RESEARCH ARTICLE

The influence of Ag_2O/NbO_2 nanocomposites on the optical properties of PVA/PVP lend in biomedical applications

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Abstract

Objective: To study the optical properties of nanocomposites as well as antibacterial activity.

Method: The experimental study was conducted at the University of Babylon, College of Science and College of Education for Pure Sciences, Babylon, Iraq, from September 2021 to February 2022. Impregnation of transparent matrix polyvinyl alcohol and polyvinyl pyrrolidone nanocomposites was done by silver oxide and niobium oxide nanoparticles. The nanostructures were created using different ratios of polymer matrix, silver oxide nanoparticles and niobium oxide nanoparticles. The optical features of these nanocomposites were examined, whereby the latter type of properties was tested within the wavelength range of 220-820nm. The determination of the anti-microbial activity was done by disc diffusion method. The anti-bacterial activity involved gram-positive and gram-negative organisms. Different bacteria were cultured with Muller-Hinton medium.

Results: Absorbance, absorption coefficients and optical conductivity of the nanocomposites increased with the increase in nanocomposite concentrations. The energy gap for silver oxide and niobium oxide nanoparticles decreased when the concentrations of the nanoparticles increased.

Conclusion: Promising outcomes may be achieved for the nanocomposites in anti-bacterial applications as the inhibition zones increased along with increased ratio of silver oxide and niobium oxide nanoparticles.

Key Words: Dissolver oxide, Polyvinyl Alcohol, Niobium, Polyvinyl, Nanocomposites, Nanoparticles, Pyrrolidinones

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Introduction

A large number of modern fields currently examine the novel polymer nanocomposite production in nanoscale, such as the non-organic addition in food packaging, barrier fields, coating procedures, anti-microbial, sensors, anti-ballistic products, conductions, and others[1]. Polymer nanocomposites are composed of polymeric substances in addition to nanoscale materials. The latter component has shown a remarkable development regarding several aspects, including optics, mechanisms, chemical resistance and thermostability. The addition of nanoparticles also improved different material properties through several factors, especially the interfacial interaction among nanoparticles and the matrix in light of a sufficient particle dispersion[2,3]. Within the field of polymer nanomaterials, nanocomposites are regarded as a fundamental concept that has developed and demonstrated remarkable physiochemical features. The improvement of nanocomposite features could be achieved most importantly through interfacial interaction and fine dispersion of nanofillers and polymers[4]. The installation of the polymer-based nanocomposite is an essential feature of nanotechnology of the application of the polymers. The role of nanometric inorganic materials used as nanofillers in polymer-based nanocomposites. These nanocomposites are a new type of material that differs from traditional polymer blends because of the addition of these nanofillers. The nanofillers, due to their extremely small size, can significantly enhance the properties of the polymers, such as mechanical strength, thermal stability, and electrical conductivity[5].

Nanocomposites represent an important issue in the field of polymer nanomaterials. The interfacial interactions and fine dispersion of nanofiller with the polymer in nanocomposites are essential factors. Many applications rely on the involvement of the nanomaterial in polymers[6].

Polyvinyl alcohol (PVA) can be defined as a synthetic polymer that can be dissolved in water and is characterised by the fact that it can be prepared easily, can be bio-degraded sufficiently, and has great chemical resistance and mechanical properties. Therefore, the polymer has been used on a variety of biomaterials[6]. There are several features that distinguish PVA from alternative polymers, such as its corrosion resistance, great thermal stability and mechanic strengths. It has a carbon-chain backbone that is fixed to methane carbons and hydroxyl functional groups. The latter contribute to the hydrogen bonding to form efficient polymer

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mixtures[7,8].

Polyvinyl pyrrolidone (PVP) can be defined as a material that can be dissolved in water as well as in other solvents. In its dry state, it takes the form of a light, flaky hygroscopic powder that absorbs about 40% of its weight in humidity. When dissolved, PVP has great features with regard to the wetting and film-forming processes. These characteristics make it very suitable to be used as coatings or additives to coatings. Being a nontoxic material, its molecular weight ranges between 40,000 and 360,000. Its aqueous solutions have a range of applications in the field of pharmacy, medicine, cosmetics, biomaterials, coatings, blood plasma substitutions and macromolecular additives[9] .

Silver nanoparticles can be applied in different technological processes and may become a part of consumer products mainly because of their properties of optics, conduction and anti-bacteria. So silver oxide (SgO2) nanoparticles are used applied for the efficient use of light harvesting and improved optical spectroscopies[10]. They are used in conductive inks, as their integration within composites contributes to the improvement of thermal and electrical conductivity[11] Anti-bacterial utilisation includes apparels, footwear, paint, wound dressing, appliance, as well as cosmetic and plastic materials[10] Silver nanoparticles are commonly used as additives in different biomedical products for their capability of fighting infectious diseases, and slowing down the development of bacteria. Therefore, studies have evaluated the use of silver nanoparticles against cancer[11].

Niobium (Nb), also known as columbium or titanium, is a light grey chemical substance that represents a ductile transition metal of a crystalline structure. In its pure state, Nb has the same hardness and ductility as iron. Given the very slow oxidation of Nb, it is considered a suitable hypoallergenic substitution for nickel in jewellery. Nb oxides (NbO_2) are characterised by many different aspects, like its solid appearance and high melting point (1512◦C). It has a density of 4.47g/cm^3 as well as a molecular weight of 265.81. Besides, it cannot be dissolved in water, but can be dissolved in hydrogen fluorides (HFs). Among its potential applications are transparent conductive oxides, solid electrolytic capacitors, photo-chromic tools, and dye-sensitised solar cell applications[12].

The current study was planned to study the optical properties of PVP-PVA-Ag_2O-NbO_2 nanocomposites, and to use the prepared nanocomposites in biomedical applications for antibacterial activity.

Materials and Methods

The experimental study was conducted at the University of Babylon, College of Science and College of Education for Pure Sciences, Babylon, Iraq, from September 2021 to February 2022. This study was approved by the ethical committee of the College of Science, University of Babylon, prior to the beginning of the research project.

PVP and PVA were obtained in powder form from local markets with each having 99.8% purity. Ag_2O (Sigma-Aldrich, Massachusetts, United States) was used as powder with particle diameter 66nm and purity 99.9%. NbO_2 (Sigma-Aldrich company Massachusetts, US) was used as powder with particle diameter 66nm and purity 99.9%.

The nanocomposites were prepared by dissolving 1gm of PVA (50 wt.%) and PVP (50 wt.%) in distilled water with a magnetic stirrer. The polymers were mixed for 1 hour for obtaining a higher homogeneity at room temperature. The concentrations of the added AgO_2 and NbO_2 particles were 0.0025, 0.005, 0.0075 and 0.01 wt.%. The PVA-PVP-Ag_2O-NbO_2 nanocomposites were prepared through the casting method, after which the solution was transferred to a clean petri-dish with a diameter of 10cm. The samples were left for 1 week at room temperature to dry. The dried film was then removed easily by using tweezers clamp. The thickness of the prepared samples was measured by using digital micrometre, and the thickness ranged 100-110μm.

The optical properties of the PVA-PVP-Ag_2O-NbO_2 nanocomposites were measured using a spectrophotometer (Shimadzu, Japan, UV-18000A) on a wavelength of 220-820nm. The determination of the antimicrobial activity was done using the disc diffusion method. The antibacterial activity was performed through gram-positive and gram-negative organisms. Different bacteria, such as *escherichia (E.)* coli, *enterococcus (E.)* faecalis, *staphylococcus aureus (S)* aureus and klebsiella *pnenmoniae* (K.) pnenmoniae, are cultured in Muller-Hinton Medium. The PVA-PVP-Ag_2O-NbO_2 nanocomposite solution was put in the wells, followed by incubation for 24 hours at a 37ºC, measuring the inhibition zone diameter.

The formula used for calculating the absorption coefficient ~ was:[13]

$\alpha (\dot{v})=2.303A/T$ …………………... (1)

In the formula, A represented absorbance, and T stood for the thickness of the sample.

The energy-band gap was determined with the formula[13]:

αhѶ=B(hѶ-E_g^OPt)r ………………. (2)

In the formula, B was the constant, h↘ represented the energy of photon, Eg stood for the energy gap, and r equalled 2 and 3 for indirect allowed and forbidden transitions, respectively.

The conductivity was determined by using the formula:[14]

$$\sigma = \alpha nc/4\pi \text{ …………………………. (3)}$$

In the formula, (σ) was the optical conductivity, c is the velocity of light, α is the absorption coefficient and the refractive index.

Results

Absorbance, absorption coefficients (Figure 1) and optical conductivity (Figure 2) of the nanocomposites increased with the increase in nanocomposite concentrations. The energy gap for AgO_2 and NbO_2 nanoparticles decreased

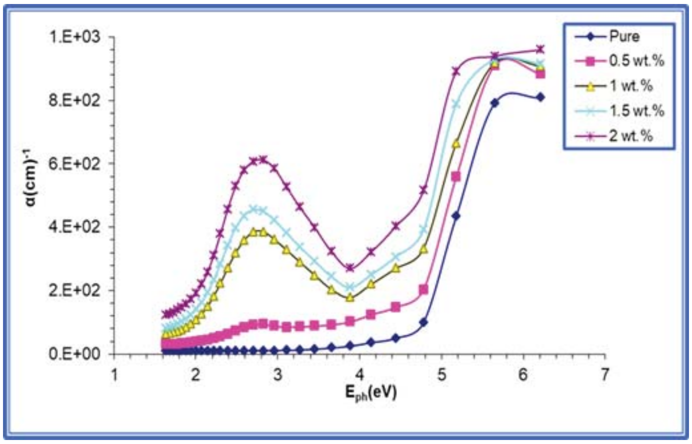

Figure-1: Varying values of the absorption coefficient (α) in PVA-PVP-Ag_2O-NbO_2 nanocomposites and the photon energy.
Polyvinyl alcohol, PVP: Polyvinyl pyrrolidone, Ag_2O: Silver, NbO_2: Niobium dioxide.

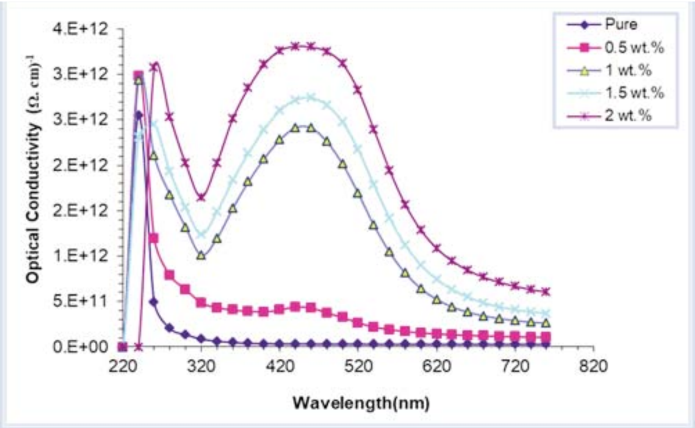

Figure-2: Varying values of optical conductivity in PVA-PVP-Ag_2O-NbO_2 nanocomposites and their wave lengths.
Polyvinyl alcohol, PVP: Polyvinyl pyrrolidone, Ag2O: Silver, NbO2: Niobium dioxide.y.

Table-1: Energy gaps in allowed and forbidden indirect transitions of PVA-PVP-Ag_2O-NbO_2 nanocomposites.).

Wt. %	energy band gap for allowed (eV)	energy band gap for forbidden (eV)
0	4.4	4.1
0.005	4.2	3.7
1	3.9	3.5
1.5	3.7	3.2
2	3.6	2.8

* PCA: Polyvinyl alcohol, PVP: Polyvinyl pyrrolidone, Ag_2O: Silver, NbO_2: Niobium dioxide.

Table-2: The diameter of inhibition for PVA-PVP-Ag_2O-NbO_2 nanocomposite antibacterial against S. aureus, E. coli, E. faecalis and K. pneumonia.

con.	S. aureus	E. coli	E. faecalis	K. pneumonia
0	0	0	0	0
0,005	19	18	17	20
0.01	21	19	17	23
0.015	21	19	18	24
0.02	21	21	18	25

Polyvinyl alcohol, PVP: Polyvinyl pyrrolidone, Ag_2O: Silver, NbO_2: Niobium dioxide. S: Staphylococcus, E: Escherichia, E: Enterococcus, K: Klebsiella.

when the concentrations of the nanoparticles increased (Table 1). The ability of antibacterial activity possessed by PVP-PVA-Ag2O-NbO2 against E. coli, E. faecalis, S. aureus and K. pnenmoniae was noted (Table 2).

Discussion

Scanning electron microscope micrographs revealed the presence of nanoparticles that were uniformly distributed inside the PVP-PVA blend where charge carriers were allowed to pass through the paths[15].

The absorption coefficient of all samples for PVP-PVA-Ag_2O-NbO_2 nanocomposites was low at low energy, which means that the electron transition had low possibility; i.e. the energy of incident photon was not enough to allow transition of electron from valence band to conduction band for the nanocomposites. However, at high energies, the absorption coefficient of all samples for PVP-PVA-Ag_2O-NbO_2 nanocomposites was high. This means that the electron transition had high possibility; i.e. the energy of incident photon was enough to allow transition of electron from the valence band to the conduction band, which, due to the energy of the incident photon, was greater than the energy band gap. The absorption coefficient indicated the nature of electron transition, and when the values of the absorption coefficient of the material were high (α>104 cm-1), direct transition of electron was expected. When the values of the absorption coefficient of material were low (α<104 cm-1), it indirect transition of electron was expected. The values of absorption coefficient of PVP-PVA-Ag_2O-NbO_2 nanocomposites were low (α<104 cm-1), and the transition of electron was indirect. The absorption coefficient of PVP-PVA-Ag_2O-NbO_2 nanocomposites increased with the increasing of the concentrations of AgO_2 and NbO_2 nanoparticles. This can be attributed to the increasing of number of charge carriers increasing the absorbance and absorption coefficient of the nanocomposites[16].

The optical energy gaps decreased for both allowed and forbidden indirect transitions.

Optical conductivity increased with the increase in photon energy for incident lights. A similarity was observed between the optical conductivity and the absorption coefficient, as the former was determined by the latter. Again, a positive correlation was found between optical conductivity and Ag_2O and NbO_2 concentrations, as both increased simultaneously. The optical conductivity was found to have increased by 34%. Such a phenomenon can be of use in a number of cases, such as photo catalysis, solar cell applications, diodes and additional optoelectronics instruments.[17]

The antibacterial tests showed that the inhibition zones increased along with increase in the ratio of Ag_2O and NbO_2 nanoparticles. The antibacterial effect of PVA-PVP-Ag_2O-NbO_2 nanocomposites can be related to the occurrence of reactive oxygen species (ROS) produced by Ag_2O and NbO_2 nanoparticles. The PVA-PVP-Ag_2O-NbO_2 mortar came into contact with the dead bacteria. Since hydrogen peroxide was produced, this further prevented the action of bacteria and carried on with creating and releasing hydrogen peroxide into the medium. The Ag_2O and NbO_2 nanoparticles in mortar have positive charges, and the microbes have negative charges. This results in a contact between the nanoparticles and the bacteria, leaving the bacteria oxidised which leads to its death[18].

Conclusion

Promising outcomes may be achieved for the nanocomposites in anti-bacterial applications as the inhibition zones increased along with increased ratio of AgO_2 and NbO_2 nanoparticles

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