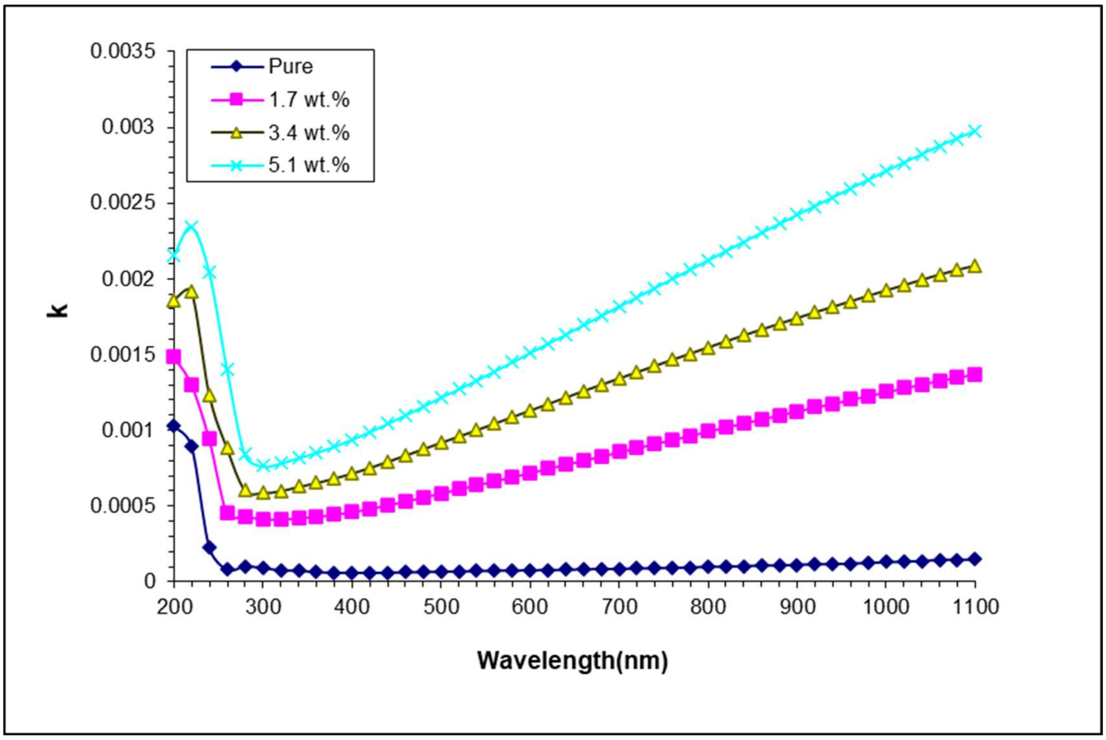

Figure (7) Extinction coefficient of PVP/Bi_2O_3 nanocomposites

Relation (6) was used to calculate the refractive index (n) of PVP/Bi_2O_3 nanocomposites. As shown in Fig (8), lower photon energies (~260 nm) result in a peak refractive index that drops off to near constant values within the visible and near infrared (NIR) regions with increasing energy. It was also noticed that The refractive index is increasing with an Increase of bismuth oxide nanoparticles. This phenomenon corresponds to the structural changes taking place in the polymer matrix, which causes a change of refractive index **[22].**

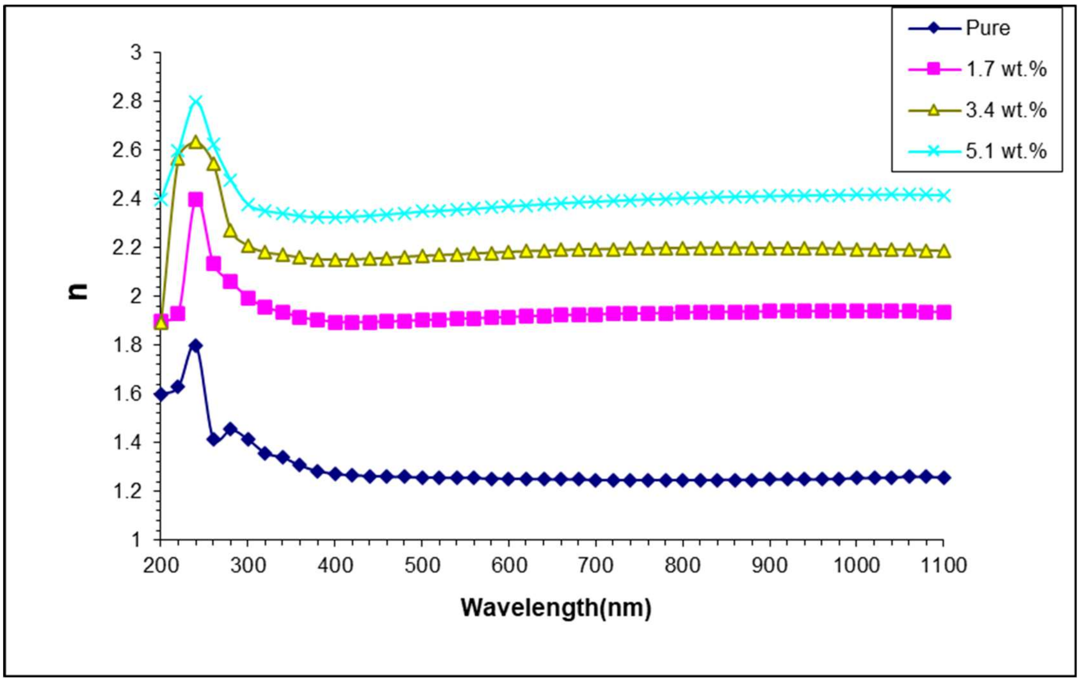

Figure (8) Refractive index of PVP/Bi_2O_3 nanocomposites

The E_1 and E_2 are real (E_i) and imaginary (E_2) parts of insulator constant for PVP/Bi_2O_3 nanocomposites were calculated using equations (7) and (8). The spectral behaviour of E and E_2 for pure PVP and PVP/Bi_2O_3 nanocomposite films at various concentrations of Bi_2O_3 nanoparticles can be seen in Figure (9) as well as Figure (10). The fact that both dielectric components begin at larger values in the higher frequencies (lower photon energies) and then have a distinct drop-off before approaching an equilibrium-like behavior in the visible and near infrared regions is confirmed by the results.

In addition, the E and E_2 are progressed as Bi2O3 nanoparticles are rising. This behaviour is largely attributed to the augmented polarization of the composite system. This similar behavior of the real part and imaginary component can be attributed to more dependence of dielectric constant on refractive index (n) than extinction coefficient (k), since k values were relatively small comparing to n, especially in squared value **[23].**

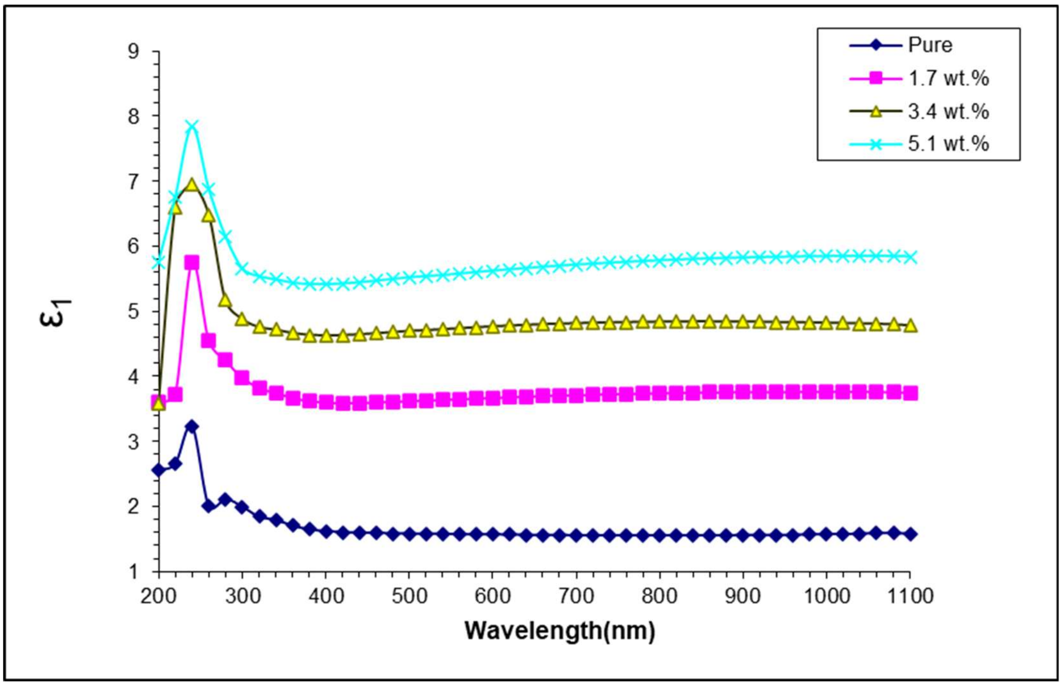

Figure (9) Real insulator constant of PVP/Bi_2O_3 nanocomposites

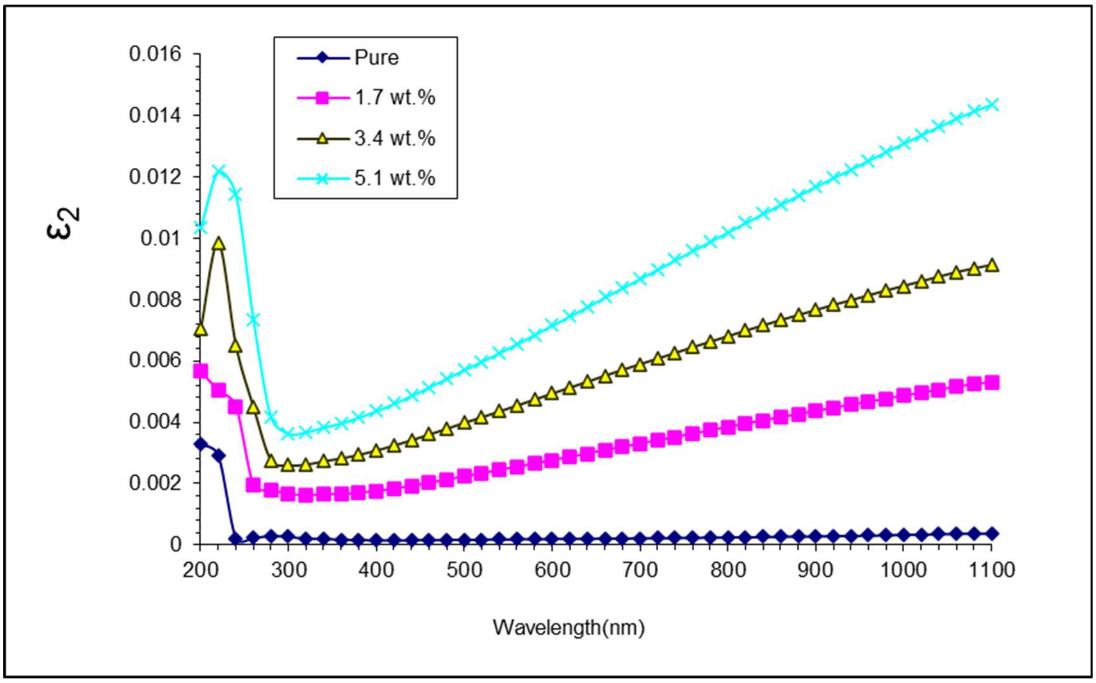

Figure (10) Imaginary insulator constant of PVP/Bi_2O_3 nanocomposites

The optical conductivity of PVP polymer and PVP/Bi_2O_3 nanocomposites modified with different concentrations of the Bi_2O_3 nanoparticles was determined using equation (9). The optical conductivity at shorter wavelengths is higher than the that, and then gradually decreases with longer wavelengths, as shown in Figure (11). This behaviour concerns mainly the experimental uncertainty regarding the absorption coefficient.

Furthermore, the increase of Bi_2O_3 nanoparticles helps also enhance the optical response because their addition leads to an increased of the conductivity. This improvement is due to rise in the absorption coefficient, which contributes substantially to improving the optical conductivity of the nanocomposite system **[23].**

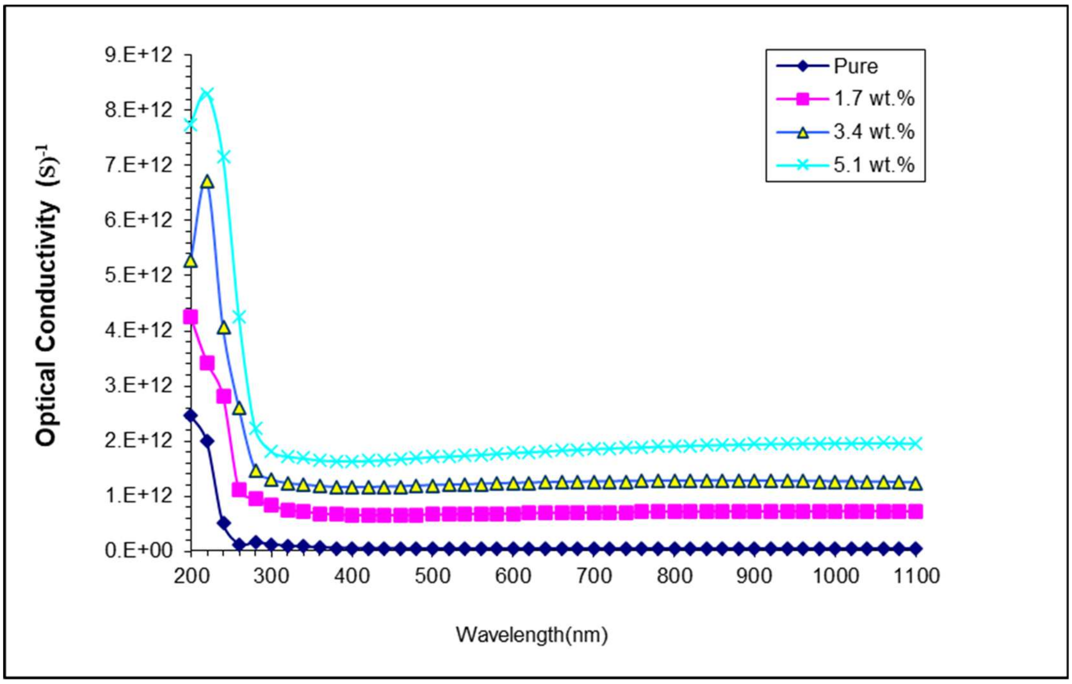

Figure (11) Optical conductivity of PVP/Bi_2O_3 nanocomposites

4. Conclusion

Here we report for the first time on the systematic solution casting strategy to prepare PVP/Bi_2O_3 nanocomposites that led to films with superior optical properties. The results demonstrate that, with increasing Bi_2O_3 nanoparticle concentration, the absorbance is increased while the transmittance is decreased due to strong interaction of light and nanocomposite structure. The addition of Bi_2O_3 nanoparticles also results in a decreased optical band gap. At 6 wt. % loading, band gap decreases from 4.8 eV (pure PVP) to 3.65 eV (allowed indirect) and from 4.58 eV to 3 eV (forbidden indirect). This decrease is mostly attributed to localized states as well as structural changes in the polymer matrix. In addition, valuable optical properties such as absorption coefficient, extinction coefficient, refractive index, dielectric constants and optical conductivity were observed to be gradually increasing with the increase of Bi_2O_3 concentration. Consequently, it is connected to effectively polarisation and stronger interactions among naïve polymer and nanoparticles.

PVP/Bi2O3 nanocomposites, in conclusion, are tunable optical materials with encouraging prospective application to optoelectronic applications and devices including optical filters, switches and coatings even at low loading of the NPs.

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