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Synthesis and Characterization of Zinc Oxide /polyaniline (ZnO/PANI) Nanocomposite for solar cell application

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Abstract
Zinc oxide/polyaniline (PANI) was synthesized by the chemical oxidation process used in this paper. ZnO nanoparticles and aniline at varying molar concentrations have been combined to create composites. Zinc oxide powder was added during the polymerization of the monomer (aniline) using an oxidizing agent (ammonium persulphate) and dopant (H_2SO_4) while stirring continuously at (0 to -2) °C. Nanocomposites demonstrate the polycrystalline nature and uniform distribution of zinc oxide in PANI. Four different probe techniques were used to measure the electrical conductivities. It is discovered that a composite containing of zinc oxide has electrical conductivity that is higher than that of any other composite and even higher than PANI. The samples' crystallinity was assessed using the powder X-ray diffraction technique.The FESEM method was used to analyze the samples' morphology. Using UV-VIS spectroscopy, the different electron transitions found in the PANI were investigated.

Keywords: Polymers, Electrical conductivity, ZnO/Polyaniline, Nanocomposites,

I. Introduction

Recently, nanocomposite (NC) materials have gained immense attention worldwide because of their demonstrated potential for various technological uses, including but not limited to efficient quantum electrical devices, magnetic recording materials, and sensors [1]. Additionally, the use of conducting polymers and oxides in nanocomposite materials has opened up new application areas, including medication delivery, solar cells, rechargeable batteries, conductive paints, toner for photocopying, smart windows, and more [2]. The morphology and interfacial features of NC materials influence their attributes in addition to those of each of their separate parents [3]. Nanocomposites (NCs) made of polymeric materials are advantageous because of their high surface area-to-volume ratio, among other factors[4]. Al so because of its intriguing electrical conductivity, unique electronic structure, and electrical conductivity mechanism [5], in addition to its potential for use as a new electronic material, polyaniline (PANI) is one of the conducting polymers that has been studied the most intrinsically [6].

To produce materials with PANI and inorganic nanoparticles that behave in a complementary or synergistic way, PANI preparation using inorganic nanoparticles is considered a possible way to enhance PANI performance [7-9]. Zinc oxide (ZnO) is one of the inorganic nanoparticles that has drawn the most attention due to its special catalytic, electrical, electronic, and optical capabilities as well as its inexpensive cost and wide range of applications [10-12]. have mentioned. It is thought that adding ZnO nanoparticles to PANI using a chemical oxidative route could produce new material with advantageous qualities [13-16]. In this working paper, we provide a facile technique for the synthesis of ZnO/PANInanocomposite systems, as well as their FESEM, XRD, UV-vis spectroscopy, and four-point probe electrical conductivity characterization applied in solar cells[17-21].

II. Experimental

2.1. Materials

Purchased from a Merck business, ANILINE monomer, zinc oxide, ammonium persulfate, acetone, methanol, and sulfuric acid were all of GR grade. These materials were employed just as supplied, requiring no additional purification steps. For the duration of this endeavor, double-distilled water was used.

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2.2. Synthesis of Zinc Oxide /polyaniline Nanoparticles

Chemical oxidative polymerization was used to create PANI in a conventional polymerization procedure. In order to oxidize 0.25 M aniline with 0.25 M ammonium persulphate in an acidic aqueous media, 60 1.0 M HCl was added to a beaker, and the mixture was continuously stirred for 20 minutes. In 60 milliliters of 1.0M HCl, ammonium persulphate (oxidant) was dissolved in a different beaker. For the purpose of polymerization, both solutions were continuously stirred. The color transitioned from colorless to light blue to dark green during the polymerization process. Stirring was stopped and the solution was allowed to rest. The PANI precipitate was gathered on filter paper the following day and cleaned with distilled water, 25 ml of 0.1M HCl, and methanol in that order. The powdered PANI (emeraldine) was vacuum-dried at 90°C. The material yield from this process is high. For the synthesis of ZnO/PANInanocomposites, a similar process was used, but this time, ZnO nanoparticles that had already been synthesized were added to an aniline solution and then sonicated.

2.3 Characterization

Sample pallets were created using a dye punch with a diameter of one centimeter in a hydraulic press (Scientific Engineering Corporation, Malaysia) operating at five tons of pressure. The electrical conductivity of palletized samples was measured using the four-probe set-model DFP-RM (SES Roorkee). The four-point probe methods, XRD, FESEM, and UV-Vis spectroscopy were used to characterize the various compositions of ZnO/PANI NCs.

III. Results and discussion

3.1. X-ray Diffraction

The X-ray Diffraction of ZnO/PANIin Figure 1. These figures show that the zinc oxide is evenly distributed throughout the polyaniline matrix. According to the XRD analysis, PANI interacts with ZnO crystallites at the interface and changes shape when it mixes. As a result, the composite materials' Four-point probe conductivity measurement confirms that the composites are more conductive than pure PANI.

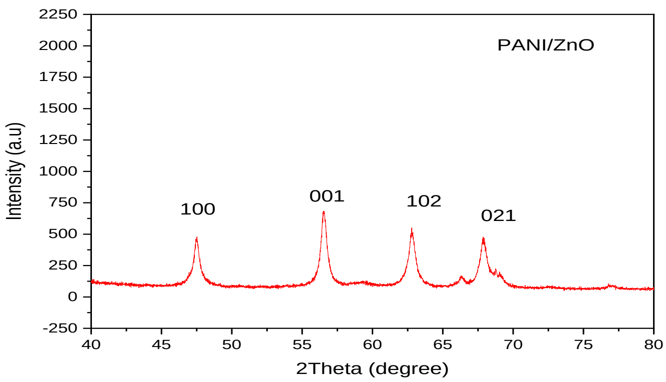

Figure: 1 X-ray Diffraction ofZinc Oxide /polyaniline nanocomposites

3.2 Field-Effect Scanning Electron Microscopy (FESEM) of Zinc oxide/Polyaniline

The shape and particle sizes of ZnO/PANI nanocomposites are determined using FESEM. Figure 2 displays the typical FESEM micrographs of ZnO nanoparticles, which have a spherical shape and a particle size range of 70-98 nm. Fig. 2 displays the typical FESEM micrographs of pure polyaniline. According to the results of the XRD study, the FESEM micrograph shows that polyaniline is deposited on the surface of ZnO particles, suggesting that the nanocomposites are made up of polycrystalline ZnO particles and PANI. It also shows that relatively few ZnO particles are clumped together and that the majority of ZnO particles are finely distributed throughout the PANI matrix. The polymer matrix is responsible for reducing the tendency of nanoparticles to aggregate.

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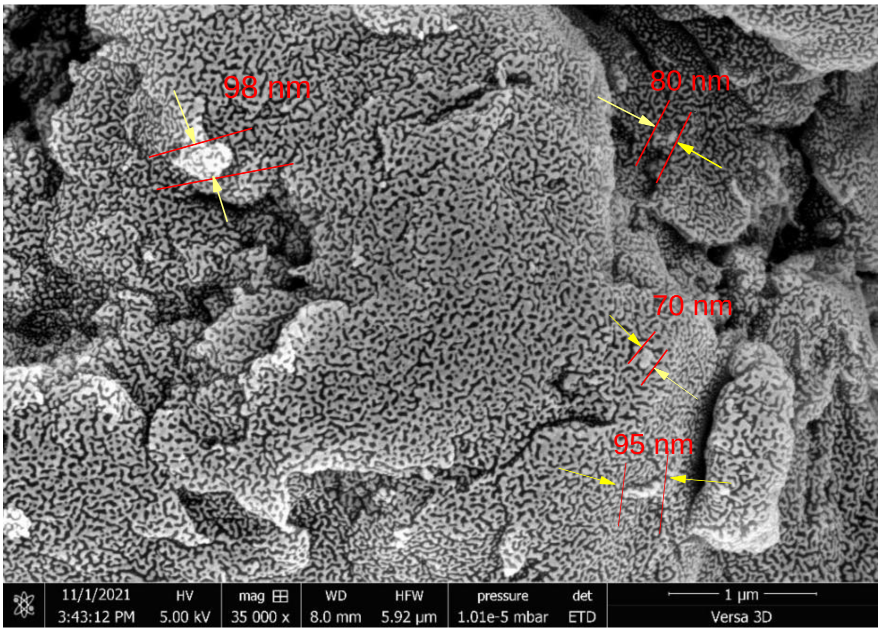

Figure 2FESEM ofZnO/polyaniline nanocomposites

3.3 UV-Vis Spectroscopy
Absorption bands are visible in the ZnO-PANI nanocomposite's UV–vis spectra (Fig. 3). The ZnO-PANI nanocomposite's UV–vis spectrum shows the first absorption band at 296 nm, which is caused by the π–π* electron transfer in the polymer chains' benzenoid units. The polaron–π* transition is responsible for the second absorption band at 366 nm, while the π–polaron transition is responsible for the third absorption band at 470 nm.

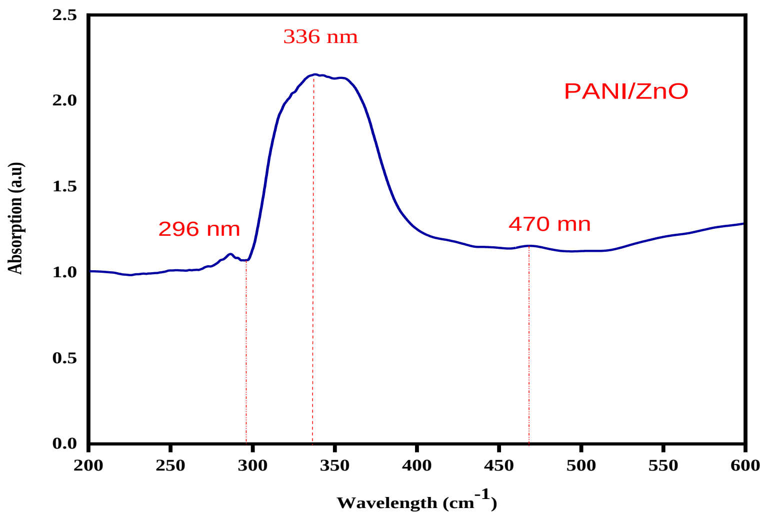

Figure 3 UV-Vis absorption spectra for ZnO-PANI nanocomposites

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.4 Optical energy band gap analysis of Zinc oxide/polyaniline
(ZnO-PANI) nanocomposites optical energy band gap analysis. Optical energy band gap of ZnO-PANI NCs produced was calculated by means of transmittance information derived from UV-visible spectroscopy. The PANI/ZnO NCs were chosen based on preliminary findings from UV-visible FESEM pictures, which displayed the best average outcome. It is crucial to realize that

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the energy difference between the valence and conduction bands in a material is its bandgap. A substance is more electrically conductive the lower its optical bandgap. The reason why there are so few electrons in the conduction bands of insulators is because they have larger band gaps than metals. The plot was used to calculate the ZnO-PANI NCs sample's bandgap. As shown in Figure 4, the optical gap was calculated by extrapolating a straight-line segment of the $(hv)^2$ versus hv figure, with the intercept on the horizontal photon energy axis. 2.77 eV is the bandgap energy of ZnO-PANI.

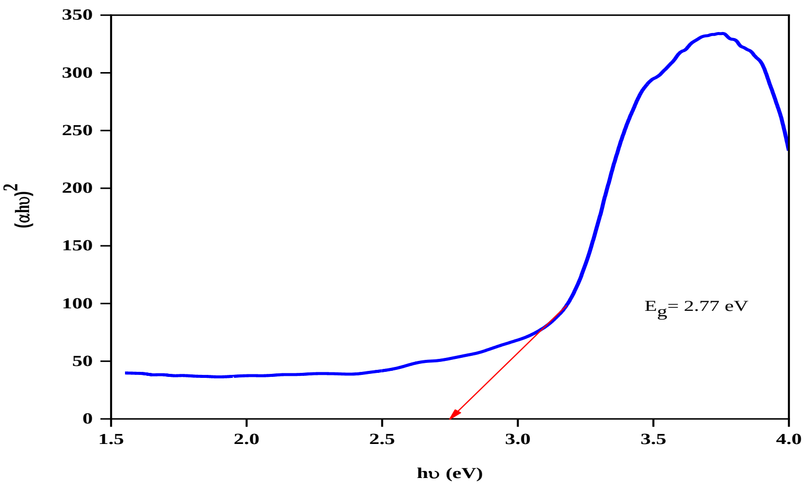

Figure 4Energy band gap for ZnO-PANInanocomposites

3.5 DC conductivity of Zinc oxide/ polyaniline analysis

The four-point probe analysis measurements were completed. For every specimen, a four-point probe was used to perform the electrical characterization of the pellet sample. This made it possible to calculate the resistivity $(\rho)^{-1}$, conductivity (σ), and sample resistance (R). Using the four-point probe technique, the electrical conductivity of zinc oxide and polyaniline was assessed; the results indicated an increase in conductivity. Zinc oxide/polyaniline nanoparticles were found to have a conductivity of 1.60×10^{-2} S cm^{-1}.

IV. Conclusion

Finally, the morphological study confirmed the formation of agglomerated ZnO nanoparticles over the PANI matrix; the XRD result revealed the presence of PANI and ZnO in the ternary nanocomposite; the UV–vis study demonstrated the structural interaction between PANI and ZnO nanoparticles. In summary, the ZnO-PANI nanocomposite was successfully prepared by the in situ chemical oxidative polymerization method. The synthesized ternary polymer was characterized using XRD, FESEM, and UV–vis techniques; all of them demonstrated that the process of synthesis was successful.The obtained values of ionic conductivity at 100 °C were 1.60×10^{-2}S cm^{-1}, indicating that conductivity increased as temperature increased. The produced nanocomposite exhibits a greater conductivity than ZnO nanoparticles, according to four-point probe measurements. Therefore, an effort has been made to investigate the new ternary nanocomposite's structure-property relationship to properly construct and process it for the right end users.

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