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Evaluation of Structural and Optical Properties of PVA/Fe₂O₃ Nanostructures for Photonic Devices

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The PVA/Fe₂O₃ nanocomposites are formed using a solution casting method with varying weight percentages of Fe₂O₃ nanoparticles: 0, 2, 4, and 6 wt.%. The optical microscopy and optical properties for films are studied; the results reveal that the nanoparticles form a continuous network in films of polyvinyl alcohol (PVA); the nanoparticles are linked in this network including routes for charge carriers to travel through it, causing a shift in the material properties. The findings reveal that, as the concentration of Fe₂O₃ nanoparticles rises, the absorbance, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constants and optical conductivity are increasing. The optical energy gap for PVA is reduced from 4.4 eV for pure PVA to 3.7 eV when Fe₂O₃ nanoparticles' concentration reaches 6 wt.%. This behaviour makes it suitable for variety optical approaches. The transmittance drops as the concentration of Fe₂O₃ nanoparticles increases.

Наноккомпозити ПВС/Fe₂O₃ формуються методом лиття розчинів з різним ваговим відсотком наночастинок Fe₂O₃: 0, 2, 4 та 6 мас.%. Вивчено оптичну мікроскопію й оптичні властивості плівок; результати показують, що наночастинок утворюють безперервну мережу в плівках полівинилового спирту (ПВС); наночастинок пов'язані в цій мережі, що включає маршрути проходження носіїв заряду через неї, викликаючи зрушення властивостей матеріалу. Одержані дані показують, що зі збільшенням концентрації наночастинок Fe₂O₃ спектральна вбирність, коефіцієнт вбирання, коефіцієнт згасання, показник заломлення, дійсна й уявна діелектричні проникності та оптична провідність зростають. Оптична енергетична щільність для ПВС зменшується від 4,4 еВ для чистого ПВС до 3,7 еВ за концентрації наночастинок Fe₂O₃ у 6 мас.%. Така поведінка робить його придатним для різноманітних оптичних підходів. Коефіцієнт пропускання спадає зі збільшенням концентрації наночастинок Fe₂O₃.

Key words: polyvinyl alcohol, iron oxide nanoparticles, nanocomposites, optical characteristics.

Ключові слова: полівініловий спирт, наночастинки оксиду Феруму, на-
нокомпозити, оптичні характеристики.

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1. INTRODUCTION

Nanotechnology has created a different part of study for the dispensation and creation of nanomaterials, which are substances that typically have crystallite sizes of less than 100 nanometers [1]. Nanotechnology is a hot theme this time, reaching, since new changes in technique, physics to precisely new fields to educating novel materials with nanometer dimensions scale [2]. That is fast emerging and rising, with vast fields in various research approaches, advancement, and industrialized activities. Nanoparticles (NPs) with higher thermal conductivity than their surrounding liquid have been found to improve deferral effective thermal conductivity [3]. Polymer matrix nanocomposites are an appealing and important part of today's materials because of their low weight, simple manufacturability, low cost, high fatigue strength, and good corrosion resistance. The addition for nanoparticles into a polymer matrix meaningfully alters its physical material properties such as structural, electrical, thermal, and optical properties [4, 5].

The polyvinyl alcohol is good host medium for an extensive variety for nanoparticles. It is motivated by the view of producing ultra-transparent films with superior optical properties. They have obtained a lot of attention due to their excellent dielectric properties. Their flexibility is exceptional, and their dielectric strength is quite robust. Due to they are created through erosion, iron oxides are intriguing due to their catalytic, magnetic, and semiconducting material properties. They can be used as high-density magnetic storage materials and as catalysts in the production of styrene. The typical stoichiometric form of iron oxides is Fe_2O_3 at room temperature. For its structural, optical, and band-gap properties, the polymer nanocomposite of ferrous oxide with PVA is included in nanocomposites [6].

2. EXPERIMENTAL PART

The PVA/ Fe_2O_3 nanocomposite films were made using the casting method at different weight percentages (0, 2, 4, and 6 wt.%) by dissolving 1 g from PVA in 40 ml of distilled water using a magnet-

ic starrier for 30 minute at temperature of 70°C. With the UV-1800 from Shimadzu at wavelengths between 220 and 800 nm, the optical properties of PVA/Fe₂O₃ nanocomposites' films were measured by a double beam spectrophotometer [nm]. The formula shown below [7] is used to calculate absorbance:

$$A = \frac{I_A}{I_O}; \quad (1)$$

I_A is the intensity of light that is absorbed by the substance, and I_O is the intensity of light that is incident.

The subsequent calculation can be used to calculate transmittance T [7]:

$$T = I_T/I_O; \quad (2)$$

I_T is the intensity of light that is transmitted through a material, and I_O is the intensity of light that is incident.

We can measure the absorption coefficient α of the current materials by use the thickness of the film [7]:

$$\alpha = 2.303A/d. \quad (3)$$

Absorbance is represented by A , and film thickness is represented by d .

The indirect transition was formed by applying the relationship [8]:

$$\alpha h\nu = B(h\nu - E_g)^r, \quad (4)$$

where $r = 2$ for transitions permitted indirectly and $r = 3$ for transitions proscribed indirectly. $h\nu$ is the incident-photon energy; B is constant value, and E_g is optical band gap.

Calculation can be used to determine the refractive index n [8]:

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

R is reflectance.

The calculation shown below [9] can be used to determine the extinction coefficient k :

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

The wavelength of the incident light is indicated here by λ .

The real (ϵ_1) and imaginary (ϵ_2) components of the dielectric con-

stant are defined by the subsequent algebraic expressions [9]:

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

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

The following calculation is used to determine the optical conductivity σ [10]:

$$\sigma = \frac{\alpha n c}{4\pi}. \quad (9)$$

Refractive index is denoted by n , while light velocity is denoted by c , and absorption coefficient is denoted by α .

3. RESULTS AND DISCUSSION

Images of PVA/Fe₂O₃ nanocomposites' films taken at a magnification power of 10× for samples of various concentrations are shown in Fig. 1. We can see (*a, b, c, d*), when the concentration of iron oxide reaches 6 wt.%, the nanoparticles form a continuous network in films of polyvinyl alcohol; inside the polymers, the nanoparticles are linked in this network, which includes routes for charge carriers to migrate through, causing a shift in the material properties [10].

The relationship between absorbance and wavelength of PVA/Fe₂O₃ nanocomposites as shown in Fig. 2. The display demonstrates that, as the wavelength increases, the absorbance of films decreases, peaking close to the fundamental absorption edge (220 nm). In general, visible and near-infrared film absorbance is minimal. We can explain this performance in this way. Near the fundamental absorption edge, the incident-photon wavelength shortens, but its energy remains sufficient to interact with atoms and transmit. Due to photon interactions with the substance, absorbance rises [11].

The relationship between transmittance and wavelength for PVA/Fe₂O₃ nanocomposites is presented in Fig. 3. We can see, if Fe₂O₃-nanoparticles' concentration rises, the transmittance decreases. This procedure results in electrons' release in their outside orbits, which is container to absorb electromagnetic energy, because the electron transported to a higher level has occupied vacant locations of energy band [12]. The pure PVA have high transmittance that allows the light to pass through while absorbing some of the incident light. This is so that the electron connection can be broken, and the electron can be moved to the conduction band [13].

The relationship between the absorbance coefficient and photon

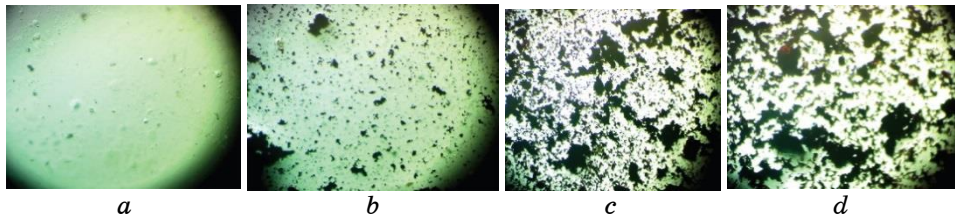


Fig. 1. The photomicrographs of PVA/Fe₂O₃ nanocomposites: (a) of PVA; (b) of 2 wt.% Fe₂O₃; (c) of 4 wt.% Fe₂O₃; (d) of 6 wt.% Fe₂O₃.

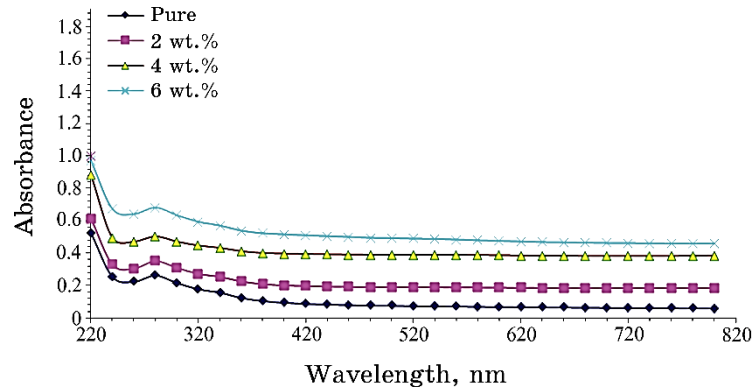


Fig. 2. Relation between the absorbance and the wavelength for the PVA/Fe₂O₃ nanocomposites.

energy for the PVA/Fe₂O₃ nanocomposites is shown in Fig. 4. We can see that this absorption coefficient is lowest at high wavelengths and low energies, indicating that there is little chance of an electron transition because the energy of the input photon is insufficient to allow the electron to pass from the valence band (V.B) to the conduction band (C.B) ($h\nu > E_g$) [14, 15]. This shows how the absorption coefficient can influence the type of electron transfer that occurs. When the absorption coefficient is high ($> 10^4 \text{ cm}^{-1}$ at high energies), a direct transition of an electron is anticipated to take place, and the energy and momentum are retained by the electrons and photons. However, because the absorption coefficients are $> 10^4 \text{ cm}^{-1}$ at low energies, it is anticipated that an electron will make an indirect transition and that the electronic momentum will be preserved with the help of the adsorption process [15]. The PVA/Fe₂O₃ nanocomposites' coefficient of absorbance is fewer than $< 10^4 \text{ cm}^{-1}$, demonstrating that the electron transition is indirect in these nanocomposites [16].

The relationship between the photon energy and the absorption

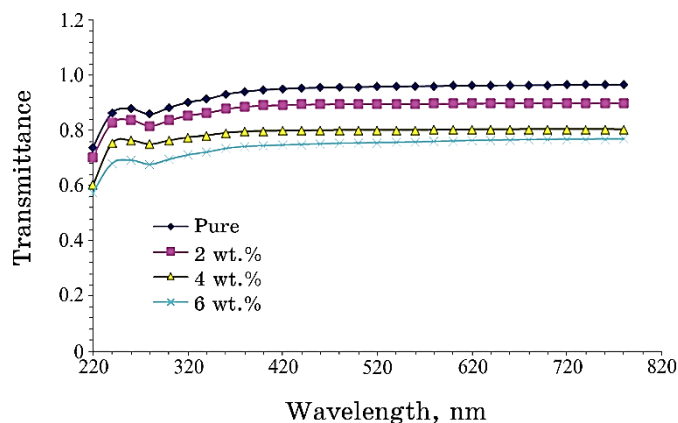


Fig. 3. Relation between the transmittance and the wavelength for the PVA/Fe₂O₃ nanocomposites.

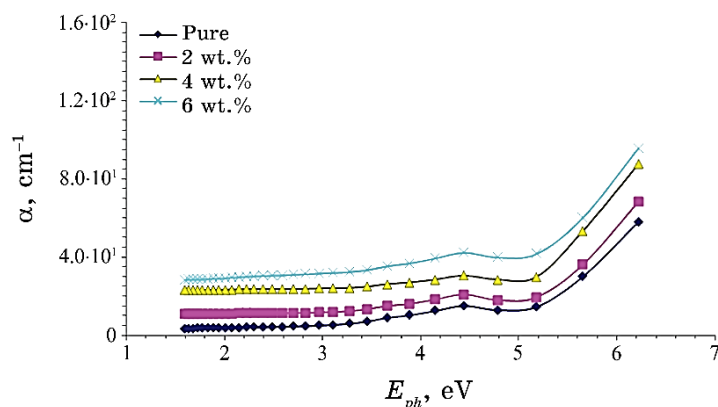


Fig. 4. Relation between the absorbance coefficient and the photon energy for the PVA/Fe₂O₃ nanocomposites.

edge $(\alpha h\nu)^{1/2}$ for the PVA/Fe₂O₃ nanocomposites is shown in Fig. 5. By connecting the higher portion of the curve on the x -axis to $(\alpha h\nu)^{1/2} = 0$, we can draw a straight line to visualize the energy gap of this permitted indirect transition.

The energy-gap values drop with weight percentages of Fe₂O₃ nanoparticles rise. The formation of localized levels in this prohibited energy gap was creditable with causing this [17]. In this instance, as the weight percentage of iron-oxide nanoparticles rises, the electron passages from V.B to these limited levels and consequently to this C.B increase. The density of the localized state rise with concentration of nanocomposites rising because they are heterogeneous (*i.e.*, electronic conduction depends on the additional concentration

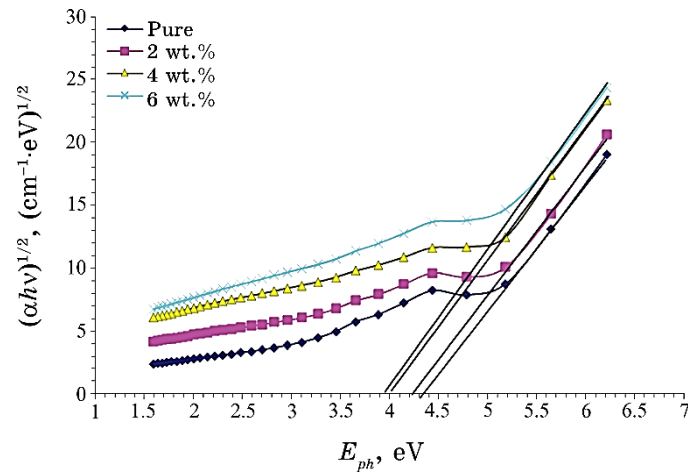


Fig. 5. Relation between the absorption edge $(\alpha h\nu)^{1/2}$ and the photon energy for the PVA/Fe₂O₃ nanocomposites.

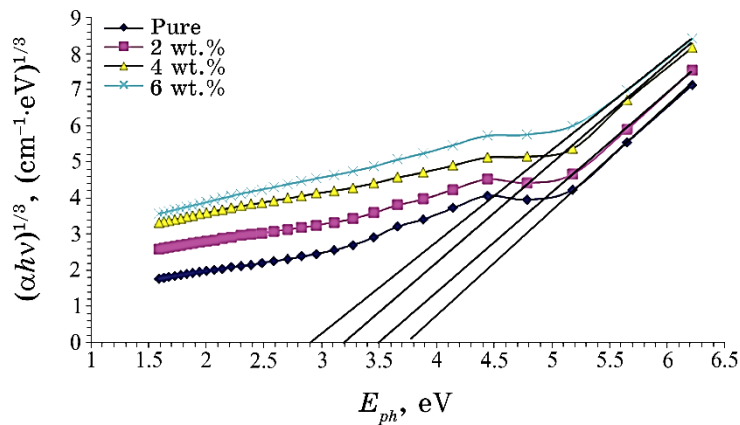


Fig. 6. Change of $(\alpha h\nu)^{1/3}$ [(cm⁻¹.eV)^{1/3}] with photon energy for the PVA/Fe₂O₃ nanocomposites.

rise as the weight percentage of iron-oxide nanoparticles increases [18]).

This similar method is used to take into account the forbidden transition for this indirect energy gap, as depicted in Fig. 6.

The relationship between wavelength and refractive index for PVA/Fe₂O₃ nanocomposites is depicted in Fig. 7. The graph demonstrates that, as density increases, *i.e.*, Fe₂O₃-nanoparticles' concentration in PVA, nanocomposites' refractive index increases. Due to its low transmittance, the UV region has high refractive-index val-

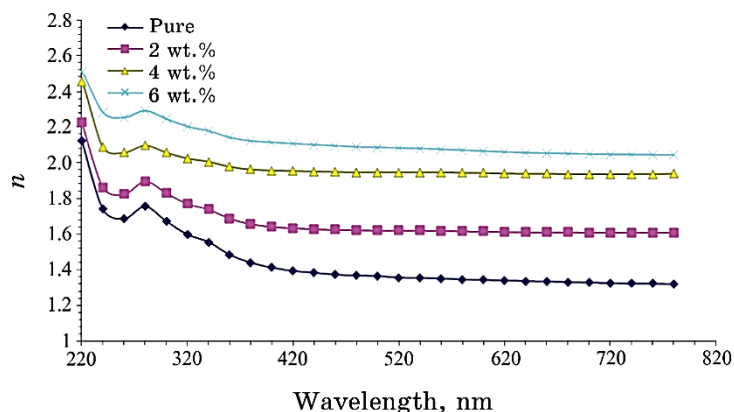


Fig. 7. Relation between the refractive index and the wavelength for the PVA/Fe₂O₃ nanocomposites.

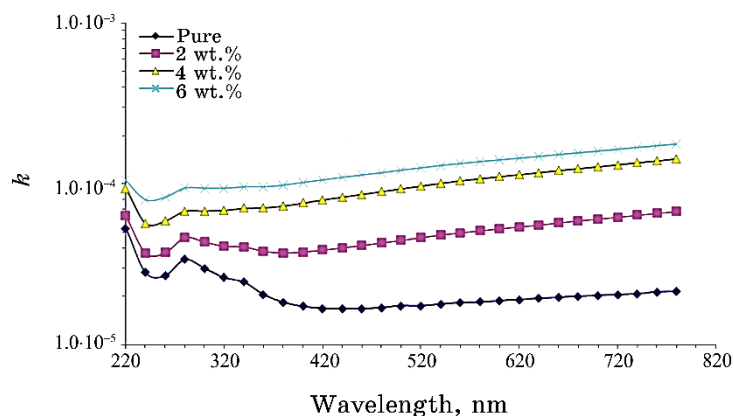


Fig. 8. Extinction coefficient as a function of wavelength for the PVA/Fe₂O₃ nanocomposites.

ues, while the visible range has little values because of its high transmittance [19].

The relationship between the extinction coefficient and wavelength for the PVA/Fe₂O₃ nanocomposites is shown in Fig. 8. We can note that the extinction coefficient rises as Fe₂O₃-nanoparticles' concentration rises. This is attributed to the increased weight percentages of Fe₂O₃ nanoparticles and the improved absorption coefficient. This reason suggests that the host polymer structure will change because of the Fe₂O₃ nanoparticles [20, 21].

The relationship between the wavelength and the real part of the dielectric constant of PVA/Fe₂O₃ nanocomposites is displayed in Fig. 9. The real dielectric constant rises with the rise of Fe₂O₃ na-

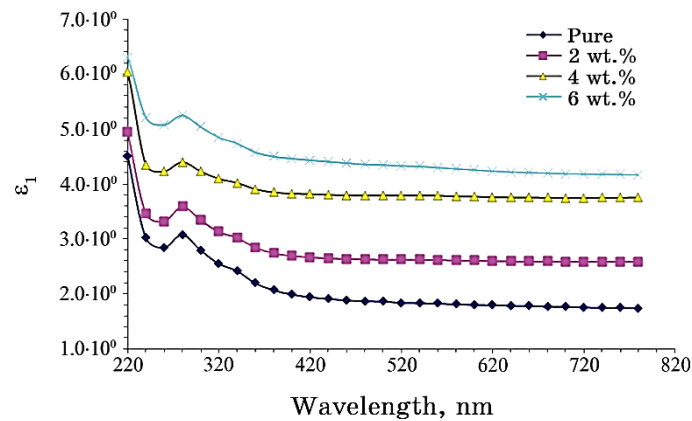


Fig. 9. Relation between the real part of dielectric constant and the wavelength for the PVA/Fe₂O₃ nanocomposites.

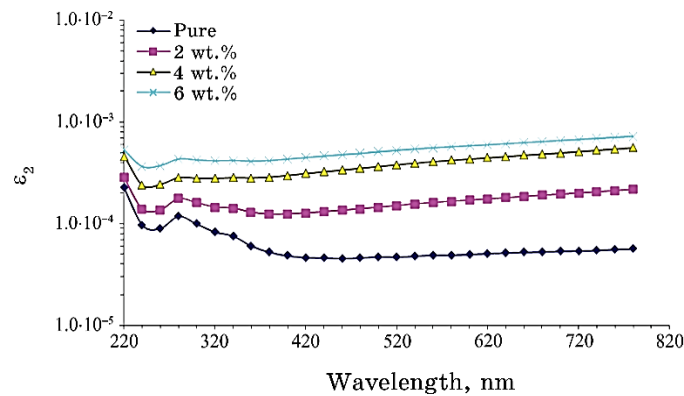


Fig. 10. Imaginary part of dielectric constant as a function of wavelength for the PVA/Fe₂O₃ nanocomposites.

noparticles' concentration. Due to the low value of n^2 , this figure demonstrates that ϵ_1 is highly dependent on it (as k^2) [22].

The relationship between the imaginary part of the dielectric constant and the wavelength for the PVA/Fe₂O₃ nanocomposites is shown in Fig. 10. We can see that the ϵ_2 values, which vary due to the absorption coefficient, are dependent on k because of relationship between ϵ_2 and k [23].

The relationship between optical conductivity and wavelength for the PVA/Fe₂O₃ nanocomposites is shown in Fig. 11. As the proportion of Fe₂O₃ NPs reached to 6 wt.%, the optical conductivity of PVA rises.

Electrons can passage from the V.B to the local levels to the C.B

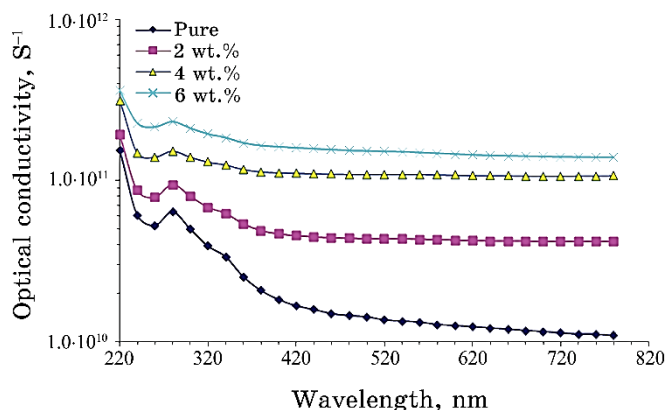


Fig. 11. Relation between the optical conductivity and the wavelength for the PVA/Fe₂O₃ nanocomposites.

more easily thanks to these new levels in this band gap. The band gap closes, as a consequence, and conductivity rises [24, 25].

4. CONCLUSION

One founding of the optical microscopy, investigators revealed that nanoparticles form a continuous network in films of polyvinyl alcohol; the nanoparticles are linked in this network including routes for charge carriers to migrate through, causing a shift in the material properties. This indicates a significant lack of interaction between the polymer and the Fe₂O₃ nanoparticles. The absorbance of PVA/Fe₂O₃ nanocomposites rises as the concentration of Fe₂O₃ nanoparticles increase, whereas the transmittance and energy gap drop as the concentrations of Fe₂O₃ rise. The rises of weight percentages of Fe₂O₃ nanoparticles increase the absorption coefficient, extinction coefficient, refractive index, real and imaginary parts of dielectric constant, and optical conductivity. Finally, the PVA/Fe₂O₃ nanocomposites may be considered as promise materials for use of it in different optical fields.

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