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Synthesis and Improved Optical Properties of PVA–In_2O_3–Fe_2O_3 Nanostructures to Use in Optical Fields

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The PVA–In_2O_3–Fe_2O_3 nanocomposites are fabricated by the casting method. Solar cells, transistors, and electronic gate units are just a few examples of the many nanoelectronic–optical systems, which can benefit from these nanocomposites. Nanocomposites including polyvinyl alcohol (PVA), indium oxide (In_2O_3), and iron oxide (Fe_2O_3) have their optical characteristics studied. The nanocomposites have significant ultraviolet (UV) light absorption properties. Moreover, the transmittance diminishes, when the In_2O_3–Fe_2O_3-nanoparticles' increase. By raising the weight percent ratio of In_2O_3–Fe_2O_3 nanosize components to 6 percent, we found that polyvinyl-alcohol average energy gap (E_g) decreases that makes it suitable for photonics applications. A number of optical characteristics are evaluated, such as the extinction coefficient (k), absorption coefficient (α), refractive index (n), optical conductivity, the real component (ε_1) and imaginary component (ε_2) of the dielectric constant.

Нанокомпозити ПВС–In_2O_3–Fe_2O_3 виготовлено методом лиття. Сонячні елементи, транзистори й електронні затвори — це лише кілька прикладів багатьох наноелектронно-оптичних систем, які можуть отримати користь від цих нанокомпозитів. Досліджено оптичні характеристики нанокомпозитів, що містять полівініловий спирт (ПВС), оксид Індію (In_2O_3) й оксид Феруму (Fe_2O_3). Нанокомпозити мають істотні властивості щодо вбирання ультрафіолетового (УФ) світла. Крім того, коефіцієнт пропускання зменшується зі збільшенням кількости наночастинок In_2O_3–Fe_2O_3. Збільшивши вагове співвідношення нанорозмірних компонентів In_2O_3–Fe_2O_3 до 6 відсотків, ми виявили, що середня ширина забороненої зони полівінілового спирту (E_g) зменшується, що робить його придатним для застосування у фотоніці. Оцінено низку оптичних характеристик, таких як коефіцієнт екстинкції (k), коефіцієнт вбирання (α), показник заломлення (n), оптична провідність, дійсна складова (ε_1) та уявна складова (ε_2) діелектричної проникности.

Key words: polyvinyl alcohol, indium oxide, iron oxide, optical properties.

Ключові слова: полівініловий спирт, оксид Індію, оксид Феруму, оптичні властивості.

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1. INTRODUCTION

The optical properties of polymers play a crucial role in various applications such as electrical transitions, insulation covers, optical filters, greenhouses, and selective surfaces. However, the primary objective of boosting the optical properties of these polymers is accomplished by improving reflection, interference, antireflection, and polarization phenomena [1, 2]. Polymers have become the preferred choice over traditional silica-based optical materials, because they are easier to process, less expensive, and can be produced in larger quantities [3, 4]. Polymers can have their characteristics enhanced and controlled by adding the right dopant. Some key points about optical properties of the intermixture composed of several metal salts interacting with PVA are shown, which are determined by refractive index and the light absorption coefficient [5, 6]. There are myriad uses for polymers. The polymeric properties such as piezoelectric, optical, semiconductor and electro-optical ones have enabled more recent developments in stretchable electronics [7]. Dopant–polymer optical properties are very sensitive with respect to electronic nature of electrolytes. For good optical properties of produced materials, it is necessary to have command over electronic mechanisms [8, 9].

2. EXPERIMENTAL PROCEDURE

The samples were fabricated using polyvinyl alcohol (PVA), indium oxide (In_2O_3), and iron oxide (Fe_2O_3). The nanoparticles composed of In_2O_3–Fe_2O_3 were incorporated into a polymer PVA by the casting method at various weight percentages: 0, 2, 4, and 6 wt.%. To create a more uniform solution, 40 ml of distilled water was used to dissolve polyvinyl alcohol (PVA). The solution was then stirred using a magnetic stirrer at a temperature of 70°C for duration of 30 minutes. The UV/1800/Shimadzu spectrophotometer is utilized for the precise measurement of the optical characteristics of PVA–In_2O_3–Fe_2O_3 nanocomposites within the wavelength range of 200 to 1100 nm.

Absorbance is the quotient of the intensity of light absorbed by a material (I_A) and the intensity of incoming light (I_0) [10, 11]:

$$A = I_A/I_0. \quad (1)$$

The transmittance (T) is defined as the ratio of the intensity of the transmitting rays (I_T) passing through the film to the intensity of the incident rays (I_0), which fall on it [12, 13]:

$$T = I_T/I_0. \quad (2)$$

Absorption coefficient (α) is defined as the ability of a material to absorb the light of a given wavelength [14, 15]:

$$\alpha = 2.303A/t, \quad (3)$$

where A is the absorption of the material, t—the sample thickness in cm. The coefficient α for this transition type is given by [16, 17]

$$\alpha h\nu = B\left(h\nu - E_g^{opt}\right)^r, \quad (4)$$

where E_g^{opt} is energy gap between direct transitions.

The refractive index (n) is given by [18, 19]

$$n = \sqrt{4R - \frac{k^2}{(R-1)^2}} - \frac{R+1}{R-1}. \quad (5)$$

The below equation can be employed to obtain the extinction coefficient (k) [20]:

$$k = \alpha\lambda/(4\pi). \quad (6)$$

The formulas for the real (ε_1) and imaginary (ε_2) components of the dielectric constant may be used to separate it [21, 22]:

$$\varepsilon_1 = n^2 - k^2, \quad (7)$$

$$\varepsilon_2 = 2nk. \quad (8)$$

The optical conductivity (σ) is determined *via* the equation given by Ref. [23]:

$$\sigma_{opt} = \alpha nc/(4\pi). \quad (9)$$

3. RESULTS AND DISCUSSION

Figure 1 shows the absorption spectra for PVA–In_2O_3–Fe_2O_3 nanocomposites *versus* wavelength. In the visible/near infrared spectrum, films often have low absorption values. This explains, why objects absorb light of longer wavelengths because few photon interacts with atoms well and transmit less energy. Therefore, since the photon interacts with matter depending on its frequency and, thus, the wavelength, there will be an increasing in absorbance as the wavelength decreases. That means that these unbound electrons will simply absorb the falling light. This leads to an increase in absorbance with increasing weight percentages of In_2O_3–Fe_2O_3 nanoparticles [24, 25].

Optical transmittance spectra at different incident-light wave-

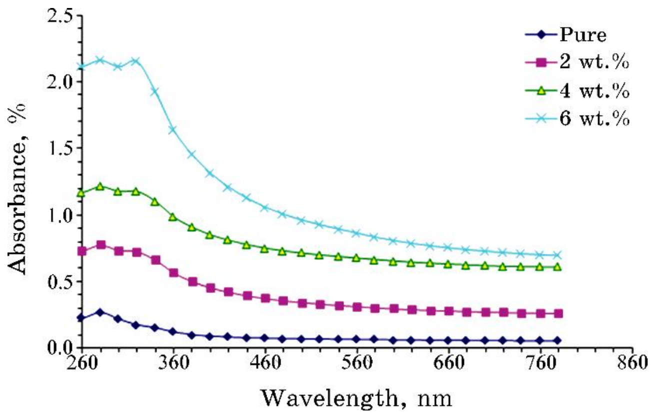

Fig. 1. The relationship between the wavelength and changes in the absorbance of PVA–In_2O_3–Fe_2O_3 nanocomposites.

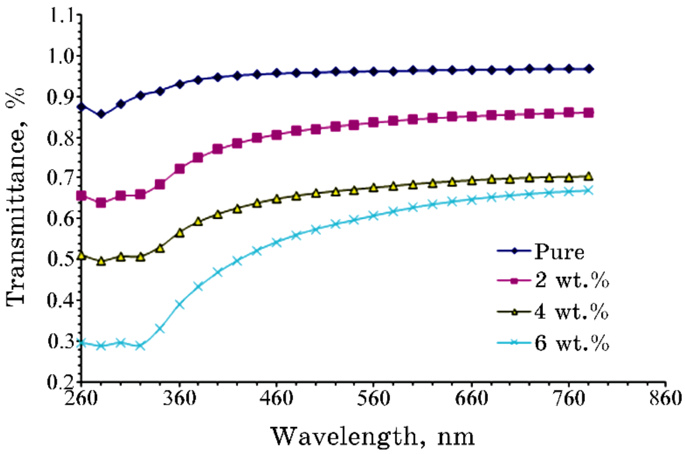

Fig. 2. The PVA–In_2O_3–Fe_2O_3-nanocomposites' transmission changes depending on the wavelength.

lengths are shown in Fig. 2 as a function of increasing the concentration of In_2O_3–Fe_2O_3 in PVA films. Transmittance drops with increasing concentration of In_2O_3–Fe_2O_3 nanoparticles, as seen in this graph. The addition of In_2O_3–Fe_2O_3, which possesses electron-accepting electromagnetic energy, has the capability to enhance the excited states of electrons [26, 27]. It also conforms to that previously was determined in other studies [28, 29].

The absorbance coefficient *versus* wavelength is drawn in Fig. 3 for PVA–In_2O_3–Fe_2O_3 nanocomposites. The low absorption coefficient at long wavelengths and low energy level 1–3 eV is revealed in Fig. 3. The probability of an incident-photon exciting an electron from the value band to the conductivity band because $h\nu$ is lower than E_g is rather small. However, if the incident-photons' energy is higher than prohibited energy gap of the material, a good absorption at high energies occurs since the electron hops to the conduction band from valence band [30]. The absorption value gives away, if it is the direct electron transition or no. Therefore, with α values more than 10^4 cm^{-1} at high energies, direct electron transition means that both the electrons and photons retain the same amount of energy and the momentum. At low energies, when the absorption coefficient is small $\alpha < 10^4$ cm^{-1}, indirect electron transition is expected, whereby phonons preserve electrons' momenta [31].

In Figure 4, we can see, how the square root of the absorption edge $h\nu$ relates to the photon energy. To calculate the size of the energy gap for an approved indirect transition by following a straight line from the peak, all the way is down the x-axis, where the square root of the product of Planck's constant and frequency is zero. A smaller energy gap is seen for higher concentrations of

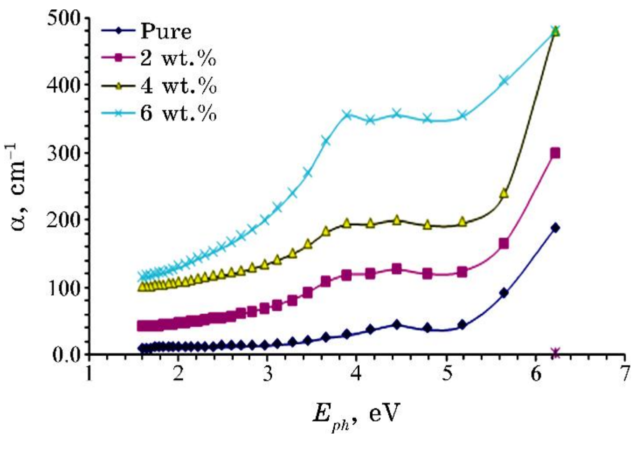

Fig. 3. The absorption coefficient of PVA–In_2O_3–Fe_2O_3 nanocomposites will change as a function of photon energy.

In_2O_3–Fe_2O_3 nanoparticles. The growth of the localized levels inside the forbidden energy gap is the corresponding reason.

The transition occurs in a two-stage process, when the amount of In_2O_3–Fe_2O_3 increases. With a rise in the amount of In_2O_3–Fe_2O_3 nanoparticles, the electron moves from a valence band passing through its local levels until it reaches the conduction band. The reason for such observation lies in the nature of these materials: since they are heterogeneous (for example, electrical conductivity depends on the degree of concentration), the density of localized states rises with the increase of In_2O_3–Fe_2O_3-nanoparticles' concen-

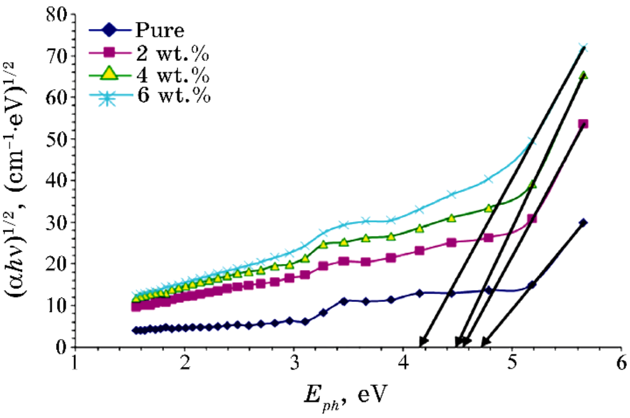

Fig. 4. The correlation between the square root of ($\alpha h\nu$) and the energy of the photons for nanocomposites consisting of PVA–In_2O_3–Fe_2O_3.

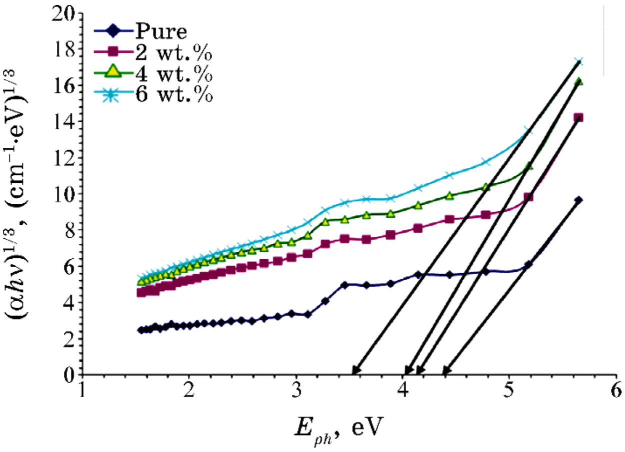

Fig. 5. The correlation between the cubic root of ($\alpha h\nu$) and the energy of photons for PVA–In_2O_3–Fe_2O_3 nanocomposites.

tration. This is that other researchers have already shown [32, 33].

Forbidden energy-gap transitions also use the same procedure to obtain them. Figure 5 depicts the forbidden transition of the indirect energy gap of PVA–In_2O_3–Fe_2O_3 nanocomposites.

Figure 6 shows the connection between refractive index and wavelength. There is a significant increment observed in the refractive index with an increase in nanocomposite density. The low transmittance in the UV region gives a higher value for the refractive index. They have high transmittance, which makes them transparent; hence, they are low in the visible zone [34, 35].

Figure 7 shows the variation of (k) for PVA–In_2O_3–Fe_2O_3 nanocomposites with wavelengths. Observed (k) values suggest that it decreases with increasing concentration of In_2O_3–Fe_2O_3 nanoparticles in a solution. The absorption coefficient increases with the percentage of In_2O_3–Fe_2O_3 nanoparticles, thus, resulting in an increase. Consequently, the structure of the host polymer will be altered by the atoms of the In_2O_3–Fe_2O_3 nanoparticles [36, 37].

The equations (7) and (8) were used to determine the real and imaginary components of the dielectric constants for the nanocomposites consisting of PVA–In_2O_3–Fe_2O_3. Figure 8 illustrates the correlation between the variable ε_1 and the wavelength. Reducing the k value results in the noticeable influence of n on the ε_1 value, as seen in this figure. The actual dielectric constant increases as the concentration of In_2O_3–Fe_2O_3-nanoparticles' increases. Figure 9 illustrates the correlation between the variable ε_2 and the wavelength. The absorption coefficient, denoted as k, governs the relationship between k and α, ultimately determining the value of k. This value of k influences subsequently [38–40].

The optical conductivity (σ_{opt}) may be calculated using Eq. (9). Nanocomposites made of PVA–In_2O_3–Fe_2O_3 show wavelength-

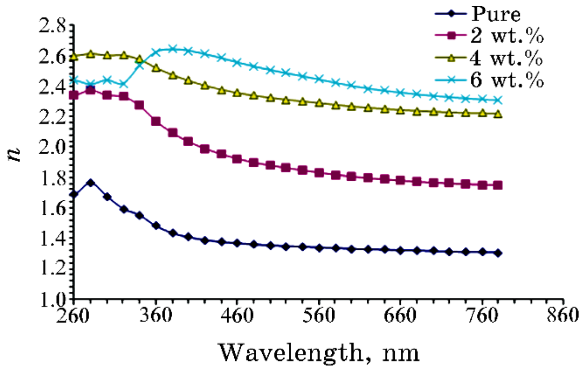

Fig. 6. Relationship between the refractive index and wavelength for PVA–In_2O_3–Fe_2O_3 nanocomposites.

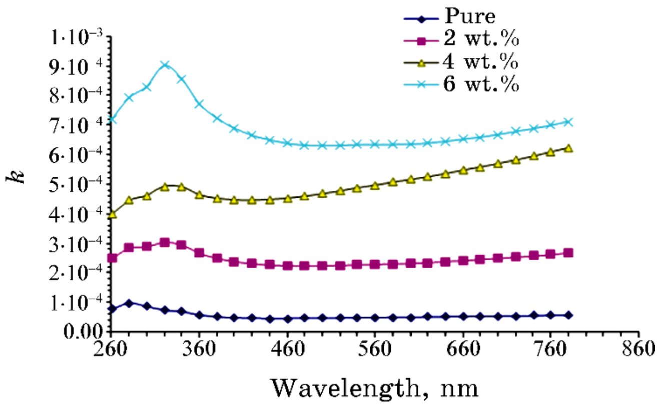

Fig. 7. The relationship between the extinction coefficient and wavelength for the nanocomposites PVA–In_2O_3–Fe_2O_3.

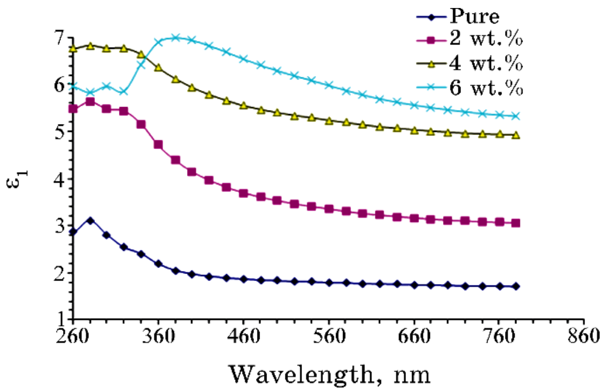

Fig. 8. Relationship between the wavelength and the real part of the dielectric constant of nanocomposite consisting of PVA, In_2O_3, and Fe_2O_3.

dependent changes in optical conductivity (Fig. 10). Improving optical conductivity may be achieved by increasing the iron oxide to iron trioxide weight ratio in PVA polymer to 6 weight percents. Elevated electron mobility is the result of expanding the band gap to include additional energy levels [41, 42]. Therefore, electrons can go from the valence band to the newly formed energy levels and, then, into the conduction band. So, the band gap narrows and conductivity grows [43].

4. CONCLUSIONS

Through the casting approach, nanoparticles of In_2O_3–Fe_2O_3 were

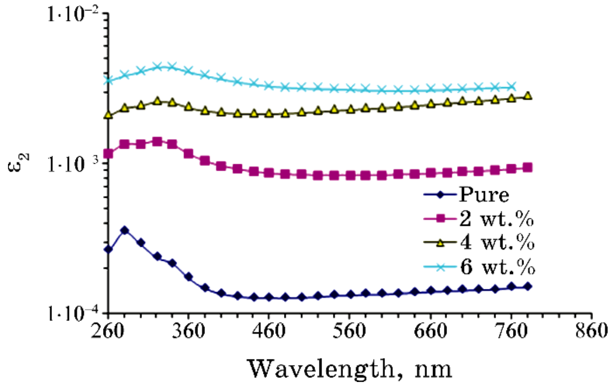

Fig. 9. The variation of imaginary part of the dielectric constant of PVA–In_2O_3–Fe_2O_3 nanocomposites with wavelength.

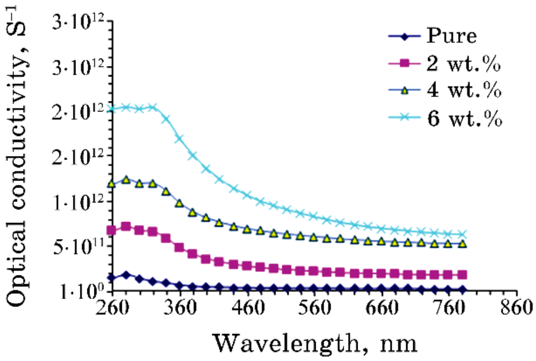

Fig. 10. The variation of optical conductivity of PVA–In_2O_3–Fe_2O_3 nanocomposites with wavelength.

integrated into polyvinyl alcohol (PVA), resulting in the development of cost-effective optoelectronic nanocomposites. The percentage of In_2O_3–Fe_2O_3 nanoparticles in PVA–In_2O_2–Fe_2O_3 nanocomposites determines how much light the composites absorb. At 6 weight percent (wt.%) of In_2O_3–Fe_2O_3 nanoparticles, the energy gap of PVA for permitted indirect transitions dropped from 4.75 eV to 4.15 eV and, for prohibited indirect transitions, from 4.4 eV to 3.55 eV.

Optoelectronics is one of numerous optical areas and nanoscale technologies, which will benefit greatly from this finding. These enhancements are closely related to the variables of extinction coefficient, absorption coefficient, optical conductivity, refractive index, imaginary and real dielectric constants, and concentrations of In_2O_3–Fe_2O_3 nanoparticles. Happening more often, nanocomposites made of PVA–In_2O_3–Fe_2O_3 show outstanding optical properties, which increase their prospective applications in electric and opto-electronic fields, according to these results.

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