Study the Optical Properties of (PVA-PVAC-Ti) Nanocomposites

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Abstract: In the present research, the effect of titanium nanoparticles on optical properties of (PVA-PVAC) has been studied. For this purpose, many samples were prepared with different weight percentages of titanium nanoparticles, the samples were prepared by casting method. The absorption spectrum has been recorded in the wave length range 200-1100 nm, the optical energy gap of the indirect allowed and forbidden transition, absorption coefficient and optical constants, such as (extinction coefficient, refractive index and real and imaginary dielectric constants) have been determined. The optical constants are increase with increasing of titanium nanoparticles concentration, also the energy gap decreased with increasing the weight percentages of titanium nanoparticle.

Key word: Nanocomposite, optical properties, poly (vinyl alcohol), poly (vinyl acetate), titanium nanoparticles

INTRODUCTION

The study of composite materials, i.e., mixtures consisting of at least 2 phases of different chemical compositions has been of great interest from both fundamental and practical standpoints (Rashid et al., 2013). Composites made of polymer with a conducting filler phase allow the combination of the mechanical properties of polymers and its ease of processing with electrical applications requiring significant conductivity, polymer-based electrically conducting materials have several advantages over their pure metal counterparts which include cost, flexibility, reduced weight, ability to absorb mechanical shock, corrosion resistance, ability to form complex parts and conductivity control. Filled conducting polymer composites are used for electromagnetic shielding of computers and electronic equipment’s (Callister, 2003). In addition, they are used as conducting adhesives in electronics packaging flip-chips, cold solders, switching devices, static charge dissipating materials and devices for surge protection (Dahshan, 2002). In the recent years, conjugated conducting polymers have been main focus of research throughout the world. Since, the discovery led by 2000 chemistry Nobel winners, Shirakawa, Macdiarmid and Heeger, the perception that plastic could not conduct electricity has changed now-a-days, conducting polymers also known as conductive plastics are being developed for many uses such as corrosion inhibitors, compact capacitors, antistatic coating, electromagnetic shielding and smart windows which capable to vary the amount of light to pass.

Composites are used in making solar cells, optoelectronic device elements, laser, diodes and Light Emitting Diodes (LED), industrial applications in aircraft, military and car industry (Richardson, 1977). PVA is one of the earliest and best known polymers, it was seen to use in a variety of applications and is currently used extensively in semiconductors applications. The transmission for visible light is very high. Polymeric composites of PVA are known for their importance in technical applications (Tawansi and Zidan, 1991). Further, polymers on doping with noble metal nanoparticles show brand new distinctive properties obtained from unique combination of the inherent characteristics of polymers and properties of metal nanoparticles (Qian and Hinestroza, 2004). The advantage of poly vinyl alcohol that has the ability to blend into the water which is resistant to do solvents, oils and has the ability to relax materials cellulose so uses his wide is used in making paper and textile industries in the manufacture of membranes resistance to oxygen in the coating photographic film (Mark, 1999). Poly (vinyl acetate) polymer is a thermoplastic which researchers got from the polymerization of vinyl acetate using an appropriate beginning in a solvent or with water installation of polymer (PVAC) which is white color and the rmoplast (Murray, 1997). The Polyvinyl Acetate (PVAC) discovered in 1912 by Dr. Fritz Klatte in Germany. It is one of the most commonly used resins water on a large scale, since 1945 has used water-based emulsions of polyvinyl acetate and paints in homes and adhesives (Jelinska et al., 2010).

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Enjoy minutes titanium nanoparticles qualities make them useful in the uses of visual and electrical insulators, anti-bacterial and chemical stability, as well as high catalytic properties useful in industrial applications. Kolobag, chock materials, auxiliary materials and stimulation of photosynthesis, titanium strong and light weight but also high resistance to corrosion. Thus, it can be used in military and space applications, it is the main applications of the particles of titanium nanoparticles are anti-microbial, antibiotics, antifungal medications, space materials, used in aluminum alloys, optical filters, paint, nanofibers, bandages, wires and textiles (Jelenska et al., 2010).

**Experimental part:** The materials used in this study are polyvinyl alcohol, Poly (vinyl acetate) and titanium nanoparticles. The solution of (PVA, PVAC) was prepared by solved (0.7, 0.3 g) in (40 mL) of distilled water, respectively. The (magnatic stirrer) is used to maxsid and the solution more homogeneous at (70°C). The weight percentages of nanotitanium are 0, 4, 8 and 12 wt.%. These are mixed for 120-180 min. The samples were prepared using casting technique. The absorbance spectrum was recorded of the wave length range 200-1100 nm by using the double-beam spectrophotometer (UV-1800 shimedza).

**RESULTS AND DISCUSSION**

**The absorbance of nano composites:** Absorptance can be defined as the ratio between absorbed light intensity (I_a) by material and the incident intensity of light (I_v) (Hashim, 2012).

$$A = \frac{I_a}{I_v}$$  \hspace{1cm} (1)

Figure 1 shows the variation of the optical absorbance with wavelength of the incident light for (PVA-PVAC-Ti) nanocomposites, it is noticed that the absorbability increases with increasing concentration of titanium nanoparticles. The absorption at any wavelength depends on the number of particles along the route of the incident light (based on concentration) and also depends on the length of the optical path passing through the form in addition to the temperature (AL-Humairi, 2013).

**The absorption coefficient and energy gap of nanocomposites:** Absorption coefficient is defined, as a ratio decrement in flux of incident rays energy relative to the distance unit in the direction of incident wave length. The absorption coefficient ($\alpha$) depends on incident photon energy ($\hbar$).

$$\alpha = 2.305 \frac{A}{d}$$ \hspace{1cm} (2)

Where:

- $A$ = Absorbance of sample
- $d$ = The thickness of sample

Figure 2 shows the relation between the absorption coefficient versus the photon energy of the (PVA-PVAC-Ti) nanocomposite, we can be see noticed that the change in the absorption coefficient is small at low energies, at high energy the change of absorption coefficient is large this is indicates to the large probability of electronic transitions (Jassim, 2013).

The absorption coefficient helps to conclude the nature of electronic transitions when the high absorption coefficient values ($\alpha \sim 10^6 \text{ cm}^{-1}$) at the high energies indicate to direct electronic transitions and the energy and momentum preserve of the electron and photon when the values of absorption coefficient is low ($\alpha \sim 10^5 \text{ cm}^{-1}$) at low energies indicate to indirect electronic transitions, the momentum of the electron and photon preserves by phonon helps, the optical energy gap can be calculated from this formula (George, 2004; Rashid et al., 2013).

Fig. 1: The variation of optical absorbance for (PVA-PVAC-Ti) nanocomposites with wave length

![Fig. 1](image1.jpg)

Fig. 2: The variation of absorption coefficient for (PVA-PVAC-Ti) nanocomposites with photon energy

![Fig. 2](image2.jpg)
\( (\alpha h\nu) = B(\nu - E_g)^r \) 

(3)

Where:
- \( B \) = Constant depending on the transition probability
- \( r \) = Index that characterizes the optical absorption process and is theoretically equal to 1/2, 2, 1/3 or 2/3 for indirect allowed, direct allowed, indirect forbidden and direct forbidden transition, respectively (Ahmad et al., 2007)

The usual method to calculate the band gap energy is to plot a graph between \( (\alpha h\nu) \) and photon energy \( (h\nu) \) and find the value of \( B \) which gives the best linear graph (Jelinska et al., 2010). This value of \( r \) decides the nature of the energy gap or transition involved. If an appropriate value of \( r \) is used to obtain linear plot, the value of \( E_g \) will be given by intercept on the \( h\nu \)-axis (Hashim, 2012).

The relation between \( (\alpha h\nu)^2 \) (eV/cm)\(^2\) and photon energy of nanocomposites shown in Fig. 3, from this researchers note that the value of optical energy gap decrease by increasing of weight percentage of titanium nanoparticles, this is due to the creation of localized levels in the allowed energy gap and have a go at this case through 2 steps include transmission electron from the valence band to the localized levels and from the localized levels to the conduction band as a result of increasing weight percentage of titanium nanoparticles (Al-Humairi, 2013), also the transition which occurs in the samples is allowed indirect transition as shown in Table 1.

**Table 1: Values of energy gap for indirect transition (allowed, forbidden) of (PVA-PVAC-Ti) nanocomposites**

<table>
<thead>
<tr>
<th>Sample</th>
<th>Allowed (eV)</th>
<th>Forbidden (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure</td>
<td>5.1</td>
<td>4.5</td>
</tr>
<tr>
<td>4 (wt.%)</td>
<td>4.6</td>
<td>4.5</td>
</tr>
<tr>
<td>8 (wt.%)</td>
<td>4.1</td>
<td>3.8</td>
</tr>
<tr>
<td>12 (wt.%)</td>
<td>3.6</td>
<td>3.2</td>
</tr>
</tbody>
</table>

When the value \( r = 3 \) indicates to forbidden indirect transition shows the relationship between \( (\alpha h\nu)^3 \) (eV/cm)\(^3\) and photon energy of nanocomposites in Fig. 4, researchers can see from Fig. 4, the value of forbidden energy gap decreases by increasing weight percentage of titanium nanoparticles, this is due to the creation of localized levels in the forbidden energy gap and have a go at this case through 2 steps include transmission electron from the valence band to the localized levels and from the localized levels to the conduction band as a result of increasing weight percentage of titanium nanoparticles (Jassim, 2013), as well as this value of forbidden indirect transition is less than the one value which is represent allowed indirect transition as shown in Table 1.

**Optical constants:** Figure 5 shows the variations of extinction coefficient with photon energy for (PVA-PVAC-Ti) nanocomposites. The extinction coefficient \( k \) is directly proportional to the absorption coefficient \( \alpha \) (Hadi et al., 2011; Haseeb, 2011):

![Fig. 3: The relationship between \((\alpha h\nu)^{1/2}\) (eV/cm)\(^{1/2}\) and photon energy of (PVA-PVAC-Ti) nanocomposites](image1)

![Fig. 4: The relationship between \((\alpha h\nu)^3\) (eV/cm)\(^3\) and photon energy of (PVA-PVAC-Ti) nanocomposites](image2)

![Fig. 5: The relationship between extinction coefficient (PVA-PVAC-Ti) nanocomposites with photon energy](image3)
Fig. 6: The relationship between refractive index (PVA-PVAC-Ti) nanocomposite with photon energy

\[ k = \frac{\alpha \lambda}{4\pi} \] (4)

Where \( \lambda \) is wavelength of light. Figure 5 shows that extinction coefficient \( (k) \) value increases with increasing of titanium nanoparticles concentration, this behavior can be described according to high absorption coefficient.

Figure 6 shows the variation of refractive index of nanocomposites as function of photon energy. The refractive index \((n)\) has been calculated by using this equation (Neamen, 1992):

\[ n = \sqrt{\frac{4R}{(R-1)^2} \left( R + 1 \right)} \] (5)

Where:

\( n \) = Refractive index
\( R \) = Reflectance index

Researchers have been found that the value of refractive index increases with increasing the concentration of titanium nanoparticles which is a result of increasing the number of atomic refractions due to the increase of the linear polarizability in agreement with Lorentz-Lorentz formula (Hadi et al., 2011).

Figure 7 and 8 show the variation of real and imaginary parts of dielectric constants \((\varepsilon_r, \varepsilon_i)\) of (PVA-PVAC-Ti) nanocomposites. The real and imaginary parts of dielectric constants have been calculated by using this equation:

\[ \varepsilon_r = n^2 - k^2 \] (6)

\[ \varepsilon_i = 2nk \] (7)

The variation of \( \varepsilon_r \) mainly depends on \((n^2)\) because of small values of the \((k^2)\) while the \( \varepsilon_i \) mainly depends on the \((k)\) values which are related to the variation of absorption coefficients (Ahmad et al., 2007; Habeeb, 2011).

Fig. 7: The relationship between realparts of dielectric constant (PVA-PVAC-Ti) nanocomposite with photon energy

Fig. 8: The relationship between imaginary parts of dielectric constant (PVA-PVAC-Ti) nanocomposite with photon energy

CONCLUSION

- The absorption coefficient for all (PVA-PVAC-Ti) samples increases with increasing of Ti (wt.% ) concentration
- The energy gap of indirect (allowed, forbidden) transition decreases with increasing of Ti (wt.% ) concentration
- The extinction coefficient, refractive index and dielectric constant (real and imaginary) increased with increasing of Ti (wt.% ) concentration

REFERENCES
