

Particles Size effect of Reinforced Iraqi Bentonite Kara Tepe on Optical Properties of Polystyrene

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Abstract: In this study, Iraqi bentonite Kara Tepe was used as reinforcing phase in Polystyrene (PS) matrix to form composites. Bentonite clay was prepared as a powder for particles size <45 and <75 μm , followed by calcinations process at 450°C for 2 h. PVA solution used as a coated layer covered the bentonite applied as a filler. Reinforced bentonite powder were added to PS solution at certain quantities. The optical study showed good transmittance value of PS, inter VIS and NIR region but it decreases with the increasing particles size of reinforced bentonite additive. The values of allowed and forbidden indirect transition optical energy gap decrease with the increasing particles size of reinforced bentonite additive up to (2.6, 2.38, 2 eV) and (2, 1.8, 1.30 eV), respectively which it is possible to apply in transistor, capacitors, solar cells, electrical equipment, etc. Optical constants such as refractive index, extinction coefficient, real and imaginary part of dielectric constant of polymer reinforcement bentonite were done. we discovered that these constants are influenced by the bentonite additive ratio and particle size.

Key words: Polystyrene, bentonite, optical properties, composite materials, solar cells, polymer

INTRODUCTION

The composite material is a mixture of two or more substances combined by a bond material, noting that there is no chemical reaction between the components of this mixture. The requirements of industrial development in the world led to the development of the science and technology of composite materials and the entry into the manufacture of new materials with special specifications determined by the required use (Umair, 2006; Hashim *et al.*, 2016).

Polystyrene (PS) is a thermoplastic polymer. Polystyrene is in a solid (glassy) state at RT but flows if heated above about 100°C , its glass transition temperature (T_g). It becomes rigid again when cooled. It is resists the action of many chemicals material (Anonymous, 2012).

Bentonite is a smectic clay which has a high montmorillonite content and the amount of less than other clay minerals. Other smectic group minerals include hectorite, saponite, beidelite and nontronite. Bentonite has a specific layer structure each layer is composed of a central sheet of octahedrally coordinated cations (called octahedral sheet) and two sheets of tetrahedrally coordinated cations (called tetrahedral

sheet) (Rautioaho and Korkiala Tantt, 2009). Bentonite group minerals show a colloidal structure in water, due to their internal structure and small particles size. They have a large adsorption capacity for polymer compounds due to their unique crystal structure.

The polymer concentration, molecular weight, hydrolysis degree of polymer, clay particle's size, shape, surface charge, clay concentration in dispersion, clay's pH and temperature are effective factors when clay particles interact with the polymers (Grim, 1970, 1978). The aim of present research is to investigate the effect of particle's size of Iraqi bentonite Kara Tepe on the optical properties of PS, for used in different applications.

MATERIALS AND METHODS

The main material used in this research is Polystyrene (PS). It has a simple repetitive structure as in Fig. 1. Because it is arranged in this form of linear polymer, it is a thermoplastic material. Its dissolved in many solvents and that the user solvent is benzene in certain proportions and a temperature of 80°C .

Bentonite Kara Tepe clay used in this study was supplied by state company of geological survey and

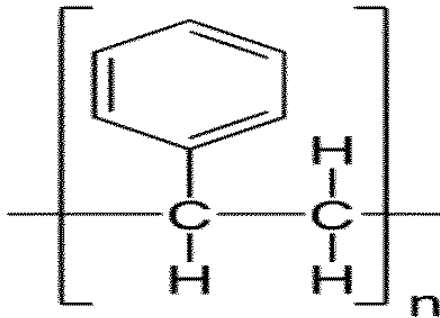


Fig. 1: Polystyrene structure

Table 1: The chemical analysis of Iraqi bentonite Kara Tepe

Constituent	Wt. (%)
SiO ₂	58.58
Fe ₂ O ₃	2.00
Al ₂ O ₃	15.80
MgO	6.10
CaO	2.77
Na ₂ O	0.70
SO ₃	0.10
Loos on ignition	12.48

Table 2: The mineralogical analysis of Iraqi bentonite Kara Tepe

Minerals	Percentage
Montmorillonite ([OH] ₂ Al ₂ SiO ₁₀)	97.54
Quartz (SiO ₂)	2.46

minority in Iraq have the general structure consisting mainly $Al_2O_3 \cdot 4SiO_2 \cdot H_2O$ (Al-Gohary *et al.*, 1987). The chemical analysis of Iraqi bentonite Kara Tepe is listed in Table 1. The mineralogical analysis of the final powder of Iraqi bentonite Kara Tepe is listed in Table 2.

The bentonite particles were dispersed in de-ionized water (PH = 7.09 measured at RT) which has electrical conductivity 23.6 μS and shaken extensively for 24 h at RT. The washing process was repeated seven times, during which the floating water was reduced every 24 h. The result of the test of the electrical conductivity of the bentonite clay after the last wash was 30 μS which is an acceptable result. The product was dried at 100°C for 24 h by using the dryer type F. G. BODE and CO-Laboratory-Equipment-Hamburg-90. Particle sizes selected for Iraqi bentonite Kara Tepe is <45 and <75 μm and the calcinations process was performed at 450°C for 2 h.

The addition of PVA has pH = 6 is one of the requirements to obtain the best adsorption on the surface of the clay before applied it as filler (Bussetti and Ferreiro, 2004). The mixture was mixed (using a magnetic sterile type-Sturt-Germany manufacture) with heat treatment in 80°C continued to get slurry form and to insure homogeneity with high viscosity (the mixing process was adopted according to the method of green

land (Greenland, 1963) then dried, milled and sieved to particle sizes <45 and <75 μm . A solution of 1.5 g have been prepared by solving 1.5 g of PS in 30 mL of the benzene and using magnetic stirrer to mix the materials to obtain more homogeneous solution at 80°C for 30 min. The reinforced bentonite of <45 and <75 μm sizes were added to PS with weight of percentage 4wt.% using a delicate electronic scale of up to 10^{-4} g and mixed for 30 min to make the mixture more homogenous. The casting method is used to get the composites cast on glasses betray dish and then left to dry for one day.

The absorption spectrum of (PS-Iraqi bentonite) composites at thickness 0.32 mm to size 45 μm and 0.35 mm to size 75 μm (by using electronic digital device-micrometer to measure thickness) have been recorded in the wavelength range 280-1100 nm by using the double beam spectrophotometer (Shimadzu, UV-1800 Å, Japan). The absorption spectrum have been recorded at RT. A computer program (UV Probe Software) was employed to obtain the absorption coefficient, extinction coefficient, refractive index, dielectric constant (real and imaginary parts) and optical energy gaps.

Basic relations: At the absorption edge, the absorption coefficient (α) can be calculated using the expression Eq. 1 (Pankove, 1971):

$$\alpha = \ln(1/T)/t \quad (1)$$

where, t is the sample thickness. The reflectance (R) of thin films was calculated from the Eq. 2 (Pankove, 1971):

$$R = 1 - \sqrt{T \exp(\alpha t)} \quad (2)$$

The refractive index (n) was calculated from the Eq. 3 (Pankove, 1971):

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

The extinction coefficient (K) is related to the exponential decay of the wave as it passes through the medium and it is defined to be Eq. 4 (Chopra *et al.*, 1969):

$$K = \frac{\alpha \lambda}{4\pi} \quad (4)$$

where, λ is the wavelength of the incident radiation. The real (ϵ_r) and imaginary (ϵ_i) parts of the dielectric constant related to (n) and (k) values can be written as in following Eq. 5 and 6:

$$\epsilon_r = n^2 - K^2 \quad (5)$$

$$\varepsilon_i = 2nK \quad (6)$$

The optical energy gap (E_g^{opt}) for indirect transition type is given Eq. 7 by Kittel (1981):

$$\alpha h\nu = B(h\nu - E_g^{opt} \pm E_{ph})^r \quad (7)$$

Where:

E_{ph} = Energy of phonon

(-) = Phonon absorption

(+) = Phonon emission

r = The exponential constant, its value depends on the type of transition

$r = 2$ = The allowed indirect transition

$r = 3$ = The forbidden indirect transition

The optical conductivity was determined using the relation Eq. 8 (Pankove, 1971):

$$\sigma_{opt} = \alpha nc/4\pi \quad (8)$$

RESULTS AND DISCUSSION

Figure 2 shows the optical transmittance spectrum versus wavelength of incident light on pure PS and (PS-Iraqi bentonite) films. The optimum value of transmittance about 65% for pure PS film at high wavelength (VIS-NIR). The transmittance decrease with the increasing articles size of reinforcement bentonite additive. This result can be attributed to what follows; the chemical analysis of bentonite indicates that the enforcement clay powder additive consists of oxides of varying proportions Table 1 and that the electrons available in it can absorb the electromagnetic energy of the incident light and travel to higher energy levels. This process is not accompanied by emission of radiation because the traveled electron to higher levels have occupied vacant positions of energy bands, thus, part of the incident light is absorbed by the substance and dose not penetrate through it. This is because the breaking of electron linkage and moving it to the conduction band needs to photon with a high energy (Dahshan, 2002).

Figure 3 shows the absorption coefficient α (cm^{-1}) versus photon energy for (PS-Iraqi bentonite) films. It can be seen that the absorption coefficient is the smallest at a low energy. This means that the possibility of electron transition is little because the energy of the incident photon is not sufficient to move the electron from the valence band to the conduction band. The values of the absorption coefficient is $<(10^4) \text{ cm}^{-1}$. This explains that the electron transitions is indirect.

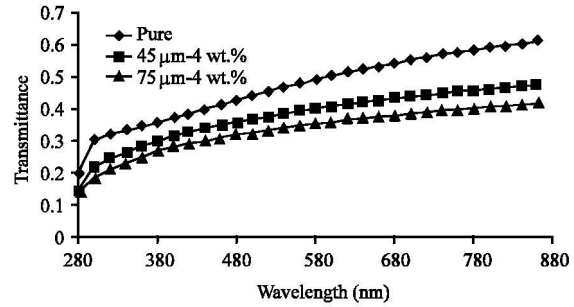


Fig. 2: Transmittance versus wavelength for PS and (PS-Iraqi bentonite) films

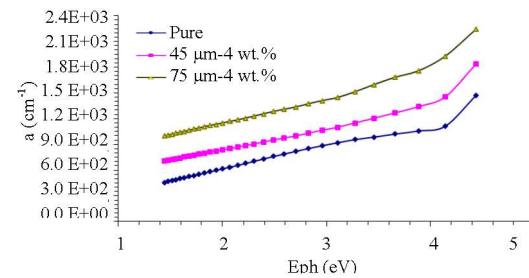


Fig. 3: Absorption coefficient α (cm^{-1}) versus photon energy for PS and (PS-Iraqi bentonite) films

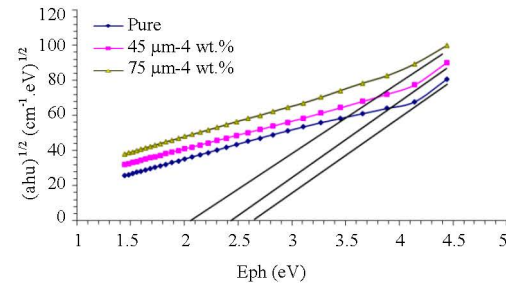


Fig. 4: Energy gap for the allowed indirect transition $(\alpha h\nu)^{1/2}$ versus photon energy of PS and (PS-Iraqi bentonite) films

Both the allowed and forbidden indirect transition optical energy gap are shown in Fig. 4 and 5, respectively. The values of optical energy gap decrease with the increasing particles size of reinforced bentonite additive (Table 3) which it is possible to apply in transistor, capacitors, solar cells, electrical equipment, etc. This results attributed to the creation of localized levels in the forbidden energy gap.

Figure 6 shows the change in refractive index for pure PS and (PS-Iraqi bentonite) films versus wavelength. In visible region (above the value of 580 nm), the refractive index increase with increasing particles size of reinforcement bentonite. This attributed to the high transmittance of pure PS in compare with that values of composite (PS-Iraqi bentonite) as in Fig. 2.

Table 3: Values of the optical energy gap for the allowed and forbidden indirect transition of PS and (PS-Iraqi bentonite) films

Samples(PS-Iraqi bentonite)	Particale size (μm)	Allowed indirect transition (eV)	Forbidden indirect transition (eV)
Pure PS	-	2.6	2
PS-4 wt.%bnt.	45	2.38	1.8
PS-4 wt.% bnt.	75	2	1.30

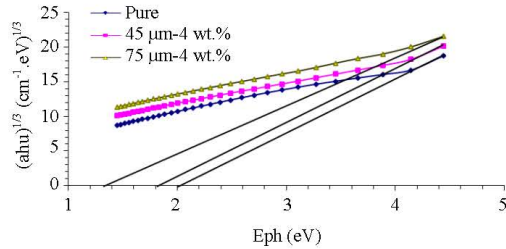


Fig. 5: Optical energy gap for the forbidden indirect transition $(\alpha h\nu)^{1/3}$ versus photon energy of PS and (PS-Iraqi bentonite) films

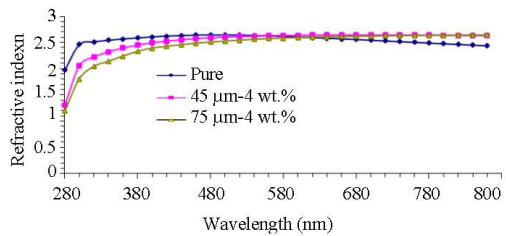


Fig. 6: Refractive index (n) versus wavelength for pure PS and (PS-Iraqi bentonite) films

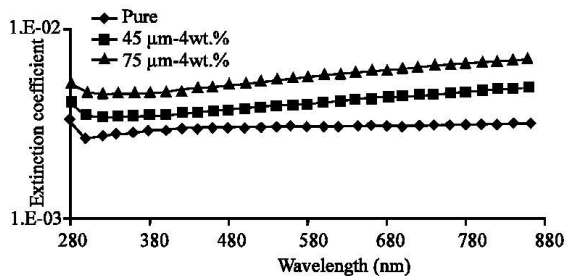


Fig. 7: Extinction coefficient (k) versus wavelength for pure PS and (PS-Iraqi bentonite) films

Figure 7 shows the change of extinction coefficient (k) for pure PS and (PS-Iraqi bentonite) films versus wavelength. It can be noted that k increase with increasing particles size of reinforcement bentonite in all regions. This is attributed to increase absorption coefficient with the increase of the particles size of reinforcement bentonite. Absorption coefficient (α) has a direct related with k as in the Eq. 4.

The dielectric constant for two parts real ϵ_1 and imaginary ϵ_2 for pure PS and (PS-Iraqi bentonite) films versus wavelength are shown in Fig. 8 and 9, respectively.

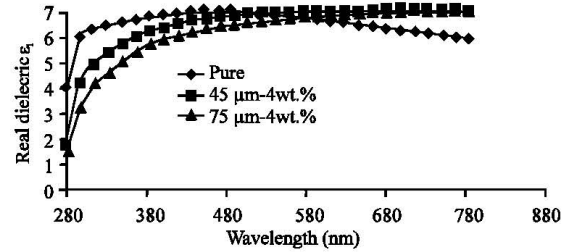


Fig. 8: Real dielectric constant (ϵ_1) versus wavelength for pure PS and (PS-Iraqi bentonite) films

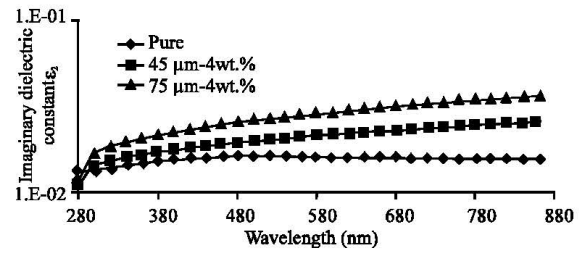


Fig. 9: Imaginary dielectric constant (ϵ_2) versus wavelength for pure PS and (PS-Iraqi bentonite) films

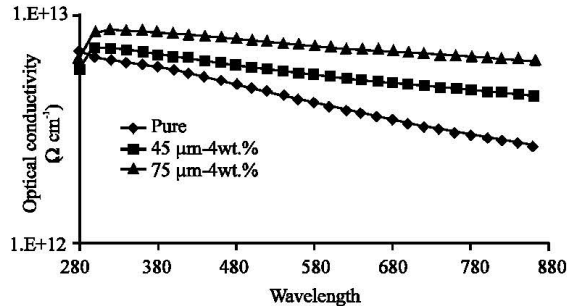


Fig. 10: Relation between the optical conductivity (σ_{opt}) and wavelength for pure PS and (PS-Iraqi bentonite) films

It can be seen that ϵ_1 considerably depends on n^2 due to low value of K^2 , so in visible region (over 580 nm), the ϵ_1 increased with the increase of the particles size of reinforcement bentonite.

The change of ϵ_2 dependent on K values that change with the absorption coefficient due to the relation between α and K .

Figure 10 illustrate optical conductivity versus wavelength for pure PS and (PS-Iraqi bentonite) films. The increase in optical conductivity with decreasing wavelength in the range of visible reign is due to electron excited by photon energy.

CONCLUSION

The optical study showed good transmittance value of PS, inter VIS and NIR regions but it decreases with the increasing particles size of reinforced bentonite additive.

The energy gap for indirect transition (allowed and forbidden) decreases with the increasing particles size of reinforced bentonite and which it is possible to apply in transistor, capacitors, solar cells, electrical equipment, etc.

The optical constant of pure PS and (PS-Iraqi bentonite) films such as refractive index, extinction coefficient and dielectric constant (real and imaginary) are increasing with the increase of particles size of reinforced bentonite.

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