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# Influence of both $VCl_3$ Concentration and Gamma Rays on the Optical and Mechanical Character of PVA/$VCl_3$ Composite, for the Application in Optoelectronics Devices

*S. K. Alghamdi* *

Physics Department, Faculty of Science, Taibah University, Al-Madina al Munawarah, Saudi Arabia.

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**Abstract:** One of the methods used to fabricate composites is the solution casting procedure. We synthesized composite with different $VCl_3$ concentrations (5, 10, 15 and 17.5 %) doped polyvinyl alcohol (PVA) films. Ligand field theory was used for identifying the structural properties. Results show an enhancement of the optical and. mechanical strength with raising the $VCl_3$ loads. The influence of γ rays on the optical and mechanical character was presented. The $VCl_3$ is well dispersed into the PVA matrix leading to an enhanced material. Also, the addition of $VCl_3$ procedure was employed to evaluate the mechanical properties of composites. Besides, the hardness of the composite samples showed a non-monotonic trend with raising the γ dose up to 150 kGy. This could be due to the preceding of cross-linking process in the composite that improves its optical and mechanical properties that allows PVA/$VCl_3$ to be suitable candidate for optoelectronics device applications.

**Keywords:** Ligand field theory, Gamma radiation, Polymer, Optical, Hardness, PVA.

## 1 Introduction

The production of new materials recent years has great importance in many research efforts which centered to produce novel matter with distinctive character that fits the optical applications [1]. In recent research, polymeric substances play an important role as working in several optoelectronic requests. They possess several rewards as a function of forte, light weight, abundant, cheap and the possibility of using it in isolation. One of the significant polymers that act as an excellent host matter is the polyvinyl alcohol (PVA) [3, 4]. Similarly, PVA possesses excellent physical and chemical characteristics that increased its stability [5]. The existence of OH groups in its backbone gives a nasty of $H_2$ bonding which is important for the manufacture of polymers [6]. PVA is a semi crystalline polymer that has great importance in industrial fields [7]. We have to treat the defects induced in polymers, by fillers, to improve its performance in industry. That is because the combination of two or more different elements in the compound gives the feasibility of using it in preparing new matter [8]. Polymer composites have a great position in photo-electric devices [9]. The addition of metals to polymers induces distinct alternation in their physical properties [10–16].Radiation effects on polymeric matter affect the structural and physical properties. The produced effects depend on the irradiation settings. The resultant effect will be degradation followed by crosslinks. The aim of the current study is to investigate the effect of both $VCl_3$ concentration and γ radiation on the optical and mechanical characteristics of PVA/$VCl_3$ composite to be suitable candidate for different industrial applications.

## 2 Experimental Section

### *2.1 Synthesis of Samples*

Pure PVA film and three films doped with $VCl_3$ at different concentration by weight were prepared using the cheap-cost casting technique. PVA powder of 35.000 g/mol MW was purchased from Laboratory Ras Ayaan, Cairo, Egypt. We dissolved PVA in DD water with rousing for 4 h at 60°C till we got transparent solution. After that, salt of vanadium chloride $VCl_3 \cdot 2H2O$, obtained from (supplied by Merck, Germany) solutions were prepared by desired wt % content (0, 5, 10, 15, and 17.5 % by weights) in twice-distilled water, are applied as inorganic fillers. Then, we mixed each weight with the PVA solution with rousing for 10 min; then casting the solution in Petri dishes and dried in an oven at 36°C for 48 hours to get rid of traces. The obtained films were nearly 0.3 mm thick.

*Corresponding author e-mail: skghamdi@taibahu.edu.sa

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### 2.2 Optical Measurements

The transmission of the films was scanned at the range of wavelength 200-2500 nm applying Carl Zeiss PMQ 11 spectrophotometers.

### 2.3 Mechanical Measurements

The hardness was measured applying a Wolpert Hardness Tester. The load fixed on the indentation was 3.6 kilo pound for 30 s. The average of 5 reading was considered. The hardness was estimated from:

$$H= Fr/3.925\ (Nmm^{-2}) \quad (1)$$

$$Fr=(0.21/(h-0.04))\ F$$

Where h is reading on the tester/100, and F is the load in Newton.

### 2.4 Irradiation tool

Cobalt 60 source produced by Bhabba Atomic research Center Bombay, India, was used. The dose rate was 4 kGy/h in air.

## 3 Results and Discussion

### 3.1 Absorbance study

Fig (1) illustrates the recorded spectrums of PVA doped with different concentrations of (5%, 10%, 15%, and 17.5% by weights) $VCl_3$ polymer films. Three absorption bands were observed at 11765cm$^{-1}$, (850 nm), 16667 $\mathrm{cm}-1$ (600nm), and 22727cm$^{-1}$ (440 nm).

All bands are characteristic for $V^{3+}$ Ions in an octahedral symmetrically field.

No shift in the positions of the bands was observed by increasing Vanadium concentration.

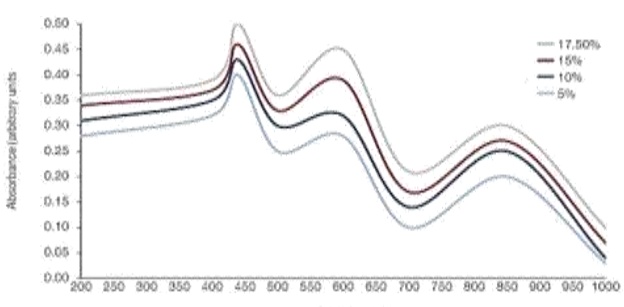


**Fig (1):** UV absorbance of PVA films doped with different $VCl_3$ conc.

It is clear from Fig. 1 that the intensity of the spectrum increased with the PVA conc. This indicates an excellent interaction among the V3+ ions and the OH grouping of PVA [19, 20]. Additionally, the peaks at 600 and 850 nm are due to the bi-polaronic states produced by $VCl_3$ [21]. The observed increase of the peak intensity above 600 nm indicates the molecular accumulation of $VCl_3$.

The first band is located at 11765 cm$^{-1}$ (850 nm) was assigned to the

$$^3T_{2g} \overset{v_1}{\leftarrow} {}^3T_{1g}$$

Transition, while the high energy band at 22727 cm-1 (440 nm) is due to

$$^3A_{2g} \overset{v_2}{\leftarrow} {}^3T_{1g}$$

Transition. The third band at 16667 cm-1 (600 nm) is due to

$$^3T_{1g}(p) \overset{v_3}{\leftarrow} {}^3T_{1g}$$

The equations governing such transitions are (16)

$$v_1 = 8D_\mathrm{q} \quad (1)$$

$$v_2 = 18D_\mathrm{q} \quad (2)$$

$$v_3 = 6D_\mathrm{q}(av) + 15B \quad (3)$$

**Table 1.** B and 10Dq values of dopes PVA (poly vinyl alcohol with VCI3 with different concentrations weights.

| $VLC_3$ content (wt%) | B(cm$^{-1}$) | 10 $D_q$(cm$^{-1}$) |
|---|---|---|
| 5 | 564 | 13670 |
| 10 | 564 | 13670 |
| 15 | 564 | 13670 |
| 17.5 | 564 | 13670 |

Where B is the reach constant, $D_q$ ligand field strength, $D_\mathrm{q}$ (av) is the average of the $D_\mathrm{q}$ values obtained from e equations (1) and (2). Data are listed in table 1.

Such values agree well with those given for V+3 in references [17, 18].

The data obtained indicate that, this composite is of octahedral structure and PVA acts as weak ligand. The correlation diagram for V+3 ion in an octahedral field is shown in fig (2).

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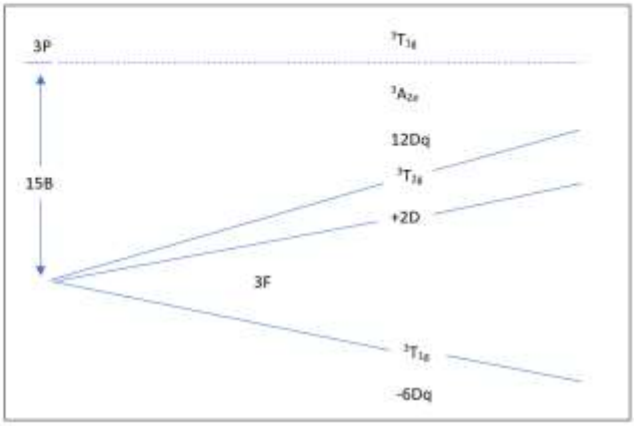


**Fig (2):** Scheme energy level diagram of □$^{3+}$Ion in an octahedral field.

The correlation diagram for $V^{3+}$ Ion in an Octahedral field is illuminated in Fig (2). One can conclude that. Vanadium ions exist in the divalent state and are acted on an octahedral symmetrical field.

### *3.2 Optical absorption spectrums of PVA doped with different concentration of $VCl_3$ irradiated with $\gamma$ doses*

The γ radiation effects on the UV-visible Spectrum of PVA/$VCl_3$. When PVA/$VCl_3$ films are subjected to γ-irradiation, the optical properties are the net result of the electronic transition of the two materials.

Figures (3-6) show w UV-visible absorption spectra of PVA filled with difference concentrations of $VCl_3$ irradiated with γ ray doses of 50, 100, and 150 kGy. Increasing the $VCl_3$ content, we observe the changes in the UV absorbance, In order to explain the observed results, one should consider the effect of γirradiation on the polymer, γ-irradiation causes cross linking and degradation.

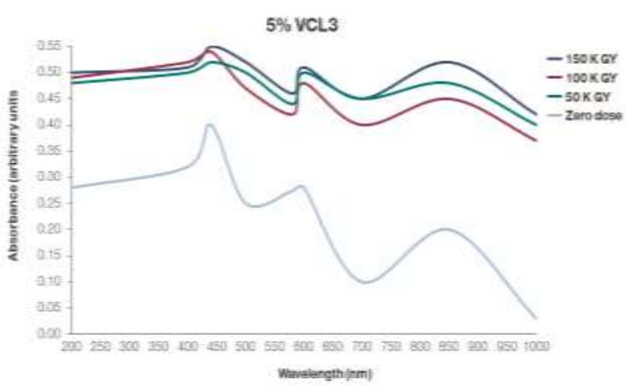


**Fig (3):** UV-visible absorption spectra of PVA doped with 5% wt. $V^{3+}$Irradiated with γ doses.

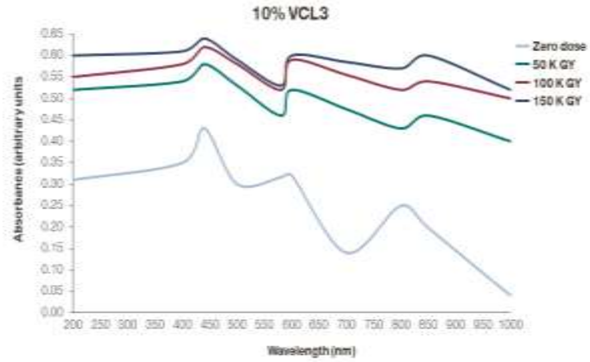


**Fig (4):** UV-visible absorption spectra of PVA doped with 10% wt. □$^{3+}$Irradiated with gamma doses.

Crosslinking of PVA macromolecules was achieved with increasing the dose. This causes a distinct rise in MW. At high dose, both degradation and crosslinking occur until crosslinking prevails.

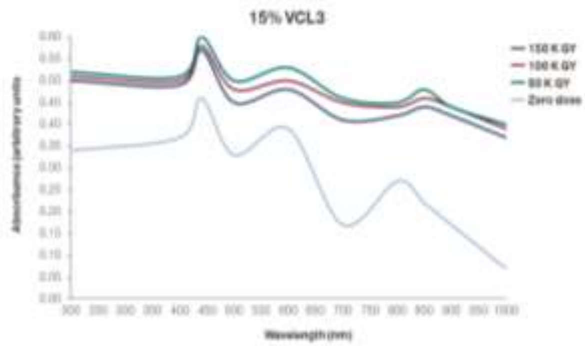


**Fig (5):** UV-visible absorption spectra of PVA doped with 15% wt. □$^{3+}$Irradiated with gamma doses.

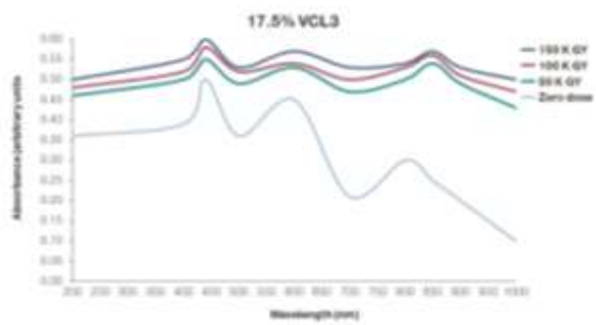


**Fig (6):** UV-visible absorption spectra of PVA doped with 17.5% wt. □$^{3+}$Irradiated with gamma doses.

After irradiation, for samples with concentrations of 10%, 17.5% $VCl_3$ by wt. the cross-linking dominates than degradation and the degree of absorption intensity increased with the increasing absorbed dose. But samples with concentrations of 5% ,15% VCl3 by wt. the effect of oxidative degradation is predominant than cross-linked effects, so by γ irradiation to dose 50 kGy the cross-linking effects is the predominately than cross linking effects.

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While at dose 150 KGy at samples with 5% cross linking is the predominant. But samples with 15% by increasing γ doses there is oxidative degradation.

### *3.3 Mechanical properties of PVA doped with different concentrations of $VCl_3$*

The hardness test was followed (Wolpert Hardness Tester type) for PVA filler by ($VCl_3$) with different weight ratios (5, 10, 15, 17.5 wt.%) as displayed in figure (7), which illustrates the dependence of hardness number (H) versus $VCl_3$ concentrations. The hardness number increases with increasing $VCl_3$ content. As shown in table 2.

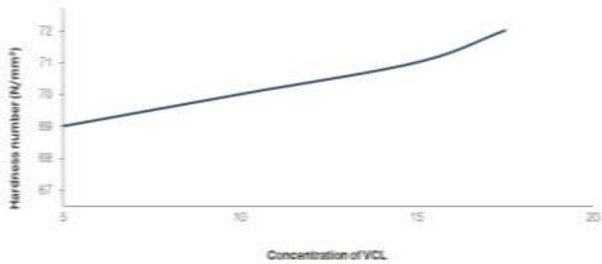


**Fig (7):** Hardness number (H) as a function of $VCl_3$ concentrations.

The hardness of the PVA increased on raising the $VCl_3$ conc. due to the bonding between PVA and $VCl_3$ which improves the density of the mechanical bond and the packing and interlocking, which reduces the movement of the base material molecules, thus raising the resistance to scratching and cutting [16].

One can then visualize that the polymer in its simplest form consists of linear chain bonds between atom of the same chain is stronger than that between atoms belongs to different chains, by increasing vanadium content it formed free radicals which leads to cross-linking i.e., the interaction between atoms of different chains become stronger. It seems that the addition of vanadium leads to increase the number of cross-linking between different chains giving rise to increase the hardness of polymer. This, in turn, can be directly correlated with variations in mechanical behavior of the polymer (22).

The investigated samples have been observed to exhibit the first signs of the high-elastic state, I.e., chain flexibility, along of increase of $VCl_3$ content.

**Table 2.** The hardness values of (PVA - $\boldsymbol{VCL_3}$), Composite films at different weight ratio of ($\boldsymbol{VCL_3}$).

| $VLC_3$ content (wt%) | Hardness number ($N/mm^2$) |
|---|---|
| 5 | 69 |
| 10 | 70 |
| 15 | 71 |
| 17.5 | 72 |

### *3.4 Mechanical properties of PVA doped with different concentrations of $VCl_3$ irradiated with γ doses*

The effect of γ radiation on the hardness is shown in fig (8). The observed effect is termed Cyclic effect, (23, 24).


**Fig (8):** Hardness number (H) as a function of γ dose.

In which the hardness rose as the γ dose is rises until maximum value, based on the VCl3 conc. then behaved in the opposite trend. After that it increased. This trend is explained the ionizing effect of γ radiation [25-27].

## 4 Conclusions

The composite films are suitable for being used in photo-electronic applications. ($VCl_3$) interacts with the OH group of PVA which was reflected in an enhancement of the hardness of the composite films.

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