Some Optical Parameters of PS Films Doped with CuO

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Abstract:

In the present work, we have studied the effect of CuO_2 dopant on the optical properties of (Polystyrene) (PS) polymer. The CuO doped PS films were prepared using solvent casting method. Optical energy band gap E_g was estimated by using UV-VI-NIR spectra and it was classified as an indirect allowed transition. In general E_g was found to decrease with the increasing of dopant concentration. The refractive indices of the samples were measured and it was found to increase with the increasing of dopant concentration. Optical transmittance, reflectance and extinction coefficient were also investigated and correlated with the action of doping process.

بعض المعلمات البصرية لاغشية البولي ستايرين المشوب بؤكسيد النحاس

طارق جعفر علوان و محمد حميد عبدالله

الخلاصة:

في البحث الحالي ،تمت دراسة تأثير الشائبة CuO على الخواص البصرية للبوليمر PS .حضرت أغشية PS المشوبة بـ CuO بأستخدام طريقة صب المحلول. حسبت فجوة الطاقة البصرية (Eg) بأستخدام طيف UV-VI-NIR ، وصنفت كانتقال غير مباشر مسموح. بصورة عامة قلت قيمة (Eg) بازدياد تركيز الشوائب. قيست معاملات الانكسار للعينات ووجد ان معامل الانكسار يزداد بازدياد تركيز الشوائب. النفاذية البصرية ، الانعكاسية ومعامل الخمود فحصت بتأثير عملية الاشابة .

Keywords: Optical Parameters, CuO, PS, band gap, reflectance, optical transmittance

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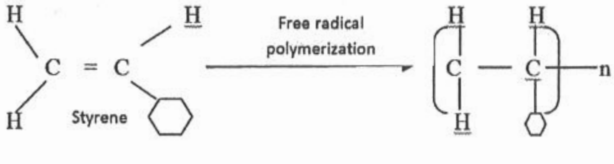
Introduction

Traditionally, polymer matrix composites have been thought as insulating materials and have been used in applications like power tools handles, cables, jackets, capacitor films and electronic packaging materials [1]. Especially the electrical and optical properties of polymers have been extensively investigated due to their applications in optical devices recently. Polymeric materials have unique properties such as low density, light weight, and high flexibility and are widely used in various industrial sectors [2]. In recent years the great progress in understanding polymer surface phenomena and developments in their theoretical description have been done. Forces occurring on polymer surfaces depend on interactions between macromolecules, which are different inside the material and on the phase boundary. Several reactions occur at the polymer surface during modification such as oxidation, crosslinking, degradation and isomerisation (rotation of functional groups) [3]. The determination of the optical constants of polymers such as refractive index and extinction coefficient is also important for optical applications. Furthermore, the refractive index and optical band gap are the fundamental parameters of an optical material, because these are closely related to the electronic properties of the material [4].

The polymer used in this work is polystyrene. The polystyrene is an inexpensive and hard plastic and is more common used in our everyday life [5]. The body of computers we are using now is probably made of polystyrene, and is also used in toys, and the housing of things like hairdryers and kitchen appliances [6]. Polystyrene is vinyl polymer. structurally, it is a long hydrocarbon chain, with a phenyl group attached to every other carbon atom is produced by free radical vinyl polymerization:-



Polystyrene is perfect for optical measurements [7] and immunological assays. it is soluble in aromatic hydrocarbon solvants, cyclohexane and chlorinated hydrocarbons. In the last two decades, many scientists have studied the electrical behavior of modified polymeric materials. These polymers are important for modern technology applications.

In this paper an attempt was introduced to obtain the effect CuO additive on the some optical constants of PS.

Experimental procedure

A high purity PS from BDH was used as a host polymeric material in this research. Chloroform ($CHCl_3$) of purity (99.998 %) and CuO from BDH were used as a solvent and dopant respectively. PS grains of weight (0.2g) were dissolved in (5) Vl of Chloroform ($CHCl_3$) to obtain a solution of (4% wt./vol). The mixture was then shaken well by stirring for about (30 min), in order to obtain homogenous solution, (5ml) of the prepared solution was transferred into a clean glass Petri dish with (6 cm) diameter and dried at a temperature of (50°C) in an oven for at least (2 hours), and then left to cool slowly to room temperature. The dried films were then removed easily by using tweezers clamp. Other similar films were casted in order to ensure dried samples without bubbles and thermal damage. The measured thickness of the prepared films was about (0.05 mm) found by using a digital micrometer.

Doped films were fabricated by dissolving CuO in Chloroform of Concentrations (0, 0.02 and 0.04 w/w). Absorptance and transmittance measurements were carried out by using a double beam UV/VIS spectrometer (Shimadzu Japan) in the wavelength range (190-900) nm.

Results and discussion

Fig. (1-a & b), shows the optical transmission (T%) and reflection (R%) of CuO doped PS films . The reflectance R can calculate from the relationship that correlating the absorptance A, Reflectance R and the Transmittance (T) as below:-

$$R=1-A-T \qquad (1)$$

From Fig (1), it is clear the transmission of the PS films decreases with dopaing, while the reflection of the films increases with doping. The optical absorption coefficient (α) of PS is very important because it provides information on the electronic band structure, the band tail and energy gap. The absorption coefficient (α) can be determined as a function of frequency using the formula [8]:

$$\alpha = \frac{2.303\,A}{d} \qquad (2)$$

Where:

d = the film thickness, A = absorbance.

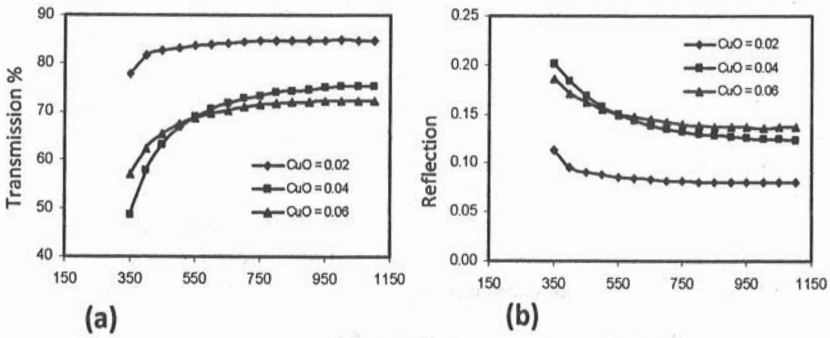


Fig. (1) a- Transmission (%). b- Reflection (%) of, 2, 4, 6 wt% CuO doped PS.

The absorption coefficient is connected with the nature of electronic transitions. Type of the electron transitions can be known by dependence on the values of the absorption coefficient; if the values of ($\alpha > 10^4$ cm^{-1}), this means the direct transitions takes place in material, while indirect transitions occur for ($\alpha < 10^4$ cm^{-1}) [9]. The optical absorption spectra could reveal the energy gap E_g between the Conduction Band (CB) and the Valence Band (VB) due to direct and indirect transitions of both crystalline and amorphous materials. The results show the value of (α) for CuO doped PS films is less than (10^4 cm^{-1}). In order to confirm the nature of optical transition the optical data was analyzed using the relation:

$$\alpha h\nu = B(h\nu - E_g)^m \quad (3)$$

Where:

h = Planck constant.

E_g= Optical energy band gap.

B = A constant known as the disorder parameter which is nearly independent of the photon energy. Parameter (m) is the power coefficient with the value that is determined by the type of possible electronic transitions, i.e., m = 1/2, 3/2, 2or 1/3 for direct allowed, direct forbidden, indirect allowed and indirect forbidden respectively [8]. The plot of the product of absorption coefficient and photon energy $(\alpha h\nu)^{1/2}$ versus the photon energy at room temperature shows in Fig.(2). Extrapolation of the linear portion of this curve to a point $(\alpha h\nu)^{1/2}$ =0, gives the optical energy band gap (E_g) for the doped PS films.

The plots in Fig (2) show E_g decreases with increasing the concentration of CuO. It was found that E_g decreases from 4 eV for 2 wt% CuO concentration, to 3.9 eV for 6 wt% CuO concentration.

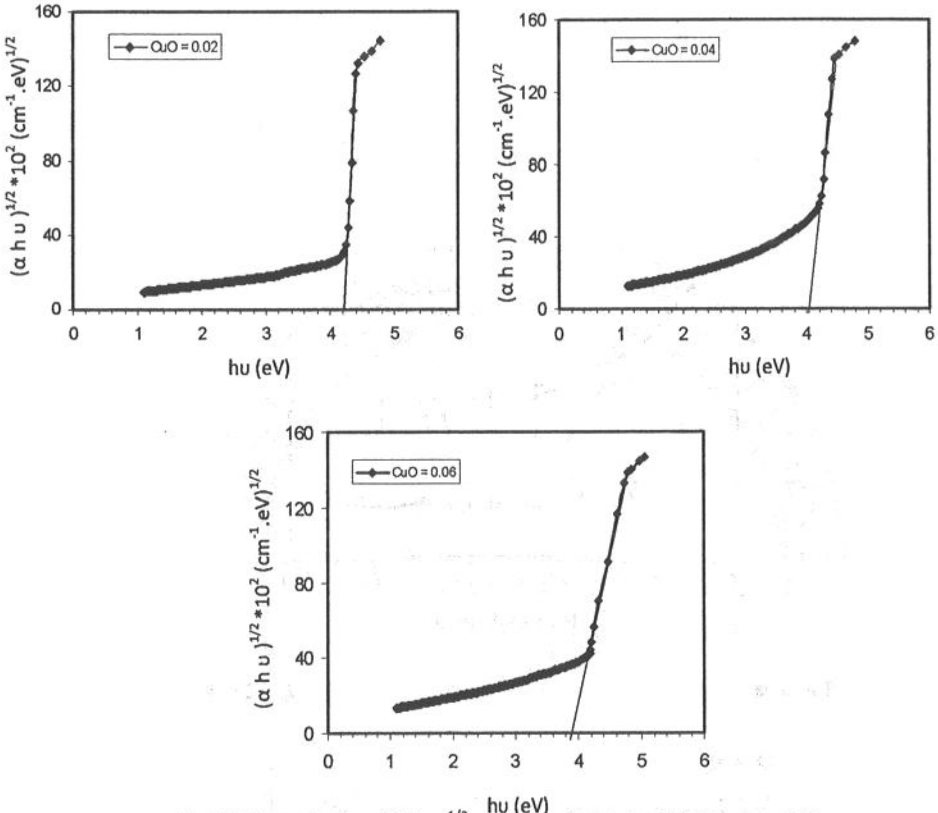


Fig. (2) The variation of $(\alpha h\nu)^{1/2}$ with hν of 2, 4, 6 wt% CuO doped PS.

The extinction coefficient can be calculated by the relation [10]:

$$k = \frac{\alpha\lambda}{4\pi} \qquad (4)$$

Where (λ) is the wavelength, (α) is the absorption coefficient.

The refractive index (n) of the film was calculated by the following equation [11]:

$$n = \left[\left(\frac{1+R}{1-R}\right)^2 - \left(k^2+1\right)\right]^{1/2} + \frac{1+R}{1-R} \qquad (5)$$

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Where k is the extinction coefficient and R is the reflectance.

The evaluation of refractive index of an optical material is important for many applications especially in optical devices. Fig.(3)and (4) shows the variation of refractive index n and extinction coefficient k with wavelength, from which it can be noticed that, in general, we can see from this figures that the values of n and k in general increased with doping.

All the change in optical parameters of PS after doping can attribute to the effect of CuO doped on the structure of PS, which creates a localized energy states in the forbidden band gap acts as a tail to the conduction band which reduced the energy gap.

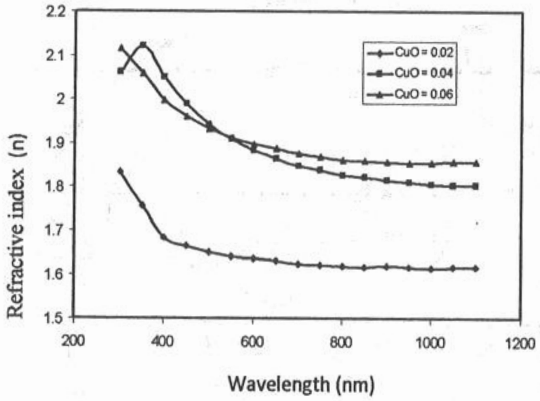

Fig.(3) The variation of refractive index (n) with Wavelength (nm) of 2, 4, 6 wt% CuO

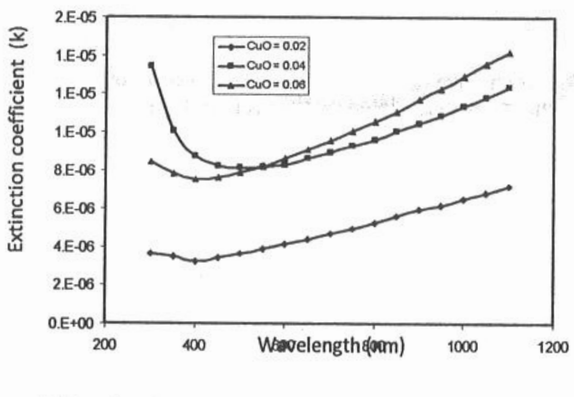

Fig.(4) The variation of extinction coefficient (k) with Wavelength (nm) of 2, 4, 6 wt% CuO doped PS films

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Conclusions:

From the present work, the followings can be concluded:-

1- The doping process decreases the transmission, while the reflection increases with doping.
2- The type of electronic transition was found to be an indirect allowed transition.
3- Optical energy band gap decreases with doping.
4- Refractive index and extinction coefficient increases with doping.

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