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Polymer carbon nanotube nanocomposite films as a new nanotechnology application in the development of optoelectronic devices

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Abstract

Our research, detailed in this paper, introduces a novel method for fabricating and characterizing PVA-CNT polymeric nanocomposite films, aiming to make them suitable candidates for optoelectronic applications. The dispersion of multi-walled carbon nanotubes in an aqueous solution can be challenging; however, effective dispersion can be achieved using an appropriate amount of tannic acid (30 mg in 100 mL of deionized water) followed by sonication. In this study, we examined CNT concentrations of 0.125% and 1% by weight. The PVA-CNT films exhibited significant improvements in their band gap, Urbach energy, and overall optical properties.

Keywords: PVA-CNT nanocomposite films; tannic acid; Urbach energy; band gap; optical conductivity;

1. Introduction

Recently, polymer-based nanocomposites have garnered significant attention in both research and practical applications for next-generation optoelectronic devices. Researchers have focused on high refractive index polymers due to their promising potential in developing various optoelectronic devices, including Organic Light-Emitting Diodes (OLEDs), Light-Dependent Resistors (LDRs), and advanced display technologies [1]. Polyvinyl alcohol (PVA), a water-soluble polymer, is renowned for its exceptional film-forming properties, compatibility, consistency, and high ductility and plasticity [2]. Carbon nanotubes (CNTs) play a crucial role in modern technology due to their unique optoelectronic, electronic, and electrical capabilities. These properties facilitate the development of diverse interfacial structures within complex nanocomposites [2].

A novel aspect of this study involves treating CNTs with tannic acid before fabricating polymer nanocomposite films. The optical constants, including the band gap, Urbach energy**,** refractive index, and the optical conductivity. Although many studies in literature investigated the influence of different ratios of CNT (up to five) on nanocomposites, our study carried out with two concentrations as lower and higher ratios (0.125% and 1.0% by weight) and their effect on the optical properties of nanomaterial films. The dispersion of carbon nanotubes (CNT) in an aqueous solution with different acids and surfactants has been the subject of numerous studies in the literature, but effective dispersion is still difficult to achieve [3]. Tannic acid was selected because it is able to crosslink macromolecules at hydrogen bonding and $\pi-\pi$ interactions that can overcome the Van der Waals forces between carbon nanotube (CNT) bundles [4].

2. Preparation of PVA-CNT Polymer Nanocomposite Films

Dispersion of carbon nanotubes (CNT) in an aqueous solution can be challenges. To prepare the dispersion, 100 mg of multi-walled carbon nanotubes (MWCNTs) was dissolved in 30 mg of tannic acid in 100 mL of deionized water. This mixture was then sonicated for 4 hours using an ultrasonic probe. In the next step, 4 g of polyvinyl alcohol (PVA) was dissolved in 100 mL of deionized water while being stirred with a magnetic stirrer for 2 hours at constant temperature at 80°C. Afterwards, in order to study the effect of CNTs on the physical properties of PVA matrix, the synthesized CNT suspensions with different concentrations (0.125% and 1.0% by weight) were added to the PVA solution, and the combined mixture was stirred magnetically at 80°C for 30 minutes. Finally, the solutions were carefully poured onto a glass substrate and dried at 30°C for 48 hours. The resulting nanocomposite films had an estimated thickness of 30 µm as shown by SEM image (**Figure 1(a)**). Our study carried out on fixed thickness of the film. Although many studies in literature investigated the influence of the thickness on the physical properties of materials.

3. Results and discussion

Figure 1(b&c) show the dispersion of CNTs in aqueous solutions with and without tannic acid. **In Figure 1(b)**, CNT dispersed in water only, it is clear that despite CNTs having little effective dispersion, CNTs aggregated as ball-like bundles in an aqueous solution. **In Figure 1(c)**, CNTs, conversely, were efficiently distributed and separated in the tannic acid-containing aqueous solution. Tannic acid and sonication-treated CNT bundles exhibited minimal agglomeration, manifesting as spherical clusters, and were primarily dispersed.

A SEM image of the PVA-CNT nanocomposite film's morphology is displayed in **Figure 1(d)**. In this nanocomposite film, the CNTs showed a well-established network-like structure after being uniformly distributed throughout the PVA matrix.

The optical energy direct band gap (**Figure. 2(a)**) could be analysed using Tauc's model (Tauc–Lorentz model is a mathematical formula can be used to estimate the band gap of materials from the optical absorption spectra) [5]:

$$\alpha h\nu = B(h\nu - E_g)^{0.5} \qquad (1)$$

As the content of carbon nanotubes (CNTs) increased in the nanocomposite films, the band gap decreased. At a CNT loading ratio of 1.0 percent by weight, the direct energy gap (E_g) value for PVA-CNT films was significantly lower at 4.14 eV compared to 4.40 eV for pure PVA. At a CNT loading ratio of 1.0 percent by weight, the direct energy gap (E_g) value for PVA-CNT films was significantly lower at 4.14 eV compared to 4.40 eV for pure PVA. A higher proportion of CNTs by weight was found to reduce the E_g, likely due to the formation of localized states in the band gap associated with Van Hove singularities (Van Hove singularity is a singularity (non-smooth point) in the density of states (DOS) of a crystalline solid). This decrease can be attributed to charge transfer occurring at the interfaces between PVA and CNTs.

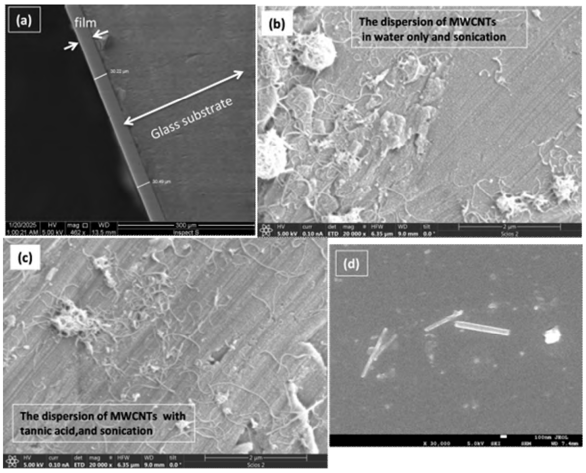

Figure 1. (a) Cross-section SEM images of the film's thickness , (b) SEM images of the dispersion of MWCNT in water and (c) in the aqueous solution with tannic acid, (d) SEM micrograph of PVA-CNT nanocomposite film

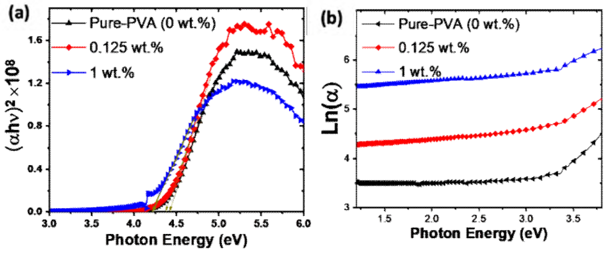

Figure 2. (**a**) direct band gap and (**b**) Plot of Ln(α) versus $h\nu$.

Table. 1 Indirect E_g and E_u for PVA and PVA-CNTs nanocomposite films

PVA-CNT	E_g (eV) Direct	E_u(eV)
Pure-PVA	4.40	0.50
0.125wt%	4.34	0.59
1.0wt%	4.14	0.91

Urbach energy E_u or Urbach edge (EU) is below the band gap energy governed by the structural disorder at the surface. The Urbach energy E_u, sometimes referred to as the Urbach tail or the width of the band tail, can be calculated using the following equation [6].

$$\alpha = \alpha_0 \exp\left(\frac{h\nu}{E_u}\right) \qquad (2)$$

Figure 2. (b) shows the plot of *Ln(α)* versus *hv*. The Urbach energy E_u values were determined from the reciprocal slope, as listed in **Table 1**. The value increased with increasing wt% of CNTs, which implied a higher concentration of localised energy states in the forbidden band gap and more significant disorder within the polymer film structure.

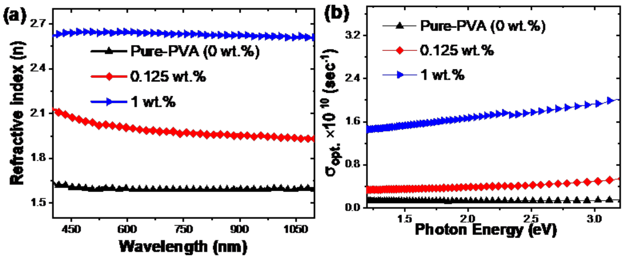

Figure. 3 (a) The calculated refractive index for PVA and PVA-CNT nanocomposite films with different wt.% CNT **(b)** the value of optical conductivity ($\sigma_{opt.}$)

The refractive index n(λ) can be calculated in terms of the reflectance R(λ) as the following equation [5]:

$$n(\lambda) = \frac{1+\sqrt{R(\lambda)}}{1-\sqrt{R(\lambda)}} \qquad (3)$$

As shown in **Figure 3. (a)**, the value of n(λ) in the PVA structure increased with the rose CNT concentration. The higher weight percentage of CNTs in the host polymer leads to an increased packing density, which accounts for this improvement.

The optical conductivity σ_{opt} of polymer composites describes how the material helps charge carriers move when photons hit it. The optical conductivity can be determined using the following equation:

$$\sigma_{opt} = \alpha\, n(\lambda) c/\pi \qquad (4)$$

Figure 3. (b) shows the optical conductivity value of the PVA matrix with different amounts of CNTs. It is apparent that optical conductivity increased primarily with loading 1.0 wt% of MWCNTs compared to others. The PVA-CNT films exhibited an increase in charge carriers due to a general increase in CNT content. This improvement can be explained by the formation of extra energy states within the forbidden band gap, which transports more electrons from one energy state to another.

4. Conclusion

PVA and nanocomposite films including varying weights of MWCNTs (0.125 and 1 wt.%) were produced. The optical characteristics enhanced with increasing CNT concentration due to the emergence of novel states in the band gap region. The optical band gap, Urbach energy, optical conductivity, and refractive index were improved.

5. Future work

The results indicate that PVA-CNT nanocomposite films may be advantageous for the development of novel optoelectronic and photoelectric devices. Further investigation is required to address the aggregation of carbon nanotubes in nanocomposites.

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