**Effect of Doping in MnxZn1-x-yFeyO that Fluctuate its Structural and Optical Properties**

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**Abstract:**

MnxZn1-x-yFeyONPs are synthesized by route precipitation method. Zinc oxide is a vast purposeful material due to its numerous different exciting properties, an infinite range of UV absorption, and wide photo stability. The various characterizations are applied on these nanoparticles to recognize its properties. X-Ray diffraction (XRD) is told about structural properties of NPs that explained only hexagonal crystalline phase of wurtzite formation for both the cases. As dopant ratio increasing which is responsible for the decrease in lattice parameters in calculated parameters. This decrease can be credited to the smaller ionic radii of Mn (0.785Å), Fe (0.78Å) and as compared to Zn (0.88Å). The crystalline size is evaluated for doped ZnO determined by both Scherrer equations. In term of optical ratio, these defects decrease the band gap but after that results in ordering and increment in band gap values.

Keywords: XRD; nanoparticles; Optical properties.

1. **Introduction:**

ZnO has been generally reviewed because of its properties; bandgap semiconductor and binding energy etc so mostly discussed in spin electronics, chemical sensors, transparent UV protection films, varistors, visible conductors, and so on [1–4]. For the production of ZnO, diverse methods together with Ball milling, vapor/thermal decomposition and route/chemical precipitation were used in the past decade [5-6]. The dramatic change has been produced in optical and magnetic properties arise due to this doped (i.e. replacement of doped element with Zn ion) as evaluated by the undoped ZnO nanoparticles. It has been necessary to produce the physical and structural properties according to their need, which are fulfilled by growing the ZnO-based ferromagnetic material [7]. The synthesis techniques and environmental condition affect strongly on the ferromagnetism during the process of synthesized sample. B. N. Dole et. al. Mn doped ZnO nanoparticles having Zn1−xMnxO were synthesized by gel route. An (XRD) study indicates preserved wurtzite structure till 8% of Mn doped samples, no extra peaks deducted. The structural properties helpful for find out lattice parameters, and other detail. In case of lattice parameters (a=b, c) were increase linearly determined with the Mn content it means Mn ions doped clearly into main element sites from XRD data. A hexagonal crystal structure found by XRD result as same as crystal structure of ZnO [8].

Jayakumar et. al. Mn-doped ZnO nanocrystalline (2 and 5 at.% particles) prepared by co-precipitation method [9]. Monophasic wurtzite structure explained with Rietveld refinement of XRD of Mn-doped ZnO crystallizes. Ciciliati et. al. Fe-ions mixed in Zn site were absolute formed by gel method [10]. XRD determined that the wurtzite structure, no extra peak.

Kumar et. al. Zn1−xFexO diluted with PVP NPS as followed co-precipitation process [11]. Senol et. al. Mn/Cu co-doped ZnO NPs were prepared by reaction method to find out the relation among Eg (energy gap) and µ ([refractive index](https://www.sciencedirect.com/topics/materials-science/refractive-index)) through different properties investigations [12]. XRD was shows that hexagonal Wurtzite structure which find out the c/a ratios. Sharma et. al. rietveld refinement showed the single phase wurtzite formation by XRD results for ZnO and Fe/Co co-doped ZnO [13]. As constract to XRD, energy band gap values decreases that clearly observed through the absorption spectra.

In this work, MnxZn1-x-yFeyO(1 ≤ x ≤ 2%)NPs were synthesized by following the route precipitation method through substitution of Ag and Al dopant. These samples were analytical grade having extremely pure (>99%) that why were no need for further any purification apply on used oxides.

1. **Experimental techniques:**

Mn and Fe nitrate (dopant) was mix properly in Zn acetate solution by using magnetic stirrer and each of these oxides were essential to dissolve properly by using ethanol and distilled water then after in above solution add ammonia solution for adjusting PH value, for precipitation mix NaOH solution and the effect of mixing was allowable for hours following total submission of ammonia solution. Wait for the completion of solution mixing, the solution was acceptable to stay down by using temperature water bath and then filters out by using filter paper and heat treatment was applied on these filtered particles around 900 0C in muffle furnace. With X'Pert PRO were used for powder diffraction studies performed via Cu-Kα having 2θ range lies in between 20°-80° and difference in size is 0.013°/min at room temperature.

**3.1 X-ray diffraction analysis:**

Fig shows diffraction (XRD) pattern of MnxZn1-x-yFeyO. Most of the diffraction peaks in the present studied samples can be matched with the ICDD card (036-1451) all the peaks corresponds to the hexagonal wurtzite of zinc oxide nanoparticles (a=3.236nm and c=5.1817nm) similar XRD pattern. No peak is present in the present patterns, so it can be concluded that no extra phase is present in these samples. By comparing the present data with standard card (ICDD Card No.036-1451) data, the lattice parameters of the present composition have been calculated. The calculated parameters have been presented in table 3.1 decrease in lattice parameters with increasing dopant concentration has been observed as contract to undoped ZnO. The decrease can be accredited to the minute ionic radii of Mn (0.785Å) and Fe (0.78Å) and as compared to Zn (0.88Å) [14]. Scherrer’s method as

D=Kλ/βCOSθ

A result of XRD are told that only hexagonal crystalline phase for wurtzite formation. With decrease occurs in lattice parameters with increase dopant ratio and decrease concentration of ZnO [15]. This decrease can be accredited to the smaller radius of Mn (0.785Å), Fe (0.78Å) and as compared to Zn (0.88Å). By Scherrer Method, The falls occur in crystalline size with increase in dopant concentration.



**Fig3.1 X-ray diffraction pattern of (MnxZn1-x-yFeyO)**

**Table 3.1 Structural properties obtained for Zn1-x-yMnxFeyO**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Structural properties** | | | | **Optical properties** |
| **Sample name** | **Lattice parameter** | | **Volume**  **V=3√3/2 a2c** | **D (nm)** | **Eg (direct) (ev)** |
| a(=b) | c |
| Mn0.01Zn0.98Fe0.01O | 3.24496 | 5.1969 | 142.171773 | 48 nm | 2.55 ev |
| Mn0.02ZnO0.96Fe0.02O | 3. 2378 | 5.1817 | 141.136303 | 40 nm | 2.70 ev |

**3.2 UV-Visible spectroscopy**

According to Tauc relation for the absorbance [16].

(αhv) = A(hv-Eg)n

The straight portion of the graphs ((αhv)2 vs hv) has been linear fitted and extrapolated to hv=0 for finding the Eg values. The higher concentration dopant concentration, the band gap values gain shows in increasing trend. This can be attributed to the generation of defects in the samples due to dopant. Upto certain concentration, these defects decrease the band gap but after that results in ordering and increment in band gap values.





**Fig 3.2 Plot between (αhv)2 Vs (hv) of (a) Mn0.01 Zn0.98Fe0.01O (b) Mn0.02ZnO0.96Fe0.02 O**

**4. Conclusion:**

The results of XRD are told that only hexagonal crystalline phase for wurtzite formation. With decrease occurs in lattice parameters with increase dopant ratio and decrease concentration of ZnO. This decrease can be accredited to the minute radius of Mn (0.785Å), Fe (0.78Å) and as compared to Zn (0.88Å). By Scherrer Method, The falls occur in crystalline size with increase in dopant concentration. As contract to XRD, these defects decrease the band gap in optical ratio but after that result in ordering and increment in band gap values.

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