

Neodymium doped Zinc Oxide Nano Particles as Photocatalyst

Shanthi Karidas, B.Kalyani, K.Srikanth, C.P.Vardhini

Abstract: Neodymium doped Zinc Oxide Nano Particles were prepared with co-precipitation method. Structural and morphological properties were studied using XRD, FESEM. Spectroscopic properties were studied using FT-IR spectrometer. Optical properties were studied using DRS UV-VIS, PL spectrophotometers. Crystallite size was found from XRD peaks. FESEM pictures show the hexagonal structure of the prepared Nano Particles. As the Neodymium concentration increases the Band gap of the prepared doped Zinc Oxide Nano Particles decreases.

Index Terms: Zinc Oxide Nano Particles, Co-precipitation method, Crystallite size, Band gap

I. INTRODUCTION

The scientific community has successfully synthesized nanostructures like nanoparticles, nanocubes, nanoribbons, nanofibers, nano tetrapods, nanoflowers etc. Compared to bulk counterparts nanostructures have unique properties. Zinc Oxide is widely used in semiconductor industry. Zinc Oxide Nano Particles (ZnO NP's) are doped with several elements like Mn, Co, Fe, Al, Nd, Ce etc. Doped Zinc oxide Nano Particles have high electron mobility, wide band gap, strong room temperature luminescence and ferromagnetism. Due to these properties they have applications in solid state lighting, gas sensing, optoelectronic devices, photo catalysts etc. Neodymium doped zinc oxide nano particles acts as good photo catalysts and helps in photo degradation of some dyes.

II. EXPERIMENTAL PROCEDURE

All the Chemicals, Zinc Nitrate Hexa hydrate $Zn(NO_3)_2 \cdot 6H_2O$, Neodymium Nitrate Hexa hydrate $Nd(NO_3)_3 \cdot 6H_2O$, Sodium Hydroxide pellets were purchased from Central Drug House, New Delhi. Neodymium doped ZnO NP's at various concentrations were prepared using $Zn_{(1-x)}Nd_xO$ where 'x' varies as $x=0.01, 0.03, 0.05, 0.07, 0.09, 0.1$. The particles were named as ZnNd1, ZnNd2, ZnNd3, ZnNd4, ZnNd5, ZnNd6 respectively. $Zn(NO_3)_2 \cdot 6H_2O$ and $Nd(NO_3)_3 \cdot 6H_2O$ were added to deionised water in stichiometric ratios. The solution was thoroughly mixed with magnetic stirrer. Sodium

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hydroxide was added till the pH of the solution became 10. The solution was washed several times to remove impurities. Then the solution was kept in hot air oven, overnight, to make it dry powder. Dried powder was grinded. The grinded Nano Particles were characterized to study structural, morphological, spectroscopic, optical properties.

III. CHARACTERISATION

Structural analysis of the Nd doped ZnO Nano Particles was studied using Rigaku Ultima IV X-Ray Diffractometer (XRD) with Cu target and λ radiation having 1.5418 Å wavelength in the range 20° to 80°. The morphology was studied using Gemini 500 FESEM. Spectroscopic properties were studied using Jasco 4200 FTIR spectrometer. Optical properties were studied using Jasco V-670 Diffuse Reflectance UV-VIS spectrophotometer and SHIMADZU RF6000 PL spectrofluorometer with 280 nm excitation.

IV RESULTS AND DISCUSSION

A

Fig 1 shows the XRD peaks for pure and Nd doped ZnO NP's. The sharp peaks confirm the crystalline phase of the prepared NP's. All the peaks are at same angles as in JCPDS 36-1451, which confirm that formed particles are ZnO NP's. All the peaks are indexed with h,k,l values using Powd software. The crystallite size of the pure and Nd doped NP's was calculated using Debye Scherer equation. Crystallite size was found in range of 33-51 nm. Lattice parameters; strain and X-ray density values were calculated and are given in Table -1. The X-Ray density values increases as the Nd doping concentration increases, showing that more Nd atoms are incorporated in the NP's. As the Nd doping concentration increases the lattice parameters 'a', 'c' decrease anisotropically, may be due to increase in strain. Fig 2 shows the variation of lattice parameters 'a', 'c' with change in Nd concentration.

B.

Morphology of Pure ZnO and Nd doped ZnO NP's show that the formed NP's have hexagonal Wurtzite structure as shown in fig 3(a-g). All the pictures are taken at 200 nm scale. Nd doped ZnO NP's have slight change in the shape. Also we see that grain size and agglomeration increases as the Nd concentration increases.

C.

Fig 4 shows the FT-IR graph of pure ZnO and Nd doped ZnO NP's.



FTIR spectra consists of various well defined peaks observed at 3452, 1389, 1464, 858 and 453 cm^{-1} . The absorption peak appearing at 3452 cm^{-1} corresponds to the stretching vibration of O-H band. This absorption peak appeared due to surface absorption of water molecules. The peaks at 1389 cm^{-1} and 1464 cm^{-1} correspond to C-H bending vibration. Nd-O absorption peak is obtained at 858 cm^{-1} . The absorption peak appearing at 453 cm^{-1} could be attributed to Zn-O stretching.

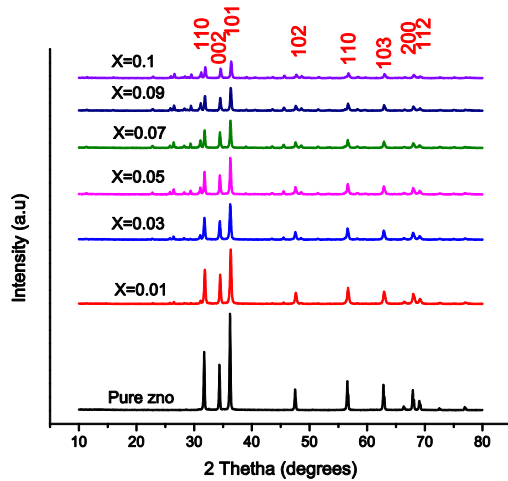


Fig 1 XRD graph of pure and Nd doped ZnO NP's

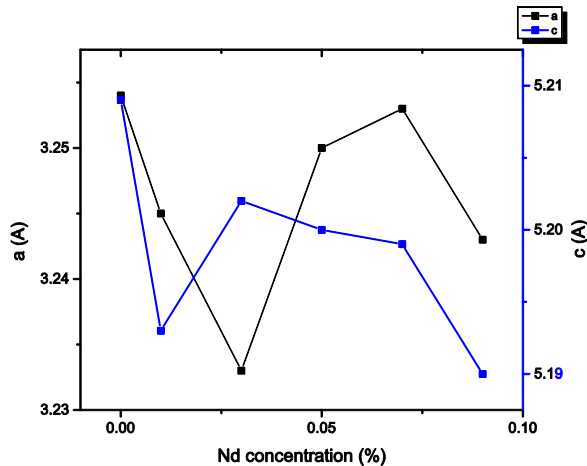


Fig 2 shows variation of lattice parameters 'a', 'c' with change in Nd concentration

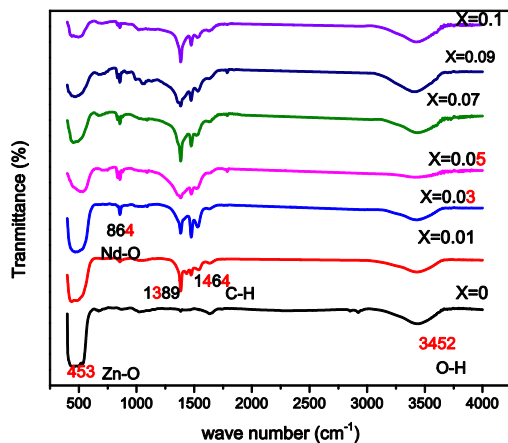


Fig 4 FT-IR absorption peaks of pure and Nd doped

ZnO NP's

D.

Fig 5 shows Diffuse reflectance UV-VIS absorption spectra for the prepared particles. Strong absorption peak is observed at 365 nm for pure and Nd doped ZnO nanoparticles. As the doping percentage increases there is shift to lower wave lengths side. For Nd doped ZnO nanoparticles absorption peaks are observed in visible region at 533nm,590 nm,747 nm,806 nm,885 nm. Intensity of absorption at these peaks increases as Nd concentration increases. Band gap was calculated using the relation [1]

$$(\alpha h\nu)^2 = k(h\nu - E_g) \quad (1)$$

where ' α ' is absorption coefficient, ' h ' is Planck's constant, ' E_g ' is band gap, ' K ' some constant, ' ν ' is frequency. Extrapolation of the Tauc plot between $(\alpha h\nu)^2$ and $h\nu$ gives the band gap. For pure ZnO NP's the value is 3.210 e.v. . For Nd concentrations at X=0.01, 0.03, 0.05, 0.07 and 0.09 the band gap values are 3.081, 3.169, 3.098, 3.104, 3.192 and 3.139 e.v. respectively. Decrease in band gap with Nd doping shows that doped ZnO NP's can be used for photo degradation [1].

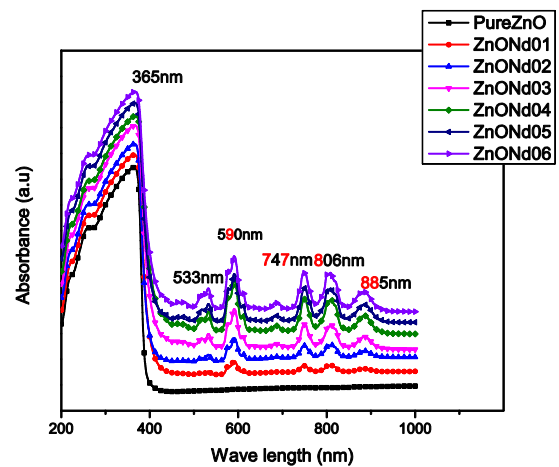


Fig 5 UV-VIS absorption peaks for pure and Nd doped ZnO NP's

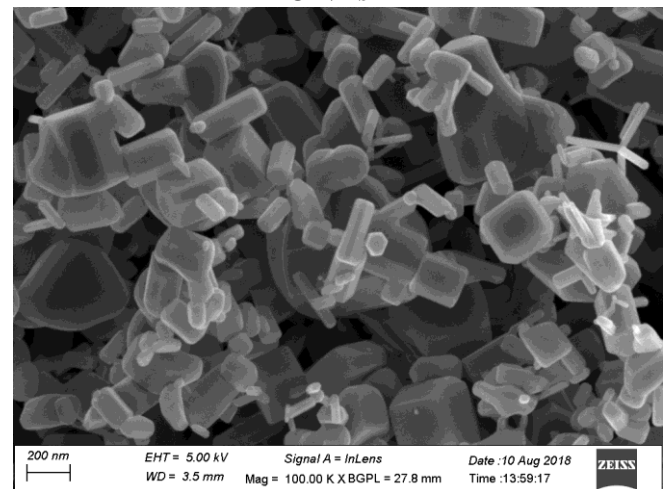


Fig 3a) FESEM image of Pure ZnO Nano Particles

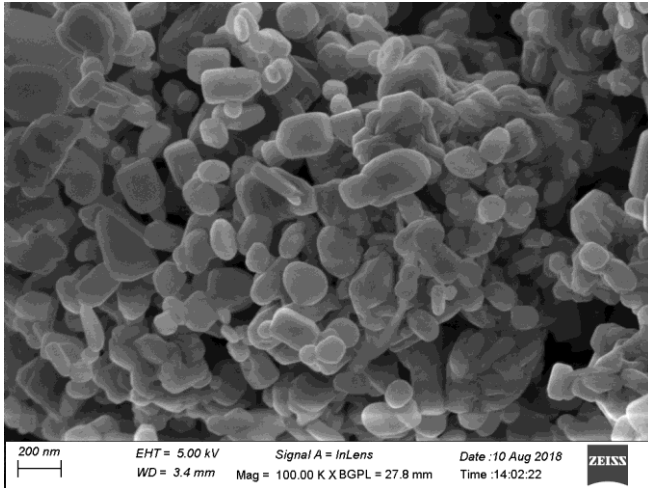


Fig 3b) FESEM image of ZnONd1 Nano Particles

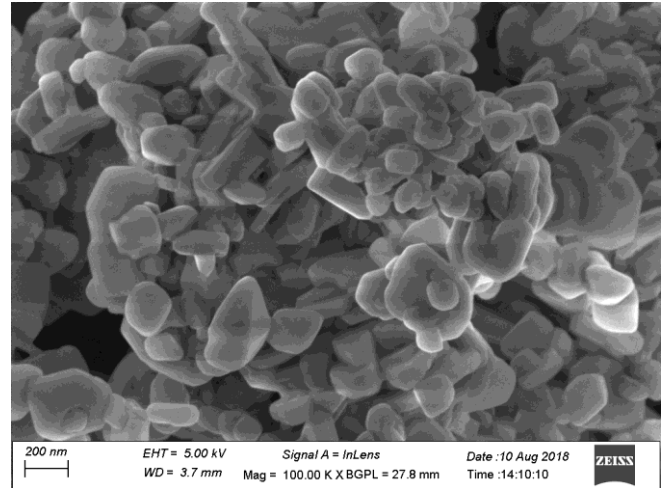


Fig 3e) FESEM image of ZnONd4 Nano Particles

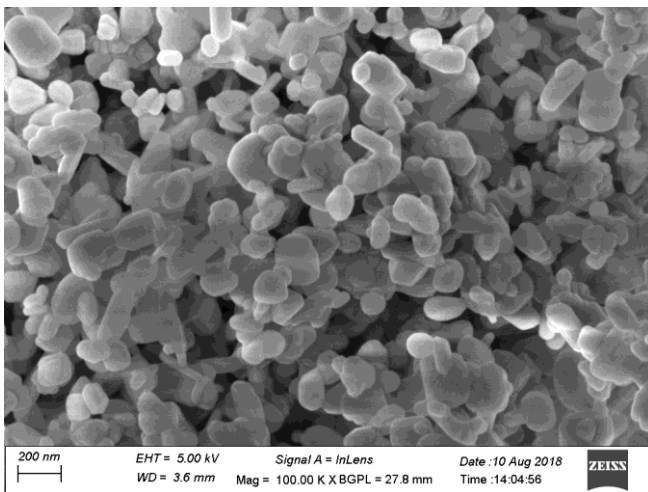


Fig 3c) FESEM image of ZnONd2 Nano Particles

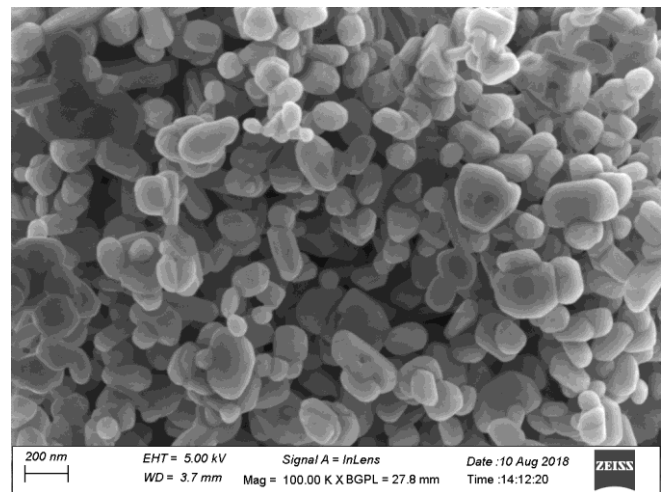


Fig 3f) FESEM image of ZnONd5 Nano Particles

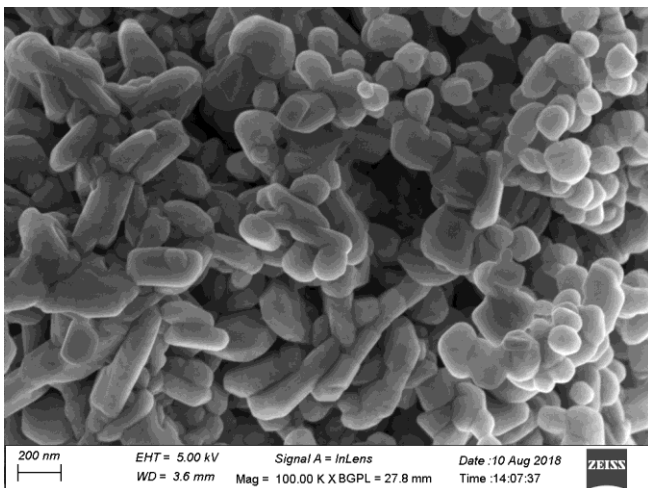


Fig 3d) FESEM image of ZnONd3 Nano Particles

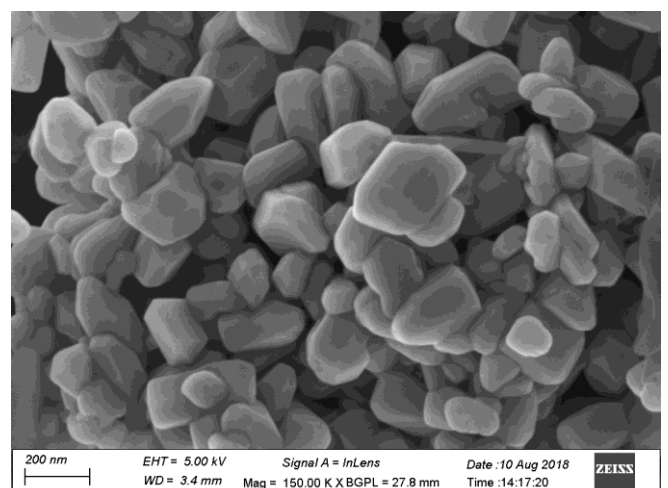


Fig 3g) FESEM image of ZnONd6 Nano Particles

TABLE 1 gives the values of lattice parameters 'a', 'c', X-Ray density, Crystallite size, Strain with varying Nd concentrations.

Nd Concentration (Wt %)	Sample name	Lattice Parameter a (°A)	Lattice Parameter c (°A)	X-Ray density (gm/cm ³)	Crystallite size D (nm)	Strain ε
X=0	Pure ZnO	3.254	5.209	16.97	51.89	0.0044
X=0.01	ZnONd1	3.245	5.193	17.33	35.15	0.0065
X=0.03	ZnONd2	3.233	5.202	17.77	33.76	0.0068
X=0.05	ZnONd3	3.250	5.200	17.92	41.82	0.0055
X=0.07	ZnONd4	3.253	5.199	18.23	41.62	0.0055
X=0.09	ZnONd5	3.243	5.190	18.70	39.47	0.0058
X=0.1	ZnONd6	3.236	5.181	18.98	36.39	0.0063

E.

Photoluminescence of the pure and Nd doped NP's was analyzed by exciting wave length of 280 nm .Fig 6 shows photoluminescence spectra of pure and Nd doped ZnO NP's. All the particles show strong emission in visible region at 565 nm. This green deep-level emission is attributed to the vacancies of zinc and oxygen, zinc interstitials in the crystal

V CONCLUSIONS

Pure ZnO and Neodymium doped ZnO NP's have been prepared by Co -Precipitation method. XRD analysis reveal the crystalline nature of doped ZnO NP's. The crystallite size of Nd doped decreased compared to pure ZnO NP's. FESEM pictures show the hexagonal wurzite structure. The grain size of Nd doped NP's increases as concentration increases. FT-IR analysis shows absorption peak at 453 cm⁻¹ corresponding to Zn-O stretching . Nd-O absorption peak is obtained at 858 cm⁻¹.DRS UV-VIS plot shows strong absorption peak at 365 nm Decrease in band gap with Nd doping shows that doped ZnO NP's can be used for photo degradation [1] and hence

acts good photocatalysts.PL graph shows peak at 565 nm in the visible region.

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