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STRUCTURAL AND OPTICAL PROPERTIES OF (ZnO/MgO) NANOCOMPOSITES

K. Anandan[1*], D.Siva[2,3], K. Rajesh[1]
[1]Department of Physics, AMET University, Chennai 603 112, Tamilnadu, India
[2]Department of Physics, Presidency College, Chennai 600 005, Tamilnadu, India
[3]Physics, Government Higher Secondary School, Andampallam, Thiruvannamalai - 606 804, Tamilnadu, India

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ABSTRACT
Different solvents such as ethanol, ethanol-water and water mediated zinc oxide/magnesium oxide (ZnO/MgO) nanocomposites have been successfully synthesized by the facile precipitation process. The structure, purity, crystallite size and the phase of the synthesized ZnO/MgO nanocomposites are confirmed by the powder XRD patterns. The functional groups of the samples are confirmed by the FTIR analysis. The optical properties of the prepared ZnO/MgO samples are characterized by the UV-visible absorption and the PL emission spectroscopies. The UV and PL studies are used to determine the band gap, impurity, material quality and defect levels in the metal oxide nanocomposites.

Keywords: Nanocomposites; ZnO/MgO; Precipitation; Structural; Optical properties

I. INTRODUCTION
Mixed metal oxides have found increasing research focus and applications in physics, chemistry, materials science and engineering. The combination of two or more metals in an oxide matrix can produce materials with novel physical and chemical properties leading to relatively higher performance in various technological applications. During the last few years, synthesis of metal oxide nanocomposite materials have been attracted considerable attention [1–5]. The metal oxides nanocomposites are extremely important technological materials for use in optoelectronic and photonic devices and as catalysts in chemical industries. Zinc oxide (ZnO) is a wide band gap n-type semiconductor with an energy gap of 3.37 eV at room temperature. It has been used considerably for its catalytic, electrical, optoelectronic, and photochemical properties [6]. MgO is typical wide band gap semiconductor; it possesses unique optical, electronic, magnetic, thermal, mechanical and chemical properties due to its characteristic structures [7]. These two oxides have been widely used in almost the same application areas. Developing a new composite material by combining them into one could open up a new direction for research and applications. In recent years, researchers have focused more on the synthesis of nanocomposite of ZnO/ MgO due to their application in advanced technologies. Various physicochemical techniques have been employed to construct nanosized ZnO/MgO nanoparticles [8-19]. Several techniques have been also developed to prepare nanocomposite of ZnO/MgO. This nanocomposite has attracted much attention because it has a larger band gap than ZnO [20-22]. However, most of the techniques need high temperatures and perform under a costly inert atmosphere. Our goal in this research is to suggest an easy method to synthesize zinc oxide/ magnesium oxide nanocomposite. Considering the importance of luminescent materials in interdisciplinary materials science and future optoelectronic applications, the present work is focused on the synthesis of zinc oxide/magnesium oxide (ZnO/MgO) nanocomposites. They have attracted increasing interest in fabricating nanostructures with the size and the optical properties could be achieved by varying the solvents. With this motivation, ZnO/MgO nanocomposites were prepared by simple precipitation process and their structural, size and optical properties were studied. The as-synthesized samples are subjected to the different characterization techniques such as the powder X-Ray Diffraction (XRD), the Fourier Transform Infrared (FTIR), the Ultraviolet-visible (UV-vis) absorption and the Photoluminescence (PL) analyzes.

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II. EXPERIMENTAL PROCEDURE

Synthesis of ZnO/MgO nanocomposites

The zinc oxide/magnesium oxide nanocomposites were prepared by the facile precipitation process. All the chemical reagents were commercial with AR purity, and used directly without further purification. In a typical experiment, 0.1M of zinc acetate dehydrate ($Zn(CH_3COO)_2{\cdot}2H_2O$) and magnesium acetate tetrahydrate ($Mg(CH_3COO)_2{\cdot}4H_2O$) were dissolved in 100 ml ethanol. The precipitates were obtained by the addition of 0.4 M of sodium hydroxide (NaOH) pellets to the above solution, which was stirred for one hour. The resultant precipitate was filtered, washed with distilled water and absolute ethanol to remove the impurities, and dried at 120ºC for 15 hrs. Then, ash colored ZnO/MgO sample was obtained, when dried sample was calcined at 450ºC for 2h. The same procedure was followed for the preparation of ZnO/MgO in ethanol-water and water as solvents. The formation of ZnO/MgO nanocomposites is given in the equation below:

$$\left.\begin{matrix} Zn(CH_3COO)_2{\cdot}2H_2O \\ + \\ Mg(CH_3COO)_2{\cdot}4H_2O \end{matrix}\right] + 4NaOH \xrightarrow{120°C} Zn(OH)_2/Mg(OH)_2 + 4Na(CH_3COO) + 6H_2O \quad \text{---------- (1)}$$

$$Zn(OH)_2/\ Mg(OH)_2 \xrightarrow{450°C} ZnO/MgO + 2H_2O \quad \text{---------- (2)}$$

Characterization of synthesized nanocomposites

The characterization of metal oxide nanocomposites is essential for understanding of their structural and optical properties. Due to the inherent difficulties involved, the scientific experiments for the characterization should have the ability for rapid collection of data of several parameters with good precision and accuracy. The development of novel tools and instruments is one of the greater challenges in nanotechnology. The different solvents mediated samples were characterized by adopting various physico chemical methods namely XRD, FTIR, UV-vis and PL. The prepared ZnO/MgO samples were characterized by using the powder X-ray diffractometer, XPERT PRO with Cukα X-ray radiation (λ=0.15496 nm). The FTIR spectrum of the as-prepared sample was recorded, with a Bruker IFS 66 W Spectrometer using the KBr-pellet technique at a resolution of 4 cm^{-1} over the range 4000–400 cm^{-1}. The absorption study of the prepared samples has been carried out using the Varian Cary 5E UV-vis spectrophotometer. The PL analysis of the prepared samples was carried out, using the Fluoromax 4 spectrofluorometer, with an Xe lamp as the excitation light source.

III. RESULTS AND DISCUSSION

X-ray diffraction (XRD) is a rapid analytical technique primarily used for the phase identification of a crystalline material, and can provide information on unit cell dimensions. This method uses a monochromatic source of X-rays and measures the pattern of diffracted radiation, which is a result of the constructive interference due to the crystalline structure of the powder. The crystallite size can be obtained either by direct computer simulation of the X-ray diffraction pattern or from the Full Width at Half Maximum (FWHM) of the diffraction peaks using the Debye-Scherrer's formula [23].

$$D=0.9\lambda/\beta\cos\theta$$

where,

λ - Wavelength of X-rays,

β - FWHM in radian,

θ - Peak angle.

Figure 1 (a-c) shows the XRD patterns of ZnO/MgO nanocomposits prepared in ethanol, ethanol-water and water, respectively. All the peaks in the patterns could be indexed to the ZnO/MgO nanocomposites. The existence of strong diffraction peaks at 2θ values located at 31.76º, 34.6º, 36.25º, 47.53º and 67.96º corresponding to (100), (002), (101), (102) and (112) hexagonal wurtzite structure of ZnO crystal planes (JCPDS Card No.79-205) and peaks at 42.9º, 47.6º , 62.28º and 74.65º, corresponding to (001), (100), (102) and (110) cubic structure of MgO crystal planes (JCPDS Card No. 45- 0946), respectively [24]. This fact indicates that the prepared samples are not a single phase but a composite. Moreover, no impurity such as Zn $(CH_3COO)_2$, $Zn(OH)_2$, $Mg(CH_3COO)_2$ and $Mg(OH)_2$ were detected. Peak broadening indicates that the smaller crystallites size of the prepared ZnO/MgO nanocomposites.

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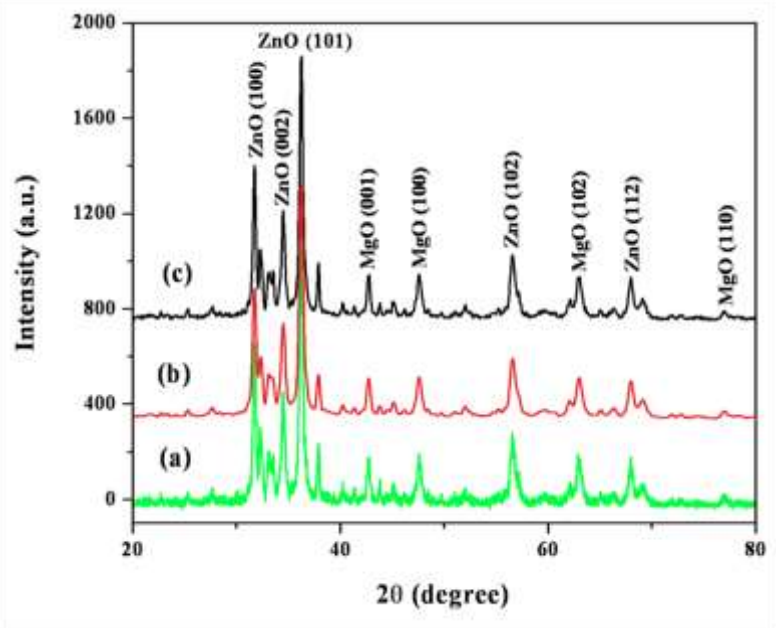

Fig. 1 XRD patterns of ZnO/MgO nanocomposites prepared in (a) ethanol, (b) water-ethanol and (c) water.

In any preparation of nanomaterials, the solvent is an important parameter for determining the crystal size. In the present work, the organic mediated samples (Fig. 1(a-b)) show a slight broadening of peaks compared to the peaks of the aqueous mediated sample, as shown in Fig.1 (c). This clearly reveals that using organic media can produce fine particles. Using Scherrer's formula, the average crystallite sizes of the ZnO/MgO samples synthesized in ethanol, ethanol-water and water are found to be 22, 23.91 and 26.82 nm, respectively. From the result it is concluded that the ethanol mediated ZnO/MgO nanocomposites are most ultra-fine, owing to their best dispersing and capping ability.

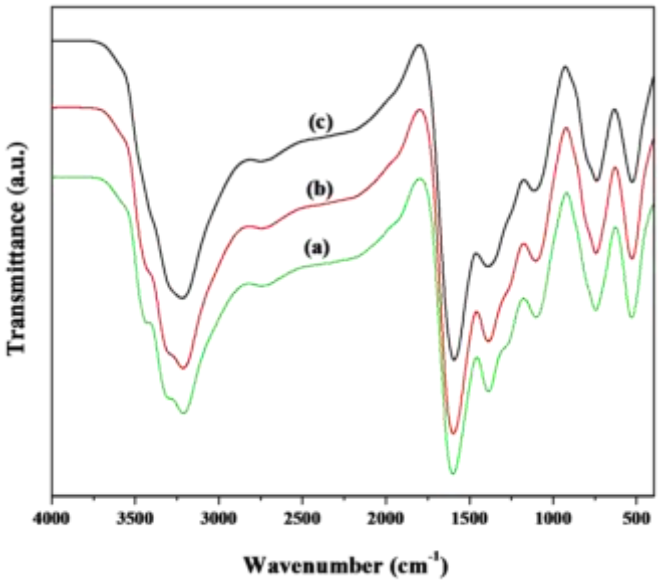

Fig. 2 FTIR spectra of (a) ethanol, (b) water-ethanol and (c) water mediated ZnO/MgO samples dried at 120°C

Fourier Transform Infrared (FTIR) spectroscopy is a powerful tool for identifying the types of chemical bonds (functional groups) in a molecule by producing an infrared absorption spectrum that is like a molecular "fingerprint". The wavelength of the light absorbed is characteristic of the chemical bond as can be seen in this annotated spectrum. Figure 2 shows the FTIR spectra of as-prepared ZnO/MgO samples dried at 120ºC. The

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peaks observed in the spectra at 3685-2840, 1604 and 1390 cm^{-1} are the stretching and bending vibrations of –OH groups, which are associated with the adsorbed water on the surface of the ZnO/MgO particles [25]. The band appeared at 1096 cm^{-1} was assigned to the C–N stretching vibration [26]. Generally, the metal oxides give absorption bands below 1000 cm^{-1}, arising due to the inter-atomic vibrations. Further, the strong bands located at 746 and 530 cm^{-1} indicate the stretching vibration mode of Mg–O and Zn–O, respectively, which confirm the formation of ZnO/MgO nanocomposites [27].

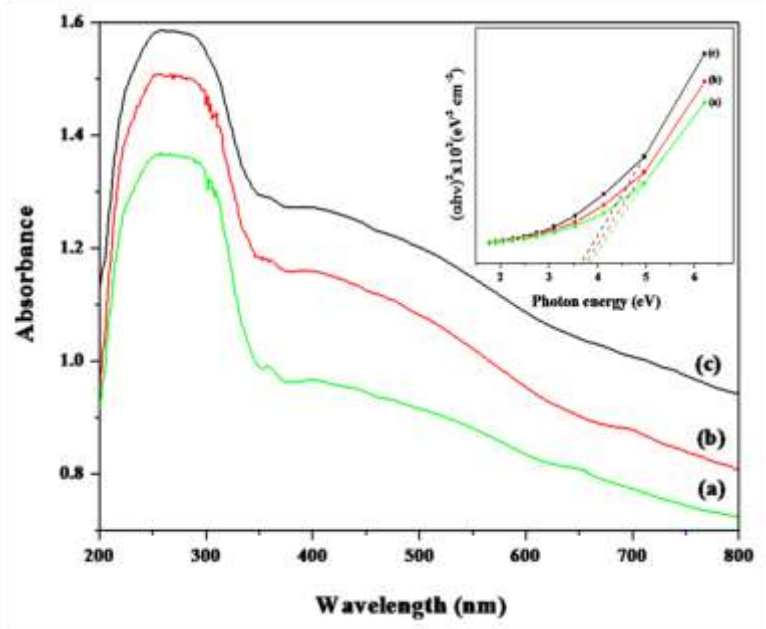

Fig.3 UV-vis absorption spectra of ZnO/MgO nanocomposites prepared in (a) ethanol, (b) water-ethanol and (c) water

Figure 3 (a-c) shows the UV-vis absorption spectrum of the ZnO/MgO nanocomposites prepared in ethanol, ethanol-water and water, respectively. It can be seen in all the spectra that the strong absorption peaks were appeared at around 280 nm, which is attributed to the band gap absorption in ZnO/MgO nanocomposites. The calculated values of the band gap energies of ethanol, ethanol-water and water mediated ZnO/MgO nanocomposites are 3.83, 3.75 and 3.66 eV respectively, which are good agreement with reported band gap values of ZnO/MgO nanocomposites. Moreover, MgO is more ionic compared to ZnO, because of 3*s* energy level in Mg and 4*s* energy level in Zn. Consequently, the energy difference between these *s* levels and O 2*p* level is smaller in ZnO and larger in MgO. Thus, ionicity is lowest in ZnO and largest in MgO. This is now consistent with larger band gaps for ZnO/MgO as compared to ZnO [28]. According to the data of the absorption spectra, the optical band gap (E_g) of the ZnO/MgO nanocomposites can be estimated, by using the following equation:

$$\alpha h\nu = C\,(h\nu - Eg)^n$$

here α is the absorption coefficient, hν is the photon energy, C is the constant, and n=1/2 for a directly allowed transition. For the indirect transitions, the plots of $(\alpha h\nu)^2$ versus photon energy of the ZnO/MgO nanocomposites are shown in the inset of Fig. 3. Hence, the optical band gap for the absorption peak can be obtained by extrapolating the linear portion of the $(\alpha h\nu)^2$–hν curve.

Optical investigations can reveal very useful information for understanding the physical properties of materials. They also demonstrate the possibility of extending the potential application of ZnO/MgO nanocomposites in optoelectronic devices. Therefore, the photoluminescence emission measurement was performed with an excitation wavelength of 300 nm. Figure 4 (a-c) shows the room-temperature PL emission spectra of ethanol, ethanol-water and water mediated ZnO/MgO nanocomposites. Generally, ZnO/MgO nanocomposites grown in the chemical solution has two kinds of defects, i.e., intrinsic defect and surface defects. The PL emission spectra of all the samples show the broad and strong deep level emissions (DLE) in the green emission region centered at ~513–548 and 560 nm, respectively, indicating that the prepared nanocomposites have a good crystal quality

[29]. The DLE is associated with the intrinsic defects in the ZnO/MgO nanocomposites, and is attributed to the radiative recombination of photo-generated holes with electrons [30]. Moreover, the DLE bands are mainly attributed to the intrinsic defects, such as oxygen vacancy, zinc vacancy, magnesium vacancy, oxygen interstitial, zinc interstitial and magnesium interstitial or surface-related defects [31, 32].

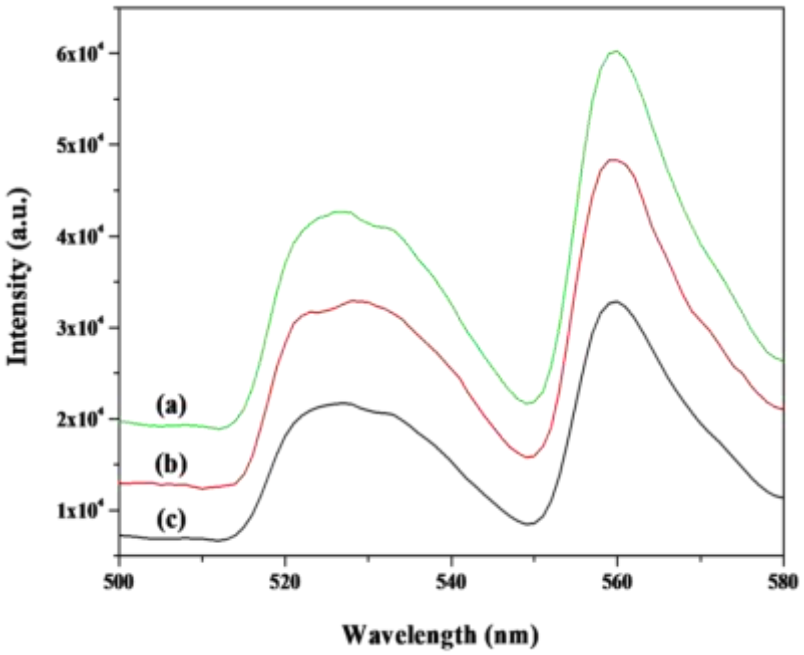

Fig. 4 PL emission spectra of ZnO/MgO nanocomposites prepared in (a) ethanol, (b) water-ethanol and (c) water

Since, it was observed from the PL emission spectra that there was a change in the intensity of the emission peaks by the alcoholic medium mediated samples (Fig.4.a-b)) than that of aqueous medium, which lead us to conclude that the alcoholic solvents changed the crystalline size or increased the intrinsic and surface defect [33, 34].

IV. CONCLUSION

Different solvents such as ethanol, ethanol-water and water mediated ZnO/MgO nanocomposites have been successfully synthesized by the facile precipitation process. The hexagonal/cubic structure of ZnO/MgO nanocomposites was confirmed by the powder XRD patterns and the average particle size of the samples calculated to be 22, 23.91 and 26.82 nm. It was found that the solvents played important roles in the preparation of size of nanocomposites. The presence of functional groups of synthesized ZnO/MgO samples was confirmed by the FTIR spectrum. The optical properties of the nanocomposites were studied by UV-vis and PL spectroscopies. The band gap energies of ethanol, ethanol-water and water mediated ZnO/MgO nanocomposites are 3.83, 3.75 and 3.66 eV respectively, which are good agreement with reported band gap values of ZnO/MgO nanocomposites. The PL emission studies showed deep level emissions (DLE) in the green emission region, indicating that the prepared nanocomposites have a good crystal quality. Moreover, the DLE bands are mainly attributed to the intrinsic defects, such as oxygen vacancy, zinc vacancy, magnesium vacancy, oxygen interstitial, zinc interstitial and magnesium interstitial or surface-related defects. Hence, it should be suitable for optoelectronic devices.

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