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Optical Properties of ZnO/PVC Composites

Abeer D. Adaileh
Applied Sciences Private University, Amman, Jordan

Abstract: The optical properties of prepared ZnO/PVC composites with different concentration: 0, 2, 6, 9 wt.% of ZnO have been investigated. The optical spectra were obtained in the UV wavelength range (400-800 nm) using a spectrophotometer. The absorption coefficient and the optical Energy gap (E_{opt}) have been obtained from indirect allowed electron transitions in k-space at room temperature. The tail widths of localized states in the band gap (E) were evaluated using the Urbach-edges method. It was found that both E_{opt} and E vary with the concentration of ZnO in the composite.

Key words: ZnO, PVC, composites, absorption, energy gap, transitions

INTRODUCTION

In recent years, polymers with different optical properties have been attracted much attentions due to their applications in the sensors, light emitting diodes and others. The optical properties of polymers can be suitably modified by the addition of particulate fillers. One of the fascinations of working in the field of particulate-filled polymer composites is the wide variety of materials used as fillers from relatively simple chalks and limestones to complex rare earth magnetic powders (Rothon, 2003; Callister, 2007; Mitchell, 2004).

This study is concerned with the study of some optical properties of ZnO/PVC composites. The optical energy gaps andenergy tails of the prepared composites are studied as a function of ZnO concentration.

MATERIALS AND METHODS

Experimental work

Composites preparation: PVC-ZnO composites with different filler concentrations (2, 6 and 9 wt.% ZnO) and neat PVC were prepared. PVC and ZnO powders were blended together in Tetrahydrofuran (THF) as a convenient solvent. Then, for 2 days the mixture was mixed by using a rotary magnet to get a homogeneous mixture. On to a glass mould the mixture was directly casted to delicate films. At room temperature by waiting for two days the Tetrahydrofuran (THF) was permitted to evaporate perfectly. All samples were dried at room temperature for 2 days (Elshabini *et al*., 1998; Shi, 2003).

Optical measurements: The study of optical absorption gives informationabout band structure of solids. The optical Absorbance (A) of the sample's sheets was taken in the wavelength (λ) range (400-800 nm) at room temperature by usingthe Cary spectrophotometer. The absorption coefficient α(λ) was calculated from the Absorbance (A) spectra using the relation (Ismail *et al*., 2012; Deshmukh *et al*., 2008; Al-Ani and Hogarth, 1984):

$$I = I_o \exp(-\alpha x) \quad (1)$$

Hence:

$$\alpha(\lambda) = (2.303/x)\log(I/I_o) = 2.303x^{-1}A \quad (2)$$

Where:

- I and I_o = The incident and transmitted intensity UV-radiation, respectively
- x = The sample thickness which was 75 μm

It was measured by a sensitive digital vernier caliper.

RESULTS AND DISCUSSION

At high absorption levels where, $\alpha(\omega)>10^4$ cm^{-1}, the absorption coefficient for non-crystalline materials has the following frequence dependence (Ramadin *et al*., 2000; Sbeih and Zihlif, 2009):

$$\alpha(\omega)\hbar\omega = B(\hbar\omega-E_{opt})^r \quad (3)$$

where, B is a constant, E_{opt} is the optical energy gap and the exponent r is an index determined by the type of electronic transitions causing the optical absorption, and can take values 1/2, 3/2 for direct and 2, 3 for indirect transitions (Sbeih and Zihlif, 2009).

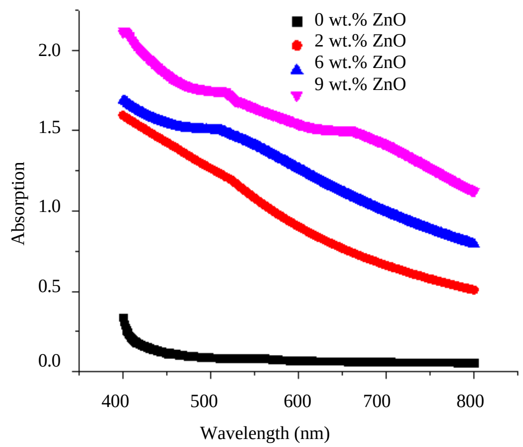

Fig. 1: Absorption spectra for ZnO/PVC composites

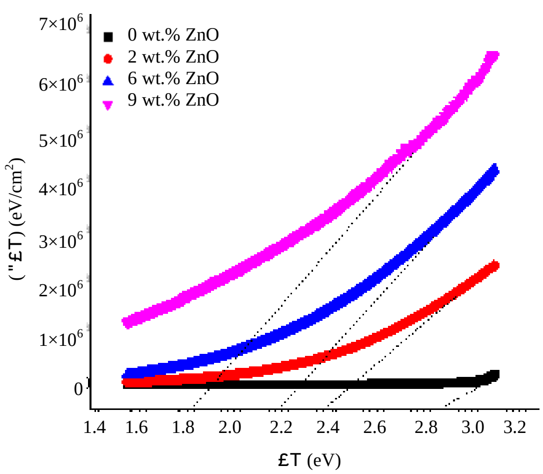

Fig. 2: $(\alpha\hbar\omega)^2$ vs. the incident photon energy for ZnO/PVC composites

Figure 1 shows comparative graphs of absorption spectra for the four samples neat PVC, 2, 6, 9 wt.% composite samples. One can clearly notice that absorption decreases rapidly with an increase in the wavelength.

Figure 2 shows the product of absorption coefficient (α) and photon energy $(\alpha\hbar)^{1/r}$ vs. photon energy ($\hbar\omega$) at room temperature for four samples. A good straight line is obtained with r = 2. This indicates that the transition energy for electrons is indirect in k-space. The values of E_{opt} extrapolated from the linear portion in the high region are listed in Table 1. The decrease in E_{opt} with filler content can be understood by considering the mobility gap variation in composites as proposed by Davis and Mott. The variation of the optical energy gap with the filler concentration is shown in Fig. 3. The values of the constant B are obtained from the slope of the linear part

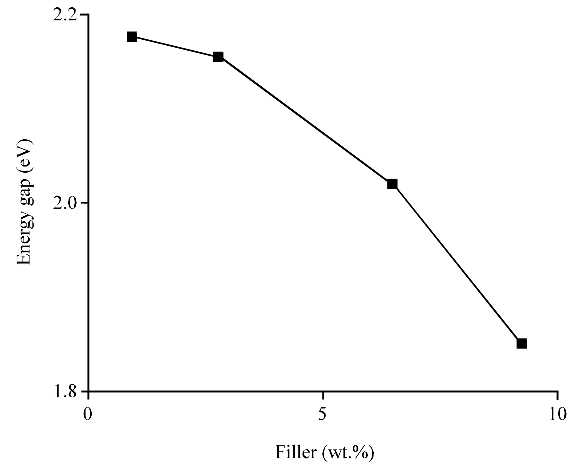

Fig. 3: Variation of the optical energy gap with oil ZnO concentrat

Table 1: Optical results

Materials	E_{opt} (eV)	ΔE (eV)	B (eV/cm^2)
Pure PVC	2.31	0.27022	2.621×10^3
ZnO/PVC (2/98 wt.%)	2.28	0.29207	1.63891×10^5
ZnO/PVC (6/94 wt.%)	2.10	0.39039	6.13186×10^5
ZnO/PVC (9/91 wt.%)	1.87	0.45171	2.00825×10^6

of these figures and also listed in Table 1 (Sbeih and Zihlif, 2009; Saq'an *et al*., 2004; Ayesh and Abdel-Rahem., 2008; Ahmed, 2009).

At lower absorption level in the range of 1-10^4 cm^{-1}, the absorption coefficient $\alpha(\omega)$ is described by the Urbach formula:

$$\alpha(\omega) = \alpha_0 \exp(\hbar\omega/\Delta E) \quad (4)$$

Where:

α_0 = A constant

ΔE = The Energy gap tail (or energy which is interpreted as the width of the tail of localized states in the forbidden band gap)(Sbeih and Zihlif, 2009)

Figure 4-7 present the Urbach plot for the four composite samples. The values of ΔE were obtained and listed in Table 1. The exponential dependence of $\alpha(\omega)$ on $\hbar\omega$ for these samples indicates that they obey the Urbach's rule. These tails become higher as the concentration of the ZnO increases which is consistent with E_{opt} variation (Table 1). The increase of the tail width with the ZnO concentration can be explained by the fact that the increase in ZnO concentration could lead to the creation of disorder and imperfections in the structure of the composites.

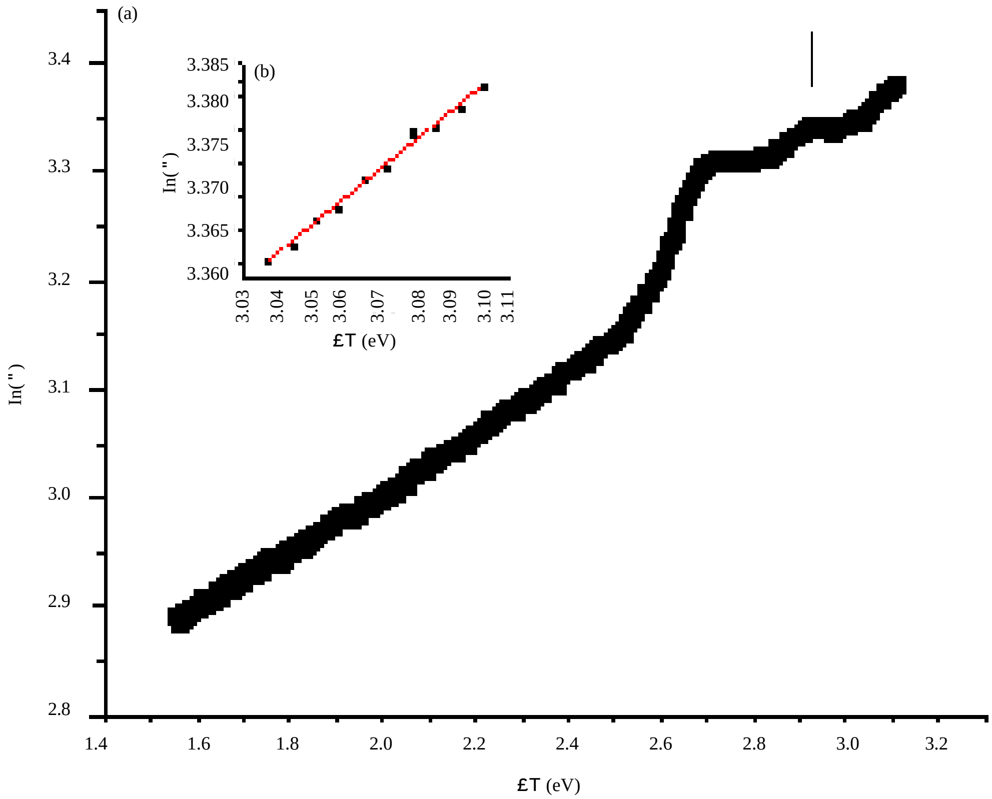

Fig. 4a, b): Natural logarithm of a vs. the incident photon energy for neat PVC

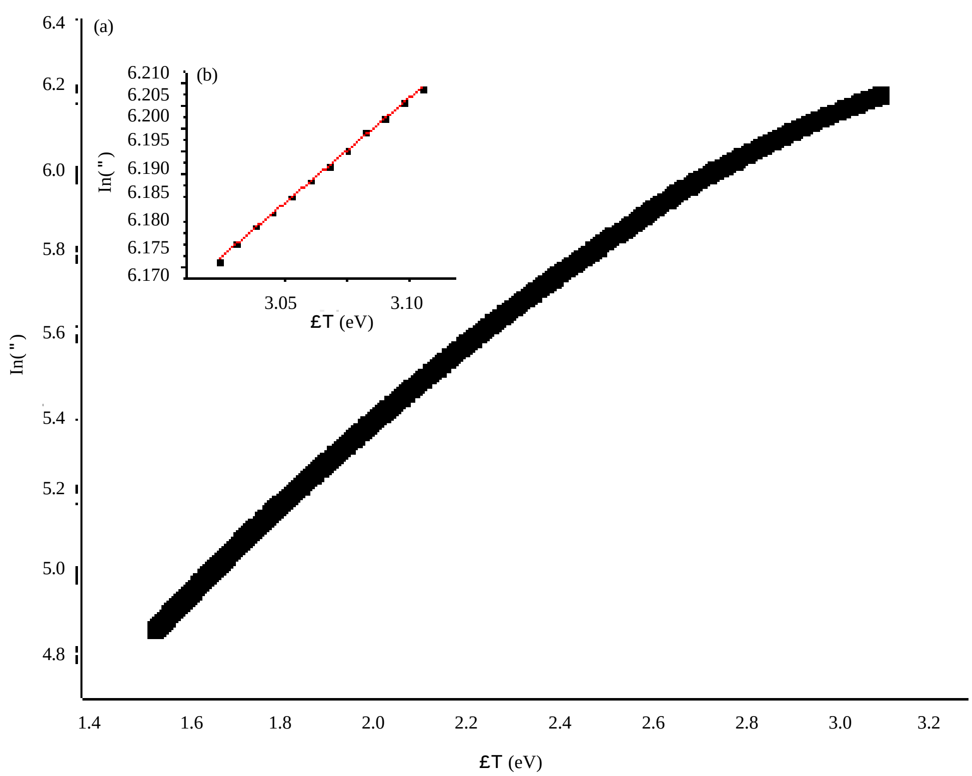

Fig. 5a, b): Natural logarithm of a vs. the incident photon energy for 2 wt.% ZnO composite

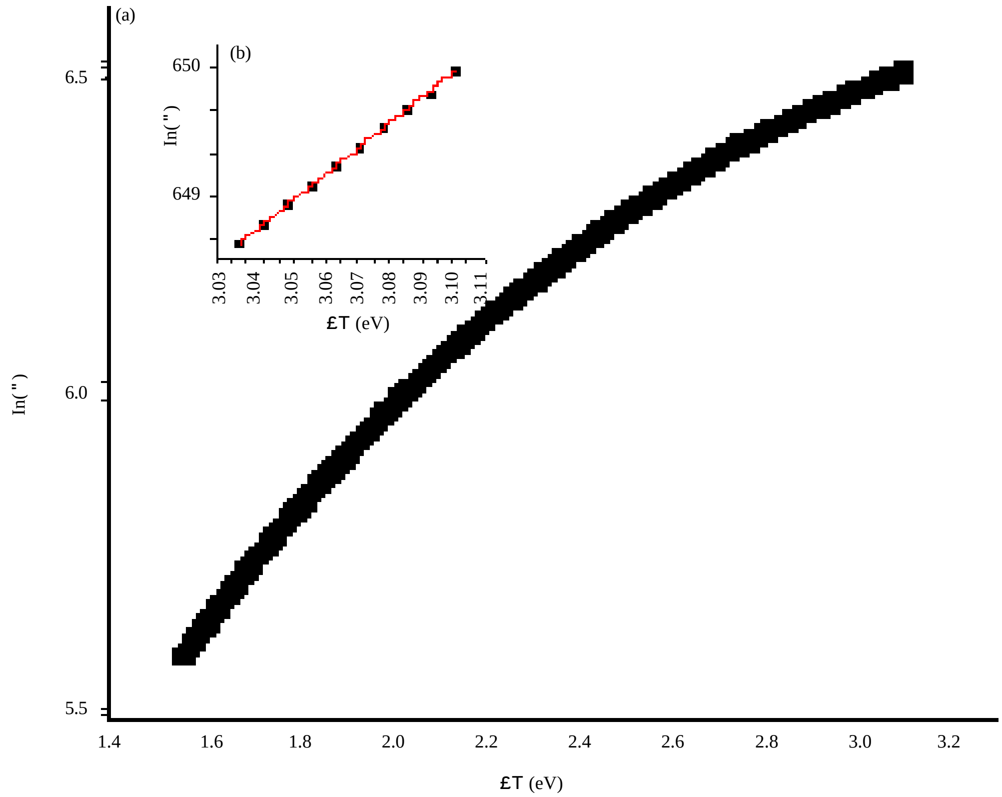

Fig. 6a, b): Natural logarithm of a vs. the incident photon energy for 6 wt.% composite

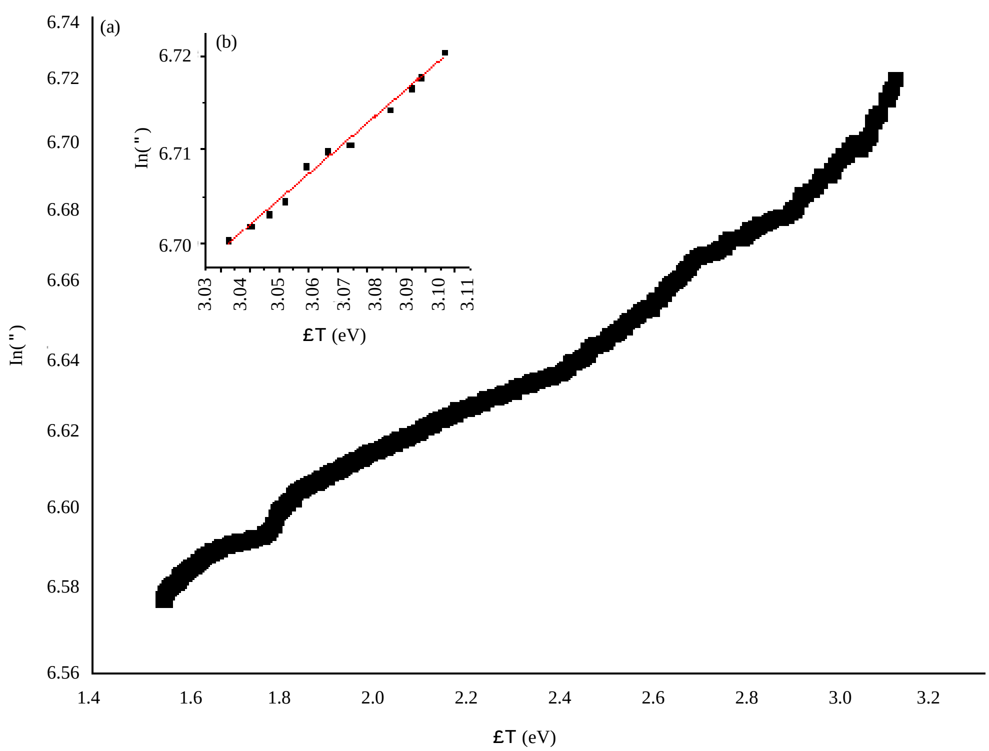

Fig. 7a, b): Natural logarithm of a vs. the incident photon energy for 9 wt.% composite

CONCLUSION

The optical properties of ZnO/PVC composites were studied as a function ZnO concentrations. From the results obtained, we conclude the followings: analysis of the optical results indicates that the electrons transition energy is indirect in k-space. The optical Energy gap (E_{opt}) values decreases with increasing the ZnO concentration. The band Energy tail (E) increases with increasing the ZnO concentration.

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