Research Journal of Chemical Sciences E-ISSN 2231-606X
Vol. **6(12),** 32-39, December **(2016)** *Res. J. Chem. Sci.*

Preparation and Study of Some Optical Parameters of (Polyvinyl Alcohol - KI) Composite Films

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Available online at: www.isca.in, www.isca.me
Received 28th September 2016, revised 3rd December 2016, accepted 13th December 2016

Abstract

Polyvinyl Alcohol - potassium iodide composite films have been prepared by using casting technique with different dopant concentrations of (2, 4, 6, 8, and 10) wt%. Some optical parameters of all films were studied. The UV-Vis spectra have been recorded in the range of (250-1100) nm. The results show that the filler content has significant effect on the transmittance, absorbance and other optical parameters of all samples. Furthermore, the results also show that the pure and PVA-KI have allowed indirect energy gap (E_g).

Keywords: PVA Films, Potassium Iodide, Composite, Optical Properties, Direct Transition.

Introduction

Polymers, as plastics and rubbers, pervade our lives and we come across them in many different forms. As such, their physical properties have great importance and an understanding of them is vital for their uses in technology and engineering[1]. Plastics are the most versatile materials used in different chemical industries such as aircraft, packaging, electrical equipment and as electrical insulators. They have increasingly important role in the manufacture of satellites, space researches and thermal barriers[2,3].

Plastics have replaced metals in many applications. They have superseded steel and many other metals in being erosion resistant and chemically inert, having higher temperature extension and specific heat than metals. Plastics have been used for constructing and lining of reactors, absorption towers and the manufacture of pipes and valves. Because of the chemical and physical properties of PVA, it has been used in many medical and industrial applications[4]. Composite polymers also have many and wide applications because additives can make changes in the molecular configuration and the microstructure of the undoped polymer which consequently change its properties[5].

Materials and Methods

PVA powder with high purity (99.9%) and potassium iodide (KI) salt powder with high purity (99.5%) supplied by Gerhard Bachmann kG Barcelona/Espana were used as the raw materials this study. One gram of mixtures of PVA and KI powders (with KI weight percentages of 2, 4, 6, 8 and 10) was dissolved in double distilled water (15 ml) and poured in a 5 cm diameter Petri dish for the preparation of the polymer films. The films were dried in air and the resultant films were of 45 µm thickness. The UV-Vis spectra of PVA-KI films have been measured in the range of (250-1100) nm by using double beam spectrophotometer provided by Shimadzu, (UV-1800).

Results and Discussion

Transmission Spectra: Transmittance spectra of the prepared films of PVA-KI composite films are shown in Figure-1. The figure shows that the transmittance has a rapid increasing behavior in the short wavelengths for all the composite films and as the wavelength increases further the transmittance remains almost constant. It can also be seen that the transmittance has a decreasing trend as the weight percentage of the KI salt increases. This can be attributed to the fact that the electrons in the outer orbit of KI may absorb the incident light resulting in the electrons transition to higher energy levels to occupy vacant positions in the conduction band, thus some photons of the incident light are absorbed by the films material and do not transmit. It is important to mention here that the pure (PVA) films are transparent because they don’t possess free electrons because all electrons are strongly joined in their atoms by covalent bonds[6].

Absorption Spectra: The absorbance of PVA-KI composite films as a function of wavelength is shown in Figure-2. It can be clearly observed that KI salt filler percentage alters the intensity of the absorbance and causes a red shift in the peaks position of. These results can be attributed to the absorption of incident photons by KI salt ions[6,7].

Absorption Coefficient: The absorption coefficient of PVA-KI composite films as a function of wavelength is illustrated in Figure-3. The absorption coefficient can be estimated by th following equation[8]:

$$\alpha = 2.303 \left(\frac{A}{t}\right) \quad (1)$$

Where α, A and t represent the absorption coefficient, the absorbance and thickness of the film respectively.

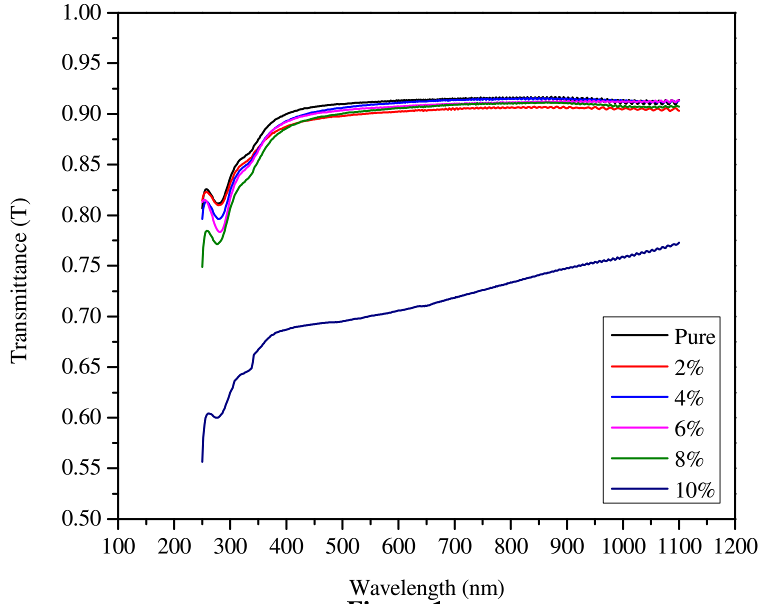

Figure-1
Transmittance versus wavelength of PVA-KI composite films

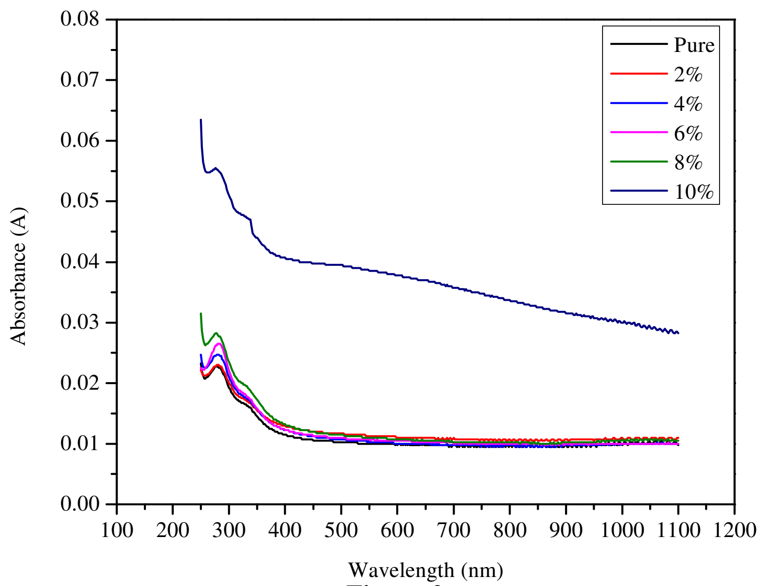

Figure-2
Absorbance versus wavelength of PVA-KI composite films

It is clear that the values of α are high at short wavelengths which leads to that the electronic transitions are more likely to occur at this region of the spectrum. Consequently, if the incident photon energy is higher than the band gap then the electrons can absorb it to transit from the valence band to the conduction band[6]. It can be observed also that α values are less than (10^4 cm^{-1}) which means that band gap is indirect. One can also see from Figure-3 that α has an increasing trend as the percentage of the KI salt increases.

Energy Gap: Figure-4 shows the Tauc's plots of PVA-KI composite films. The allowed indirect band gap (E_g) has been estimated by using equation[9]:

$$\alpha h\upsilon = B(h\upsilon - E_g)^2 \qquad (2)$$

Where: B is constant.

If a straight line of the linear part of the plot is extrapolated to the x-axis at the zero value of y-axis, the allowed indirect band gap (E_g) can be obtained (Table-1).

It can be seen that the values of band gap (E_g) have a decreasing trend as the percentage of KI salt increases. This result is due to localized levels within the band gap (E_g) introduced by the dopants. Two stages of electronic transitions can be conducted; the first involves the electronic transitions from the valence band to the localized states and the second from the localized states in the band gap to the conduction band. This behavior is due to that the electronic conduction depends on the additives. The increase in the additive percentage makes new paths for electrons which can enhance the transition of electrons from valance band to the conduction band[10,11].

Table-1
Allowed indirect band gap (E_g) values of PVA-KI composite films

KI concentration (wt%)	E_g (eV)
Pure (PVA)	5.972
2	5.094
4	5.085
6	5.044
8	4.984
10	4.799

Urbach Energy: The Urbach energy (E_u) has been calculated by using equation[10]:

$$\alpha = \alpha_0 \exp\left(\frac{h\nu}{E_u}\right) \quad (3)$$

The Urbach energy values of PVA-KI composite films at different concentrations of KI salt were shown in Figure-5. Urbach energy can be obtained from the inverse of the slope of (lnα) versus (hυ). The magnitude of Urbach energy of these composite films has a decreasing trend as the percentage of KI salt increases. This result was reported by Davis and Mott who revealed that the filling can affect the Urbach energy significantly. The filling process can create localized states in the matrix of polymer proportional to the concentration of KI salt content[12]. The values of Urbach energy (Eu) for all films prepared in this study are depicted in Table-2.

Refractive Index: Figure-6 illustrates the variation of the index of refraction (n) as a function of wavelength for PVA-KI composite films which can be estimated using the following equation[11]:

$$n = \sqrt{\frac{4R - k_o^2}{(R-1)^2}} - \frac{(R+1)}{(R-1)} \quad (4)$$

Where R and ko represent the reflectance and the extinction coefficient respectively. From the figure one can see that the refractive index has an increasing trend as the percentage of KI salt increases.

Extinction Coefficient: The extinction coefficient (k_o) versus wavelength λ for PVA-KI composite films is shown in Figure-7. It can be estimated using the following equation[13]:

$$k_o = \frac{\alpha\lambda}{4\pi} \quad (5)$$

It can be noticed that the extinction coefficient increases as percentage of KI salt increases. This can be attributed to high values of absorption coefficient.

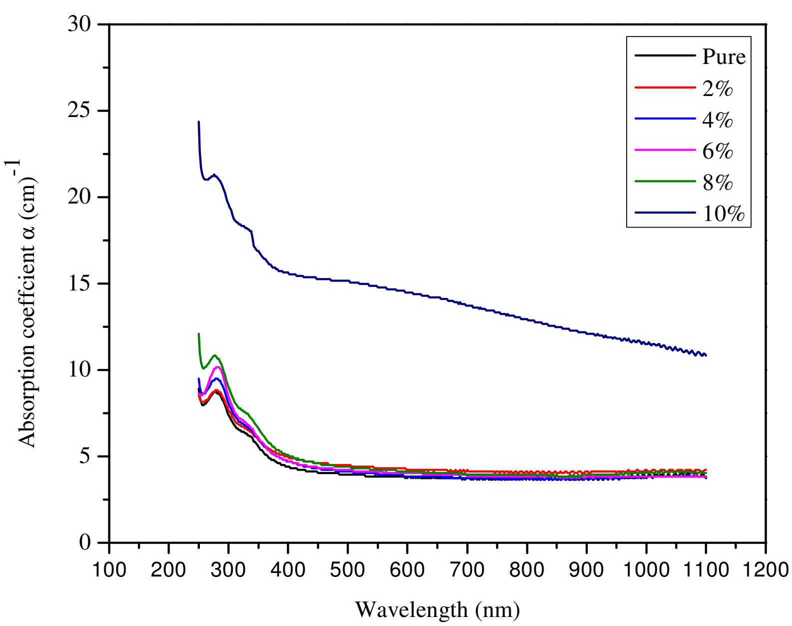

Figure-3
Variation of α as a function of wavelength for PVA-KI composite films

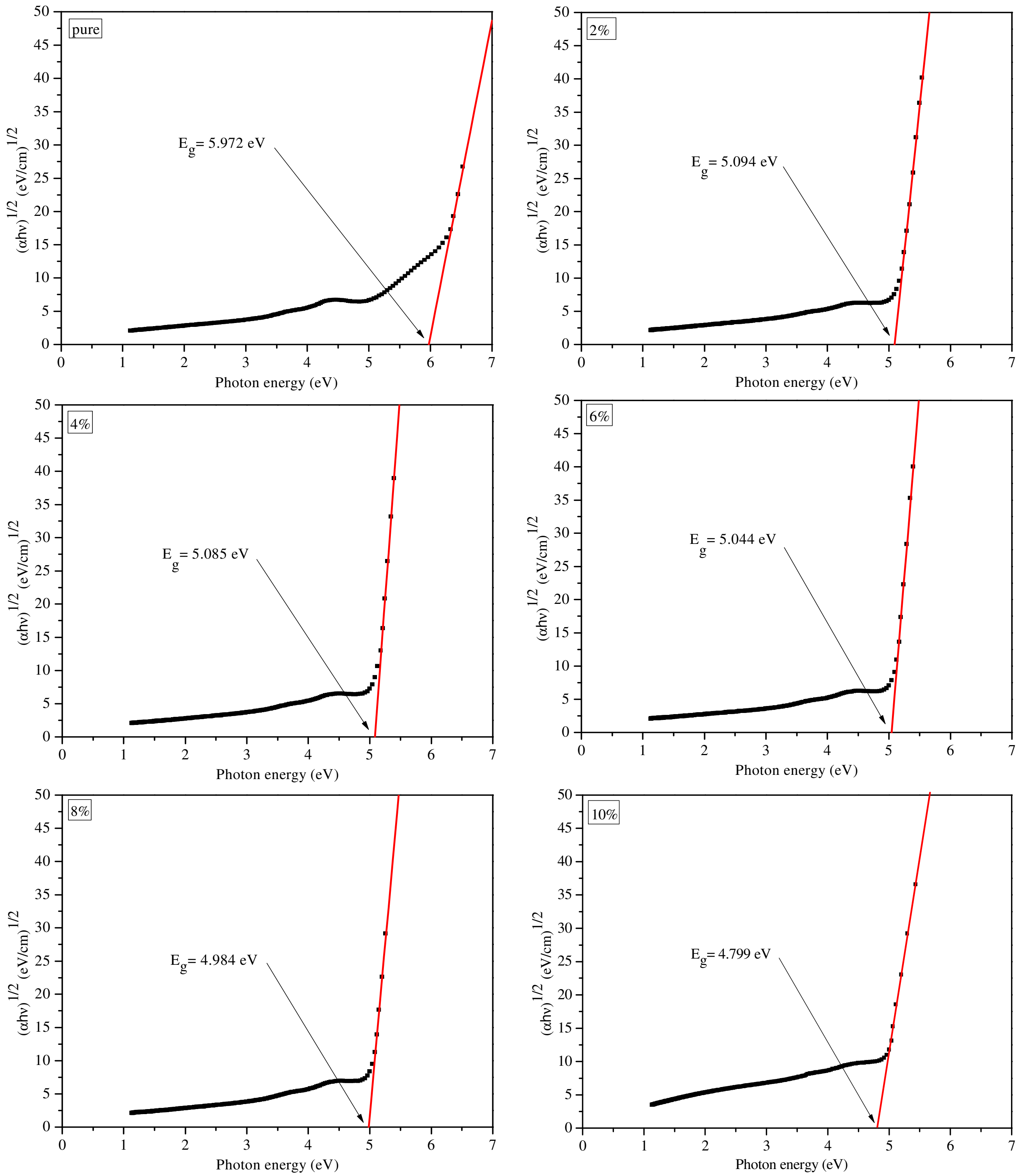

Figure-4
Energy band estimation for PVA-KI composite films using Tauc's model

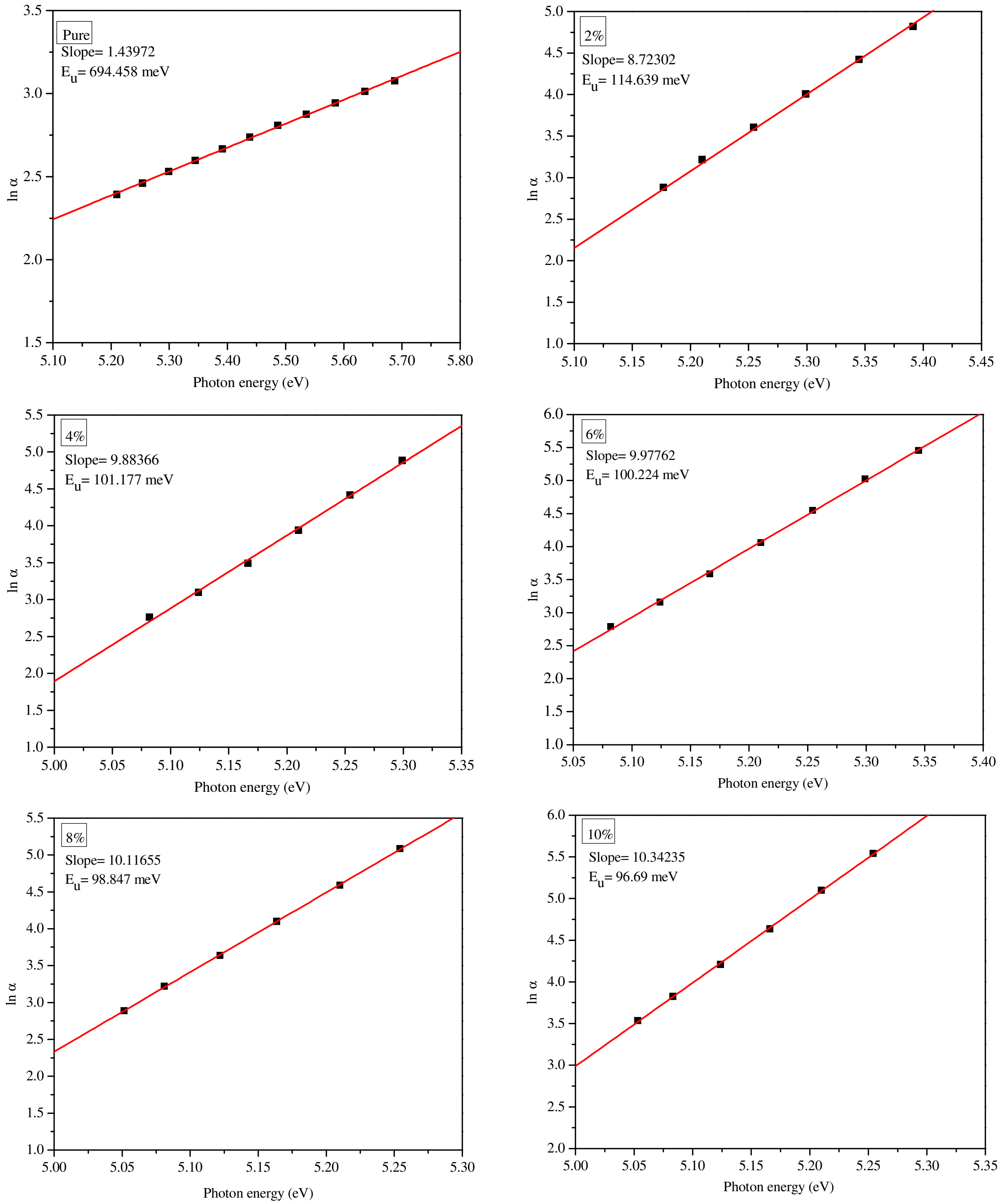

Figure-5
E_u estimation of PVA-KI composite films

Table-2
Value of Urbach energy (E_u) of PVA-KI composite films at different concentrations of KI salt

KI concentration (wt%)	E_u (meV)
Pure (PVA)	694.579
2	114.639
4	101.177
6	100.224
8	98.847
10	96.69

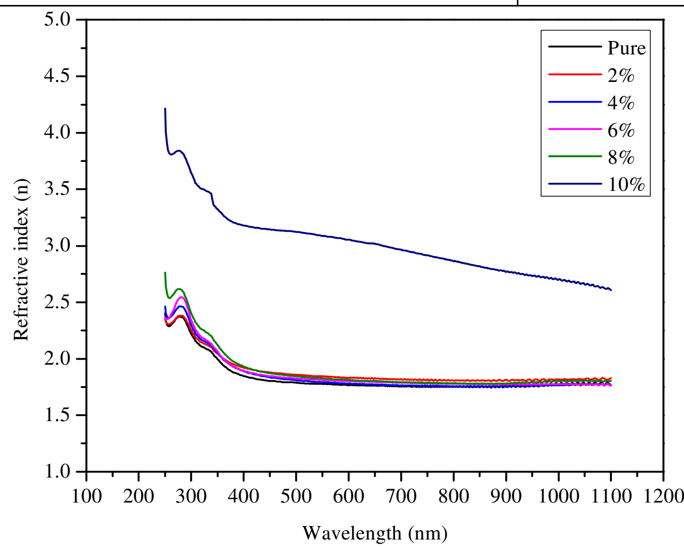

Figure-6
n versus λ for PVA-KI composite films

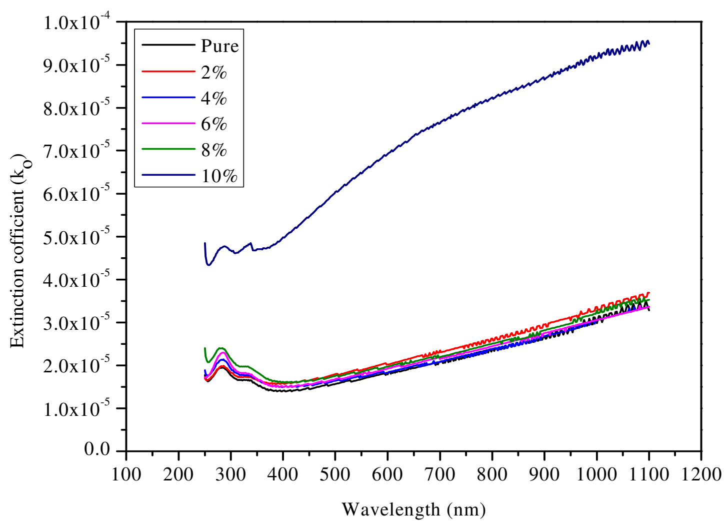

Figure-7
ko versus λ for PVA-KI composite films

Dielectric Constant: The variation of dielectric constant in its two parts [the real (ε_1) and imaginary (ε_2)] of PVA-KI composite films as a function of wavelength is shown in figures-8 and 9. These two parts can be expressed by the following equations[14]:

$$\varepsilon_1 = n^2 - {k_0}^2 \quad (6)$$

$$\varepsilon_2 = 2nk_0 \quad (7)$$

It can be seen that (ε_1) and (ε_2) increase as the percentage of the KI salt increases.

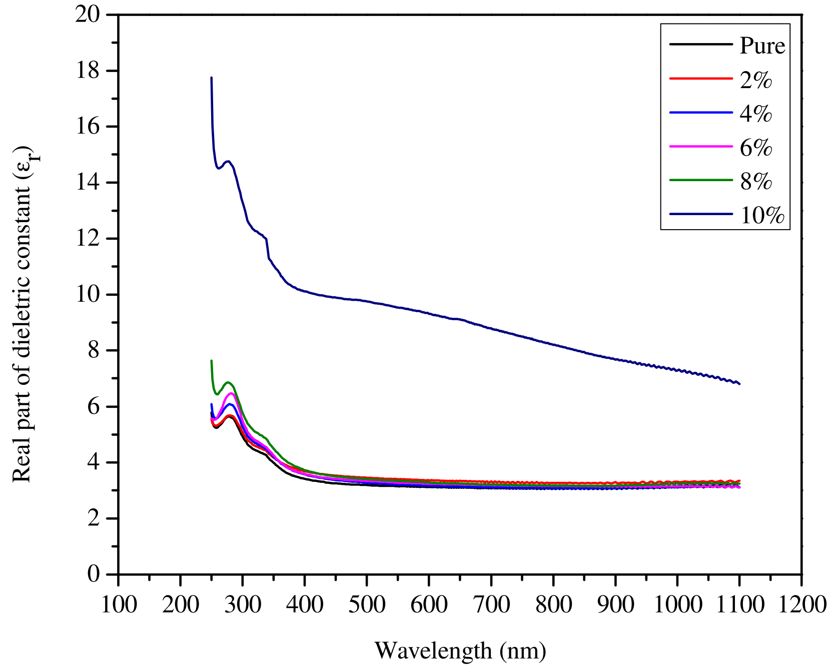

Figure-8
ε_1 versus λ for PVA-KI composite films

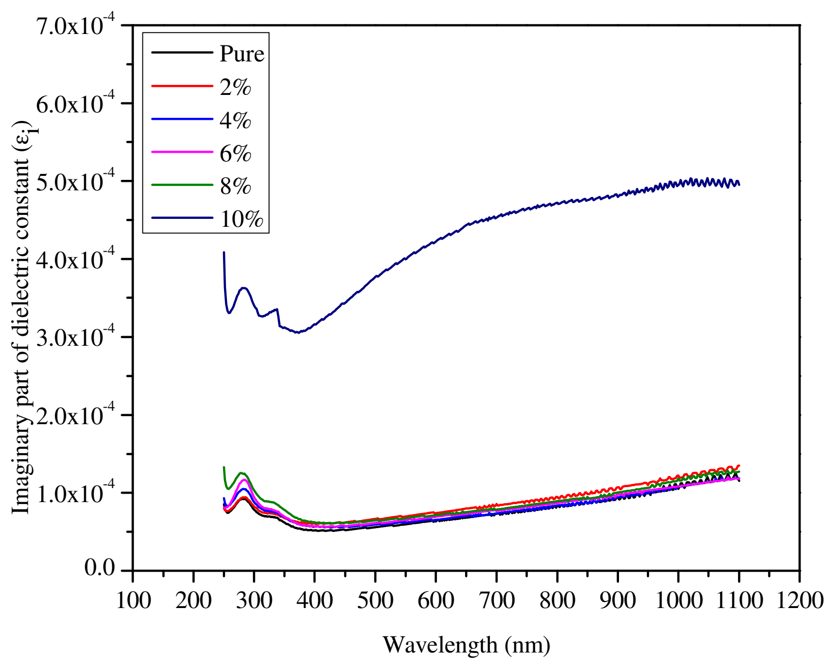

Figure-9
ε_2 versus λ for PVA-KI composite films

Conclusion

The absorbance of PVA-KI composite films has an increasing trend as the increase in KI salt content increases. The values of absorption coefficient for all films are less than (10^4 cm^{-1}) suggesting that the band gap is indirect. The allowed indirect band gap and the Urbach energy of all films have a decreasing trend as the filler content weight percentage increases. All the optical parameters of the films are highly affected by the filler content weight percentage.

References

1. Pethrick R.A., Amornsakchai T. and North A.M. (2011). Introduction to Molecular Motion in Polymers. Whittles Publishing, United Kingdom, 1-214. ISBN 1849950083

2. Kontos G., Soulintzis A. and Karahaliou P.K. (2007). Electrical Relaxation Dynamics in TiO_2 – Polymer Matrix Composites. *J. Express polymer Letters*, 1(12), 781-789.

3. Mustafa S. (2008). Engineering Chemistry, Library of Arab Society for Publication and Distribution. Jordan

4. Mahsan M., Sheng C., Isa M., Ghapur E., Ali E. and Razali M., (2009). Structural and Physical Properties of PVA/TiO2 Composite. From Malaysia Polymer International Conference 10, 21st–22nd October

5. Tawansi A., Migahed M.D. and El-Hamid M.I.A. (1986). Electrical Conduction of Poly (vinyl alcohol) films. *Journal of Polymer Science Part B: Polymer physics*. 24(12), 2631-2642

6. El-Dahshan M.E. (2002). Introduction to Material Science and Engineering. King Saud University Press, Saudi Arabia

7. A Munaim, A Hashim (2010). Electronic Transitions for (PS-LiF) Composites. From 6th Science Conference of College of Science, University of Mustansiriah, Baghdad, Iraq

8. Mwolfe C., Holouyak N. and Stillman G.B. (1989). Physical Properties of Semiconductor. Prentice Hall, New York, 1-354, ISBN 9780136699613

9. Sze S.M. and Kwok K. Ng. (2007). Physics of Semiconductor Devices. 3rd Ed., John Wiley and Sons Inc., Hoboken, New Jersey, pp 832, ISBN: 978-0-470-06830-4

10. Gabur K. (2010). Preparation and Study the Electrical and Optical Properties of (PS-Ni) Composites. (Unpublished M.Sc. Thesis). Babylon University, College of Science, Iraq

11. Ghosh D.K. and Samanta L.K. (1986). Refractive indices of some narrow and wide bandgap materials. *Infrared physics*, *26*(5), 335-336

12. Chopra K (2012). Thin Films Device Applications. Plenum Press, New York, 1-300. ISBN: 978-1-4613-3684-6

13. Berglund R., Graham P. and Miller R. (1993). Applications of In-situ FT-IR in Pharmaceutical Process R & D. *Spectroscopy,* 8, 31-42

14. Klingshirn C.F. (2012). Semiconductor Optics, Springer Berlin Heidelberg. 1-560. ISBN: 978-3-642-28361-1