Effects of FeCl₃ additives on optical parameters of PVA

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Abstract. PVA doped FeCl₃ have been deposited utilizing casting technique. Absorption spectrum was registered in the wavelengths (300-900 nm) utilizing UV-Visible spectrophotometer. Optical constants behavior such as, absorbance, absorption coefficient, and skin depth were studied. It was found these parameters were increased as Fe content increase. While the extinction coefficient and optical conductivity was decreased. The energy gap of PVA-Fe films were decreased from 4 eV for the PVA film to 3.5 eV for the PVA: 4 % Fe film.

Keywords: Poly (vinyl alcohol), Optical parameters, optical energy gap.

1. Introduction
Poly (vinyl alcohol) (PVA) has gained great importance, as it has a unique properties such as, crystalline polymer, solubility in water is high, its dissolution needs the breaking of the crystal structure and poverty to be carried out at high temperature [1-4]. Ionization of atoms and separation of molecules occur leading to the formation of charged species both ionic and free radicals [5].

Different composite materials latterly synthesized by starting from different polymers and a broad assortment of dopants like metals, oxides and inorganic salts [6]. Polymeric films have been widely used in industry especially in the measurement of electron beam dosimetry [7]. The motivated physical and chemical characteristics of polymer-metal composites showing the composites as conductive or semiconductor materials, hence it gives the chance to use these materials in many applications, like, design the integrated circuits, optoelectronic devices, solid-state batteries [8,9]. In this study, the PVA-Fe composite by casting solution method is prepared in order to study the optical properties of this composite.
2. Materials and Methods

Polymeric solution of high purity Poly (vinyl alcohol) (molecular weight 10000 g/mol) was used as a matrix element in this work, which was supplied from (BDH Chemicals). FeCl₃ supplied from (Merck chemicals Germany) with a volumetric percentage of (2% and 4%) was used to obtain Films of PVA:Fe utilizing casting method. Absorbance spectrum in the wavelength range (300-900 nm) was calculated to obtain the optical constants.

3. Results and Discussion

Absorbance spectra of PVA with various content of Fe (0, 2, and 4% wt.) were depicted in Figure 1, which was recorded by spectrophotometer in the range of 300-900 nm, using casting method as a film with thickness 1.5 µm. The absorbance decreased with the increasing of wavelength, while it increased with the increasing of Fe content in the PVA-Fe films.

![Figure 1. Absorbance versus wavelength of PVA-Fe composite with various content of Fe.](image)

The absorption coefficient ($\alpha$) of PVA-Fe was estimated by the following formula [10]:

$$\alpha = \frac{2.303A}{d} \quad (1)$$

Where (A) is the absorbance and (d) is the film thickness. Absorption coefficients via wavelength was presented in Figure 2, from this figure, it can be seen that absorption coefficient were increased by increasing Fe content in the PVA-Fe films.
Figure 2. The absorption coefficient of PVA-Fe composite with various content of Fe.

The extinction coefficient (k) of PVA-Fe films were calculated from the following equation [11]:

\[ k = \frac{\alpha \lambda}{4\pi} \]  \hspace{1cm} (2)

Where (\(\alpha\)), (\(\lambda\)) are the absorption coefficient and incident photon wavelength respectively. Extinction coefficient versus wavelength was presented in the Figure 3. Same behavior of absorption coefficient was noticed in extinction coefficient with the increment of Fe content.

'Figure 4' depicts the relation between refractive index (n) and wavelength (\(\lambda\)) that obtained from the formula [12]:

\[ n = \left[ \left( \frac{4R}{(R-1)^2} \right) - K^2 \right]^\frac{1}{2} + \frac{(R+1)}{(R-1)} \]  \hspace{1cm} (3)

Where (R) denoted reflectance. Refractive index of PVA-Fe films were decrease with the increase of Fe content up to 500 nm of wavelength, and then the changes in refractive index seem slightly increase up to 900 nm of wavelength.
Figure 3. The extinction coefficient of PVA-Fe composite with various content of Fe.

Figure 4. The absorbance spectra of PVA-Fe composite with various content of Fe.

The optical conductivity (σ) was calculated using the following formula [13]:

\[
\sigma = \frac{\alpha \cdot n \cdot c}{4\pi}
\]  

(4)
Where (c) is the velocity of light in the vacuum. The optical conductivity versus wavelength was presented in Figure 5, which was increase with the increasing of Fe content in the PVA-Fe films.

Figure 5. The optical conductivity of PVA-Fe composite with various content of Fe.

The skin depth increased with the increasing of Fe content in the PVA-Fe films as shown in the 'Figure 6'.

Figure 6. The skin depth of PVA-Fe composite with various content of Fe.
The optical band gap of PVA-Fe composites were estimated from absorption spectra. The energy gap is found from Tauc relation [14]:

\[ a\nu = B(h\nu - E_g)^m \]  

(5)

Where (h\nu) represent photon energy, (B) is a parameter depends on transition probability [15], and m = 1/2 or 2/3 [16]. By plotting (a\nu)^2 versus h\nu, the band gap value can be obtained from Figures 7 - 9. From the figures, the energy gap decreased from 4 eV for the film PVA to 3.5 eV for the film PVA-4%Fe. The Fe content makes a network inside the PVA films leads to decrease the energy gap.

**Figure 7.** Energy gap of PVA polymer.

**Figure 8.** Energy gap of PVA-2% Fe composite.
4. Conclusion
The films of PVA-Fe for various content of Fe are prepared by solution casting method. The absorbance spectra are recorded in the range of 300-900 nm. Absorbance, absorption coefficient, and skin depth increase with the increasing of Fe content in the PVA-Fe films, but extinction coefficient and optical conductivity are decreased. The energy gap of PVA-Fe films are decreased from 4 eV for the film PVA to 3.5 eV for the film PVA-4%Fe, make these films suitable in solar cell application.

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