International Journal of Recent Research and Review, Vol. XVIII, Issue 3, September 2025
ISSN 2277 – 8322

INVESTIGATION of STRUCTURAL, OPTICAL and PHOTOCATALYTIC PROPERTIES OF ZnO-25wt% CNTs NANOCOMPOSITES

Ramanand Sharma[1,2*], Madhu Yadav[2,3], Chhagan Lal[2,3], Amanpal Singh[2]

[1]Kamla Modi, Govt. Girls College, Neem Ka Thana-332713, Rajasthan, India
[2]Department of Physics, University of Rajasthan, J.L.M. Marg, Jaipur-302004, Rajasthan, India
[3]Centre for Non-Conventional Energy Resources, University of Rajasthan, J.L.N. Marg, Jaipur-302004, Rajasthan, Jaipur
*Corresponding author: rnsharmanmr@gmail.com

Abstract - Nanocomposites composed of zinc oxide (ZnO) have attracted a lot of attention due to their ability to remove the pharmaceutical pollutants that don't break down in the environment. In this study, ZnO–25 wt% CNT nanocomposite were synthesized and studies to find out its structure, optics, and photocatalytic properties. XRD confirmed that ZnO was in a crystalline phase with nanoscale crystallite size and that the CNTs were well integrated into the matrix. UV–visible spectroscopy revealed a strong absorption edge in UV region, with the optical band gap estimated at approximately 3.12 eV, which is lower than that of pure ZnO, suggesting improved light-harvesting capacity. The photocatalytic activity has been evaluated through the decomposition of methylene blue (MB) dye while under UV irradiation. The composite had a remarkable ~85% degradation efficiency for this nanocomposite. The better performance is due to the efficient separation of charge carriers and the increased mobility of electrons that come from adding CNT. These results show that ZnO–CNT nanocomposites could be very useful and cheap photocatalysts for treating wastewater.

Keywords: ***Nanocomposites, CNTs, photocatalytic activity, MB dye.***

1. INTRODUCTION

Nanocomposites based on ZnO have shown considerable potential as materials for processing the wastewater, especially when it comes to breaking down artificial dyes. Their performance is mostly due to their strong photocatalytic activity when they are in the light [1,2]. Combining ZnO with other materials that work well with it, such as graphene oxide (GO), copper oxide (CuO), titanium dioxide (TiO_2), or silver (AgNPs) nanoparticles, can make it work even better [3–14]. These hybrid systems usually have a larger surface area, better band gap alignment, and better charge carrier separation. All of these qualities help the catalyst to break down dyes faster and be easier to recycle [15].

Recent studies indicate that ZnO can be modified into nanoscale structures to improve surface reactivity, charge transport, and light absorption, all of which are crucial for photocatalytic efficiency. Dopants, heterojunctions, and composites fabricated with materials like carbon nanostructures or noble metals may enhance functions by lowering the band gap and stopping electron-hole recombination. These changes proved ZnO nanomaterials very useful for breaking down the harmful drug residues in wastewater over time. This is an environmentally friendly approach to clean up the environment [16].

When exposed to light, structural features like surface area, shape, and crystallinity are important for breaking down organic dyes and killing bacteria. ZnO/TiO_2 composites are a good and long-lasting way to clean up wastewater that has both chemical and biological pollutants in it [17].

Since their discovery, carbon nanotubes (CNTs) have been the focus of a lot of research around the world because of their unique structural and electronic properties. The electronic properties of CNTs depend strongly on their chirality and tube diameter. These properties can be semiconducting, semi-metallic, or metallic [18]. A novel approach for producing ZnO/CNT nanocomposites has been reported to improve their ability to break down malachite green dye when exposed to visible light. This research demonstrates that ZnO/CNT nanocomposites are a promising material for photocatalysis utilizing visible light to eliminate hazardous dyes from wastewater [19].

In the present study, ZnO-25wt% CNTs nanocomposite were synthesized using a hydrothermal method. Then, these compsoites were structurally and optically characterized and evaluated for degradation applications with the MB dye.

II. EXPERIMENTAL SECTION

A. Synthesis of ZnO/MWCNTs Nanocomposites

To make zinc hydroxide gel, 4.39 gram of $Zn(CH_3COO)_2.2H_2O$ was dissolved in 50 mL of distilled water. A sodium hydroxide solution (1.6 gram in distilled water) was added drop by drop while stirring constantly. This made a white zinc hydroxide precipitate. We filtered the precipitate and washed it with ethanol to get rid of any contamination. To make the nanocomposite, 0.74 gam of zinc hydroxide gel and 0.20 gram of multi-walled carbon nanotubes were mixed with 70 mL of distilled water and sonicated for an hour. Then, the suspension was put into an autoclave lined with Teflon and treated with 3 mL of acetic acid. It was kept at 80 °C for 24 hours. The product was spun in a centrifuge at 5000 rpm for 30 minutes in three cycles: first with water, then with ethanol, to get rid of any residual solvents. The solid was dried at 100 °C until all the solvent had evaporated. Then, it was ground into a fine powder with a mortar and pestle. Finally, it was calcined at 400 °C for 2 hours in a muffle furnace to make it more crystalline and create the ZnO/MWCNTs nanocomposite.

B. Characterization of ZnO-25wt% CNTs nanocomposite

Here, we used XRD, UV–Vis spectroscopy, and followed by MB dye degradation tests to understand further application of ZnO-25 wt% CNT nanocomposite. X-ray diffraction (XRD) is used to confirm that the ZnO is crystalline and the CNTs are well-dispersed and have nanoscale crystallite sizes. We used UV–Visible spectroscopy to measure absorbance and the Tauc plot to estimate the band gap from the absorbance data. Photocatalytic studies were conducted to demonstrate enhanced MB degradation efficiency under UV light exposure.

III. RESULTS AND DISCUSSIONS

A. Structural analysis of ZnO-25wt% CNTs

Figure 1 shows the diffraction pattern of a ZnO-CNT nanocomposite. The peak around 25.82° is connected to the (002) plane of graphitic carbon from the carbon nanotubes (CNTs). The peaks' width suggests nanocrystallinity and possibly strain effects, might become broader because of the factors like lattice deformation, changes in structure, or a higher concentration of defects in the composite material. The peaks at 33.56°, 51.520°, and 53.670° show that ZnO has formed in the composite and might have maintains its characteristic hexagonal wurtzite structure. 8

The peak at 43.14° in the diffraction pattern shows that the carbon material (CNTs) has been successfully added to the ZnO matrix, making the desired nanocomposite. The presence of the various corresponding peaks confirms that ZnO has a crystalline structure in the composite. When added to the CNT concentration, it shows that the ZnO-CNT nanocomposite has been successfully produced. This indicates that ZnO–CNT nanocomposite probably has nanometer-sized crystallites with some lattice strain caused by the addition of CNT. This may enhance photocatalytic activity better by creating more defect states and improving electron transport.

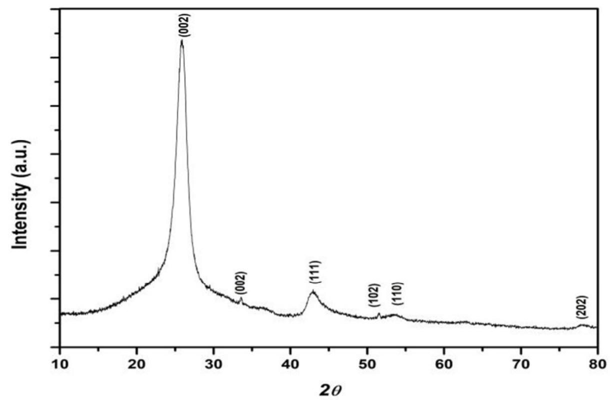

Fig. 1 Diffraction pattern of ZnO-25wt% CNTs nanocomposite

B. Optical properties of ZnO-25wt% CNTs nanocomposite

The absorbance of the ZnO-25wt% CNT nanocomposite is shown in Figure 2. Optical properties have been employed to determine the absorbance activity and the band gap. It is clear from figure, that It strongly absorbs UV light (λ ~238 nm below 400 nm) and has a long tail that expands into the visible range. The visible tail is common in ZnO–CNT composites, where π–π* absorption of CNTs and defect/charge-transfer states add absorption below the band gap.

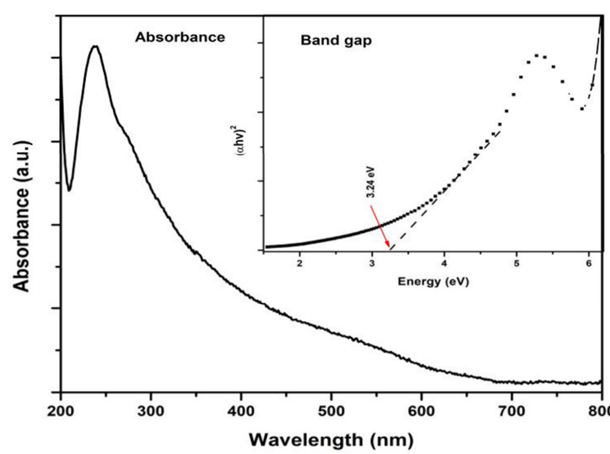

Fig. 2 Absorbance and band gap (inset figure) of ZnO-25wt% CNTs nanocomposites

Here, the Tauc equation is used to find the optical band gap for a direct band gap semiconductor:

$$(\alpha h\nu)^2=A(h\nu-E_g)^2 \quad \text{(I)}$$

where α, $h\nu$, A and E_g are the absorption coefficient, photon energy, a constant and the optical band gap, respectively. The band gap can be estimated by extending the line along the energy axis, when $(\alpha h\nu)^2$ is plotted against $h\nu$. The intercept gave us Eg =3.24 ± 0.05 eV, which is slightly lower than bulk ZnO (~3.37 eV). It could be due to interfacial charge transfer or defect states caused by CNT coupling and nanostructuring.

C. Functional groups in ZnO-25wt% CNTs nanocomposites

The FTIR spectrum of the ZnO–25 wt% CNT nanocomposite are shown in Figure 3, which illustrates several distinct absorption characteristics and confirm the existence of both ZnO and CNTs within the hybrid material. A broad band in the region around 3400 cm^{-1} is likely caused by the stretching vibrations of hydroxyl groups. These groups probably come from water molecules that have stuck to the surface. The low-frequency signals between 2900 and 3000 cm^{-1} correspond to C–H stretching vibrations, which indicates that there are carbon-based elements in existence. The weak and broad absorption features are seen in the 2000–2500 cm^{-1} range of the ZnO–25 wt% CNT FTIR spectrum, which are not unique to ZnO or CNTs. The spectrum primarily displays CO molecules that have adhered to the surface, rather than chemical bonds between the molecules in the material.

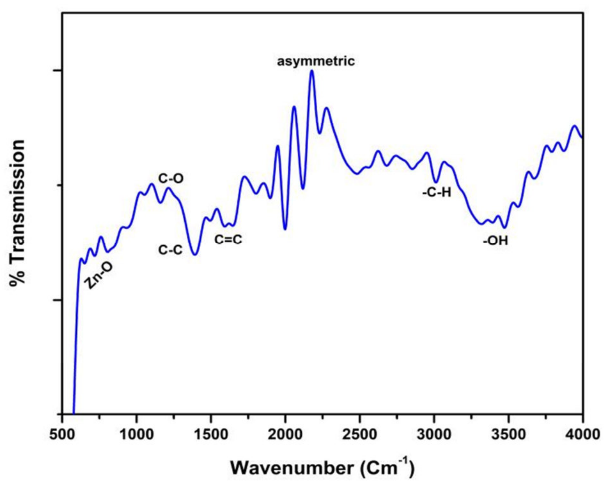

Fig. 3 FTIR Spectra of ZnO- 25wt% CNTs nanocomposites

The peaks observed around 1500 - 1700 cm^{-1} are due to C=C stretching vibrations in the graphitic structure of CNTs. The absorption feature below 600 cm^{-1} is also a unique fingerprint of Zn–O stretching vibrations, which shows that ZnO has formed successfully. The presence of both Zn–O and carbon-related functional groups indicates that CNTs and ZnO can work effectively in combination. This combination is expected to improve charge transfer and stability in photocatalytic applications.

D. Morphology of ZnO-25wt% CNTs nanocomposites

This SEM micrograph with elemental mapping are shown in Figure 4, which provides information about the sample's surface structure and chemical composition. The SEM image in (a) shows a structure that is porous and agglomerated, with particles that are not perfectly round in shape. This means that the surface is rough. The overlay mapping in (b) shows where the detected elements are located in the environment, which confirms that the elements are spread out evenly across the surface. The individual elemental representations illustrate that carbon (C), nitrogen (N), oxygen (O), and zinc (Zn) are all spread out evenly throughout the structure. Zn, on the other hand, seems to be more concentrated and evenly spread out. This means that the material is made up of a Zn-rich phase that is mixed with C, N, and O. This typically indicates that a composite or doped structure with good elemental intermixing has formed.

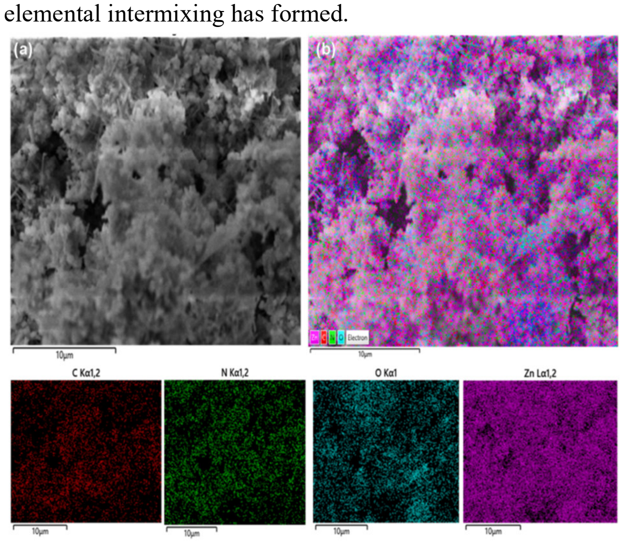

Fig. 4 SEM (a) micrograph (b) mapping with elemental composition of ZnO-25wt% CNTs nanocomposite

E. MB Dye degradation using *ZnO-25wt% CNTs nanocomposite*

This study examined the photocatalytic decomposition of methylene blue (MB) using ZnO–25 wt% CNT nanocomposites under UV light by monitoring how the absorbance changed over time. Figure 5(a) illustrates the concentration of MB dye in the presence of a ZnO-25wt% CNTs catalyst under UV light exposure. It is clear from the observed data, At first, the dye solution had a strong absorbance peak (P), but this peak become weaker over time as the irradiation period increased.

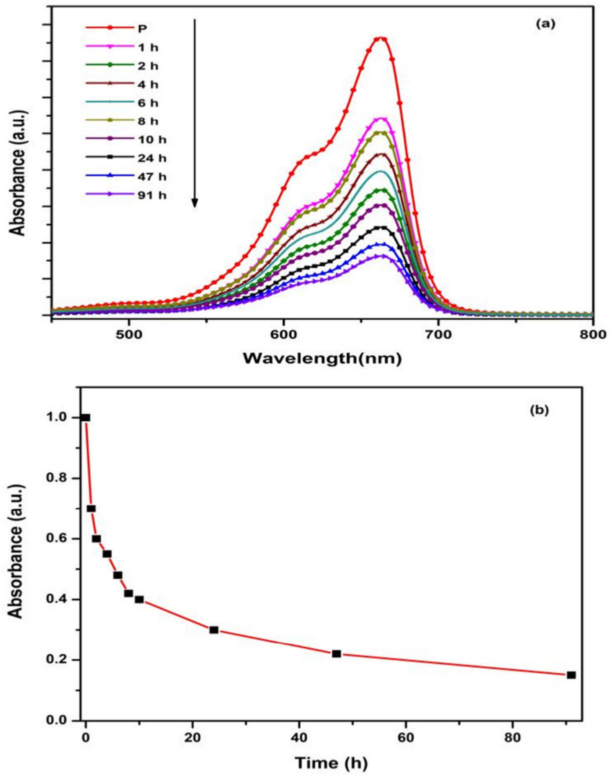

Fig. 5 (a) Absorbance under UV light (b) Change in absorbance over time for ZnO-25wt% CNTs nanocomposite

As the irradiation time increased, the absorption intensity of MB at ~664 nm slowly decreased. Additionally the formula

$$\left(1 - \frac{A_t}{A_0}\right) X\ 100 \qquad \text{(II)}$$

is used to determine the degradation percentage. Where A_0 and A_t are the absorbance values at the start and at the end of the time period. The decrement in concentration of MB dye is shown in Figure 5(b). The results showed that the dye concentration continued to decline, with almost 30% degradation after 1 hour, about 60% after 10 hours, and nearly 85% degradation after 91 hours. This shows how well the photocatalytic process worked to break down methylene blue (MB) when it was exposed to UV light. The improved performance is due to the synergistic effect of ZnO and CNTs, where CNTs absorb electrons, which lowers charge recombination and makes ZnO's photocatalytic efficiency better. This showed that the nanocomposite was able to break down MB effectively.

IV. CONCLUSIONS

XRD analysis of the structure of the ZnO–25 wt% CNT nanocomposite showed that ZnO was in the crystalline hexagonal wurtzite phase. The addition of CNTs did not change the crystal structure, but it caused the peaks to broaden slightly, by suggesting that the crystallites are very small. This crystallite size was in the nanometer range, which is good for photocatalytic uses. Optical studies showed a clear absorption edge, and the estimated band gap was lowered to about 3.12 eV compared to pure ZnO. This means that CNT incorporation has improved light absorption and electronic interactions. The FTIR measurements confirm the structural properties by illustrating the different functional groups that are in the ZnO-CNTs nanocomposite. The study used methylene blue (MB) degradation under UV light to determine how well the composite worked as a photocatalyst. The ZnO–25 wt% CNT nanocomposite degraded by about 85% in 95 hours of UV light, while pure ZnO did not degrade as quickly. The conductive CNT framework makes it easier for charge carriers to separate, stops recombination, and speeds up electron transfer. This is what makes the degradation efficiency better. The results show that combining CNTs with ZnO greatly improves both the optical and photocatalytic properties. This makes the nanocomposite a good choice for removing dyes and treating wastewater.

V. ACKNOWLEDGMENT

The authors thank the Centre for Non-Conventional Energy Resources and the Department of Physics at the University of Rajasthan, Jaipur, Rajasthan, India for the synthesis facility and optical characterization. Also, thank you to S.S.J. Subodh PG College, Jaipur, Rajasthan, India for XRD characterization.

REFERENCES

[1] S. Kumar, K.V. Rao, N.L. Reddy, ZnO-Based Nanostructures for Photocatalytic Degradation of Organic Dyes: A Review. *J. Environ. Chem. Eng.*, *8* (4), 103958, 2020.

[2] J. Singh, A. Kumar, K.-H. Kim, Graphene Oxide–ZnO Nanocomposites for Enhanced Photocatalytic Degradation of Dyes under Visible Light. *Appl. Catal. B, 243*, 575–590, 2019.

[3] W.Ma, M. Lv, F. Cao, Z. Fang, Y. Feng, G. Zhang, Y. Yang, H. Liu, Synthesis and Characterization of ZnO–GO Composites with Their Piezoelectric Catalytic and Antibacterial Properties. J. Environ. Chem. Eng. 10 (3), 107840, 2022.

[4] Y. Lin, R. Hong, H. Chen, D; Zhang, J. Xu, Green Synthesis of ZnO–GO Composites for the Photocatalytic Degradation of Methylene Blue. J. Nanomater. 2020, 2020, 4147357.

[5] A.G. Bekru, L.T. Tufa, O.A. Zelekew, M. Goddati, J. Lee, F.K. Sabir, Green Synthesis of a CuO–ZnO Nanocomposite for Efficient Photodegradation of Methylene Blue and Reduction of 4-Nitrophenol. ACS Omega, 7 (35), 31128–31138, 2022.

[6] X. Li, J. Yu, J. Low, Y. Fang, J. Xiao, Chen, X. Engineering Heterogeneous Semiconductors for Photocatalytic Water Splitting and Environmental Remediation. Chem. Rev., 119 (6), 3962–4179, 2019.

[7] M. Jeevarathinam, I.V. Asharani, Synthesis of CuO, ZnO Nanoparticles, and CuO–ZnO Nanocomposite for Enhanced Photocatalytic Degradation of Rhodamine B: A Comparative Study. Sci. Rep., 14, 9718, 2024.

[8] T. T. T. Nguyen, Y. N. N. Nguyen, X. T. Tran, T. T. T. Nguyen, T. V. Tran, Green Synthesis of CuO, ZnO, and CuO/ZnO Nanoparticles Using Annona glabra Leaf Extract for Antioxidant, Antibacterial, and Photocatalytic Activities. J. Environ. Chem. Eng., 11 (5), 111003, 2023.

[9] M. M. Ali, M. J. Haque, M. H. Kabir, M. A. Kaiyum, M. S. Rahman, Nano Synthesis of ZnO–TiO_2 Composites by Sol–Gel Method and Evaluation of Their Antibacterial, Optical, and Photocatalytic Activities. Results Mater., 11, 100199, 2021.

[10] R. Chong, F. Qian, Z.-H. Sun, M.-J. Wei, W.-Y. Zhou, J. Zhang, M.-Y. He, Q. Chen, J.-F. Qian, Catalytic Behavior of a ZnO/TiO_2 Composite in the Synthesis of Polycarbonate Diol. RSC Adv., 13 (8), 5070–5079, 2023.

[11] F. Pinzari, Synthesis, Photocatalytic and Bio Activity of ZnO–TiO_2 Nanocomposites: A Review Study. Reactions, 5 (4), 680–739, 2024.

[12] J. Maity, D. Roy, T. Bala, Template-Free Synthesis of Hexagonal ZnO Disk and ZnO–Ag Composite as Potential Photocatalyst. Hybrid Adv., 3, 100055, 2023.

[13] V.-E. Podasca, M.-D. Damaceanu, ZnO–Ag Based Polymer Composites as Photocatalysts for Highly Efficient Visible-Light Degradation of Methyl Orange. *J. Photochem. Photobiol. A Chem.*, *406,* 113003, 2021.

[14] J. Han, N. B. T. Pham, K. Oh, H.-K. Choi, Robust Biobased Membrane: Self-Entangled Cellulose Nanofibrils–ZnO–Ag Composite with High Photocatalytic Performance for Efficient Dye-Contaminated Water Treatment. ACS Omega, 9 (6), 5589–5599, 2024.

[15] K. M. Mohamed, J. J. Benitto, J. J.Vijaya, M. Bououdina, Recent Advances in ZnO-Based Nanostructures for the Photocatalytic Degradation of Hazardous, Non-Biodegradable Medicines. *Crystals*, *13* (2), 329, 2023.

[16] H. T. Truong, H. B. Truong, T. C. Nguyen, ZnO/TiO_2 Photocatalytic Nanocomposite for Dye and Bacteria Removal in Wastewater. *Mater. Res. Express*, *11* (8), 085003, 2024.

[17] S. Iijima, Helical Microtubules of Graphitic Carbon. *Nature*, *354*, 56–58, 1991.

[18] A. Nasser, B. Sina, J.S.A. Abuali Maryam, New Method for Preparing ZnO/CNT Nanocomposites with Enhanced Photocatalytic Degradation of Malachite Green under Visible Light. *J. Photochem. Photobiol. A: Chem.*, *361,* 100061, 2022.

[19] R. Vyas, R. Sharma, P. Sharma, V. Sharma, XRD pattern of pure ZnO and ZnO–MWCNT nanocomposites. Adv. Mater. Res., 585, 235–239, 2012.