

# INVESTIGATE OPTICAL PROPERTIES OF PURE AND NI DOPED ZnO NANO PARTICLES

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## ABSTRACT

In this paper Pure and Ni doped Zinc oxide nano particles were synthesized by hydrothermal method using zinc acetate as a precursor and varying the dopant concentration ( $x = 0.02, 0.04, 0.06$ ) at 72 hours. The effects of dopant concentration, on the crystallite size, electrical property and absorption properties have been studied. The X-ray diffraction results confirm the formation of hexagonal wurtzite structure and crystallite size decreases with increasing dopant concentration. Optical property and bandgap values were calculated for the prepared samples using UV- Visible spectrophotometer.

## INTRODUCTION

In recent years, nanosized-inorganic semiconductor materials, such as TiO<sub>2</sub>, ZnO, ZnS, CdS, WO<sub>3</sub> have gained considerable research interest as photocatalyst. Zinc oxide (ZnO) is one of the most widely studied photocatalysts owing to its properties such as wide band gap energy (3.2 eV), large exciton binding energy of 60 meV [1], ability to absorb large range of solar spectrum, environmental friendliness, etc. However, the photocatalytic efficiency of ZnO gets affected to a great extent due to the rapid recombination of the generated charge carriers. Among the strategies for overcoming the limitation of charge carrier recombination, doping with transition metals is an effective way which will facilitate the efficient transportation and separation of electron-holes by introducing energy levels in between the conduction and valence band of the nanostructure [2-4]. For the last decades, there is an increased interest for zinc oxide (ZnO) because of their wide variety of applications. Zinc oxide is n-type semiconductor [5-6] which is considered as promising candidate for optical and optoelectronic applications in nanoscale devices [7-8]. It is used as a transparent electrode in solar cells [9], chemical and gas sensors [10], spintronic devices [11], and light emitting diodes [12]. In order to enhance the versatility of ZnO to meet the different requirements of application, structural modifications have usually been utilized, among which metal ion doping is well-known and the most effective approach [13-15]. ZnO is well-known as n-type

semiconductor where its electrical conductivity is due to the excess of zinc interstitial position [16]. Doping with various amount of Ni not only enhances electron-hole pair separation by decrease the band gap to make advantages of shifting the absorption to the visible light spectrum, but also decrease the average grain size [17,18]. In this study we have used Ni doping to improve optical property.

## EXPERIMENTAL PROCEDURE

### Materials used

Zinc acetate Zn (CH<sub>3</sub>CO<sub>2</sub>)<sub>2</sub> .2(H<sub>2</sub>O), Nickel-nitrate Ni(NO<sub>3</sub>)<sub>2</sub> .6(H<sub>2</sub>O), sodium hydroxide (NaOH) were procured from Loba-chemicals, Maharashtra, India. These chemical compounds were utilised in their original form, without any further purification.

### Synthesis of Nickel doped zinc oxide:

In this work, Pure zinc oxide and Nickel doped zinc oxide nanoparticles have been synthesized by Hydrothermal method using Zinc acetate as a precursor. Stoichiometric amounts of the metal precursor and dopant used to synthesize the nanoparticles. Zinc nitrate was diluted with 100 ml of distilled water and stirred to obtain homogenous solution. Then dopant were added varying concentration ( $X = 0.02, 0.04, 0.06$ ), the solution was stirred using magnetic stirrer upto dopant dissolved in the solution. Then NaOH solution were added drop by drop for maintain the pH. The solution was taken in a tefflon container and kept in a preheated oven maintained at 120 °C for 72 hours. The obtained powder was filtered using distilled water and

acetone and the sample was kept in oven for dried the sample. Finally obtained the powder grounded by using an agate mortar and pestle and at last, the final product of Zinc nickel oxide nanoparticles was obtained.

#### Results and Discussion:

Figure 1 shows the XRD patterns for the undoped and Ni doped ZnO samples with various doping concentration. Using X'Pert High Score plus software, the observed XRD patterns were indexed as hexagonal wurtzite structure of ZnO which are in good agreement with the ICDD Reference Pattern: zinc oxide, 01-079-2205. In the diffraction pattern of the doped samples, no additional peak corresponding to metal Ni and its oxides phases were observed which reveals that the Ni atoms successfully replaced the Zn atoms from the lattice sites of ZnO without disturbing the wurtzite structure of ZnO. The average grain size

of the Ni doped and undoped sample was calculated using

Debye-Scherrer formula  $D = \frac{0.9\lambda}{\beta \cos\theta}$ , where D is the grain size,

$\lambda = 1.5405 \text{ \AA}$  for Cu  $K\alpha$  radiation,  $\beta$  is the Full width at half maximum and  $\theta$  is the Bragg's diffraction angle. The grain size of the undoped sample is 40 nm which increases to 78 nm for  $x = 0.02$ . With increase in doping concentration, the grain size decreases for 57nm for  $x = 0.04$  to 53 nm for  $x = 0.06$ . This reduction in particle size with increasing Ni doping in ZnO is primarily due to lattice strain, inhibited grain growth, and altered nucleation dynamics induced by the incorporation of smaller  $Ni^{2+}$  ions into the ZnO crystal lattice.

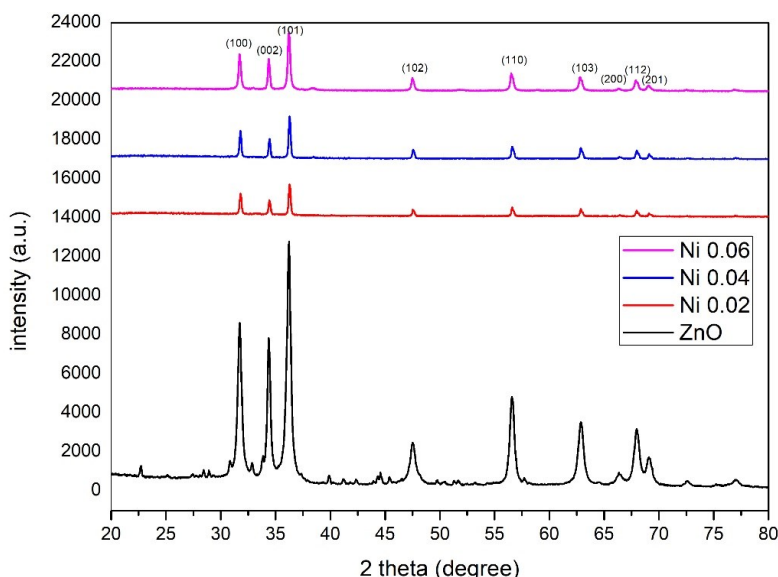


Figure. 1: XRD pattern of the pure ZnO and Ni doped ZnO

The optical characteristics of pure and Ni -doped ZnO nanoparticle become decreasingly prominent when particle size is pushed to the nanoscale. UV-visible spectroscopy has been used to comprehensively evaluate the optical properties of pure and Ni-doped ZnO nano particles. Since different dopants can produce different crystal defects in the ZnO crystal structure, the band gap of these compound semiconductor nanoparticles varies accordingly. Figure 2 depicts the UV-Visible transmission spectra of the pure and Ni-doped ZnO nanoparticles. The transmission spectra of the nanoparticles have been recorded over the wavelength range from 300 to 800 nm. The nano particles are found to be almost transparent to the radiations in the 400 to 800 nm wavelength range. When compared to pristine ZnO, the absorption edge of Ni-doped ZnO thin films exhibits

substantial blue shift. Because of the inclusion of Ni ions, the observed blue shift suggests a change in the band structure in Ni-doped ZnO films. Bandgap value for the nanoparticles having Ni content 0, 0.02, 0.04 and 0.06 is found to be 289, 264, 285 and 261 eV, respectively. Band gaps are observed to vary with an increase in concentration. The band structure might be caused by the sp-d exchange interaction between ZnO band electrons and localised d electrons associated with doped  $Ni^{2+}$  cation.[19]. The widening of the optical energy band gap and the blueshift of the absorption edge can also be attributed to an increase in carrier concentration and are explained in theory by the Moss-Burstein band filling phenomena, which is commonly observed in n type semiconductors. [20,21].

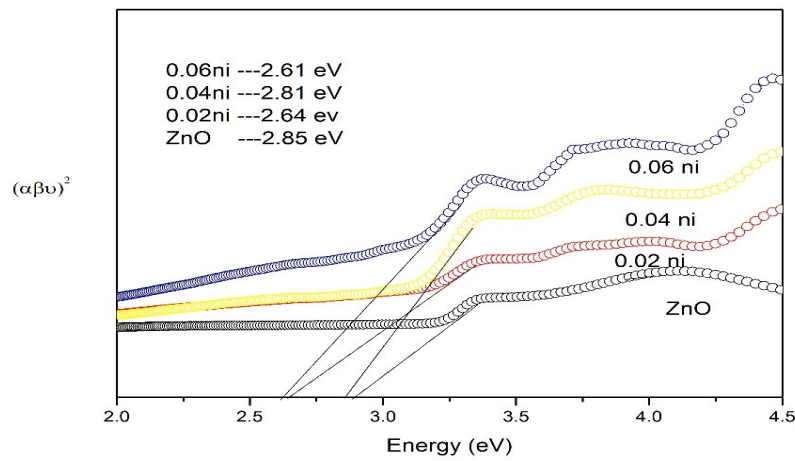


Figure. 2: Tauc plot of pure and Ni doped ZnO

From PL investigations on pure ZnO and  $\text{Zn}_{(1-x)}\text{Ni}_x\text{O}$  samples to study their relationships between oxygen defects and optical property. Fig. 3 shows PL spectra of pure ZnO and  $\text{Zn}_{1-x}\text{Ni}_x\text{O}$  ( $x = 0.02, 0.04, 0.06$ ) samples. All emission spectra are banded spectra, with one violet band (peaking at 465 - 467 nm) and one broader weaker green band (peaking around 530-550 nm) and occur the yellow emission (peaking around 550 nm) increasing the doping concentration of nickel ( $x = 0.04, 0.06$ ). The violet emission is band-edge exciton transition, whose luminescence intensity is determined by crystalline quality. We can see from Fig. 3 that the violet emission intensity decrease with Ni doping concentration, suggesting the crystal quality becomes worse which is consistent with the XRD results. [22] It is also noted that ZnO is a N-type material which easily absorbs oxygen on surface. This absorbed oxygen captures electron to become oxygen ion to form electron depletion layer on ZnO surface. The surface band

bends to separate photo-generated electron-hole pairs and decrease their recombination rate, therefore, the violet emission is reduced [23,24]. The mechanism of visible light is generally believed to be generated by deep level defects. Different defects in ZnO like Zn vacancy ( $\text{V}_{\text{Zn}}$ ), O vacancy ( $\text{V}_{\text{O}}$ ), Zn interstitial ( $\text{Zn}_i$ ), O interstitial ( $\text{O}_i$ ), and anti-site O ( $\text{O}_{\text{Zn}}$ ) can all lead to green emission, but which one is dominant is always under dispute. However, it is generally believed that O vacancy ( $\text{V}_{\text{O}}$ ) is the main reason for green emission [25]. It is proposed, for example, the green emission come from the composite transition of O vacancy and valance band holes, the transition of O vacancy and Zn vacancy, etc. As shown in Fig. 3, the green emission intensity increases significantly when Ni doping concentration is increased. This is most likely caused by O vacancy.

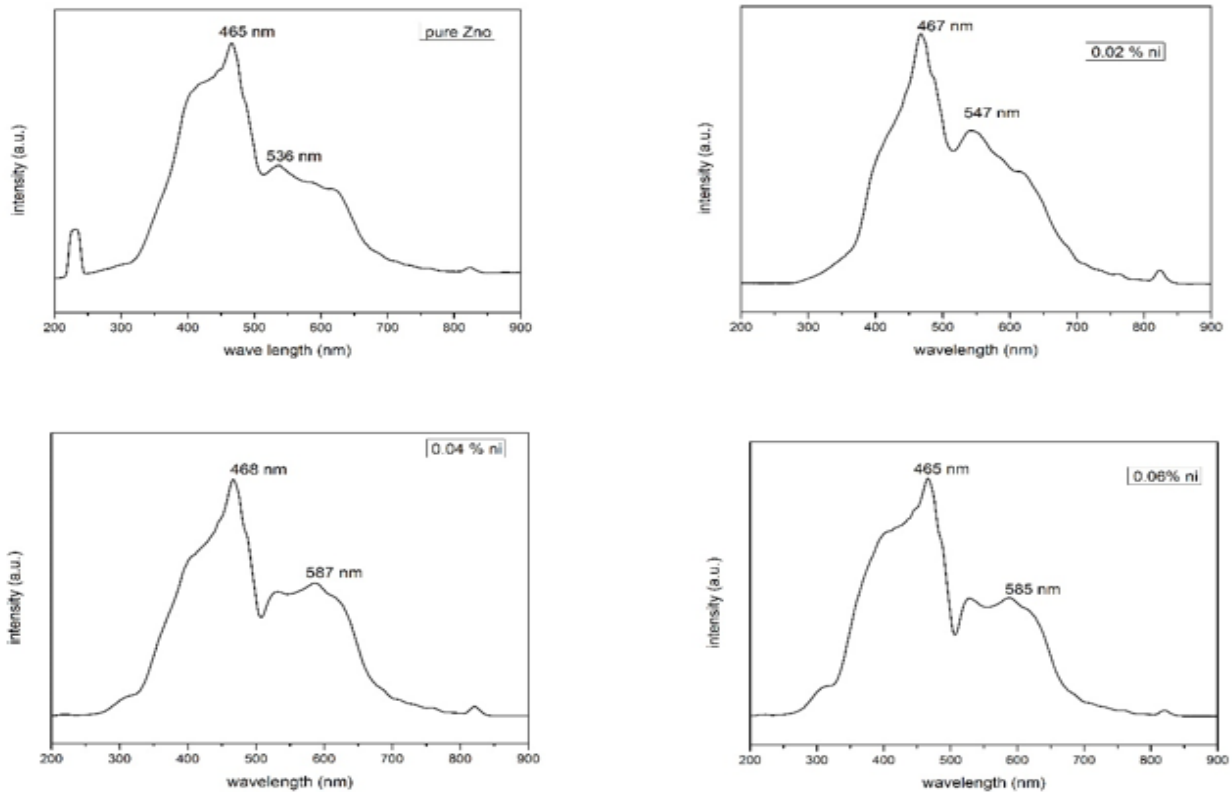


Figure.3: PL spectra of pure and Ni doped ZnO nanoparticles

## CONCLUSION

Pure ZnO and Nickel doped zinc oxide nano particle were synthesized by Hydrothermal technique. The average D-size was found and lattice Strain, nucleation growth modified with increasing doping concentration of Nickel. UV-VIS spectroscopy showed, The optical band gap of Ni-doped ZnO varies from 2.85 eV to 2.61 eV with various Ni doping concentration, indicating band gap narrowing due to dopant-induced defect states. Photoluminescence (PL) spectra of Ni-doped ZnO show prominent emission peaks around 460 nm, 540 nm, and 580 nm, which correspond to blue, green, and yellow-orange emissions, respectively. These emissions arise from various intrinsic and Ni-induced defects such as zinc interstitials, oxygen vacancies, and oxygen interstitials. The incorporation of Ni modified the defect landscape of ZnO, enhancing deep-level emissions and modifying its optical properties.

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