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Study the Influence of TiO_2-Nanoparticles Doped in Polyvinyl Alcohol by Measuring Optical Properties of PVA Films

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Abstract

It was investigated how titanium dioxide nanoparticles affected the optical properties of polyvinyl alcohol. Polymer nanocomposites (PVA-TiO_2) are created via stirring and casting. The results demonstrate that transmittance improves from 75% to 95% while titanium dioxide concentration enhances the absorbance of nanocomposites. Nanocomposite films made of PVA and TiO_2 had reflectance values of 12 and 16 percent (weight percent=0.15 and 0.85%).The refractive index and coefficient of extinction rise with increasing density, and optical absorption and photon dispersion in the nanocomposite (PVA-TiO2) also rise as the concentration of titanium dioxide nanoparticles rises. Real dielectric (r) and imaginary dielectric I constants also rise as titanium dioxide nanoparticle concentration does. The results show that when the weight % of (TiO2) nanoparticles increased, the energy gap decreased from 3.32 to 2.23. Additionally, optical conductivity increased with the concentration of (TiO2) NPs. Nanocomposites of PVA and TiO2 are essential for optical applications.

Introduction

Like a conventional composite, a nanocomposite consists of a matrix and filler. While the filler in a conventional composite is often a fiber, like carbon fiber or fiberglass, in a nanocomposite the filler is a nanomaterial. CNTs, carbon nanofiber, and nanoparticles made of gold, silver, diamond, copper, and silicon are some types of nanomaterials. By mixing material NPs with polymers, the optical

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characteristics of the polymer composite are improved while the mechanical behavior is altered [1]. The use of optically transparent polymers for many applications such as encapsulation of electronic devices and Coating with optical characteristics, and the reason for this is their low cost, superior processability, and high transparency in the visible region. [2]. Manufacturing, commercial, medical, and food are just a few of the industries that employ PVA.Medical sutures, corrugated paper, and components for food packaging have all been made with it. Because of its enticing film-forming capabilities, as well as its processability, biocompatibility, and chemical resistance, PVA has sparked a lot of attention [3].PVA might effectively prevent the nanoparticles from agglomeration. Polymers have drawn a considerable interest in device fabrication because of their extraordinary inherent properties [4]. One of the most important technologies of now and tomorrow is nanotechnology [5].The chemical compound titanium dioxide is sometimes called titanium (IV) oxide or titania. The remarkable electrical and optical properties of TiO2-NPs, as well as their security, chemical stability, and photocatalytic activity, were all factors in their selection. To mention a few uses, the designer of a computer disk, sensors, and optoelectronics employed TiO2 nanoparticals film. [6]. This type of polymer might be one of the materials utilized in gas sensors [7]. Other materials, such as graphene, have been employed as gas sensors [8]. The optical characteristics of the manufactured(PVA-TiO_2) films made of nanocomposites, such as transmission (T percent), absorption (A), reflectance(R), energy gap(E_g), coefficient of optical constants (α), refractive index (n), coefficient of extinction (k), and functions of optical dielectrics (ε_r, ε_i), are the focus of this research.

Experiment Specifics

1. Materials

Titanium dioxide nanoparticles, purity > 99.7% , particle size 30±5, it's molecular weight(79.866 g/mol) panichem.Co.,LTD . Made by Korea · Polyvinyl Alcohol (PVA) is used as granular white forms its molecular weight is in the range (26,300-30,000) g/mol. Polyvinyl alcohol is a product of Shanghai Kaidu Industrial Development Co, Ltd, China.

2. Preparation of (PVA-TiO_2) Nanocomposites

1 gram of (PVA) was dissolved fully in 30 ml distilled water for an hour and a quarter under continual stirring and the fluid was heated to 70°C. Then, when the pure sample had been dissolved, various amounts of (TiO_2) nanoparticles are added little by little (0, 0.15, and 0.85) wt percent, and diverse samples have been formed. The pure and each nanocomposites concentrations were poured in a petri dishes with a diameter of 10cm and thoroughly cleaned with ethanol and distilled water as

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stated in table-1. The movies were produced after this period had gone, which have been disjoined from the casting glass and cut into pieces for testing and thickness (45□m±5) measurement using a micrometer. These ratios of the nanomaterial to the polymer have been selected to examine the connectivity between the two materials in proportions that differ noticeably and have been more fully explored.

Table (1) percentages of (PVA-TiO2) nanocomposites by weight

PVA (wt %)	TiO_2 (wt %)
1	0
1	0.15
1	0.85

Theoretical Part

Our understanding of the internal structure of polymers, the nature of their linkages, and the range of potential applications for polymers is expanded by the study of their optical properties. The absorption and transmittance spectra of a polymer may be used to identify a number of optical properties over a broad range of wavelengths. By looking at them in the ultraviolet spectrum, we can identify the kind of bonds, orbits, and energy beams that are there. Research on the visible spectrum provides sufficient understanding of a material's behavior for solar applications [9]. Planar waveguide devices and small optical components need optical materials, therefore polymers with nanoparticles like metal oxides are being researched. Utilized polymer nanocomposite structures' advantages in production and processing are fueling their growth. [10]. The well-known Beer–Lambert relationship describes their optical linear absorption coefficient.

$$\alpha = \frac{2.303\,A}{t} \qquad (1)$$

A = log (I_0/I_T), I_0 and I_T indicate the intensity of the incident and transmitted beams, and t represents test width [11]. The complex dielectric function is used to characterize the optical characteristics of solid film material. (ε_r and ε_i), coefficient of extinction (k), refractive index (n), and reflectivity of incident [12]

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \qquad (2)$$

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$$n = \sqrt{\frac{4R - k^{2}}{(R-1)^{2}}} - \frac{(R+1)}{(R-1)} \qquad (3)$$

In the strong absorption spectral region, using an appropriate straight line. Tauc equation may be utilized to determine the indirect and direct permissible optical transitions.

$$\alpha h\upsilon = B(\, h\upsilon - E_{g}^{opt.} \pm E_{ph}\,)^{r} \qquad (4)$$

The optical band gap and photon energy are Eg and h. For indirect allowed, indirect forbidden, direct authorized, and direct banned transitions, it may be between E g=3.32 and 3.16 and 2.23 [13]. The values of ($E_{g}^{opt.}$) are calculated using by (h) 1/r with h relationship [14]. The coefficient of extinction (k) is calculated using the formula below [11]:

$$K = \left(\frac{\alpha\lambda}{4\pi}\right) \qquad (5)$$

The (ε_r) and (ε_i) components of the constant of dielectric are described according to the following relationships [15]:

$$\varepsilon_r = (n^2 - k^2) \qquad (6)$$

$$\varepsilon_i = (2nk) \qquad (7)$$

The optical conductivity (σ_{op}) is the electric conductivity that causes charge carriers to flow due to the incident electromagnetic waves' intermittent electric field [16]:

$$\sigma_{op} = \frac{\alpha n c}{4\pi} \qquad (8)$$

Results and Discussion

A peak at 220nm may be seen in the spectra of pure and nanocomposites samples, this is attributed to the presence of carbonyl groups related to the unsaturation of ethylene. In such materials, UV absorption is high as a result of the utilization of photon energy to electrons are excited from the (V.B) to the (C.B) [17]**.** Theoretical algorithms are used to compute nanocomposites based on the wavelength of incoming light. As the concentration of TiO_2 nanoparticles rises, UV absorption by nanocomposites samples increases, which is owing to donor level electron excitations to the (C.B) at these energies. Absorbance grows in lockstep with additive concentration that is connected to growth

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in charge carrier numbers [18]. Fig. 2 displays the optical transmittance spectra that the PVA-grafted TiO_2 nanocomposites with 0.85 wt% loadings were exceptionally transparent over the visible range, with a transparent of nearly 95 percent. The onsets of the UV-vis transmission spectrum are also sharp, showing the TiO_2-NPs doesn't distort light in the visible range [19].

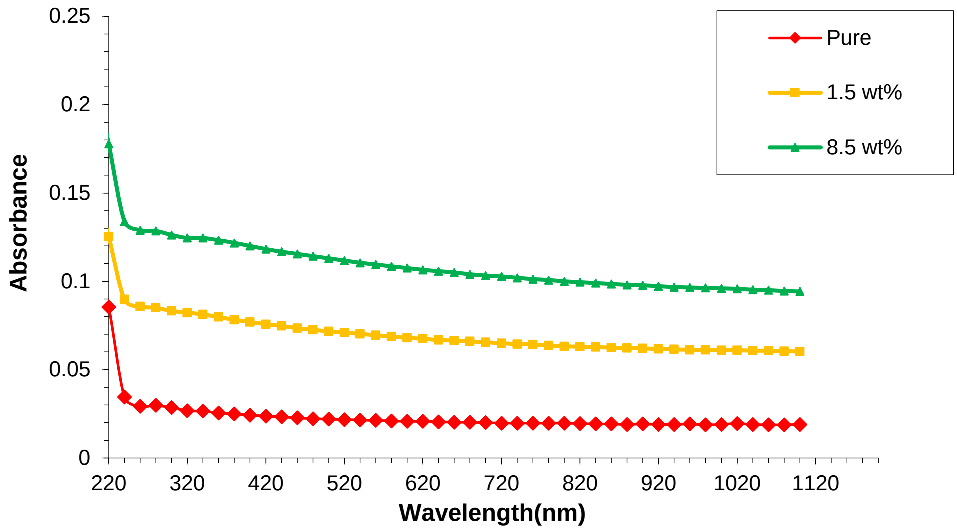

Figure 1: The (PVA-TiO_2) comparative absorbance as a function of wavelength.

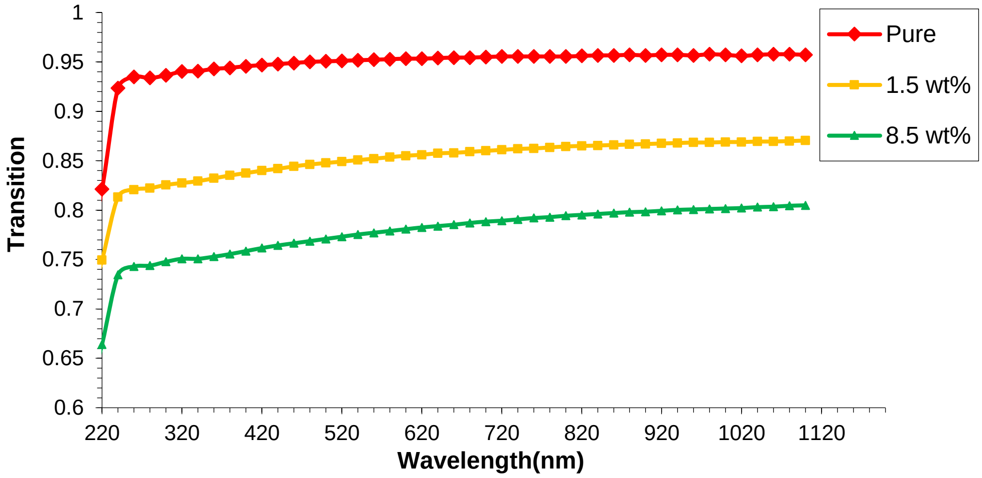

Figure 2: The (PVA-TiO2) comparative transition as a function of wavelength.

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In figure-3, a rise in absorbance coefficient (α) was seen for sample when the wavelength was increased. This might be due to transit of the electronic between the bonding and nonbonding molecular orbits [20]. It can be shown that the absorbance coefficient (α) for both nanocomposites (PVA-TiO_2) is lower (10^4 cm^{-1}). Absorbance coefficient (α) is projected to be low (10^4 cm^{-1} at low energy), meaning that an indirect electron transition happens when the electric moment the phonon conserves energy [21]. As the concentration of nanoparticles increases, more charge carriers are present, increasing the absorbance coefficient of (PVA-TiO2) nanocomposites [22]. Figure (4) illustrates how the energy band gap of a nanocomposites is calculated experimentally (4).. Theoretical Eg for indirect transitions in (PVA–TiO_2) nanocomposite [23]. The energy gap shrinks from 3.32 to 2.23 when the weight percentage of (TiO_2) nanoparticles rises, according to the findings. The most likely cause is the establishment of localized level in the prohibited energy gap as a consequence of rising the fillers nanoparticle weight percent

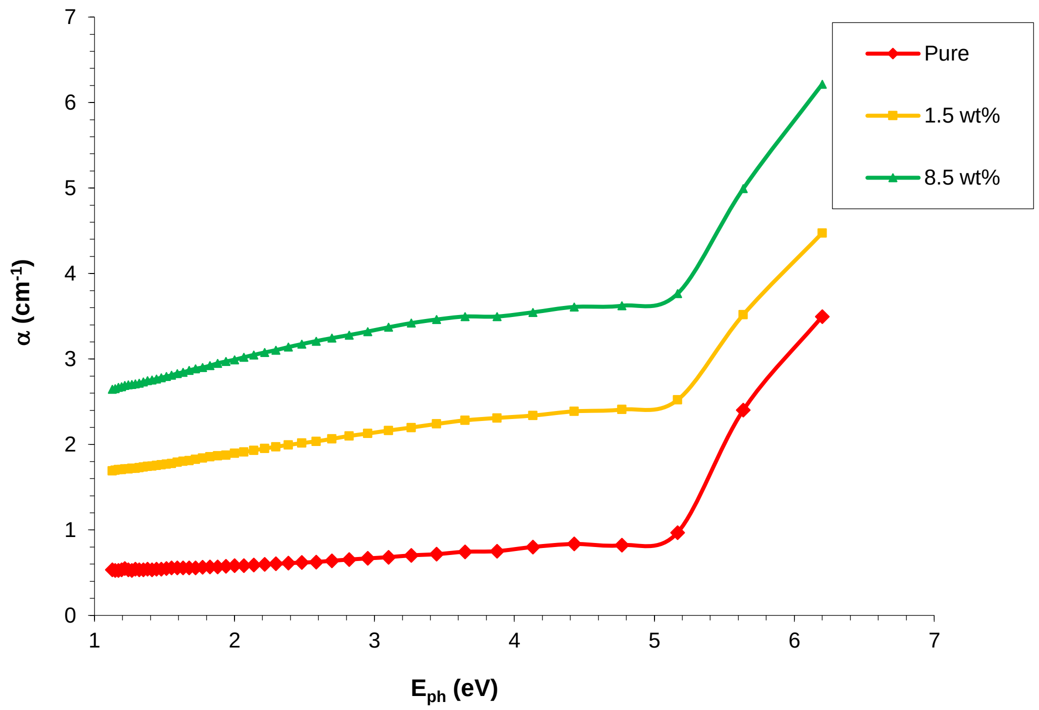

Figure 3: The (PVA-TiO2) comparative absorbance coefficient as a function of wavelength.

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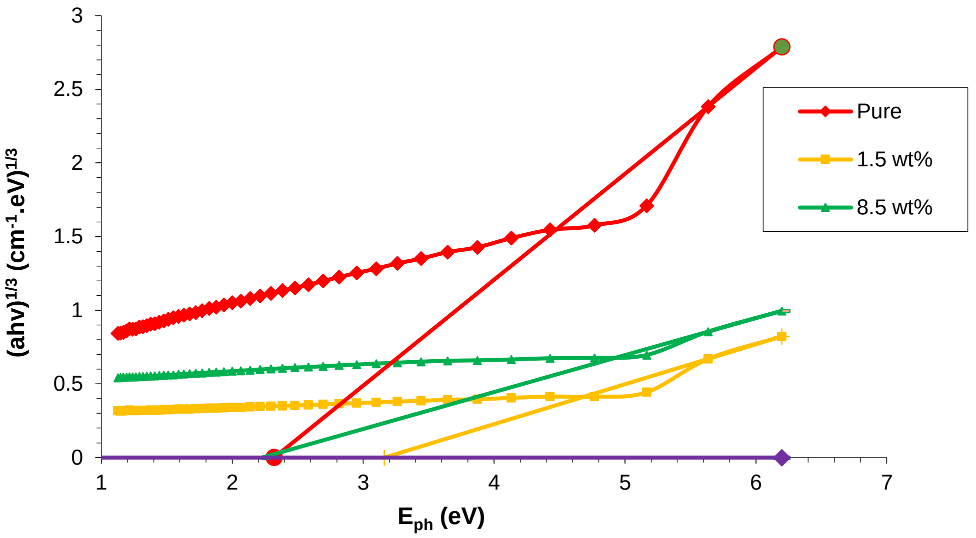

Figure 4: The (PVA-TiO2) compare the energy difference between the permissible direct and indirect transitions (αhυ)1/2

Figure 5 observed the spectrum of reflectance(R) of (PVA-TiO_2) nanocomposite film for variety TiO_2-nanoparticales fillings as a function of incoming light wavelength. As the wavelength is extended above 260 nm, the reflectance values fall marginally. Surprisingly, increasing the concentration of (TiO_2) nanoparticles in Poly (Vinyl Alcohol) polymeric films results in growth in reflectance values. As expected, the reflectance spectrum (R) behaves differently from the transmission spectrum. The values of reflectance of (PVA-TiO_2) nanocomposite films (wt. percent = 0.15 and 0.85 percent) are 12 and 16 percent, respectively, according to our findings. The average value of the sum of transmittance and reflectance is unity [24].

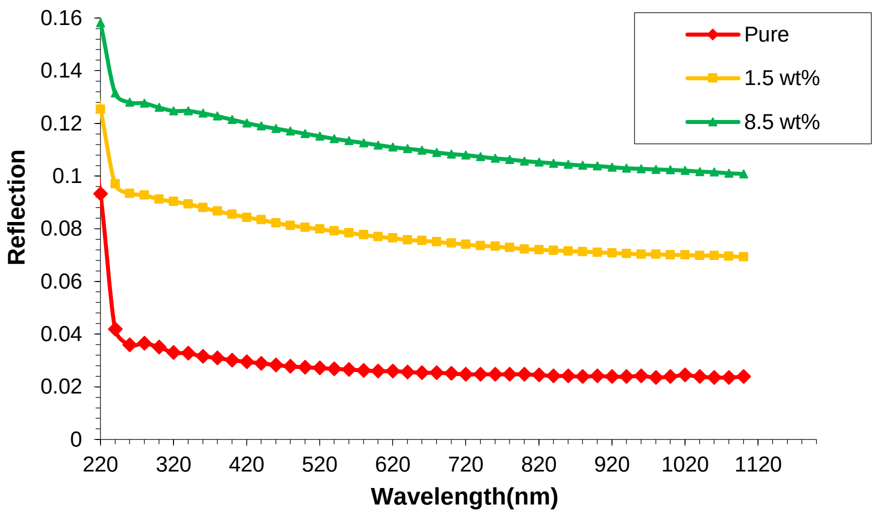

Figure 5: The (PVA-TiO2) comparative reflection as a function of wavelength

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The (ε_r), and (ε_i) components of the dielectric constant are calculated by formula 6 and 7. Figures 6 and 7 demonstrate the expected variety of the (ε_r) with wavelength for the (PVA–TiO_2) nanocomposite. There is a loss peak that can be attributable to interfacial polarization. As the concentration of TiO_2 in the composite rises, these lessening peaks shift to the lowest portion [24]. The relationship between the dielectric constant's real portion and the refractive index (*n*) computed the dielectric imaginary component of the equation7 [25].

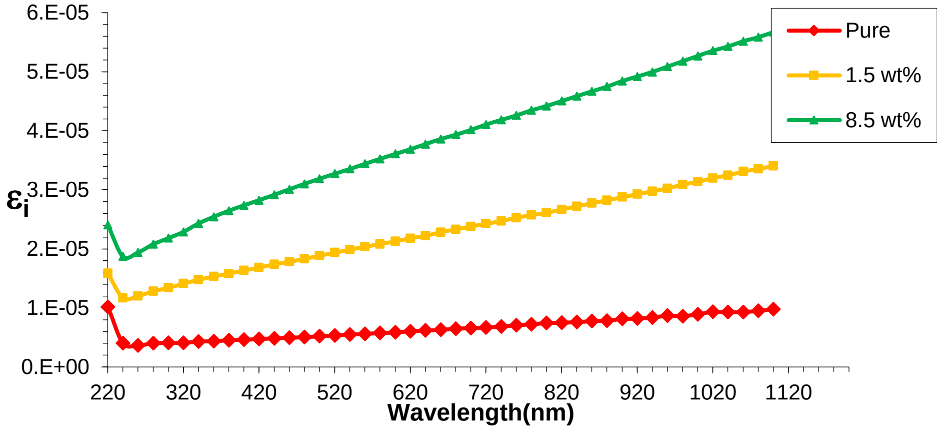

Figure 6: The (PVA-TiO2) comparative the dielectric imaginary part as a function of wavelength.

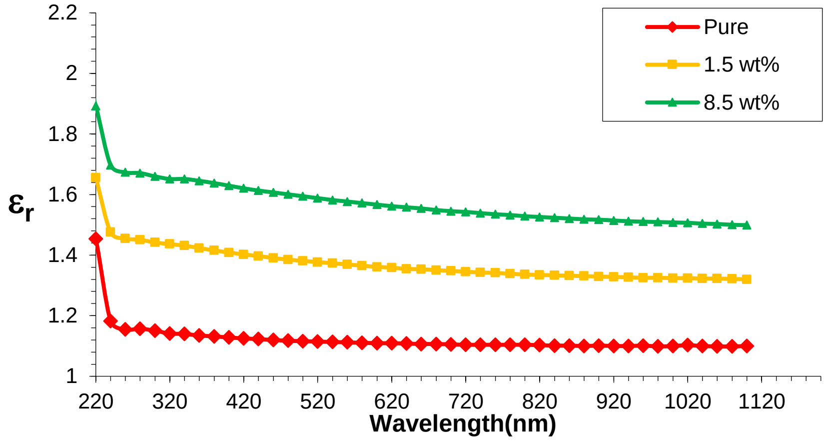

Figure 7: The (PVA-TiO2) comparative the dielectric constant real part as a function of wavelength

The extinction coefficient (k) is determined using the following formula (5). The computed extinction coefficient for the (PVA–TiO_2) nanocomposite varies as a function of wavelength, like figure-8. The coefficient of extinction of nanocomposites rises, as depicted in Figure. As the concentration of TiO_2 nanoparticles increases, so does optical absorption and photon dispersion in the nanocomposite [26].

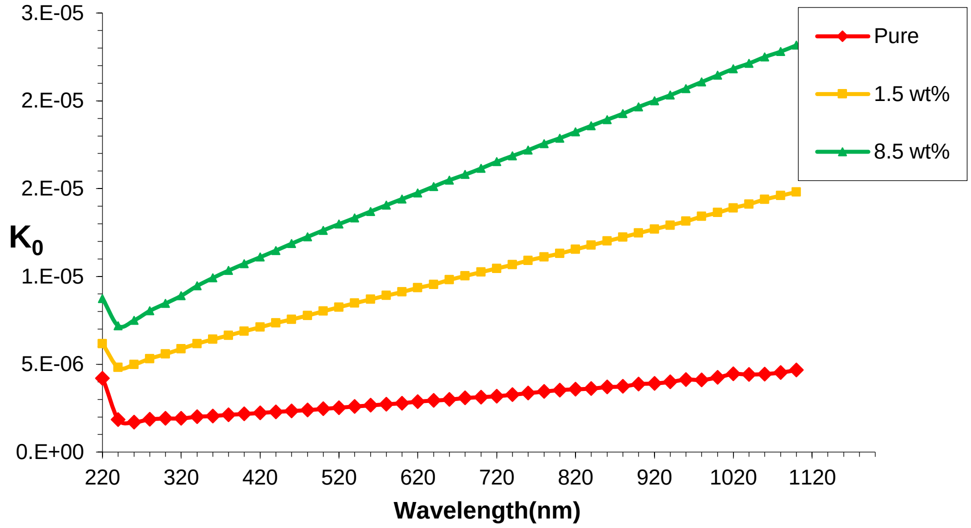

Figure 8: The (PVA-TiO2) comparative the coefficient of extinction by relation to wavelength

The computed refractive index (*n*)of (PVA–TiO_2)nanocomposite with relation to wavelength are given in figure-9. The refractive index (*n*) of a nanocomposite rises for the amount of TiO_2 nanoparticles present and falls as the wavelength increases. The rise in density is thought to be the cause of this phenomenon [27].

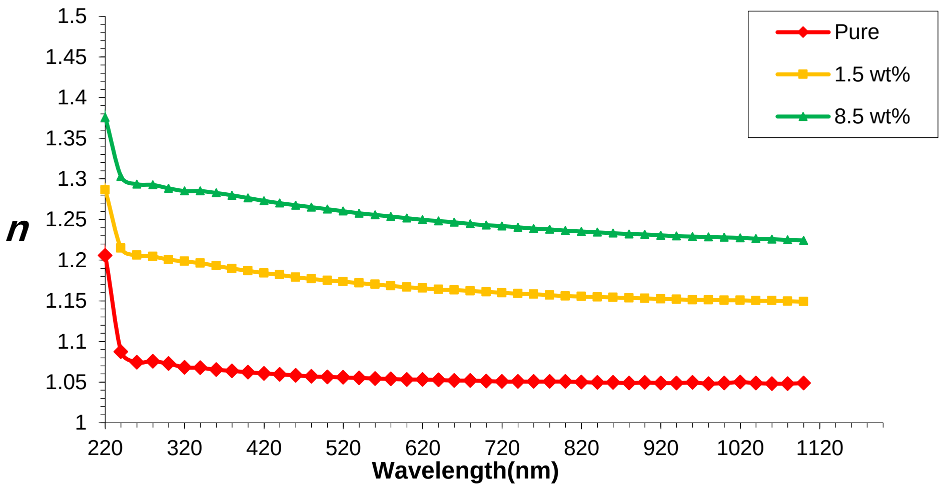

Figure 9: The (PVA-TiO2) comparative the refractive index (n) as a function of wavelength

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Figure 10 depicts the projected change in the optical conductivity (σ_{op}) with wavelength for (PVA–TiO_2) nanocomposites. As the concentration of TiO_2 nanoparticles in nanocomposites increases, so does their optical conductivity (σ_{op}). The formation of localized levels in the energy gap is linked to this phenomenon. As the concentration TiO_2 nanoparticle rises, in the band structure, the density of localized states grows. As a result, as the absorbance coefficient (α) increases, so does the optical conductivity [28] of (PVA–TiO_2) nanocomposites.

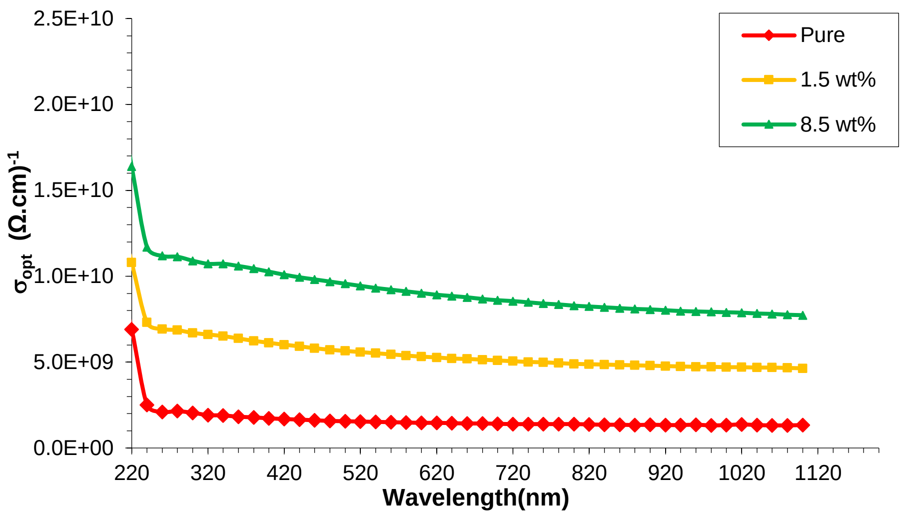

Figure 10: The (PVA-TiO2) comparative the optical conductivity (σop) as a function of wavelength.

Conclusions

The results revealed that (PVA–TiO_2) nanocomposites had a great UV absorption. The quantity of TiO2 nanoparticles improve a substance's optical conductivity, as well as its (A), (α), k, n, ε_r, and ε_i constants, and optical conductivity (PVA).When compared to other devices, the (PVA–TiO_2) nanocomposite has indirect energy gaps of (3.23 - 2.23) eV, making it beneficial for many optoelectronic applications, photovoltaics, lasers, photovoltaic cells, sensors, photocatalytic mechanisms, filters for light, Detectors of ultraviolet light, and so on are only some of the applications.

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