# Investigation of Structural and Optical Properties of $(ZnO)_x$-$(MgO)_{1-x}$ (x=1.0, 0.75, 0.50, 0.20, 0.10) Nano crystalline Thin Films

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**Abstract: In this paper, $ZnO_xMgO_{1-x}$ composites were deposited on glass and silicon substrate using E-Beam Deposition Technique. Doping of MgO is in atomic percentage for various compositions from 0% to 90%. XRD results show that MgO has been doped successfully. The investigation of Band gap has been done and the result displays as the MgO content is increased, the band gap is tuned from 3.16 eV to 3.55 eV and transmission band edge is blue shifted about 36 meV to the higher energy direction, this is closely related to formation of mesoporous structure. The Band Gap has been calculated using UV-Vis Spectroscopy. Investigation confirms that defects in surface have been increased with the increase in MgO Content.**
**Keywords:** E-Beam Deposition, transmission band edge, mesoporous structure, defects in surface, UV-Vis Spectroscopy, wurtzite hexagonal structure, cubic rock salt structure.

## 1. INTRODUCTION

Literature shows that ZnO is widely used due to its wide band gap in the range of Eg=3.17 eV to 3.37 eV at temperature 300K. ZnO has binding energy which is 60 meV [1]. ZnO based nano structured devices are used for the application of LED, Lasers and many transparent conducting electrodes of gas Sensors. ZnO can be alloyed with several materials [2]. ZnO based thin films are used in potential applications for many optoelectronics devices. Composites of ZnO are used for tuning of band gap in blue-green wavelength and ultraviolet range. MgO(Magnesium Oxide) has band gap in the range of 7.1 eV to 7.7 eV with the large binding energy of 80 meV. ZnO can be alloyed with high band gap materials like MgO to increase its Optical Band gap [3]. Mostly the phase transition problem is occurred in structure of ZnO and MgO due to having extremely different crystal structures as ZnO has wurtzite hexagonal structure whereas MgO has cubic rock salt structure. Band gap has been enhanced due to formation of ZnOxMgO1-x alloys already reported [4].

## 2. EXPERIMENTAL

$ZnO_xMgO_{1-x}$(x=1.0, 0.75, 0.50, 0.20, 0.10) has been fabricated through E-beam deposition method. Deposition was done on silicon and glass substrates with the thickness of ~150 nm. Before depositing, the material substrates have been cleaned thoroughly using RCA cleaning and rinsing in DI water for 10 times after every steps. $ZnO_xMgO_{1-x}$ alloys in different compositions(x=1.0, 0.75, 0.50, 0.20, 0.10) have been deposited homogeneously on silicon and glass substrates. The powder which is thoroughly mixed has been dried and heated in 1200 °C for around 2 hours in air atmosphere. This fine powder has been pressed into discs of 13mm diameter with the thickness 1-2 mm with steel die and hydraulic press. The $ZnO_xMgO_{1-x}$ pellets were sintered at 1230°C and cooled down at room temperature. The pellets were cleaned and Nano crystalline thin films of $ZnO_xMgO_{1-x}$ were deposited using E-beam. The grain size distribution has been analyzed by FESEM (Field Emission Scanning Electron Microscope) that has been done using technique of mean linear intercept technique. Optical band gap has been calculated through UV-VIS NIR Spectrophotometer with the range of wavelength of 400-1200nm.The spectro flourimeter Perkin Elemer LS-55 has been used to measure the photoluminescence spectra [5]. The crystalline structure was explored by X-Ray diffraction (EQ-MD10 diffractometer with a Cu-tube).Literature shows that ZnO is widely used due to its wide band

### 2.1 Two gram calculations of the appropriate Atomic Percentage Proportions weighed using an Electronic Balance

Since, atomic mass of ZnO = 81.38 g/mol and atomic mass of MgO = 40.3044 g/mol

**Table 1:** Calculations of the appropriate Atomic Percentage Proportions

| Composites | Weighing Calculation of ZnO | Weighing Calculation of MgO |
|---|---|---|
| **ZnO** | **2 gm** | **0 gm** |
| **$(ZnO)_{0.75}$-$(MgO)_{0.25}$** | $\frac{0.75\times81.38\times2}{((0.75\times81.38)+(0.25\times40.3044))}$ **= 1.7166 gm** | $\frac{0.25\times40.3044\times2}{((0.75\times81.38)+(0.25\times40.3044))}$ **= 0.2833 gm** |
| **$(ZnO)_{0.50}$-$(MgO)_{0.50}$** | $\frac{0.50\times81.38\times2}{((0.50\times81.38)+(0.50\times40.3044))}$ **= 1.3375 gm** | $\frac{0.50\times40.3044\times2}{((0.50\times81.38)+(0.50\times40.3044))}$ **= 0.6624 gm** |
| **$(ZnO)_{0.20}$-$(MgO)_{0.80}$** | $\frac{0.20\times81.38\times2}{((0.20\times81.38)+(0.80\times40.3044))}$ **= 0.6709 gm** | $\frac{0.80\times40.3044\times2}{((0.20\times81.38)+(0.80\times40.3044))}$ **= 1.3290 gm** |
| **$(ZnO)_{0.10}$-$(MgO)_{0.90}$** | $\frac{0.10\times81.38\times2}{((0.10\times81.38)+(0.90\times40.3044))}$ **= 0.3664 gm** | $\frac{0.90\times40.3044\times2}{((0.10\times81.38)+(0.90\times40.3044))}$ **= 1.6335 gm** |

## 3. RESULTS AND DISCUSSIONS

### 3.1Structural Studdy

XRD diagrams for $ZnO_xMgO_{1-x}$ (x=1.0,0.75,0.50,0.20,0.10) composites are shown in Fig.1.The sharp peaks with regular distribution shows the presence of ZnO (wurtize structure)[6] and MgO(cubic structure).On the basis of JCPDS card No. 80-0075 and 78-0430[7] , the diffraction peaks of hexagonal ZnO and cubic MgO are indexed respectively. The indexing of the pattern is according to hexagonal ZnO and cubic MgO. There is formation of composite which is indicated by the presence of (111) and (200) peaks along with the peaks of ZnO [8]. As the concentration of MgO content is increased, the respective intensity of the (111) and (200) peaks increased.

### 3.2 Morphological Properties

The scanning electron micrographs of $ZnO_xMgO_{1-x}$ composites are shown in Fig 2. The SEM micrographs show that there are some hexagonal crystal-shaped and well distributed nano structured grains. These SEM images indicate the influence of higher doping of Mg on the surface of ZnO matrix [8]. The surfaces of all the samples are rough containing grains and nano tubes having many shapes and sizes. These crystallites are randomly distributed and irregularly disoriented. When the MgO composition x varied from 0 to 50%, the grain size are found to decrease from 109 nm to 55nm shown in Fig 2(a) to Fig 2(c). From the Fig 2(d), it is found that the grain density is decreased, and there is coalescence of small grains for highly doped ZnO samples [9]. As the Fig 2(e), reveals the presence of grain boundaries and large grains covered by small crystallites.

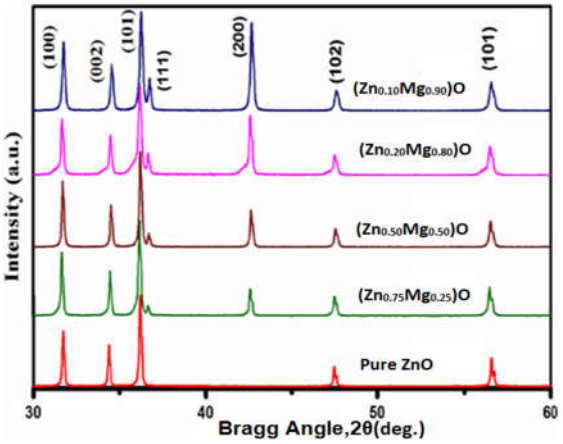


**Figure 1:** X-Ray Diffraction patterns for various content of MgO in $ZnO_xMgO_{(1-x)}$ composites

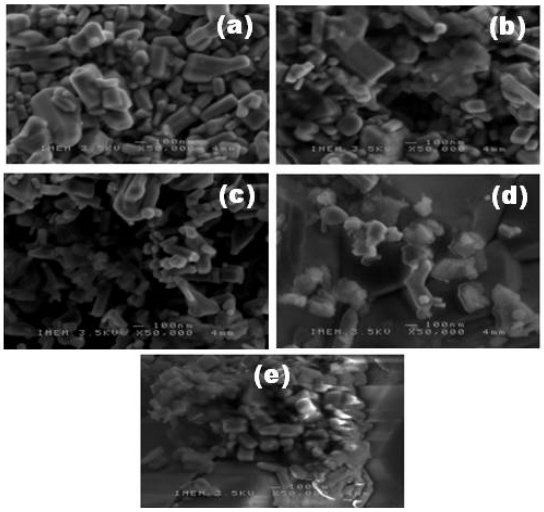


**Figure 2:** SEM images obtained for composites:(a) Pure ZnO (b) $ZnO_{0.75}MgO_{0.25}$ (c) $ZnO_{0.50}MgO_{0.50}$ (d) $ZnO_{0.20}MgO_{0.80}$ (e) $ZnO_{0.10}MgO_{0.90}$

### 3.3 Optical Properties

The optical band gap of $ZnO_xMgO_{1-x}$ (x=1.0, 0.75, 0.50, 0.20, 0.10) composites on glass substrate is obtained by Tauc Plot. The plot of $(\alpha h\nu)2$ versus photon energy shows a linear region just above the optical absorption edge[10-13]. The plot of the

photon energy (hν) and the absorption coefficient (α) are related to the direct band gap by following relation [14]:

$$\alpha h\nu = K.\ (h\nu - E_g)^2$$

Where K is a constant, α is the absorption coefficient and hν is the photon energy. Fig 4 shows the optical absorption data of $(\alpha h\nu)2$ versus hν (Tauc Plot).The band gap evaluated is found to increase with concentration of MgO. Fig 4 shows the variation of optical band gap for different content of MgO in $ZnO_xMgO_{1-x}$ (x=1.0, 0.75, 0.50, 0.20, 0.10) composites. The values of Eg for different concentration varies from x=1.00 to x=0.10 are found to be 3.16 , 3.22, 3.27, 3.34 and 3.55 eV respectively . This observation of blue shift of the band gap may be attributed to following two reasons: (i) quantum size effect [15-17] (ii) electronic structure modifications.

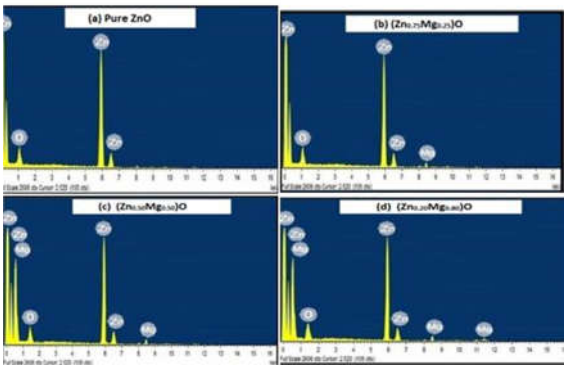


**Figure 3:** Energy Dispersive X-Ray Spectra (EDS) : (a) Pure ZnO (b) $ZnO_{0.75}MgO_{0.25}$ (c) $ZnO_{0.50}MgO_{0.50}$ (d) $ZnO_{0.20}MgO_{0.80}$

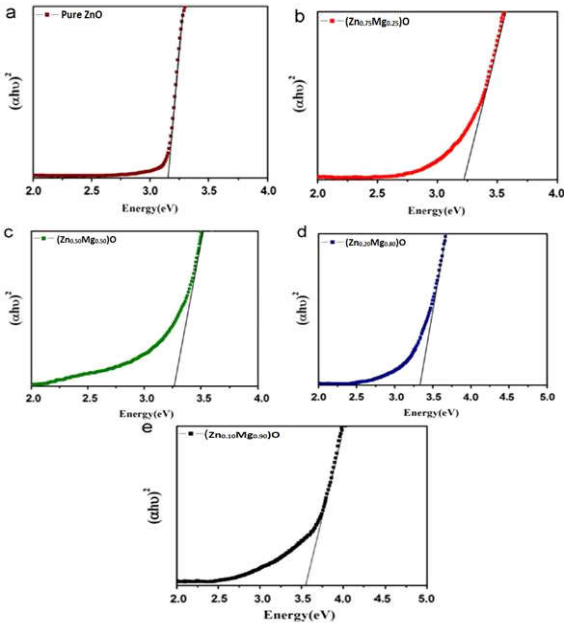


**Figure 4:** $(\alpha h\nu)^2$ versus hν plot of $ZnO_xMgO_{(1-x)}$ composites : (a) x=1.0 (b) x=0.75 (c) x=0.50 (d) x=0.20 (e) x=0.10

## 5. CONCLUSION

$ZnO_xMgO_{(1-x)}$ composites thin films are deposited by E-beam deposition technique. The XRD study reveals the formation of the composite. The SEM micrograph shows the porous nature of the samples. It also shows the rougher surfaces of the samples covered by grains having prismatic shapes and different sizes. FESEM studies confirm that the crystallite size increases with increase in Mg content. The band gap is successfully tuned from 3.16 to 3.55 eV with increasing MgO content.

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