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UDC 539

FABRICATION AND EVALUATION OF OPTICAL CHARACTERISTICS OF (PVA-MnO_2–ZrO_2) NANOCOMPOSITES FOR NANODEVICES IN OPTICS AND PHOTONICS

We study the impact of (MnO_2–ZrO_2) nanoparticles on optical properties of (PVA) polymer. Several samples were produced with different weight ratios of (MnO_2–ZrO_2) nanoparticles. To prepare the selected samples, the casting method is used. To record the absorption spectrum, wavelengths of 200–1100 nm are applied. We have determined the absorption coefficient, energy gap for indirect transitions (forbidden and allowed), optical constants (such as the dielectric constant with its imaginary and real parts, refractive index, and attenuation coefficient), and optical conductivity. The results indicate that there is a proportional relationship between the optical constants and the concentration of (MnO_2–ZrO_2) nanoparticles, which means that an increase of the concentration of (MnO_2–ZrO_2) nanoparticles leads to an increase of the optical constants, while the transmission decreases. Additionally, the optical energy gap decreases from 4.83 eV to 3.4 eV and from 4.65 eV to 3.28 eV with increasing the concentration of (MnO_2–ZrO_2) nanoparticles for allowed and forbidden indirect transitions, respectively. These results can be considered as key ones for the use of (PVA-MnO_2–ZrO_2) nanocomposites in various fields such as optoelectronics and photonics.

Keywords: nanocomposite, optical properties, polyvinyl alcohol, MnO_2–ZrO_2 nanoparticles.

1. Introduction

According to the relevant literature, the composite materials, i.e., combinations consisting of at least two different chemical compositions, are rapidly gaining the interest of researchers for its important and functional standpoints [1]. Composites formed from polymer and a conducting matter offer products that have the mechanical properties of polymers, as well as the electrical conductivity required for the product application. There are several advantages for using polymer-based electrically conducting materials which include a reduced weight, plasticity, low cost, mechanical shock absorption ability, rust tolerance, ability to form complex parts, and conduction management. In electronic devices and computers, polymer nanocomposites and conductive thin films are mainly used for the electromagnetic shielding, where they are used as conductive adhesives in refrigeration enclosures, switching devices, electronics packaging chips, surge protectors, and static charge dissipation materials [2]. The conducting polymers take an important place in the world industry after their discovery by Shirakawa, Macdiarmid, and Heeger. This discovery altered the common perception that plastic is incapable to conduct electricity. Currently, conductive polymers in the form of thin films and nanomaterial's are used for many purposes as corrosion inhibitors, embedded capacitors, antistatic coatings, electromagnetic shielding, and smart windows that can adjust the amount of light that passes through them [3]. Moreover, this revolutionary compound is essential in the production of suitable solar cells, diodes, photovoltaic components, as well as light emitting diodes (LED), manufacturing of aircrafts, military equipment, and in the car industry [4]. It is shown that polymeric samples with metallic nanoparticles possess unique and good properties due to the

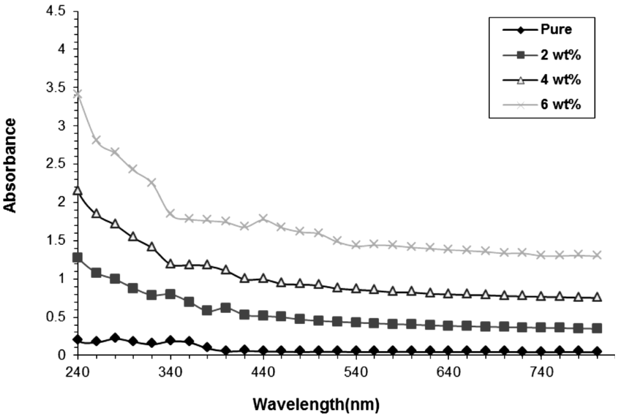

Fig. 1. Variation of absorbance for (PVA-MnO_2–ZrO_2) nanocomposites with wavelength

features of metallic nanoparticles and inherent features of polymers [6]. Poly vinyl alcohol polymer has the capacity to amalgamate with water, and this is employed in the creation of oxygen-resistant coatings that are used in photographic films [7]. Manganese dioxide is considered as a medium for the drug transportation, as well as being used as a scaffold to replace stem cells. The related research has confirmed that it is biodegradable and non-toxic and helps in stem cell differentiation [8].

The MnO_2 metal oxide can undergo and degrade the oxidoreduction reaction. This work aims to investigate the optical properties of (PVA-MnO_2–ZrO_2) nanocomposites.

2. Experimental Procedure

In this research, the materials used are nanoparticles (MnO_2–ZrO_2) and polyvinyl alcohol. The mixture (PVA) is formed by dissolving 1 g in 40 ml of deionized water (DW). The magnetic stirrer was used to mix the components, where, at (70 °C), the mixture became uniform. The weight ratios of (MnO_2–ZrO_2) are 0, 2, 4, and 6 wt.%. It is mixed for 15 min. Using the casting technique, samples were made. The absorption spectrum for the wavelength range 200–1100 nm was calculated using a UV-1800 Shimedza spectrophotometer.

The absorption coefficient α is calculated by the following formula [9]:

$$\alpha = 2.303(A/t), \tag{1}$$

where A is the absorbance. For the amorphous polymer, the indirect transition model can be computed as [10]

$$\alpha h\nu = D(h\nu - Eg)^x. \tag{2}$$

In this relation, D is a constant, $h\nu$ is the photon energy, E is the optical energy band gap, $x = 3$ for a forbidden indirect transition, and $x = 2$ for an allowed indirect transition.

Refractive index n is given by the relation [11]

$$n = (1 + R^{1/2})/(1 - R^{1/2}). \tag{3}$$

Here, c is the velocity of light in vacuum, and v is the velocity of light in a medium.

The extinction coefficient k is defined by the following formula [12, 13]:

$$k = \alpha\lambda/4\pi, \tag{4}$$

where λ is the wavelength of incident light.

We use Eqs. (5) and (6) to obtain the dielectric constant for both real and imaginary components [14, 15]:

$$\varepsilon_r = n^2 - k^2, \tag{5}$$

$$\varepsilon_{im} = 2nk. \tag{6}$$

The optical conductivity σ has been determined according to [16, 17]

$$\sigma = \alpha nc/4\pi. \tag{7}$$

3. Results and Discussion

As in Fig. 1, the differences are seen in the optical absorption spectra of the samples with (PVA-MnO_2–ZrO_2) nanocomposites under investigation and those of several (MnO_2–ZrO_2) nanocomposites. In addition, Fig. 2 shows the relationship between the transmittance spectrum and the spectrum of the nanocomposite (PVA-MnO_2–ZrO_2). We may conclude that the transmittance decreases, while the absorbance increases with the increasing concentration of (MnO_2–ZrO_2) nanocomposite, which correlates with the increase in the number of charge carriers [18, 19]. In this case, the absorption decreases, and the transmittance increases with the increasing wavelength. Figure 3 shows that the absorption coefficient of nanocomposite (PVA-MnO_2–ZrO_2) increases with the increasing concentration of nanoparticles (MnO_2–ZrO_2). and it was attributed to an increase of the number of charge

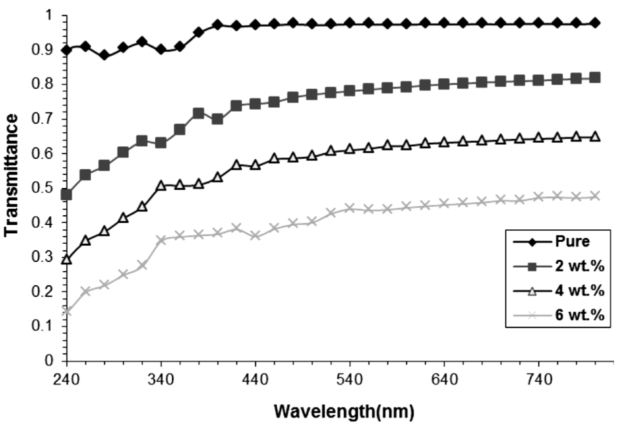

Fig. 2. Variation of the transmittance for (PVA-MnO_2–ZrO_2) nanocomposite with the wavelength

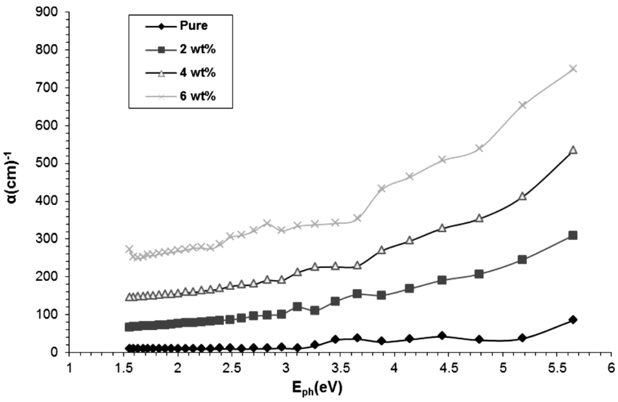

Fig. 3. Variation of the absorption coefficient α for (PVA-MnO_2–ZrO_2) nanocomposite with the photon energy

carriers, which also causes an increase of the absorption. This occurs, because it increases with the wavelength. Figures 4 and 5 also demonstrate the energy gap of the nanocomposite (PVA-MnO_2–ZrO_2) as a function of the optical absorption edge. From the values of the absorption coefficient, we assume that the nanocomposite possesses an indirect energy gap within the energy range, which decreases with the increasing concentration of nanoparticles (MnO_2–ZrO_2). This phenomenon occurs as a result of the formation of energy gap levels [20, 21]. Figure 6 gives the refractive index n for different wavelengths. When the energy of a photon increases, the refractive index increases rapidly. It is assumed that the electromagnetic radiation that passes through the material is faster for low energies of the photon. Figure 7 shows the correlation of the damping coefficient k and the photon energy. By this figure, the contrast is the lowest in the low-energy region, while the contrast increases in the high photon energy region. This phenomenon may occur as a result of the variation in the absorption coefficient, which leads to a spectral difference in the location of a charge polarization. The attenuation coefficient is related to the loss of the transition energy of charge carriers between the energy bands [22, 23, 24].

Figures 8 and 9 show that the increasing of λ leads to a decrease of the real and imaginary parts of the dielectric constant, while increasing with the (MnO_2–ZrO_2) concentration. To examine the loss factor, the data were examined by the ratio of the imaginary and

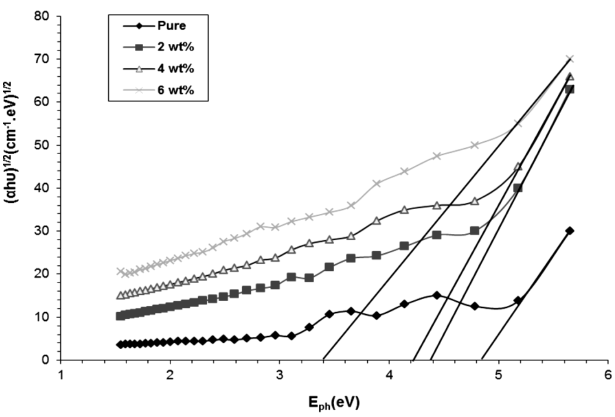

Fig. 4. Variation of $(\alpha h\nu)^{1/2}$ for (PVA-MnO_2–ZrO_2) nanocomposite with the photon energy

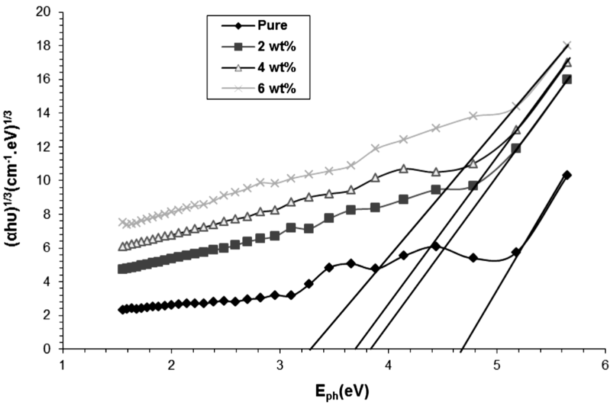

Fig. 5. Variation of $(\alpha h\nu)^{1/3}$ for (PVA-MnO_2–ZrO_2) nanocomposite with the photon energy

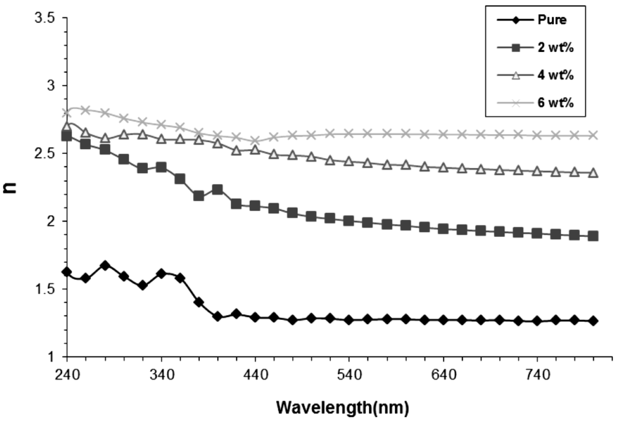

Fig. 6. Variation of the refractive index for (PVA-MnO_2–ZrO_2) nanocomposite with the wavelength

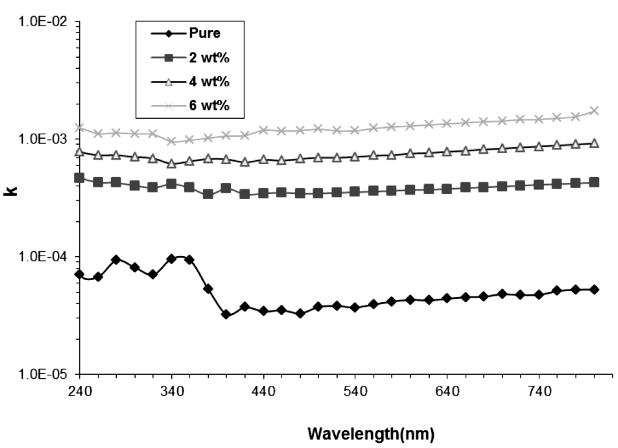

Fig. 7. Variation of the extinction coefficient for (PVA-MnO_2–ZrO_2) nanocomposite with the wavelength

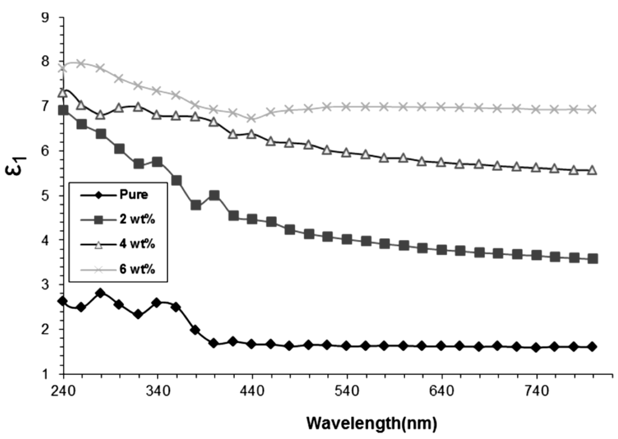

Fig. 8. Variation of the real part of the dielectric constant for (PVA-MnO_2–ZrO_2) nanocomposite with the wavelength

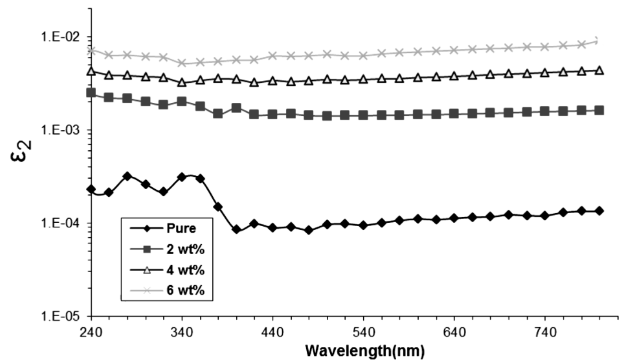

Fig. 9. Variation of the maginary part of the dielectric constant for (PVA-MnO_2–ZrO_2) nanocomposite with the wavelength

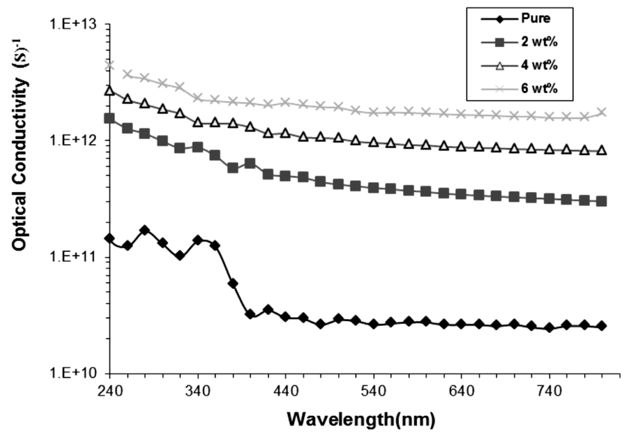

Fig. 10. Variation of the optical conductivity for (PVA-MnO_2–ZrO_2 nanocomposite with the wavelength

real parts of ε values. The findings show that, in the synthesized material, the loss factor rises with the reduction of the photon energy. In addition, the real part of the dielectric constant decreases slightly with the rise in the photon energy in the higher energy region, but it decreases slowly in the lower one. On the other hand, the (ε_{im}) of ε shrinks slowly as the photon energy rises [25, 26, 27]. To examine the electronic states in the material, the optical conductivity method was utilized. Figure 10 shows the plot of the optical conductivity of (PVA-MnO_2–ZrO_2) nanocomposite as a function of the photon energy. The figure pointed that the optical conductivity rises, which is indicative of the reduction of the direct band gap that is triggered by the addition of the dopant. This phenomenon occurs due to the generation of new states

 ISSN 0372-400X. Укр. фіз. журн. 2022. Т. 67, № 10

in the energy band gap that facilitates the charge carrier formation from the (V.B) to the (C.B) local levels [28, 29, 30].

4. Conclusions

The casting method is utilized to form (PVA-PVP-Co_2O_3) NC_S films. The increase of the (MnO_2–ZrO_2) nanocomposite concentration leads to an increases in the absorbance of (PVA-MnO_2–ZrO_2). (PVA-MnO_2–ZrO_2) has higher absorbance in the UV region. The energy band gap of (PVA-MnO_2–ZrO_2) nanocomposite decreases from 4.83 eV to 3.4 eV and from 4.65 eV to 3.28 eV with increasing the concentration pf (MnO_2–ZrO_2) nanoparticles for allowed and forbidden indirect transitions. The extinction coefficient k, absorption coefficient α, dielectric constant with the real and imaginary parts, refractive index n, and optical conductivity σ increase with the weight ratios of (MnO_2–ZrO_2) nanoparticles. The optical properties indicate that (PVA-MnO_2–ZrO_2) nanocomposites may be employed in a wide area like photonics and electronic applications

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Received 29.10.22

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ВИГОТОВЛЕННЯ ТА ОЦІНКА ОПТИЧНИХ ХАРАКТЕРИСТИК НАНОКОМПОЗИТІВ (PVA-MnO_2–ZrO_2) ДЛЯ НАНОПРИЛАДІВ У ГАЛУЗЯХ ОПТИКИ І ФОТОНІКИ

Вивчається вплив (MnO_2–ZrO_2) наночастинок на оптичні властивості полімера (PVA). Було виготовлено декілька зразків з різними ваговими відношеннями наночастинок (MnO_2–ZrO_2). Зразки було отримано методом лиття. Спектр поглинання вимірювався в діапазоні хвиль довжиною 200–1100 нм. Ми знайшли коефіцієнт поглинання, енергетичні щілини для непрямих переходів (заборонених і дозволених), оптичні константи (такі як діелектрична проникність з її уявною і дійсною частинами, показник заломлення і коефіцієнт загасання) та оптичну провідність. Отримані результати показують, що є пряма пропорційна залежність між оптичними константами та концентрацією наночастинок (MnO_2–ZrO_2), тоді як прозорість зменшується зі зростанням концентрації. Крім того, оптична енергетична щілина зменшується з 4,83 еВ до 3,4 еВ і з 4,65 еВ до 3,28 еВ зі зростанням концентрації наночастинок (MnO_2–ZrO_2) для дозволених і заборонених непрямих переходів, відповідно. Ці результати можуть бути важливими для використання нанокомпозитів (PVA-MnO_2–ZrO_2) у різних галузях, таких як оптоелектроніка і фотоніка.

Ключові слова: нанокомпозит, оптичні властивості, полівініловий спирт, наночастинки MnO_2–ZrO_2.