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Linear optical properties and energy loss function of Novolac: Epoxy blend film

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ABSTRACT

In the present work, thelinear optical properties of Novolac: Epoxy films(10 μm thicknesses) have been calculated depending on the absorbance and transmittance spectra at wavelength range (300-900 nm). The linear optical parameter include calculation (refractive index n, absorption coefficient α, extraction coefficient k.Real and imaginary part of dielectric ε_r, ε_i, and optical and electrical conductivity σ_{op}, σ_e). The surface, volume energy loss function and electronic interband transition strength have been calculated depending on dielectric constant of the bland. The values of direct and indirect energy gap have been found using Tucc procedure ,equals to [(C1 (2.295 ev), C2 (2.408 ev) , C3 (2.655 ev) and C4 (3.792 ev)], and[C1 (1.95 ev), C2 (2.025 ev) , C3 (2.06 ev) and C4 (3.553 ev)]respectively. In addition to that, ithave be foundalso that the type of electronic transmission is indirect.

Keyword:, Optical properties;refractive index;Optical Energy gap;Novolac; interband transition strength, surface and volume energy loss.

INTRODUCTION

Recently, the search for optical properties increase because of their applications in integrated optics such as optical modulation, optical information, and optical data storage [1]. The optical behavior of a material is utilized to determine its optical constants. Films are ideal specimens for reflectance and transmittance,therefore, an accurate determination of the optical constants is extremely important [2].The study of optical absorption, particularly absorption edge has proved to be very useful for elucidation of the electronic structure of the materials. It is possible to determine indirect and direct transition occurring in band gap by optical absorption spectra [3].The date transmittance can be analyzed to determine optical constants such as refractive index, absorption index and dielectric constant.The refractive index is one of the fundamental properties of a material, because it is closely related to the electronic polarizability of ions and the local field inside the material.The evaluation of refractive indices of optical materials is considerable importance for applications in integrated optics devices such as switches fillers and modulators, etc., where the refractive index of a material is the key parameter for device design [4].

Polymers are attractive materials due to their easy fabrication process and low cost [5-7] therefore manyresearchers deals with investigation of new types of polymer materials. In thisresearch epoxy is the diglycidyl ether of bisphenol –A (DGEBA) and Novolacare choosingdue to its excellent properties. The epoxy (DGEBA) is a commonly used composite material precursor and has many excellent properties, such as high electricalresistance, good mechanical properties which high workability under various processing conditions. However, sinceDGEBA degrades easily at high temperatures, the use of additives to improve thermalstabilization and flame retardantproperties is an area of great interest.[8].

we can classified the Novolacto two types of phenol resins: resold and Novolac. The first one is synthesized under basic pH conditions withexcess formaldehyde, and the second is carried out at acidic pH (with an excess of phenol).

They are widely used in industry because of their chemical resistance, electrical insulation, and dimensional stability [9].

The interaction of the photons with the material results in excitation of electrons into unoccupied energy levels in the conduction band as well as collective excitation of valence electrons. Interband transitions originate from the excitation of electrons in the valence band to empty state in the conduction band, so thesecan be identified as transition in a band structure model [10]. The excitation of the electrons valence band can be distinguished between collective plasma oscillations and single electron interband transition.The latter depend on critical point in the band structure [11]. The is two regions for electronic energy loss function. The first region is the high loss energy region (>1eV), analysis of the first (10 eV) of spectra after the ionization edge can give information about the oxidation state. The second region is the low energy loss (<1 eV) which can provide information about composition and electronic structure [10]. The energy loss function results from dielectric constant of the materials within the range of validity of the dielectric theory [12-14].

This paper reports the results of linear optical properties of Novolac film of thickness (10µm) in the wavelengthrange (300-900 nm).

MATERIALS AND METHODS

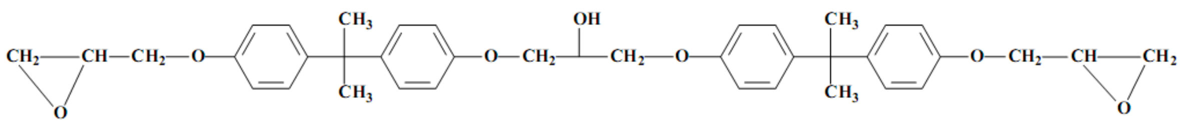
2- Experimental

Preparation Material

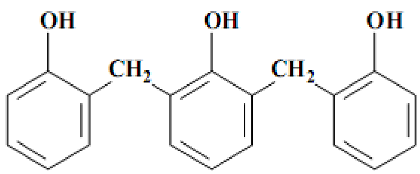
Ethanol form Fluke Co., Novolac and Epoxy from physical measurements, IR spectra were recorded on Buck 500 IR spectrophotometer using nojul in the range (4000-600 cm^{-1}) Absorption spectra are recorded using Reflactophotometer CE-3000 in the wavelength range (300-900 nm).

The Novolac (A)(0.1 mol,10.7 gm) dissolved in Ethanol (100 mol) is added to Epoxy (DGEBA) (B),(M.wt =626.77) with deferent volume ratio (1:1,1:2,1:3). The mixture is stirred for one hour at room temperature to produce polymer blend (Epoxy: Novolac)(c).

Fig.(1): Shows the chemical structure of (A)and (B).



(A) - Epoxy (DGEBA)



(B)-Novolac

Fig. 1.Chemical structures of (A) - epoxy (DGEBA), (B) –Novolac [15].

The film of Novolac: Epoxy is prepared using spin coating method using speed 2500 r/min and we cast on glass (2 cm ×2 cm) size , the film is heated at (80 ^{0}C) for one hr. In order to determine optical properties a measurement of the spectral absorption (A) and transmittance (T) are done.

IR Spectra

The IR Spectra of Novolac and epoxy compounds are recorded as liquid and the spectra data of the products are gathered in Fig. (2) and Table (1) .

The Novolac compound exhibited intense IR absorption at around (3550-2900) cm^{-1} due to ν(OH) . The presence of OH- groups involved in intramolecular hydrogen bonding for compound give the ν (OH) as a shallow, very broad band extending.

Within the (3550-2900) cm^{-1} . Compounds containing OH groups displays bands at (1190-1150) cm^{-1} ν(OH). The stretching vibrations of the aromatic C-H groups give medium to weak bands within the (3090-3020) cm^{-1} ν(OH) but the display because of the interaction with OH bands .The (C=C) gives band at 1610 cm^{-1} .The CH aliphatic gives bounds at 1480 cm^{-1}as shown in fig.(2-a) . The epoxy compound exhibited intense IR absorption at around (3500- 3430) cm^{-1} , 3070 cm^{-1}, 2970 cm^{-1}, 1600 cm^{-1} and 1475 cm^{-1} due to ν(OH) , ν(C-H) aromatic , ν(C-H) aliphatic , (C=C) aromatic and (C-H) aliphatic respectively as shown in fig.(2-b). Fig. (2-c,d,e) (Epoxy and novolac)asat deferent volume ratio(1:1,1:2,1:3) displays the bands which confirm physical blending of compounds.

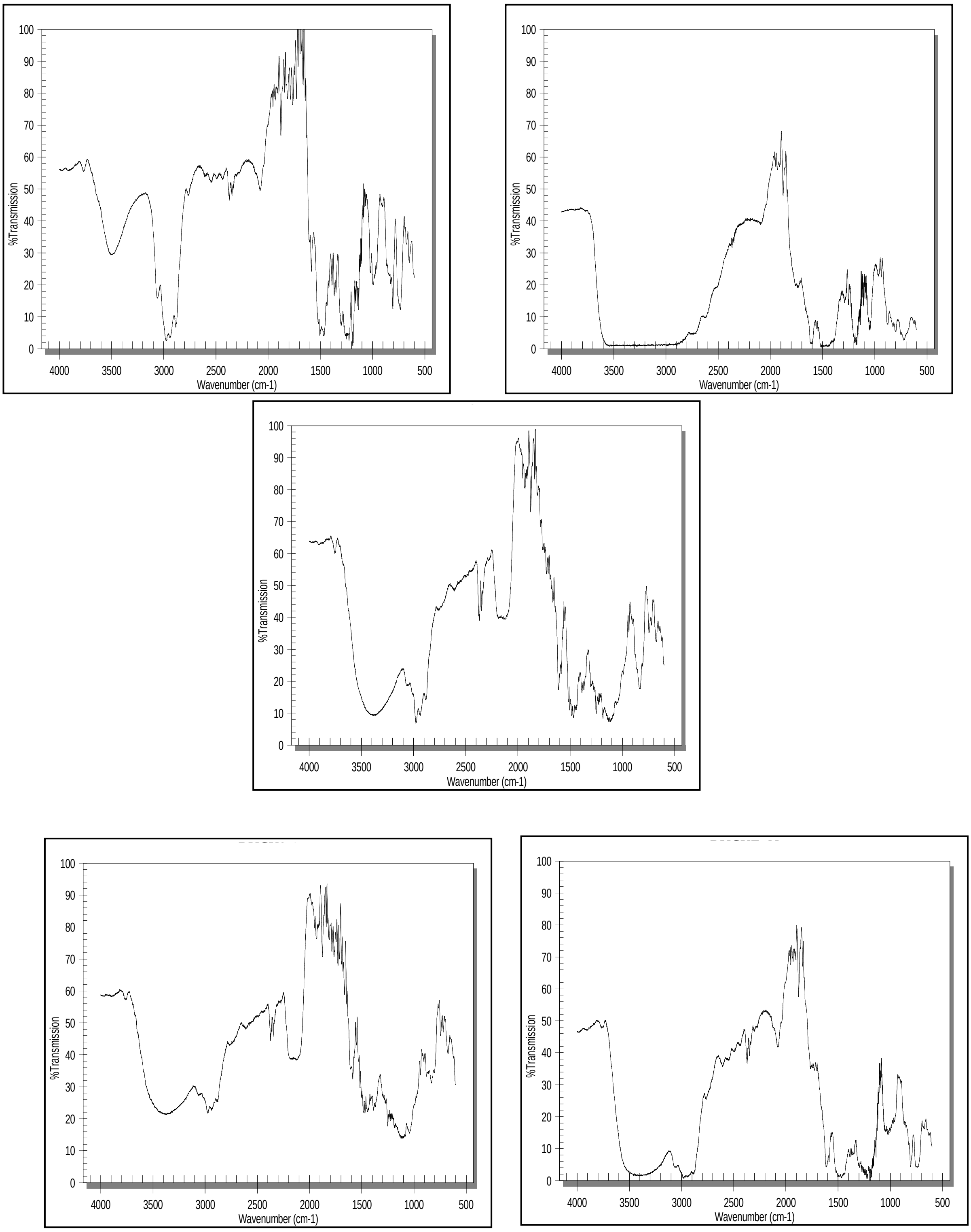


Fig.(2) IR spectra of (a) epoxy ,(b) novolac, (c),(d) and (c) epoxy and novolac for the volume ratio(1:1, 1:2, 1:3)respectively.

Table (1) : IR spectra data for novolacepoxy (c)

Materials	OH	CH(aromatic)	CH(aliphatic)	C=C
Novolac	(3550-2900)	3080	2980	1620
Epoxy	3500	3090	2950	1610
Epoxy and novolac(1:1)	3500-3300	3080	2970	1600
Epoxy and novolac(1:2)	3480-3250	3080	2970	1600
Epoxy and novolac(1:3)	3520-3140	3080	2970	1600

RESULTS AND DISCUSSION

The absorption coefficient (α) has been obtained directly from the absorption spectra using Beer-Lambert low α =2.303(A/d) [16] where (A) is the absorbance and (d) is the thickness of the film. Fig. 3 shows (a) the absorbance, (b) the transmittance (T) , (c)the Reflectance(R), as a function of wavelength, and (d) absorption coefficient (α) as a function of photon energy.

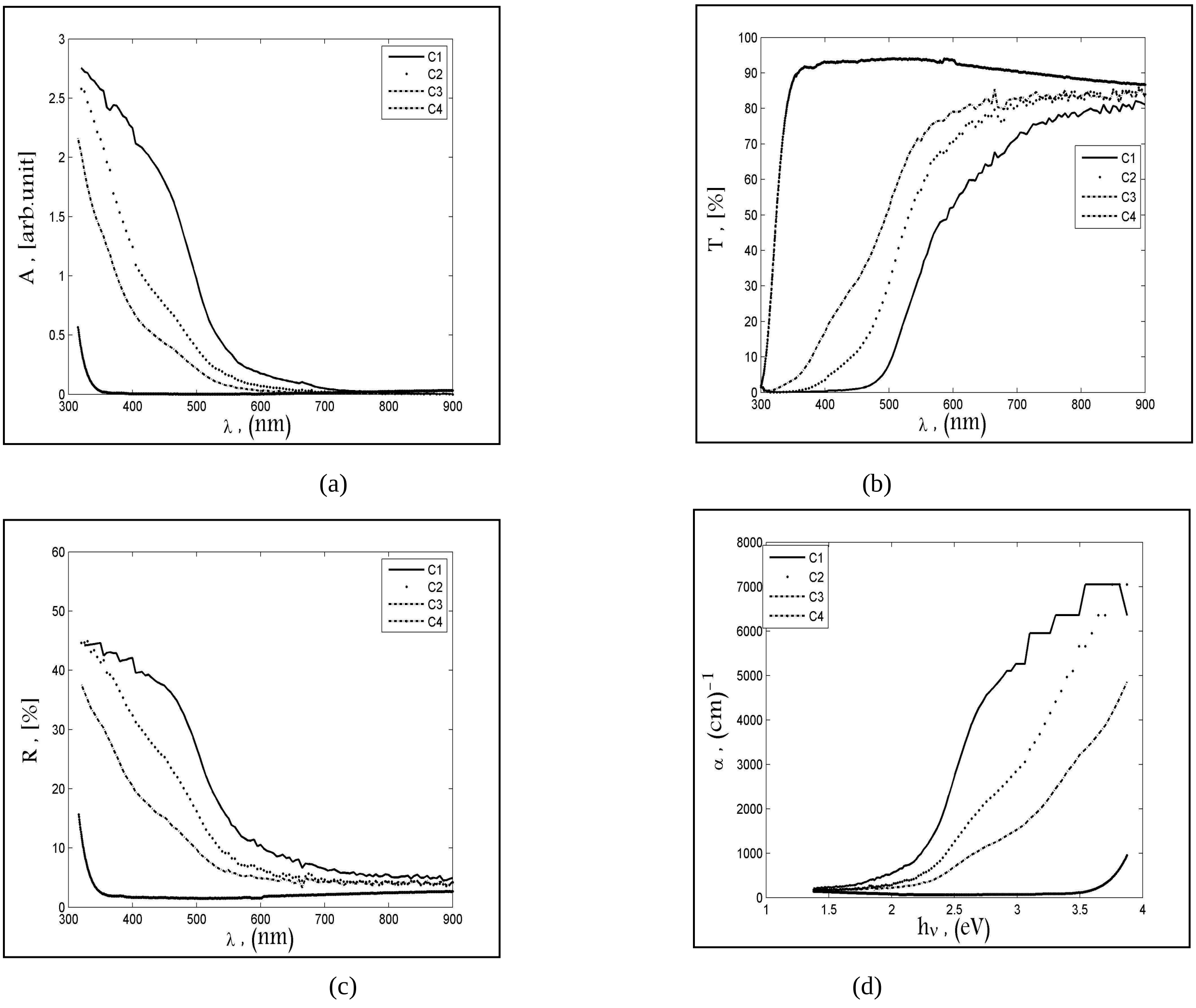


Fig. 3. (a) the absorbance, (b) the transmittance (T) ,(c) the Reflectance(R), as a function of wavelength. (d) absorption coefficient (α) as a function of photon energy for the volume ratio
C1: 1 Epoxy : 1 Novolac C2: 2 Epoxy : 1 Novolac
C3: 3 Epoxy : 1 Novolac C4: Epoxy Pure

The theory of reflectivity of light has been used to calculate the value of refractive index (n) and extinction coefficient k . The value of n and k has been calculated using the following equations[17].

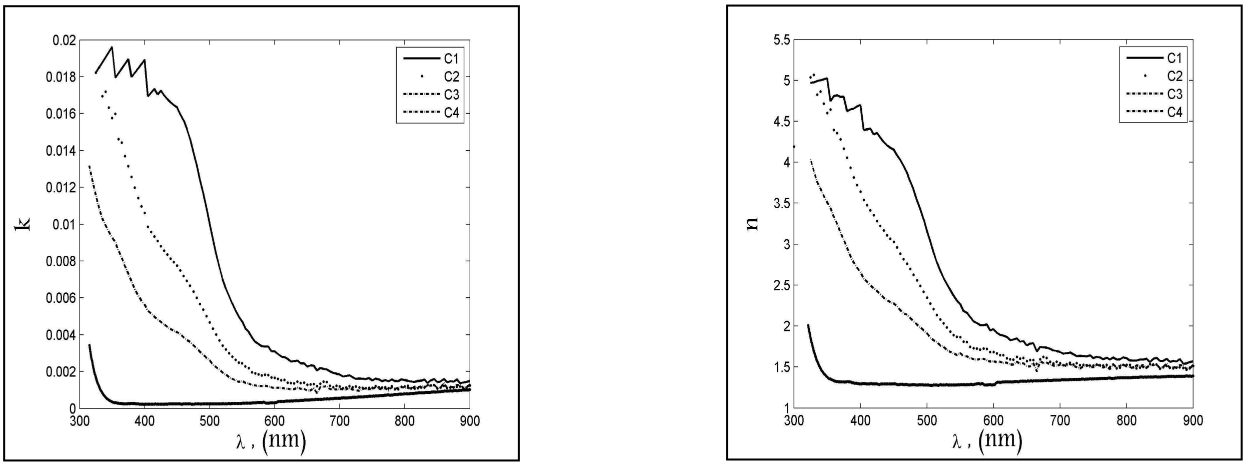
$$k = \alpha\lambda / 4\pi \qquad (1)$$

And

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

Where λ is the wavelength.

Fig. 4 shows(a)extinction coefficient (k),and(b) Refractive index (n),as a function of wavelength.



(a) (b)

Fig. 4 (a) extinction coefficient (k),(b) Refractive index , as a function of wavelength.for the volume ratio
C1: 1 Epoxy : 1 Novolac C2: 2 Epoxy : 1 Novolac
C3: 3 Epoxy : 1 Novolac C4: Epoxy Pure

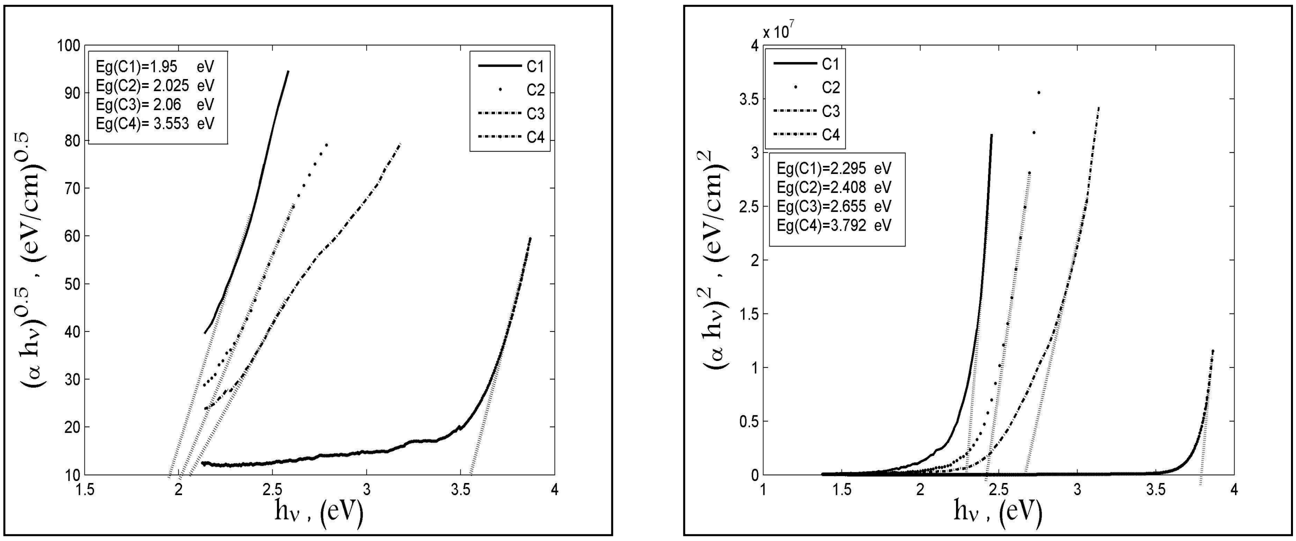
Fig.3 (a) represents the absorbance curve ofNovolac: Epoxy film as a function of wavelength and it iswell noted that the greatest value of the absorption occurs at the wavelength range 300-350 nm and then gradually decreases to reach, in the wavelength range for the volume ratio (C1,C2,C3,C4), (700-900, 650-900, 600-900, 350-900) nm,The edge of the absorption occurs at wavelength 560 nm. The optical transmittanceand Reflectancespectra, in the range of (300–900 nm) wavelength for the Novolac: Epoxy filmis depicted in Fig. 3 (b).The optical transmission data are employed to obtain various parameters which could help in having a better understanding of the optical behavior of the Novolac: Epoxy film.

The fundamental absorption edge follows an exponential law above the exponential tail, the absorption coefficient has been reported to obey the following equation[18.19]:

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

Where B is constant, $h\nu$ is photon energy, , $E_g$is optical Band gap and n is an exponent, which can be assumed to have values of 1/2,3/2,2 and 3 depending on the nature of electronic transition responsible for the absorption. n=1/2 for allowed direct transition, n=3/2 for forbidden direct transition,n=2 for indirect allowed transition, and n=3 for forbidden indirect transition. The direct and indirect energy gap is calculated by plot $(\alpha h\nu)^{0.5}$ and $(\alpha h\nu)^2$ as a function to photon energy (hν) for the film as shown in fig. (5).

E_g^d And E_g^{ind} values are obtained by extrapolating the linear portion of the plots to intercept the photon energy axis (Fig. 5) The calculated values of $E_g$are given in Table 2.



(a) (b)

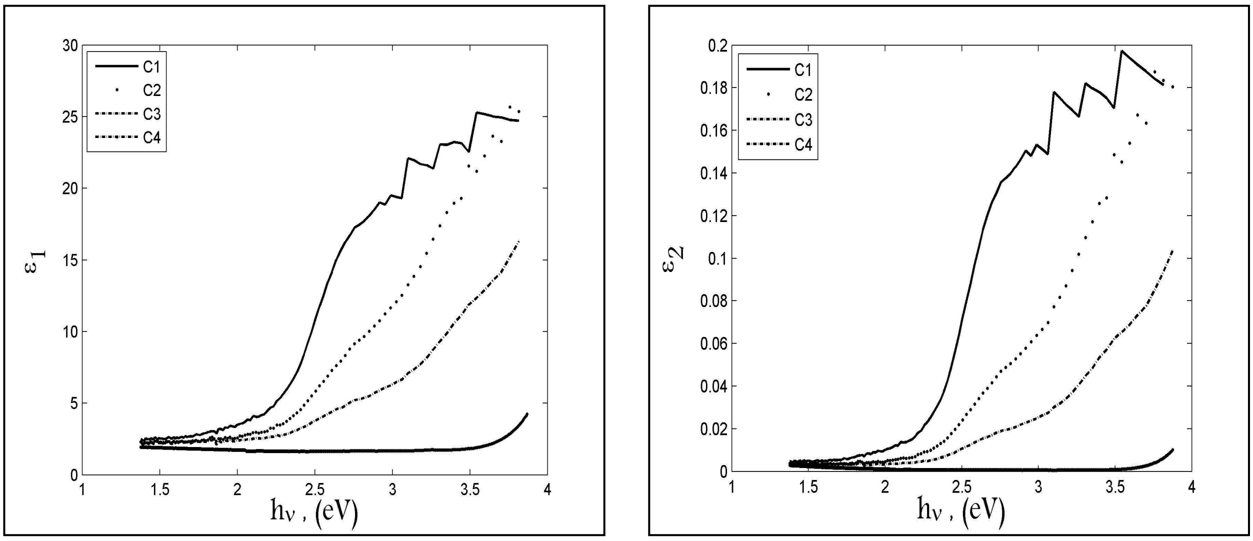
Fig. 5 plot (a) $(\alpha h\nu)^{0.5}$,(b) $(\alpha h\nu)^2$ as a function to photon energy (hν).for the volume ratio
C1: 1 Epoxy : 1 Novolac C2: 2 Epoxy : 1 Novolac
C3: 3 Epoxy : 1 Novolac C4: Epoxy Pure

Fig. (6) show the variation of real and imaginary dielectric constant fo Novolac:Epoxy film . The complex dielectric constant is a fundamental material property .the real part of it is associated with the term of how much it will slow down the speed of light in the material and the imaginary part gives that how a dielectric absorb energy from electric field due to dipole motion. The real and imaginary part of the dielectric constant was determined using the relation [20].

$$\varepsilon_r = n^2 - k^2 \qquad (4)$$

$$\varepsilon_i = 2nk \qquad (5)$$

Where ε_r and ε_i are the real and imaginary parts of the dielectric constant respectively.



(a) (b)

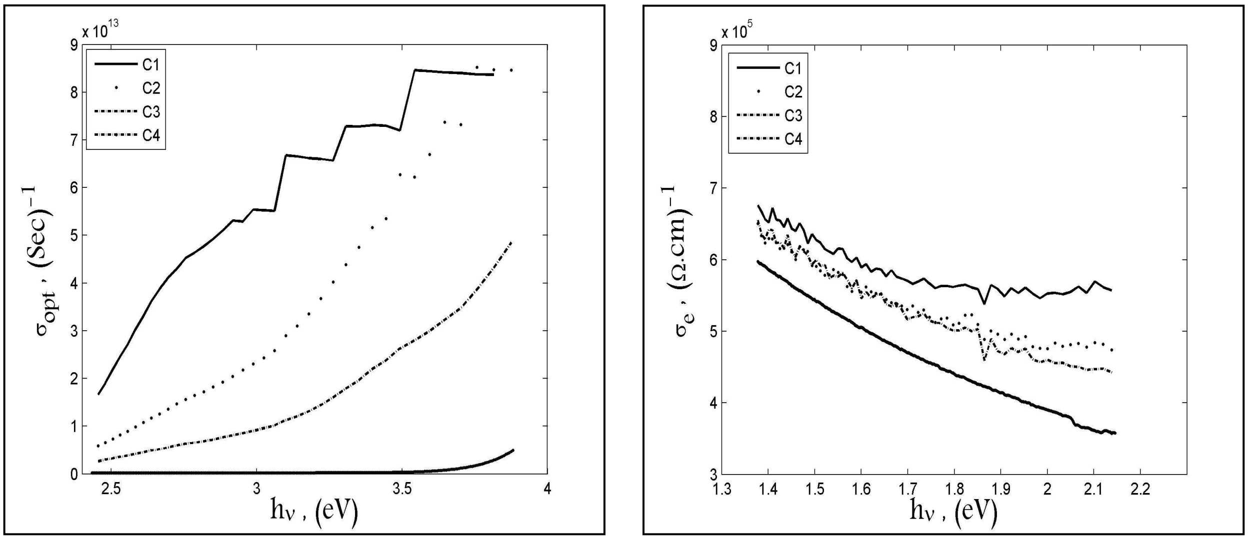
Fig.(6) Plot (a)real part ε_1 and (b) imaginary part ε_2 of the dielectric constant as a function of phonon energy for the volaume ratio
C1: 1 Epoxy : 1 Novolac C2: 2 Epoxy : 1 Novolac
C3: 3 Epoxy : 1 Novolac C4: Epoxy Pure .

The dielectric grow gradually with the photon energy which is reached to the highest value when the energy is greater than for (C1 (2.2 ev),C2(2.3 ev),C3(3.1 ev) and C4(3.5 ev)) , In addition, the value of the real part is greater than the value of the imaginary part and this indicates that the material in response to light falling on any of its response to visual and clear.The variation of optical conductivity σ_{op} and electric conductivity $\sigma_e$as a function to photon energy (hν) are show in the Fig. (7) and they are determined using the relations [20]

$$\sigma_{op} = \alpha nc/4\pi \qquad (9)$$

$$\sigma_e = 2\lambda\sigma_{op}/\alpha \qquad (10)$$

where c is the velocity of light.



(b) (a)

Fig.(7) Plot (a)optical conductivity σ_{opt} and(b) electrical conductivity σ_e of the dielectric constant as a function of phonon energy for the volume ratio
C1: 1 Epoxy : 1 Novolac C2: 2 Epoxy : 1 Novolac
C3: 3 Epoxy : 1 Novolac C4: Epoxy Pure

It can be noted from Fig.(7-a)that the optical conductivity increases with the photon energyand the value of optical about 10^{13} for all the volume ratio,this shows the optical response of the material that led to be the movement of electrons through the material and in Fig.(7-b)that the electrical conductivity decreases with the photon energy and the value of optical about $10^5$and the optical and electrical conductivity have same image by increasing photon energy and optical conductivity higher than electrical.

In general, the realand imaginary parts of the dielectric increaseswith increasing of photon energy, this behaviorleads to increased extinction and electronictransfers through the material from valence bandto conduction band. The random electronictransfers makes electronic collisions elastic andinelastic lead to increase the dielectric constant.

The interband transition strength J_{cv} is accounts for the dipole selection rules for the

Transitions [21]. J_{cv} is proportional to the probability that a transition of an electron between the filled valence band and the empty conduction band with transition energy takes place and relates to complex dielectric constant (ε)by [22]

$$J_{cv} \equiv J_{cv1} + iJ_{cv2} = \frac{m^2 4\pi^2}{e^2 h^2}\frac{E^2}{2}(\varepsilon_2 + i\varepsilon_1) \qquad (6)$$

Where J_{cv1}, J_{cv2} are the real and imaginary part of interband transition strength, m: mass of the electron, E is the photon energy, e charge of the electron and h blank constant. $J_{cv}(E)$

is proportional to the transition probability and it has units of. g .cm^{-3} For computational convenience, we take the prefactor ($\frac{m^2 4\Pi^2}{e^2 h^2}$) in Eq. (6), whose value in8.289×10^{-6}g .e V^{-2}as unity is token , J_{cv} calculated from Eq. (6) is shown in the Fig. (8).

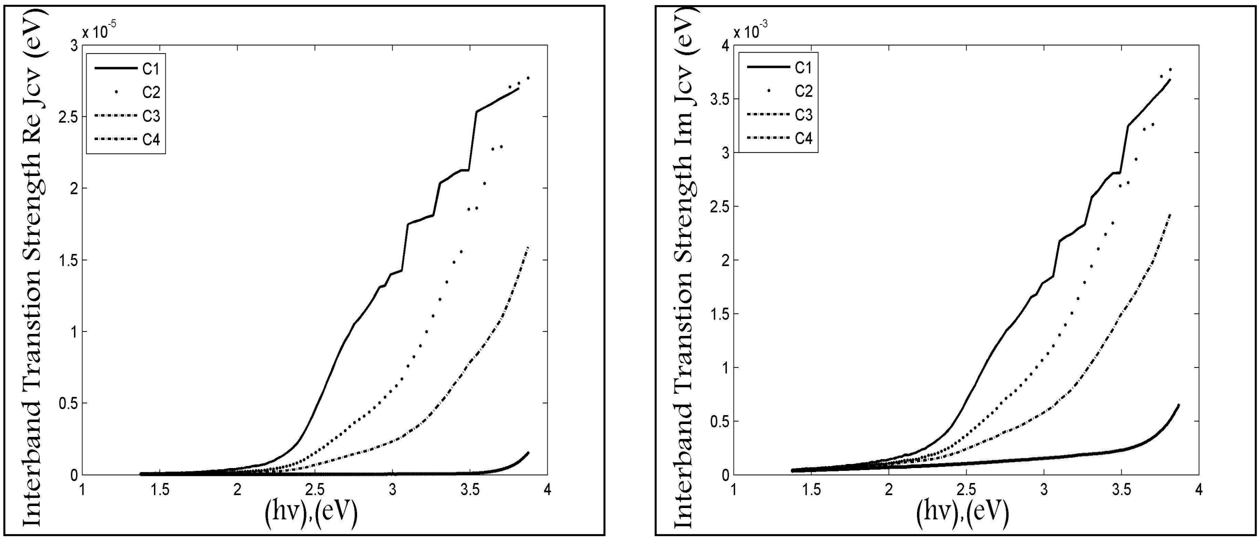
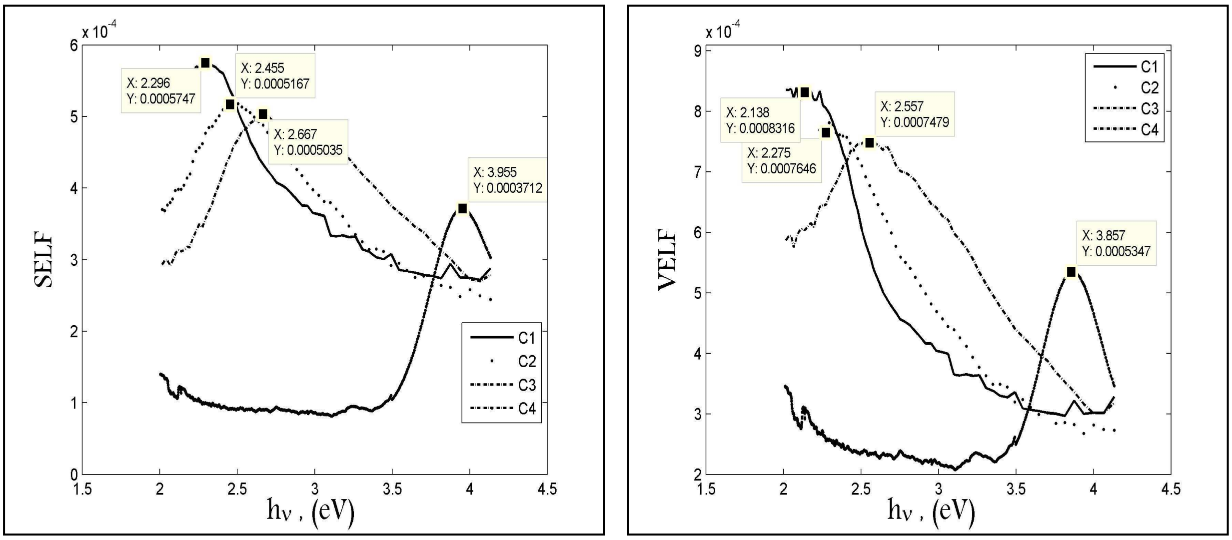


Fig.(8) Plot (a) real part of J_{cv} and (b) imaginary part of J_{cv} as a function of photon energy forthe volume ratio.
C1: 1 Epoxy : 1 Novolac C2: 2 Epoxy : 1 Novolac
C3: 3 Epoxy : 1 Novolac C4: Epoxy Pure

Fig. (8) Shows interband transition strength J_{cv} as a function of the photon energy $h\nu$. It is increases with increasing of the photon energy and this denote the probability of electronic transitions occur increasing with increasing photon energy. It is noted that J_{cv} active up for C1 to 2(ev) , C2 to 2.5 (ev) , C3 to 3 (ev) and C4 to 3.5 (ev) because the bland has large band gab (C1 has (1.95 ev), C2 has (2.025 ev) , C3 has (2.06 ev) and C4 has (3.553 ev))so absorption of more energy to result excitation and electronic transition from valance band to conduction band.



(a) (b)

Fig. (9) Plot (a) surface energy loss function SELF and (b) volume energy loss function VELF as a function of photon energy($h\nu$) for the volume ratio.
C1: 1 Epoxy : 1 Novolac C2: 2 Epoxy : 1 Novolac
C3: 3 Epoxy : 1 Novolac C4: Epoxy Pure

The fundamental optical constants calculated based on experimental absorption, transition spectra includes: real and imaginary parts of dielectric constant which are a characteristic losses of volume (bulk) $-\text{Im}(\varepsilon^{-1})$ and surface $-\text{Im}(1+\varepsilon)^{-1}$, then we surface, volume energy loss function by the relation can be determined[23]

$$Volume - -\text{Im}(\varepsilon^{-1}) = \varepsilon_2(\varepsilon_1+\varepsilon_2)^{-2} \quad (7)$$

$$Surface - \text{Im}(1+\varepsilon)^{-1} = \varepsilon_2[(\varepsilon_1+1)^2+\varepsilon_2{}^2)]^{-1} \quad (8)$$

The behavior of both surface and volume energy loss function as a function of photon energy are illustrated in the Fig.(9)(a,b). It is clear that the volume energy loss is greater than surface energy loss at incident photon energies. It is also clear that the maximum of SELF and VELF correspond to the absorption energy due to the interband transition occurs at (324 nm)(3.8) ev.

Table2. Optical properties

Quantity	*Value*			
	C1	*C2*	*C3*	*C4*
$E_g^d\ (eV)$	2.295	2.408	2.655	3.792
$E_g^{ind}\ (eV)$	1.95	2.025	2.06	3.553
SELF	0.0005747	0.0005167	0.0005035	0.0003712
VELF	0.0008316	0.0007646	0.0007479	0.0005347

CONCLUSION

The optical constants and optical band gap of Novolac: Epoxy film prepared by casting direct method onto glass substrates have been investigated by optical characterization method. Optical properties such as refractive index and extinction coefficient were determined from transmittance spectrum in the visible regions using envelope method. Where calculated the energy gap for direct transition and indirect where it's values(C1 (2.295 eV), C2 (2.408 eV) , C3 (2.655 eV) and (C4 (3.792 eV)) and for the volume ratio (C1 (1.95 eV), C2 (2.025 eV) , C3 (2.06 eV) and C4 (3.553 eV)).The interband transition strength (Epoxy: Novolac) film found active when the photon energy for (C1>2.2 eV, C2>2.4eV, C3 >2.7 eV, C4 > 3.6 eV). Bath surface, volume energy loss function have been obtained by depending on real and imaginary parts of dielectric constant, it has maximum peak at energy region (C1$\approx$2.138 eV , C2 $\approx$2.275, C3 $\approx$2.557 eV , C4 $\approx$3.857 eV) this leads to single electron excitation process that occurs in the (Epoxy: Novolac) film.From the results thatwe obtained, we find that the materialhas thenew visualresponseto light andthe nature of theelectronictransmissionwasindirectly.Greaterdielectricvalueoccurs when theenergy range(C1(2.2-3.7 eV),C2(2.3-3.7 eV),C3(3.1- 3.7 eV) and C4(3.6-3.7 eV)andMaterialhaselectricalconductivityandgood visual.

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