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Evaluation of coated Ti(Sm)O_2-NPs for antibacterial and Computed Tomographic Imaging

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Abstract: This study evaluates the structural, optical, luminescence performance and antimicrobial activities of Ti(Sm)O_2 coated with PVA nanoparticles. The measured electronic and optical properties were also examined. The bacterial strains under visible-light irradiation. The coated Ti(Sm)O_2-NPs were synthesized by Hydrothermal technique and characterized by UV–vis spectroscopy and photoluminescence (PL). The decreased band-gap energy of Ti(Sm)O_2 coated with PVA nanoparticles was examined by UV–vis spectroscopy. Photoluminescence was used to track the degree of recombination and transfer behavior of the photoexcited electron-hole pairs in semiconductors. The antimicrobial activity of the coated Ti(Sm)O_2-NPs nanoparticles was evaluated against gram-negative (*Escherichia coli*) bacteria. The absorption peak for Ti(Sm)O_2 NPS appears at 366.65 nm, which shifted more slightly in the case of PVP@Ti(Sm)O_2 NPs. The Ti(Sm)O_2 NPs, and PVP@Ti(Sm)O_2 NPs elicited cytotoeffects against *E.coli*. The CT numbers of PVP@Ti(Sm)O_2 NPs were systematically higher than that of Ti(Sm)O_2 NPs.

keywords: Ti(Sm)O_2 Nanoparticles; antibacterial; Photoluminescence; PVA.

1.Introduction

Bacterial contamination has become a major issue because of the numerous infectious diseases it has caused in storing food, surgical devices, medical settings, biosensing, and public health events [1]. Implant-associated infections (IAIs) can be avoided by imbuing the implant surface with antibacterial properties before implantation [2].

A transformation in material science has occurred during the past ten years, employing novel materials in the form of nanostructures with improved qualities for usage in several fields, particularly the field of medicine [4], the world of metal alloys has seen significant advancement in unique, multidisciplinary technologies [3], particularly in memory form, biosensors, and numerous other biomedical applications [4].

A class of nano-structured alloys that are crucial in these applications are nanoparticles coated with polymeric shells [5]. These nanoparticles develop antibacterial lethal that could help in healthcare problems as a targeted microbial resistance to infectious diseases [6].

Bacterial cell wall structure directly influences bacterial response to nanoparticles (NPS). Bacteria are classified as Gram-positive (+) or Gram-negative according to their structure and function. When compared to the Gram-negative wall, the Gram-positive wall has a thick layer of peptidoglycan connected to teichoic acids that are only found in Gram (+) [7]. The outer membrane offers hydrophobic protection and is made up of lipopoly-saccharides, which are in charge of the negative charge on the cell membrane [8].

TiO_2, a photocatalytic agent recognized for its optical and chemical stability, has been widely used to kill various groups of microorganisms, such as bacteria because of its high photoreactivity, antibiosis, and chemical stability [9,10]. TiO_2 can generate the transformation of an electron towards the conductive band in the presence of light, thereby preferring the oxidative capacity of other species by producing active agents such as radicals [11]. With bacteria being able to release a specific self-destruction mechanism when exposed to oxidative stress, it is simple to recognize that TiO_2 is a material with bactericide activity that is improved in the presence of light [12-14].

Metal doping has historically been known as one of the best methods for changing the intrinsic band structure of TiO_2, and thus improving its visible light sensitivity [15], in addition to, boosting its photocatalytic activity when exposed to UV light [16].

The NPS surfaces have a great effect on their fate and interaction within the human body in biomedical applications. The coating can effectively protect NPs from mononuclear phagocyte and protein adsorption in vivo [17].

The characteristics of the coating materials, like organic coating materials (polysaccharides, proteins, polymers, etc.) and inorganic coating materials, have a significant impact on the function of a coating (chloride, sulfides, etc) [18]. The evolution of TiO_2-coated or -incorporated food packaging has piqued the interest of researchers [19]. Chawengkijwanich and Hayata investigated the antibacterial properties of TiO_2-coated wrapping against *E. coli* in vitro and in real tests under two types of synthetic light [20].

In light of these requirements, the current study intends to establish a focused relationship between the electronic structure of the coated $Ti(Sm)O_2$-NPs through the energy gap and the action toward pathogenic bacterial grams depending on their cell wall composition.

2. Materials and Methods

2.1. Materials

Titanium Dioxide (TiO_2 =79.89 g, Min. assay (ex Ti) 99%, Max. limits of impurities, loss on drying .5 %, Iron (Fe) .05%). Sodium hydroxide (Sodium hydroxide pellets AR assay 99.5 %, MW.40.00, SO. 55592, Egypt). 10%. PolyVinylPyrrolidone(PVP), (K-30), pure, M.W. =40000, MUMBAI, INDIAN. Samarium (III) nitrate hexahydrate, 99.9% (REO), Hygroscopic. Store under Nitrogen, 10g, LOT: D12X008, FW:444.45, Germany, Clinical strains of *Escherichia coli* and *Staphylococcus aureus* were obtained from Urology and nephrology center Mansoura university. Each piece of glassware was rinsed with distilled water and dried in an oven at 40±1 °C. All other chemicals used were of analytical grade.

2.2. Synthesis of 1% Samarium-doped TiO_2

The TiO_2 particles were prepared with the hydrothermal method as we mentioned previously. In the preparation, ethanol, HCl, and deionized water were used (30 ml ethanol, 0.5 ml HCl, 2 ml deionized water, and 1% samarium) and mixed under stirring. 5 ml of titanium oxides mixed with the previous solution drop by drop under vigorous stirring for 15 min. After that was put in the autoclave at 150℃ for 3 hr. then filtered, dried at 110℃ for 2 hr, and calcination at 500℃ for 2 hr.

2.3. Sample coating

To improve the stability of TiO_2 NPs and PVP were used to enwrap the nanoparticles. Solution of 0.1g of Tio_2 with (0.1g of PVP) mixed in 100ml of deionized water. Stirred at 60℃ for 3h. The Solutions were separated by centrifugation at 60 rpm for 2 min. Then they were dried at 60℃.

2.4. Sample characterization

2.4.1 Ultraviolet-visible spectroscopy (UV-Vis)

To investigate the structure of specimens and their optical properties, UV-Vis absorption was measured in the wavelength range (200-900 nm) using a spectrophotometer (Pg instruments, T80+, UV/Vis spectrometer, China). Photon spectroscopy in the UV, visible, and neighboring ranges is included (near-UV and near-infrared). Electronic transitions happen in this area of the electromagnetic spectrum. Because molecules include both bonding and non-bonding electrons (n-electrons), these electrons can absorb energy in the form of ultraviolet or visible light to excite them to higher anti-bonding molecular orbitals [21].

2.4.2. Luminescence performance analysis

Luminescence qualities were assessed using a spectrofluorometer (Jasco FP-6500, Japan) and two-photon laser confocal microscopy

(690–1040 nm) (Xenon arc Lamp 150 watt). The excitation and emission spectra were used to analyze the nanocomposite's luminescence capabilities. Before measurement, the nanocomposite is purified by dialysis against distilled water for one week, and the purified samples are distributed in distilled water.

2.4.3. Antimicrobial activity

Two bacterial species were used to assess the synthesized TiO2-doped samarium's antibacterial effectiveness. The Urology and Nephrology Centre graciously gave microbial strains (NRC). Staphylococcus aureus and Escherichia coli, respectively gram-positive and gram-negative resistant bacterial strains, were the two separate microorganisms that were assessed. Individual bacterial strains were grown for 48 hours each in universal tubes with a 15 mL nutrient broth medium. TiO_2-doped samarium was pipetted into the sanitized filter sheets in a variety of concentrations. The cultures were then incubated for 48 hours at 28 ± 0.5 °C. The diameter (in mm) of the inhibitory zone surrounding cavities was used to interpret the results. TiO_2 in the PVP-coated solution was incubated with broth media for 48 hours at a temperature of 28 ± 0.5 °C.

3. Results and Discussion

3.1.UV/Visible optical absorption spectral data

Ultraviolet-visible (UV/Vis) absorbance spectra may be helped in evaluating the electronic structure of the optical band gap of the NPs. in the near ultraviolet region, absorption arises from electronic transitions accompanied by the sample. UV/Vis absorbance spectra of dopped Titanium dioxide nanoparticles were recorded and they are presented in **Fig. 1**. The absorption peak for samarium doped TiO_2 appears at 366.65 nm and 409.2 nm, the latter band attributed to the presence of samarium. The absorbance somewhat varies with PVP coating. Generally, the absorption edge resembles the electronic transition from the occupied valence band to the empty conduction band.

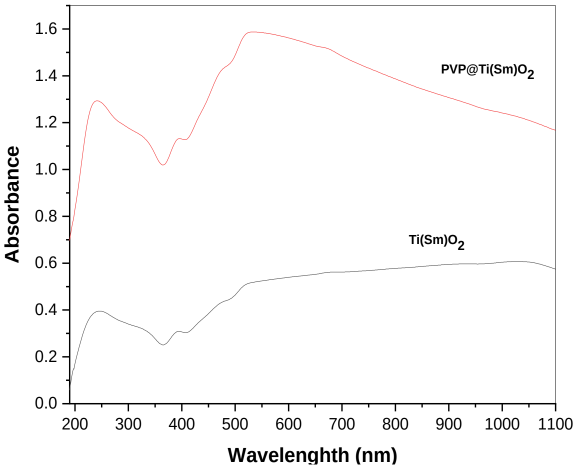

Fig. 1 UV spectra of $Ti(Sm)O_2$ and PVP@ $Ti(Sm)O_2$ nanoparticles.

3.2 PL spectrum of studied samples

TiO_2 is an indirect band gap semiconductor that displays no band gap photoluminescence. photoluminescence(PL) rising from the recombination of oppositely free carriers and charged trapped. Photoluminescence from $Ti(Sm)O_2$ suspension has two bands (600 nm, 515 nm). The band at 600 nm exhibits a strong correlation with defects, and the 515 nm band displays a close relationship with the oxygen vacancies. PL of $Ti(Sm)O_2$ in coating with PVP in **Fig. 2**. Normal emission from nano-particles is characterized by PL, which results from stored electrons and valence band holes recombining to produce a broad spectrum with a peak at 600 nm.

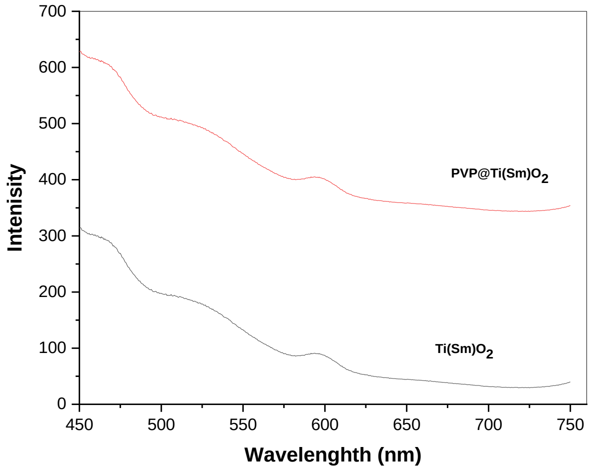

Fig. 2 Photoluminescence of $Ti(Sm)O_2$ and PVP@$Ti(Sm)O_2$ nanoparticles.

3.3. Antibacterial studies

All of the examined substances' antibacterial activity were discovered using the Agar plate method and liquid broth media. The gram-negative pathogenic bacteria *Escherichia coli*, were chosen as the test microorganisms to evaluate their antibacterial activity. In experiments, solidified material was diluted with sterilized double distilled water and added to a nutrient agar medium (DSMZ1) in sterilized Petri dishes. Study samples were laid out on an agar surface that had been seeded with test microorganisms, and the incubation period was set for 24 hours at 37± 2 °C. inhibitory zone diameter was found to be 2 mm as shown in **Fig.3**. $Ti(SmO_2)$, PVP@ $Ti(SmO_2)$ have a cidal effect on *E.coli* as shown in **Fig.4**. The antibacterial of NPs estimated through the liquid broth media by evaluating the optical band gap of the *E.coli*. Bacteria have diluted by Broth media, Nps added by concentration (0.01mM) under U.V excitation. From Fig.3 the peak (500nm) attributed to E.coli has been disappeared for $Ti(SmO_2)$, PVP@ $Ti(SmO_2)$.

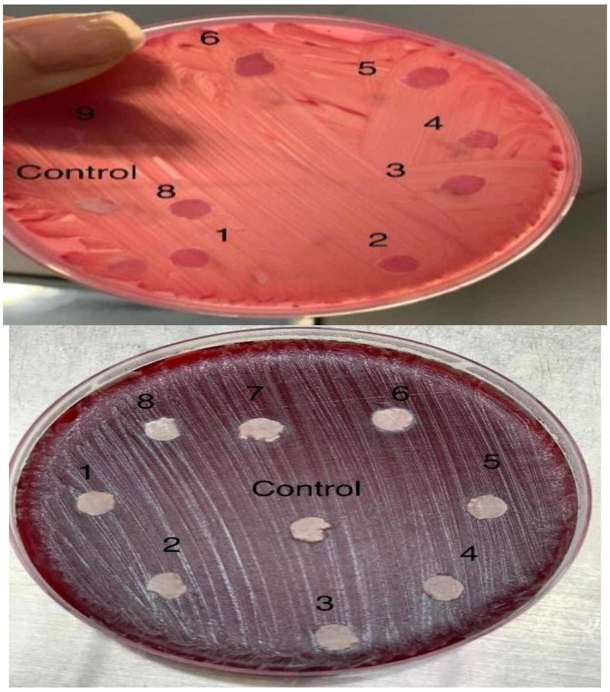

Fig. 3. Antibacterial activity of $Ti(Sm)O_2$ nanocomposites under different treatments.

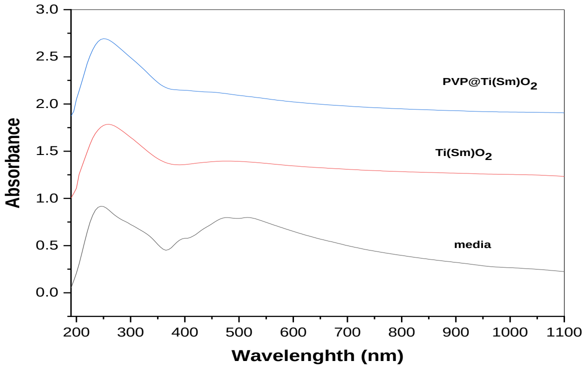

Fig. 4 UV media containing bacteria as a control sample and different treatments by $Ti(Sm)O_2$ and PVP@$Ti(Sm)O_2$ nanoparticles.

X-ray CT phantom images were captured using various concentrations of $Ti(Sm)O_2$ coated with PVP polymer diluted with distilled water **Fig.5**.

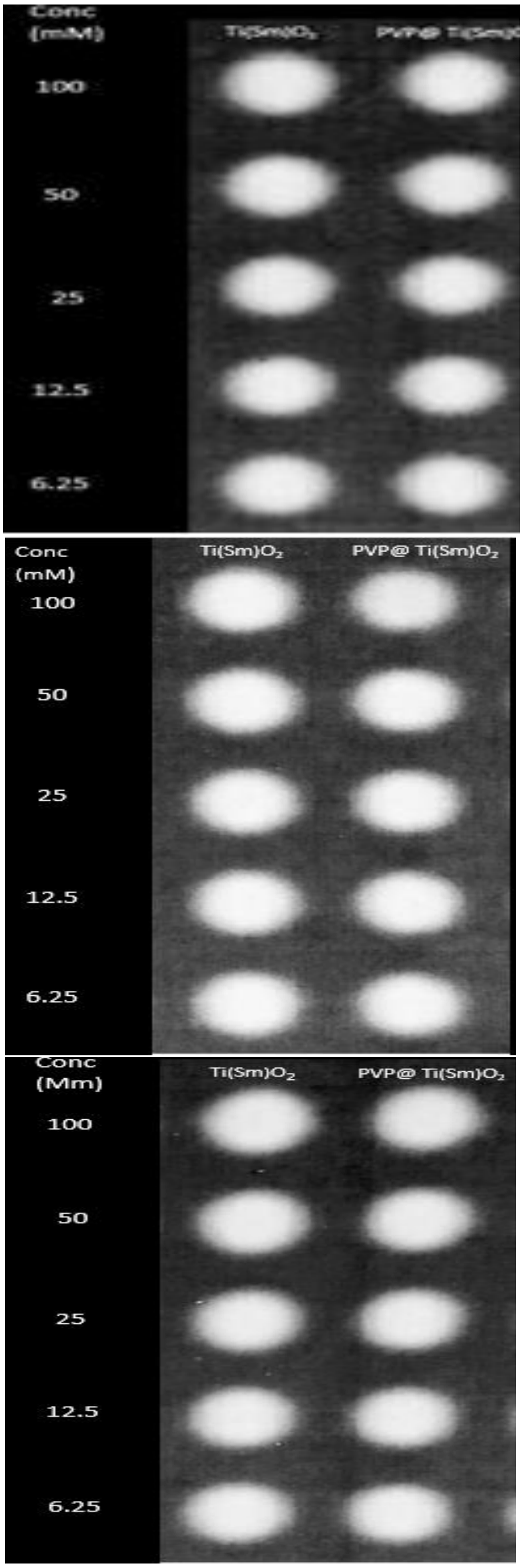

Fig. 5 CT phantom images were acquired using various concentrations of $Ti(Sm)O_2$ coated with PVP polymer.

The CT number increased as the concentration of nanoparticles increased **Fig.6**.

the variation, in contrast, is slightly varied. However, the high contrast was gained at 80 kV.

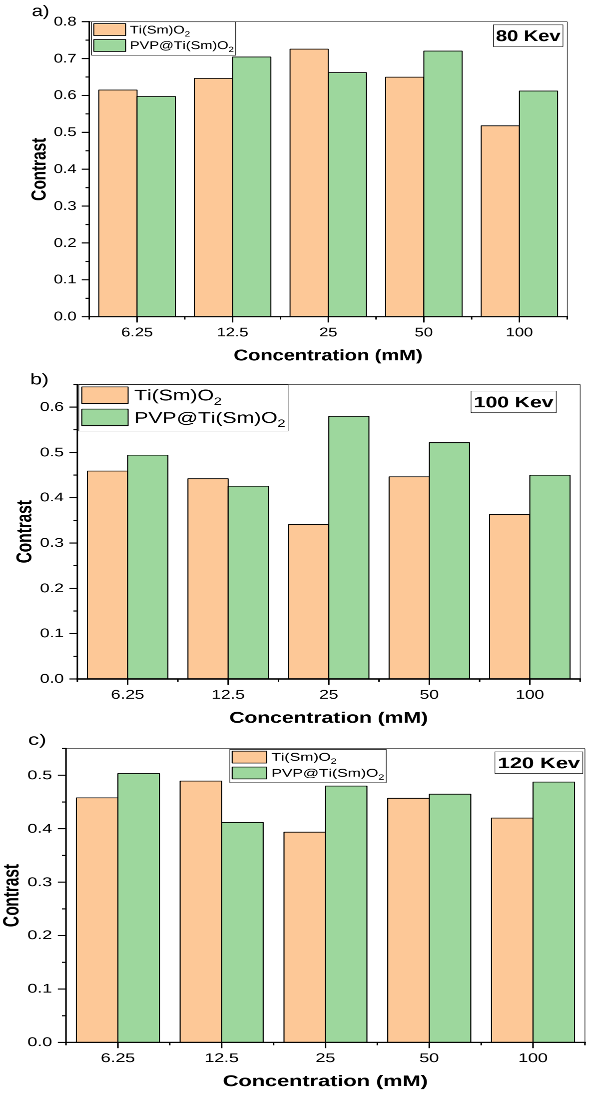

Fig. 6 Contrast of $Ti(Sm)O_2$ coated with PVP a) 80, b) 100, and c) 120 Kev.

4. Conclusion

The findings of this investigation and a prior study indicate that doping metal and metal oxides on the surface of TiO_2 nanoparticles enhances the value of the e-h+ charge separation by lowering the band-gap energy, delaying the recombination rate, and producing strong antibacterial properties. The maximum photocatalytic activity was observed in the case of PVP@$Ti(Sm)O_2$ in the TiO_2 matrix due to the decreased band-gap energy in comparison to other prepared nanoparticles. The anti-bacterial activity of the investigated colloidal solutions of $Ti(Sm)O_2$ was evaluated against Gram-negative bacterial species. The diameter of the inhibition zone is used as a measure of the antibacterial activity (mm). A larger clean region around the well - performing PVP @$Ti(Sm)O_2$ zone that demonstrated a higher diameter zone against *Escherichia coli* was associated with a greater antibacterial impact. CT number increased as the concentration of $Ti(Sm)O_2$. These findings solidify the potential role of $Ti(Sm)O_2$ as a lethal antibacterial and CT contrast agent.

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