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Hydrothermally synthesized pure ZnO and ZnO-MgO nanostructures for Solar Cell Applications

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ABSTRACT

Hydrothermal synthesis offers an efficient and eco-friendly route to fabricate nanostructures with enhanced properties for solar cell applications. In this study, pure zinc oxide (ZnO) and zinc oxide-magnesium oxide (ZnO-MgO) nanostructures were synthesized by hydrothermal method and characterized to explore their potential as photoanode materials in solar cells. The structural analysis using PXRD revealed high crystallinity and phase purity, while photoluminescence (PL) analysis highlighted reduced recombination rates due to MgO doping. Optical characterization using UV-Vis spectroscopy showed improved light absorption for ZnO-MgO nanostructures with a widened bandgap. These enhancements are critical for improving the efficiency of solar cells. The results demonstrate the promise of hydrothermally synthesized ZnO-MgO nanostructures for next-generation photovoltaic applications.

Keywords: *nanocomposites, metal oxide, PXRD, photocatalytic*

1. Introduction

Nanocomposites comprise various systems, for instance, multidimensional (1D, 2D, 3D) and amorphous materials, which are made of several different components with varied characteristics, with the dimension less than 100 nm. The incorporation of these materials serves to enhance the properties of the nanomaterials to function more effectively for the intended applications [1-3]. ZnO has a wide band gap (~3.37 eV), which makes it transparent to visible light, allowing more light to pass through to the active layers of solar cells. Its high electron mobility promotes efficient charge transport, reducing energy loss and enhancing solar cell efficiency. [4-6]. To further enhance its effectiveness, ZnO is often combined with other materials to form nanocomposites. Among these, magnesium oxide MgO emerges as a promising candidate due to its renowned stability and bandgap engineering properties. The hydrothermal synthesis method, recognized for its ability to produce high purity, defect-free nanostructure, offers a controlled and efficient method for fabricating ZnO-MgO nanocomposites. The formation of ZnO-MgO nanocomposites through hydrothermal

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synthesis produces stable, defect-free, and uniform structures that are well-suited for absorbing sunlight and sustaining efficient photovoltaic performance [7-9]. This technique enables the creation of nanomaterials with enhanced functional characteristics, making them suitable for advanced solar cell application.

2. Materials and Methods

In this project work, high-quality pure ZnO and ZnO-MgO nanostructures are synthesized by the hydrothermal method. The materials used for preparing the nanomaterials consist of zinc acetate, manganese acetate, magnesium acetate, double distilled water and hydroxide. 0.1 M of zinc acetate dihydrate and 0.1 M of $MgCl_2$ are separately dissolved in 100 ml of distilled water and then it is mixed together and the solution is under vigorous stirring for 10 minutes. Then, 3M of NaOH, dissolved in 100 ml of distilled water is slowly added to the solution in order to maintain the pH value 10 which results in the formation of white precipitate. Then the solution is stirred for 5 minutes and transferred into the autoclave and closed at 160 °C for 12 hrs and cooled at room temperature. The resultant colourless products are cleaned and rinsed with distilled water and ethanol for 3 times and placed in the hot air oven for drying and then, it is kept in the muffle furnace for 500° C and finally, the ZnO-MgO nanopowder obtained appears white in colour. ZnO nanopowder is also synthesized using the same method as mentioned above.

3. Results and Discussion

3.1 PXRD analysis

The structural properties of the pure ZnO nanoparticles and ZnO-MgO nanocomposites are analyzed by recording the powder X-ray diffraction (PXRD) spectra using X-ray diffractometer. The average grain size can be quantitatively estimated using the Scherrer equation and the diffraction peak broadening in the XRD curves.

$$D = \frac{0.9\lambda}{\beta cos\theta}$$

where λ is the wavelength of the Cu-K_α radiation [1.54060 Å], β is the full width half maximum of the diffraction line and θ is the angle of diffraction. Fig.1 depicts the PXRD pattern of the synthesized Pure ZnO nanoparticles. The peaks of ZnO are observed at (100), (002), (101), (102), (110), (103), (112) and (201) corresponding to 2θ = 31.6834°, 2θ = 34.3185° and 2θ = 36.2542°, 2θ = 47.5045º, 2θ = 56.5110º, 2θ = 62.8222°, 2θ = 67.8745°, 2θ = 69.0411°,2θ = 72.4610º and 2θ = 76.9071º respectively. The average grain size D is 30.20 nm using Scherrer equation. Fig.4.2 shows the PXRD pattern of the synthesized zinc oxide (ZnO) – magnesium (MgO) nanocomposites. The peaks of ZnO are observed at (100), (002), (102), (110), (200), (112), (201), and (202) corresponding to 2θ = 31.6617°, 2θ = 34.3215°, 2θ = 47.4385°, 2θ = 56.4840°, 2θ = 66.2877°, 2θ = 67.8421°,2θ = 68.9600° and 2θ = 76.9280° respectively and the peaks of MgO are observed at (111), (200) and (220) corresponding to 2θ = 36.1469°, 2θ = 42.6428° and 2θ = 62.7546° respectively. The MgO peak corresponding to (111) is of high relative intensity. The average grain size D is calculated as 44.22 nm using Scherrer equation [10].

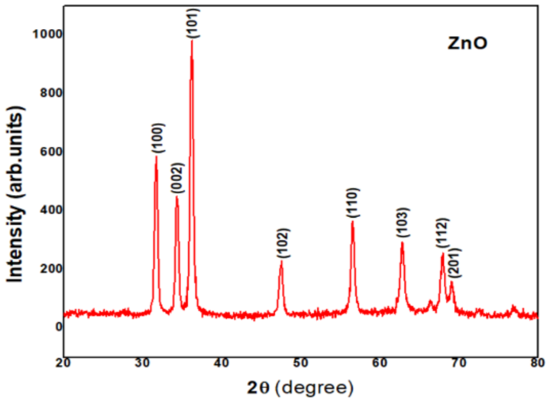

Fig. 1. PXRD pattern of pure ZnO nanoparticles

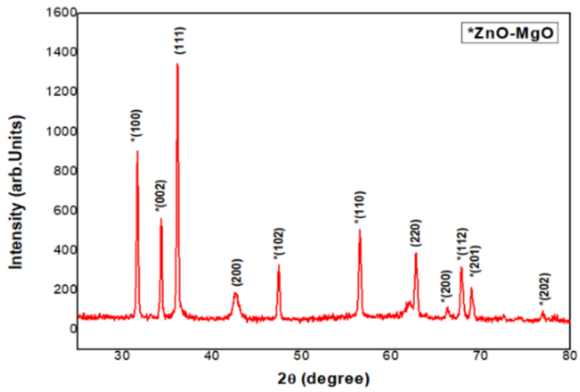

Fig. 2. PXRD pattern of ZnO-MgO nanocomposites

3.2 Photoluminescence (PL) analysis

Photoluminescence (PL) studies of the synthesized pure ZnO and ZnO-MgO nanocomposites were conducted using a photoluminescence spectrophotometer. The emission spectra were recorded at a scan rate of 600 nm/minutes employing an excitation wavelength of 320 nm. The PL emission spectrum of pure ZnO nanoparticles, presented in Fig. 3 exhibits prominent peaks at 358 nm, 392 nm, 408 nm, 436 nm, 490 nm, 521 nm, and 594 nm, each corresponding to distinct energy levels.In comparison, the PL emission spectrum of ZnO-MgO nanocomposites, shown in Fig. 4 reveals peaks at 359 nm, 390 nm, 406 nm, 491 nm, 519 nm, 540 nm, 571 nm, and 596 nm, each associated with specific energy levels. The PL emission peaks in the blue and green regions for both ZnO and ZnO-MgO nanocomposites indicate the nanoscale nature of the synthesized materials [10].

3.3 UV– Visible analysis

The absorbance of the synthesized pure ZnO nanoparticles is shown in Fig.5 which exhibits a maximum peak at 357 nm with absorbance 1.2 (a.u.). The absorbance of the synthesized ZnO-MgO nanocomposites is shown in Fig.6 which exhibits a maximum peak at 363 nm with absorbance 0.75 (a.u.) [11]. The optical band gap is calculated by using the relation

$$\alpha h\upsilon = A\,(h\upsilon - E_g)^n$$

where, A is a characteristic parameter independent of photon energy, h is Planck’s constant, υ is the frequency of light, E_g is the optical energy band gap, and n defines the type of electronic transition. For direct allowed transition, n = 2 and for indirect allowed transition n =1/2. The

Tauc plot method is a commonly used to determine (E_g) by plotting $(\alpha h\upsilon)^2$ against hυ (photon energy). The optical band gap is estimated by identifying the linear region of the plot and extrapolating it to intersect the energy axis (X-axis) at zero. Using this method, the optical band gap was determined to be E_g= 3.06eV for ZnO nanoparticles and ZnO-MgO nanocomposites (Fig. 7 & 8). These differences in bandgap values highlight the distinct electronic properties of the nanoparticles and nanocomposite, crucial for optimizing their optoelectronic performance in specific application.

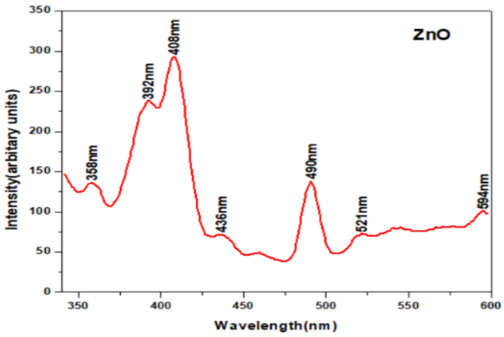

Fig. 3. PL emission spectra of ZnO nanoparticles

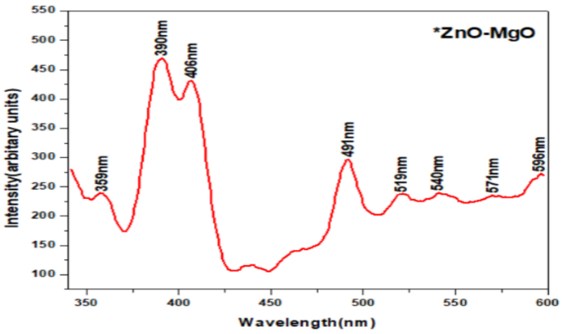

Fig. 4. PL emission spectra of ZnO-MgO nanocomposites

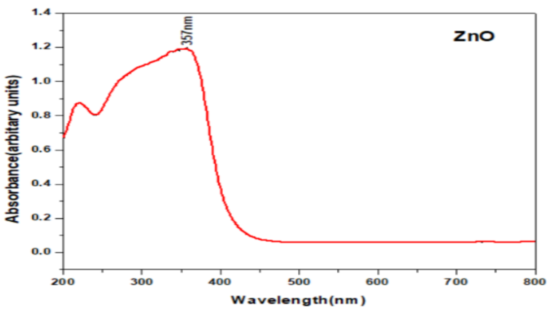

Fig. 5. Optical absorbance spectra of ZnO- nanoparticles

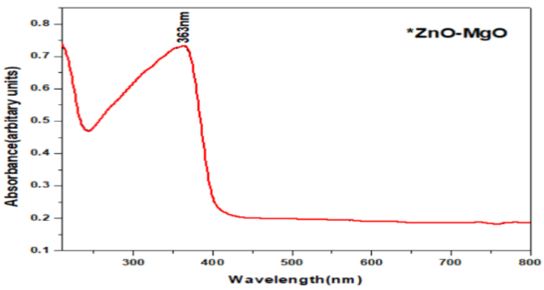

Fig. 6. Optical absorbance spectra of MgO nanocomposites

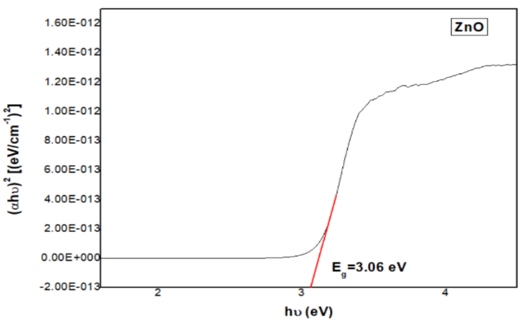

Fig. 7. Optical Energy band gap of ZnO nanoparticles

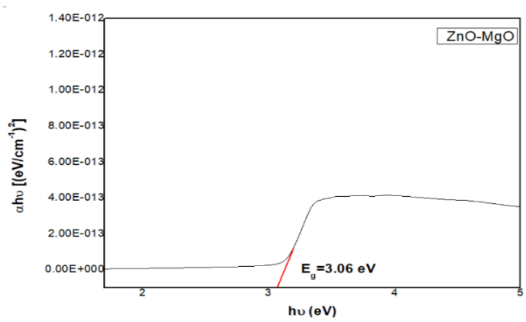

Fig. 8. Optical Energy band gap of ZnO-MgO nanocomposites

3. Conclusion

The study successfully synthesized and characterized pure ZnO nanoparticles and ZnO-MgO nanocomposites using the hydrothermal method. PXRD confirmed well-defined crystalline structures with average grain sizes of 30.20 nm for ZnO and 44.22 nm for ZnO-MgO. The addition of MgO enhanced absorption and shifted diffraction peaks, indicating successful composite formation. PL and UV-Vis studies revealed emission peaks in the blue and green regions and a band gap of 3.06 eV for both materials, highlighting their nanoscale nature and improved optical properties. These findings demonstrate the potential of ZnO-MgO nanocomposites for applications in solar cells and other photoactive devices.

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