



Fabrication and Study the Structure, Optical and Dispersion Parameters of PMMA with InCl_3 Additive

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Abstract

Polymethyl methacrylate films are prepared by casting method with various content of InCl_3 (2, 4%). X-ray diffraction (XRD) and optical microscope are used to determine the structural properties. Transmittance that determined using UV-Visible spectrophotometer and optical parameters also calculated. Urbach energy values increase with the increasing of InCl_3 and energy gap decreased from 3.849 eV of pure PMMA films to 3.230 eV of PMMA-4% InCl_3 . Dispersion parameters are determined using Wemple-DiDomenico model. Refractive index data at infinite wavelength was found to obey single oscillator model.

Keywords: PMMA, Dispersion parameters, Composite, Optical properties.

Introduction

Poly methyl methacrylate PMMA has received great attention due its unique properties such as excellent mechanical properties [1], high chemical resistance [2]. Simple synthesis low cost [3], good tensile strength and hardness [4]. Low optical loss in visible spectrum, good insulation properties and thermal stability [5]. PMMA is considered as an excellent material that affected upon doping due to their good transparency [6].

As a result of the above properties, PMMA has been extensively used in various industrial sectors, like, gas sensing, photonics and optoelectronics applications [7], in light-emitting diode applications [8]. In this work was focused on effect of InCl_3 upon structural and dispersion Parameters of PMMA composite.

Materials and Methods

Commercial poly methyl methacrylate supplied from SIGMA-ALDRICH (Germany),

average molecular weight $\sim 120,000$ by GPC with purity of minimum assay around 98% were used a raw material dissolved in chloroform to obtain a solution.

InCl_3 from the same chemical company with purity of 98 was used as doping agent with volumetric concentration of 2 and 4% in PMMA matrix utilizing the casting method in order to obtain film free from any noticeable cracks.

The thickness of the film was estimated by digital micrometer, their values were around 25 micron. Transmittance and absorbance spectra were determined by double beam spectrophotometer (Schimadsu)

Results and Discussion

Figure 1 represent amorphous structure of pure and various content InCl_3 of PMMA films.

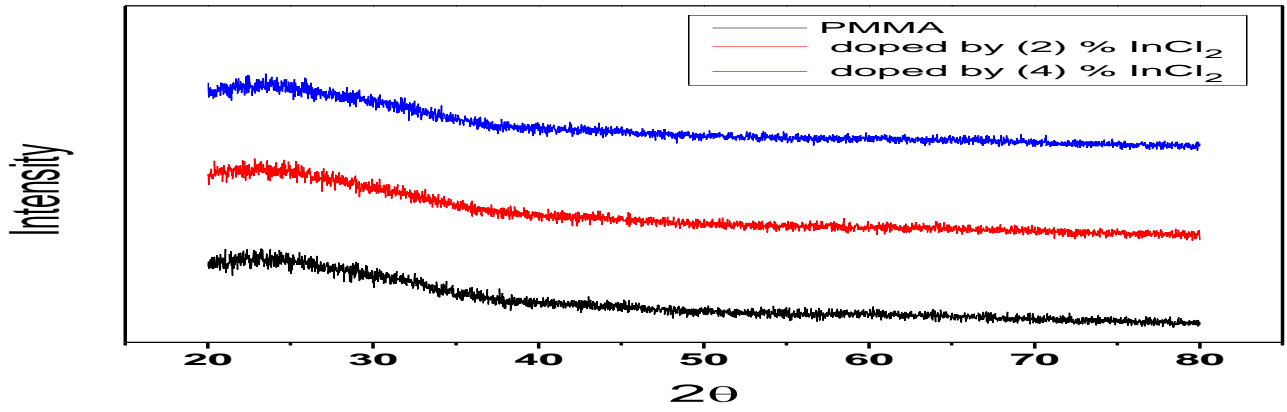


Figure -1: XRD pattern of PMMA-In films

Transmittance (T) is calculated by using equation [9]:

$$T = 10^{-A} \tag{1}$$

Where (A) is absorbance.

Transmittance versus wavelength of PMMA-InCl₃ composites as shown in Fig.2. Transmittance decreased by increasing InCl₃ doping in composite, which agrees with [10].

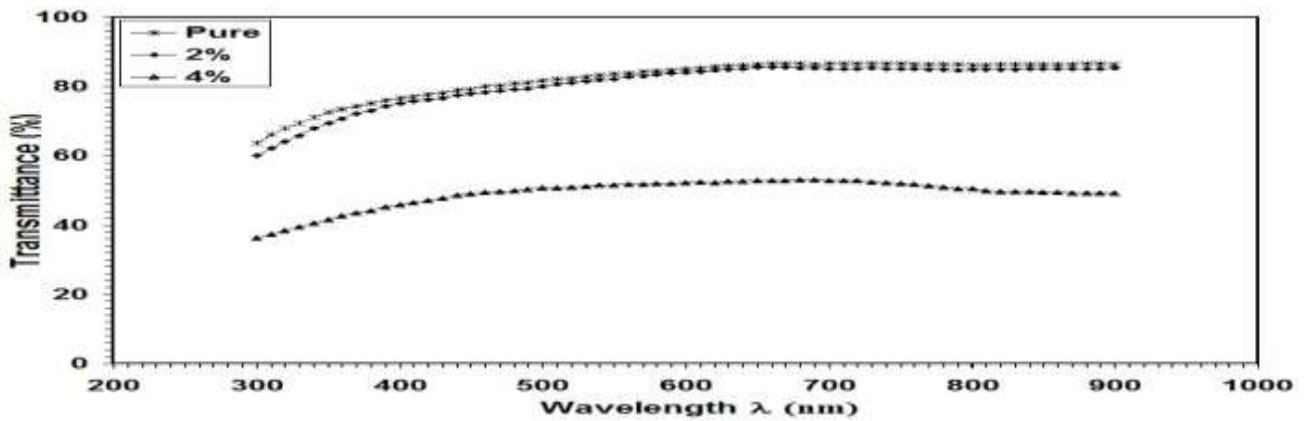


Figure -2: Transmittance versus wavelength of (PMMA-InCl₃) composites

Absorption coefficient (α) was calculated by following equation [11]:

$$\alpha = 2.303A/t \tag{2}$$

Where A: is absorbance and t: is film thickness

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From Fig. 3, α of PMMA-InCl₃ Composite decreased with increasing of InCl₃

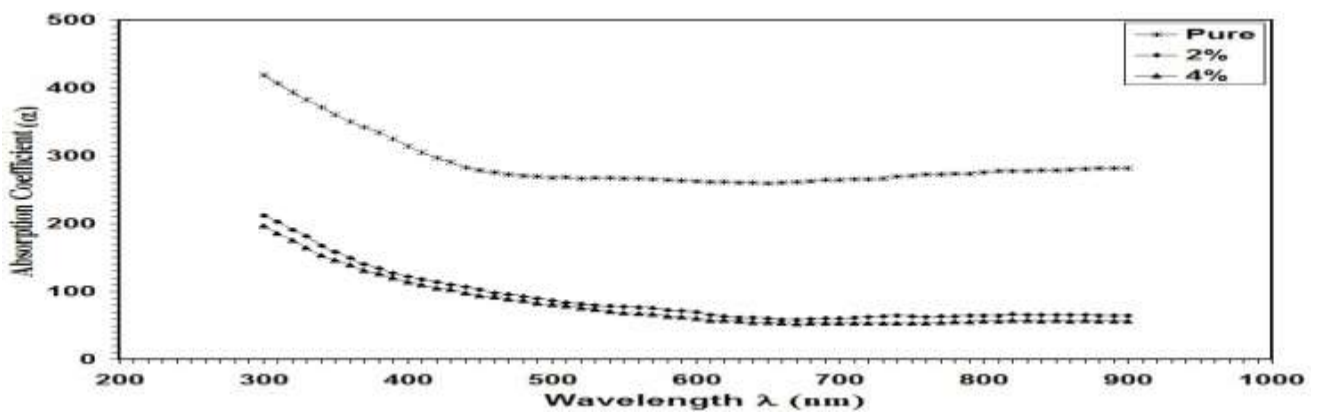


Figure -3: α of PMMA-InCl₃ composites with wavelength

Refractive index was evaluated by following relation [12]:

$$n = (1+R^{1/2}) / (1-R^{1/2}) \tag{3}$$

Where R represent reflectance

Refractive index (n) values versus wavelength are shown in Figure 4. From this Figure, n increased with increasing InCl₃ doping, this result agrees with [13].

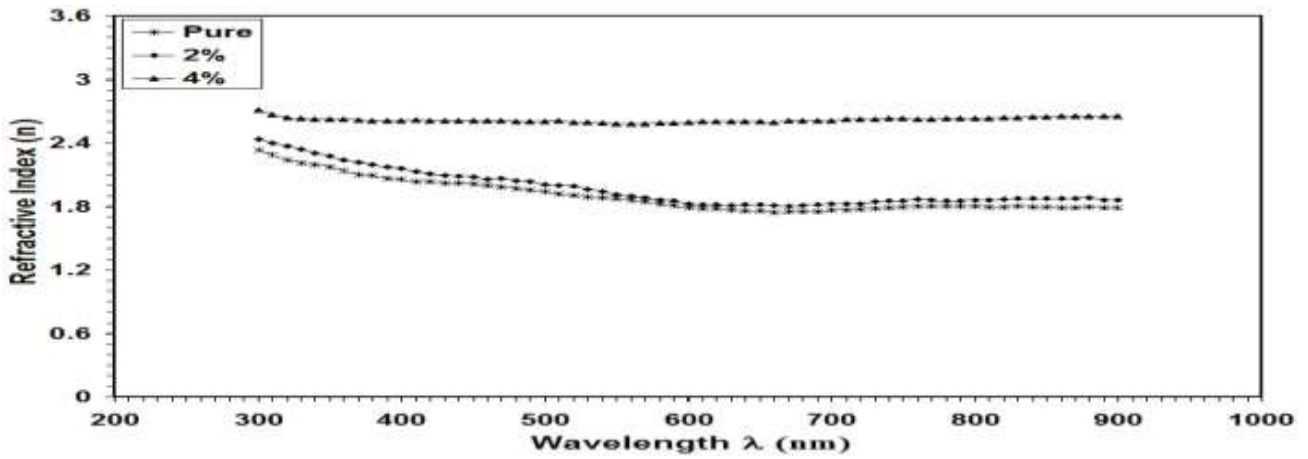


Figure -4: n against wavelength of PMMA-InCl₃ composites

Real (ϵ_1) and imaginary (ϵ_2) parts of dielectric constant of PMMA-InCl₃ composites were calculated by using equations [14]:

$$\epsilon_1 = n^2 - k^2 \tag{4}$$

$$\epsilon_2 = 2nk \tag{5}$$

Figures (5, 6) display ϵ_1 and ϵ_2 for PMMA-InCl₃ composites for different concentration of InCl₃ with wavelength. From the figures, ϵ_1 and ϵ_2 increased with the increasing InCl₃ dopant which related to increase in refractive index (n) [15].

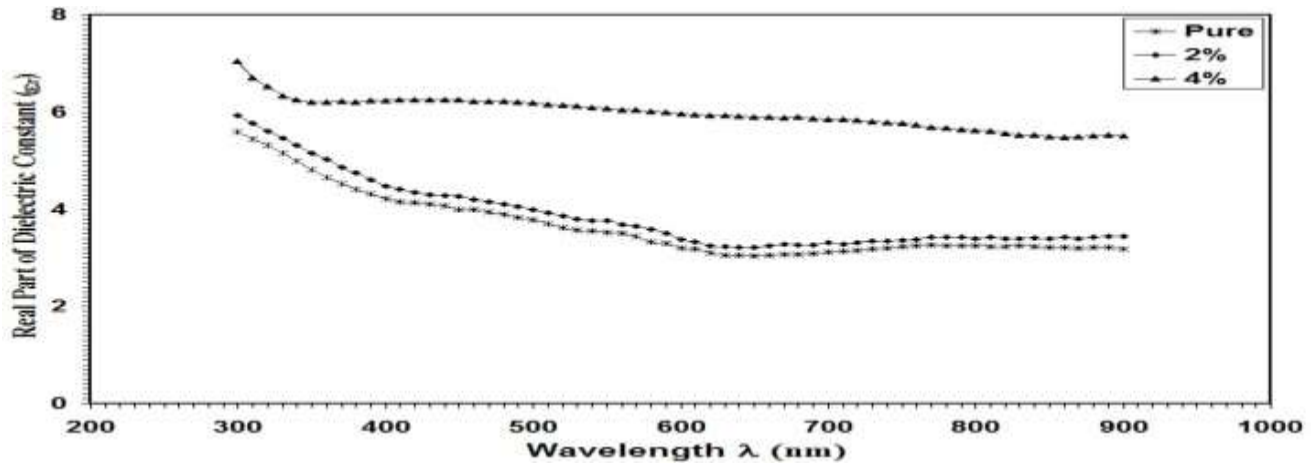


Figure -5: ϵ_1 against wavelength of pure and doped PMMA films

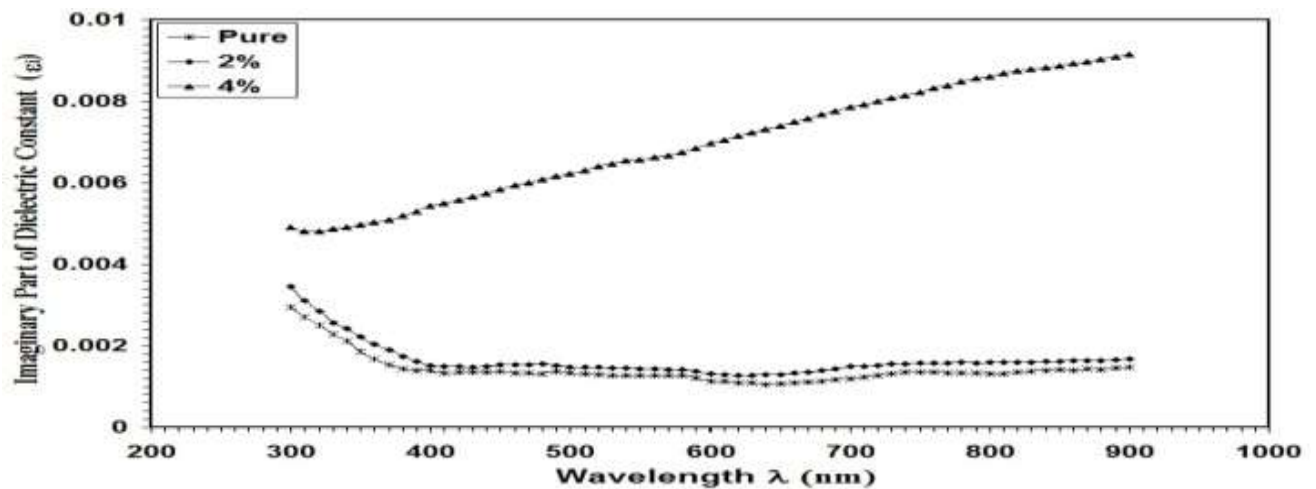


Figure -6: ϵ_2 against wavelength of pure and doped PMMA films

Optical conductivity (σ) of PMMA-In films was determined from the following relation [16]:

$$\sigma = \frac{\alpha n c}{4\pi} \tag{6}$$

Where c is speed of light in vacuum. Fig. 7 represents relationship between optical conductivity and wavelength of PMMA-In films. From Fig., Optical conductivity increased with increasing InCl₃ dopants.

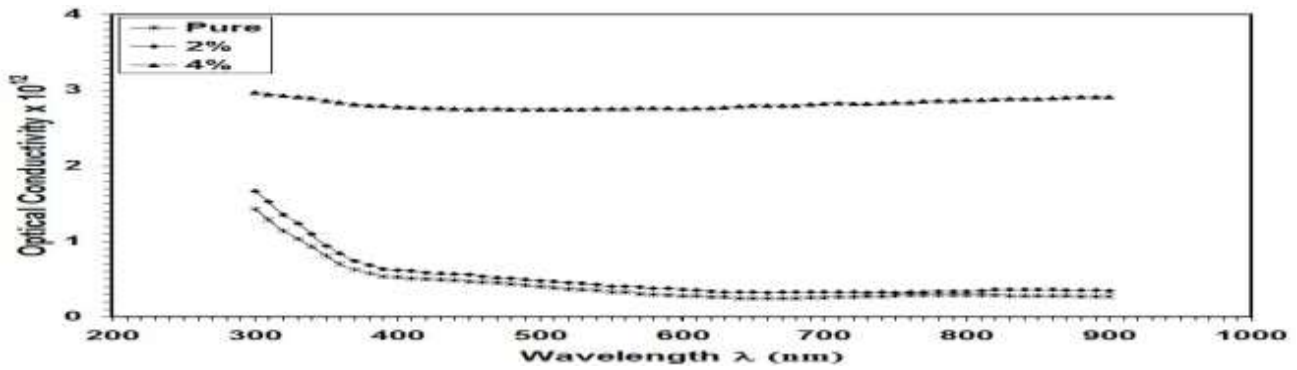


Figure -7: σ gainst wavelength of pure and doped PMMA films

Urbach tail can be determined by the following relation [17]:

$$\alpha = \alpha_0 \left(\frac{E}{E_U} \right) \quad (7)$$

Where E_U is Urbach energy, α_0 is a constant, and E is photon energy.

Relation of $\ln \alpha$ versus $h\nu$ was presented in Figure 8 to determine Urbach energy from inverse slope of these plots [18]. Urbach energy increased with increasing of InCl_3 in PMMA-In films and listed in Table (1).

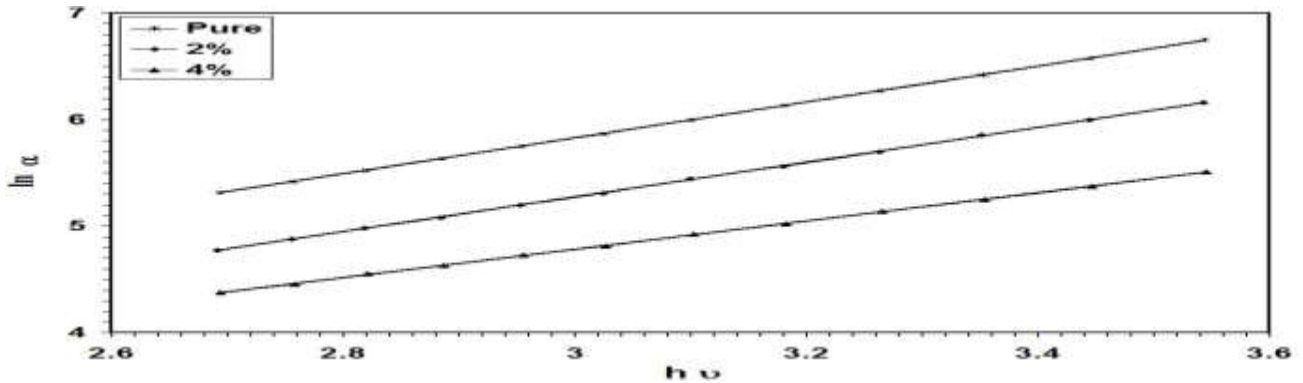


Figure -8: $\ln \alpha$ with $h\nu$ of pure and doped

PMMA films

Dispersion parameters (Caglar, et al., 1970) were estimated from single oscillator model that describes by Wemple and DiDomenico relation [19]:

$$n^2 = \frac{E_d E_0}{E_0^2 - h\nu^2} \quad (8)$$

Where E_0 and E_d are energy of effective dispersion oscillator dispersion energy respectively., Fig. 9 represent relationship between $(n^2-1)^{-1}$ and $(h\nu)^2$, Values of E_0 and E_d decrease with increasing of InCl_3 additive, these values are recorded in Table

(1).Dispersion parameters are very important in many applications (Caglar, et al., 1970). Dispersion parameters were estimated from single oscillator model that describes by Wemple and DiDomenico relation [19]:

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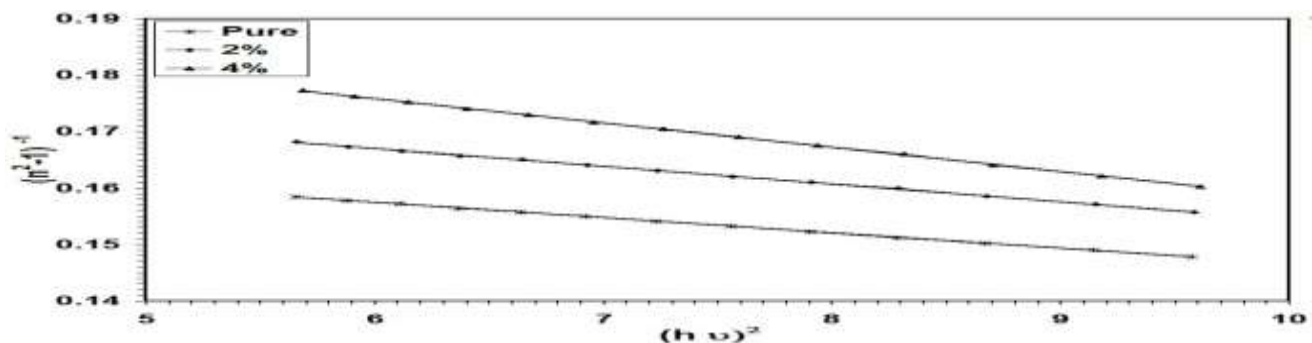


Figure -9: $(n^2-1)^{-1}$ with $(h\nu)^2$ of pure and doped PMMA films.

A single term Sellmeier relation was introduced by [20, 21]:

$$n^2 - 1 = \frac{S_0 \lambda_0^2}{1 - \lambda_0^2 / \lambda^2} \tag{9}$$

Where n is refractive index, S₀ is average oscillator strength, and λ₀ is average oscillator position. Fig.10 represent plot of (n²-1)⁻¹ with 1/λ², from figure it can determine values of S₀ and λ₀ that recorded in Table (1).

Dielectric constant can be calculated by the following classical dispersion relation [22]:

$$\frac{n_\infty^2 - 1}{n^2 - 1} = 1 - \left(\frac{\lambda_0}{\lambda}\right)^2 \tag{10}$$

Where n_∞ is refractive index (ε_∞ = n_∞²) at infinite wavelength (λ₀) (average oscillator wavelength), λ is t wavelength of incident photon. Values of ε_∞, n_∞, and λ₀ are presented in Table (1).

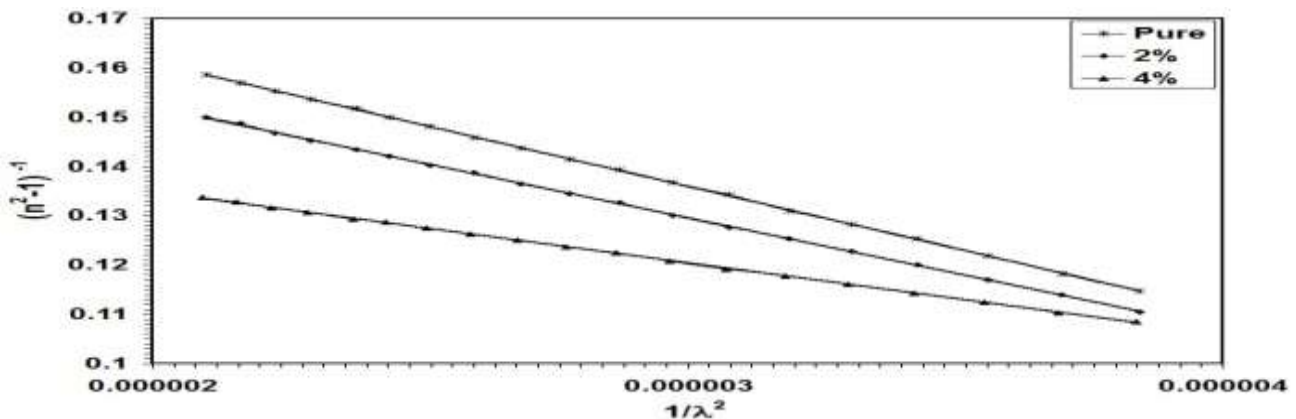


Figure -10: (n²-1)⁻¹ with 1/λ² of pure and doped PMMA films

The moments of optical spectra (M₋₁ and M₋₃) can be calculate from the following relations [21]:

$$E_0^2 = \frac{M_{-1}}{M_{-3}} \tag{11}$$

$$E_d^2 = \frac{M_{-1}}{M_{-3}} \tag{12}$$

The values of M₋₁ and M₋₃ of PMMA-In films are decreased with increasing of InCl₃ additive. These values are recorded in Table (1).

Table 1: Optical Parameters of PMMA-In films

Sample	E _d (eV)	E _o (eV)	E _g (eV)	ε _∞	n(o)	M ₋₁	M ₋₃ eV ⁻²	S ₀ x10 ¹³ m ⁻²	λ ₀ nm	U _E meV
Pure	48.11	7.69	3.849	7.25	2.690	6.25	0.107	3.95	398	588
2 %	43.56	7.40	3.700	6.88	2.623	5.88	0.107	4.46	386	609
4 %	35.94	6.46	3.23	6.56	2.560	5.55	0.032	6.60	327	769

Conclusions

PMMA films are deposited successfully by casting method with various content of InCl₃. An XRD pattern reveals that all deposited films were amorphous in structure. Urbach energy values increase with increasing of InCl₃, and energy gap decreased from 3.849 eV for pure PMMA films to 3.230 eV concluded that there is an inverse relation

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between them. Dispersion parameters were estimated. Refractive index data at infinite wavelength were established confirming single oscillator model.

Acknowledgments

Authors would appreciated Babylon, Mustansiriyah and Diyala Universities for their support in this work [23, 24].

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