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Study of Structural and Optical Properties of ZnO Doped with Aluminum for Solar Cell Applications

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Abstract

Zinc oxide (ZnO) nanoparticles were doped with aluminum (Al) in the ratio (Al: ZnO) from 0 to 10% and synthesized using the co-precipitation technique. The synthesized nanoparticles of ZnO have shown a wurtzite structure. The crystallite sizes of nanoparticles of ZnO and ZnO doped with Al, were found with the help of Scherrer's equation. With an increase in Al concentration doping, there is a reduction in the nanoparticle's average crystallite size. The synthesized nanoparticles were further characterized by using X-ray diffraction (XRD), ultraviolet-visible (UV-Vis) spectroscopy, and Fourier transform infrared (FTIR). The UV-Vis spectrum results of prepared nanoparticles have shown absorption values in the visible range (200 Hz - 800 Hz). Also, as the doping concentration increased, a remarkable increase in the optical band gap was observed.

Keywords

Nanoparticles, Fourier transform infrared, Optical materials and properties

Introduction

Energy plays a vital role in human existence and modern living. Energy can be found in many resources, the most common being electrical and thermal energy. Fossil fuels being a finite resource, can generate a large amount of electricity and is available in plenty. But the carbon dioxide emitted while burning fuels causes global warming. As these are non-renewable resources, we need a renewable energy resource, which produces diverse applications. Sunlight is the richest available carbon-neutral source of energy. The material to be used in solar cell must have a band gap above 1.8 eV, high optical absorption, and high electrical conductivity. One such material is silicon. Over recent years, as the cost of single-crystal silicon and polycrystalline silicon has increased, researchers are focusing on new materials with better optical and as well as, electrical properties.

ZnO is a semiconductor having many applications in optoelectronics like, solar energy conversion, photocatalysis, gas sensors, and light emitting diode, having a wide band gap of ~ 3.37 eV [1, 2]. ZnO exhibits three crystalline structures, namely cubic zinc blend, rock salt, and hexagonal wurtzite. The most stable crystal structure at room temperature is hexagonal wurtzite. ZnO has a large energy band gap and is transparent to visible light (400 - 700 nm) [3]. ZnO has many applications owing to its optical, acoustic, and electrical properties and they further enhance by doping with group III elements like Al, Ga, Mn, In, and B. Among these, Al doping remarkably enhances both electrical as well as optical properties [4].

Synthesis of ZnO nanoparticles doped with Al, can be done by sol-gel [5], hydrothermal [6], chemical bath deposition, combustion [7], co-precipitation

[8], and spray pyrolysis [9]. Among these, synthesis using co-precipitation was found to be more economical and easier.

Influenced by the findings from the literature survey, the present research was focused on enhancing the structural and optical properties of ZnO nanoparticles doped using Al concentrations, synthesized using co-precipitation technique, and the end products were characterized via XRD, FTIR, and UV-Vis spectroscopy methods, useful in solar cell applications.

Experimentation

Pure ZnO nanoparticles that were doped with Al concentrations, were synthesized by co-precipitation technique, at ambient temperature for different concentrations (0.01, 0.03, 0.05, 0.07, 0.09, and 0.1 moles %), the samples were renamed as ZnO, ZA01, ZA03, ZA05, ZA07, ZA09, ZA1. According to the stoichiometric ratio, to prepare 5 g of ZnO, 18 g of zinc nitrate is dissolved in 100 ml of deionized water and then stirred for 1 h using a magnetic stirrer to get a homogeneous solution. To prepare ZnO nanopowder, NaOH solution (30 g of NaOH sample, dissolved in 100 ml deionized water) was added drop by drop until the pH level reaches 12, and then precipitates. This precipitate was aged for 24 h, filtered, and then dried at 500 °C for about 24 h in an oven. Then, calcination was done at 7000 °C for 3 h. Finally, nanoparticles are formed. The same procedure is followed for all ZnO nanoparticles that were doped with Al.

Results and Discussion

From figure 1 all the XRD patterns of ZnO samples that were doped with Al, were found to exhibit hexagonal wurtzite structure. Moreover, the hexagonal-wurtzite structure shows no change after doping with Al [10], and no additional peaks were seen [11]. Furthermore, the 2θ values belonging to the most intense peak were not altered with the Al concentration. The lattice parameters were found by Powder X software and the average crystallite sizes of the prepared samples were estimated using Scherrer's equation (Equation 1) [12]. The variations observed in the XRD patterns were because of the differences in valence charges and the radius of Al^{3+} (0.53 Å) and Zn^{2+} (0.74 Å) ions. The lattice constants decrease as Al^{3+} ions are relatively smaller than Zn^{2+} ions [13-15].

$$D = k\lambda/(\beta\cos\theta) \quad (1)$$

Where 'D' is the average crystallite size, 'θ' is the Bragg angle, 'λ' is the wavelength, 'β' is the full width at the half maximum of the diffraction peak, and 'k' is a constant.

Table 1 illustrates the optical and micro-structural data of ZnO and ZnO nanostructures doped with Al, estimated by the Scherrer equation (Equation 1), assuming a 2θ value ~ 47° for the blended oxides. It is seen that the average crystallite sizes diminish from 79 nm to 54 nm with an increase in Al^{3+} content up to 1 mole % [16]. Hence, it is evident that the doping was done successfully, owing to the substitution of Al^{3+} ions with Zn^{2+} ions in the lattice crystalline structure of ZnO, which caused a decrease in the lattice parameter, and hence a decrease in the average crystallite size [17].

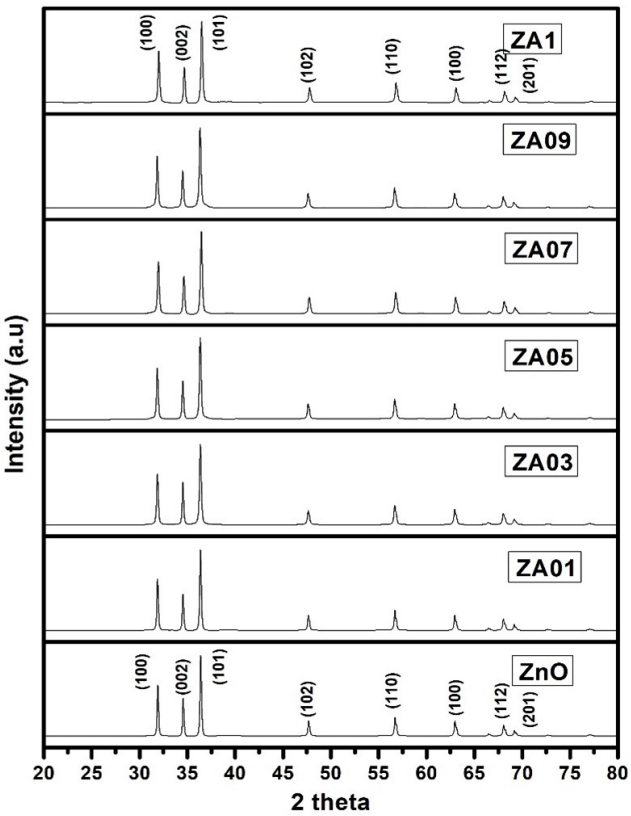

Figure 1: XRD patterns showing ZnO and ZnO nanoparticles doped with Al.

Table 1: Structural and optical data of ZnO and ZnO nanoparticles doped with Al.

Sample	Crystallite size (nm)	Lattice parameter, a (Å)	Lattice parameter, c (Å)	Energy band gap, E_g (eV)
ZnO	79	3.2353	5.6037	3.07
ZA01	72	3.2381	5.6085	3.109
ZA03	68	3.2394	5.6108	3.11
ZA05	63	3.2405	5.6127	3.139
ZA07	59	3.2298	5.5941	3.152
ZA09	57	3.2415	5.6144	3.165
ZA1	54	3.2249	5.5858	3.178

ZnO nanoparticles doped with Al samples were supported by FTIR results, at room temperature in the region 4000 - 400 cm^{-1} and the exhibited FTIR characteristics peaks of ZnO doped with Al at different concentrations of Al (0.01, 0.03, 0.05, 0.07, 0.09, and 0.1 moles %) are shown in figure 2, to study the functional groups existing in the prepared samples. The broad absorption in frequency bands was observed between 3417 and 3479 cm^{-1}, corresponding to the O-H group. The stretching vibrations indicate the existence of H_2O over the surface of the samples. The Zn-O stretching vibration band, confirms the ZnO hexagonal-wurtzite structure formation and relates to the band near 500 cm^{-1} in figure 2 [18]. The bands around 2350 cm^{-1} and 1445 cm^{-1} correspond to CO_2, absorbed by metal cations contained in the atmosphere. The band, Al-O can be seen near 683 cm^{-1}. The swing in the bands of doped samples can be attributed due to the crystal agitation created by Al atoms into the crystalline lattice sites. The band at 445 cm^{-1}, which pertains to the Zn-O bond, is observed in

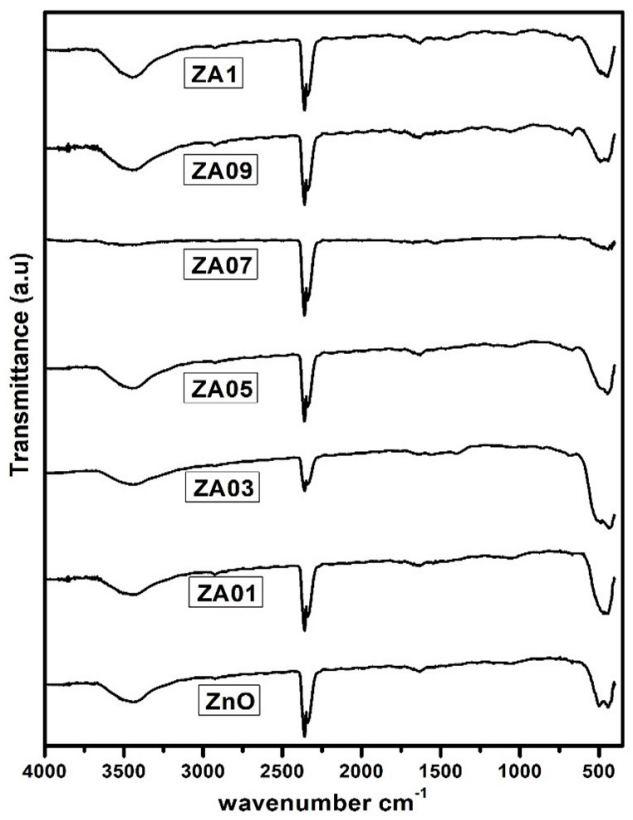

Figure 2: FTIR spectra of ZnO and ZnO nanoparticles doped with Al.

all the samples. The bands with weak intensity near 960 cm^{-1} and a sharp and strong intensity at 1122 cm^{-1} are found to enhance the intensity with Al doping. They belong to Al-O stretching vibrations.

Figure 3a shows the optical absorption spectra of pure ZnO nanostructures doped with Al, in the wavelength range of 200 nm - 800 nm. It was observed that the absorbance values increase with Al concentration. By applying Tauc's equation 2, the optical band gap of the nanopowders was estimated.

$$(h\alpha v)^2 = B(hv - E_g) \quad (2)$$

Where, 'α' is the coefficient of absorbance (α = 2.303A/t, 'A' is the absorbance, and 't' is cuvette thickness), 'B' is a constant, 'h' is Planck's constant, 'v' is the frequency of the photon, and 'E_g' is the optical band gap.

Owing to the nature of the electronic transition accountable for absorption, the value of 'n' can be 1/2, 3/2, 2, or 3 (n = 2 for direct band gap). The plot of $(h\alpha v)^2$ on the Y-axis vs photon energy (hν) on the X-axis gives the value of the optical band gap (E_g) as shown in figure 3b and tabulated in table 1 for all samples.

As Al concentration increases from 0% to 10 % the energy band gap increases from 3.07 eV to 3.178 eV, which shows the doping of Al changes the band structure of ZnO. According to quantum confinement, E_g increases with a decrease in crystallite size. However, it is not only due to quantum confinement, but the dopant may also cause a change in lattice symmetry and produce defects in the lattice which lead to a change in the optical band gap [18-20]. As the band gap of Al_2O_3 (bulk band

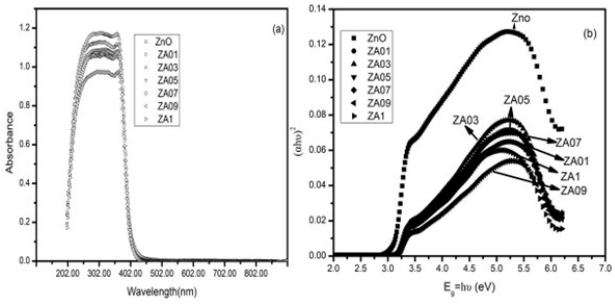

Figure 3: (a) Optical absorption spectra and **(b)** $(h\alpha v)^2$ vs $h\nu$ curves showing band gaps of pure ZnO and ZnO doped with Al.

gap is 6.4 eV) was higher than that of ZnO (bulk 3.37 eV), as per the Burstein-Moss effect, as Al concentration increases, the band gap increases.

Conclusion

ZnO nanopowders doped with different concentrations of Al have been prepared by the co-precipitation method at room temperature. The structural and optical properties of ZnO powders doped with Al were investigated and formed a pure hexagonal-wurtzite structure. The optical band gap was also enhanced with Al concentration. The present work is well suited for optoelectronic devices, such as solar cells.

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Conflict of Interest

There are no known conflicts of interest in person or financial..

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