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Williamson-Hall analysis of ZnO and Mg doped ZnO nanoparticles prepared via *Psidium guajava* leaf extract

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Abstract

ZnO and Mg doped ZnO nanoparticles (NPs) were synthesized by green method using *Psidium guajava* leaf extract. X-ray power diffraction studies confirmed that**,** synthesized nanoparticles were retained the wurtzite hexagonal structure. In addition, the crystallite development in nanostructured ZnO and Mg doped ZnO NPs by X-ray peak broadening analysis. The individual contributions of small crystallite sizes and lattice strain to the peak broadening in pure and Mg doped ZnO NPs were studied using Williamson-Hall (W-H) analysis.

Keywords: ZnO, Mg doped ZnO, Williamson-Hall, Lattice strain.

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Introduction

The optical and electrical properties of the ZnO NPs are depends on the band gap. The band gap can be modified by doping some larger band gap materials [1].

A perfect crystal would spread enormously in all directions; therefore, no crystals are perfect due to their finite size. This deviation from perfect crystallinity leads to a broadening of diffraction peaks. The two main properties extracted from peak width analysis are the crystallite size and lattice strain. The crystallite size is an amount of the size of coherently diffracting domains. The crystallite size of the particles is normally not the same as the particle size due to the creation of polycrystalline aggregates [2].

To estimate the particles size using X-ray powder diffraction measurements, the Scherer's formula is the simplest method to calculate

crystallite size, and is applicable only when there is no strain in the materials.

In present work, the average particle size of ZnO and Mg doped ZnO NPs are compared. In addition, we studied the strain of the synthesized NPs by the analytical method such as Williamson–Hall (W-H) analysis and Cyclic voltammetry characterization was carried out to study the qualitative information about the potentials at which electrochemical reactions occur.

Experimental methods

Synthesis of ZnO and Mg doped ZnO NPs was carried out using analytical grade. Zinc (II) nitrate hexahydrate (Zn $(NO_3)_2 \cdot 6H_2O$) and Magnesium nitrate hexahydrate (Mg $(NO_3)_2 \cdot 6H_2O$), were used as the precursors without further purification. The synthesis methodology was reported in our earlier paper [3].

Characterization Techniques

The ZnO and Mg doped ZnO NPs were characterized by X-ray diffractometer (model: X'PERT PRO PANalytical). The diffraction patterns were recorded in the range of 20°–80° for the ZnO samples where the monochromatic wavelength of 1.54 Å was used.

The samples were analyzed by Field Emission Scanning Electron Microscopy (Carl Zeiss Ultra 55 FESEM) with EDAX (model: Inca). The morphology of the synthesized NiO NPs was examined using HRTEM (Model: Tecnai F20). The FT-IR spectra were recorded in the range of 400–4000 cm−1 by using Perkin–Elmer spectrometer. Photoluminescence measurement was carried out on a luminescence spectrophotometer (PerkinElmer LS-5513, Perkin Elmer Instrument, USA) using xenon lamp as the excitation source at room temperature [3].

Results and discussion

The XRD pattern d-spacing of ZnO and Mg doped ZnO NPs for the corresponding diffraction peaks are well oriented with the JCPDS Card No: 79-2205[3].

The micro-strain the breadth of the Bragg peak is a combination of both instrument and sample-dependent effects. To decouple these contributions, it is necessary to collect a diffraction pattern from the line broadening of a standard material such as silicon to determine the instrumental broadening. The instrument-corrected broadening βhkl [4] can be represented by:

$$\beta hkl=[\beta hkl^2 measured-\beta hkl^2 instrumental]^{1/2} \text{----(1)}$$

The particle grain size of ZnO and Mg doped ZnO NPs are determined by the X-ray line broadening method using the Scherrer's equation,

$$D = k\lambda/\beta\ (D\cos\theta) \text{ ---------} \quad (2)$$

where D-is the size in nanometers, λ is the wavelength of the radiation (1.5406Å for CuKα), k is a constant (0.94), βD-is the peak width at half-maximum intensity and θ is the peak position. The ZnO and Mg doped ZnO NPs average particle sizes are 42 nm and 33 nm respectively [3]. The Mg doped ZnO NPs particle size decrease as compared to that of ZnO NPs, the reduction in the particle size

is mainly due to the distortion in the host ZnO lattice by Mg^{2+} ion, which decrease the nucleation and subsequent growth rate of the ZnO NPs.

The strain-induced broadening βε is given by the Wilson formula βε = 4εtanθ, where ε is the root mean square value of the micro-strain. Assuming that the particles size and strain contributing to the line broadening and independent of each other and both have a Cauchy like profile, the observed line width is simply the sum of these two, i.e., βhkl = (kλ / Dcos θ) + 4εtan θ, which becomes as

Bhkl cosθ = (kλ/D) + 4εsin θ ------ (3)

When plotting the Williamson-Hall (W-H) equation between 4sinθ Vs β cosθ the slope of the line is the strain ε. Figures 1 (a) and Figure 1(b) show the plots of Williamson-Hall equation for ZnO and and Mg doped ZnO NPs samples. From the Table 1 calculated strain values are 0.00132 and 0.00293 for ZnO and and Mg doped ZnO NPs respectively. The strain of Mg doped ZnO NPs increased as compared to that of the ZnO NPs, which is due to the relaxation of the strain in the respective unit cells. These effects change the size and shape of the particles.

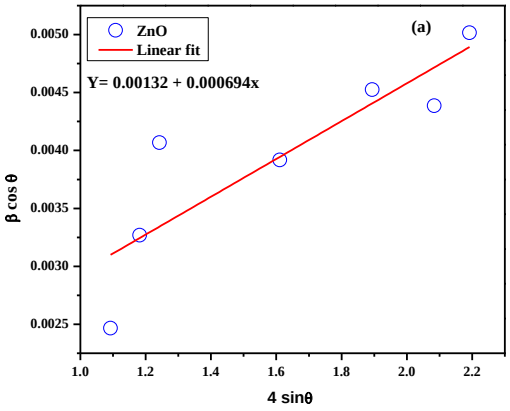

Figure 1(a) The Williamson-Hall of ZnO NPs

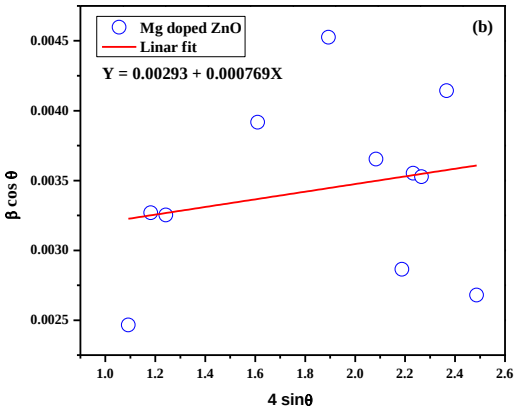

Figure 1(b) The Williamson-Hall of Mg doped ZnO NPs.

Table 1 X-ray diffraction parameter values of the pure ZnO and Mg-doped ZnO NPs.

Sample	Lattice Parameter values (Å)		Atomic Packing factor (c/a)	Volume V $(Å)^3$	Position parameter (u)	Bond length Zn-O L (Å)	Average Crystallite size D (nm)	Strain
	a	c						
ZnO	3.2598	5.2199	1.6012	48.0354	0.3799	1.9836	42	0.00132
ZnO:Mg	3.2585	5.2177	1.6054	47.9769	0.3800	1.9927	33	0.00293

Conclusions

The ZnO NPs and Mg doped ZnO NPs synthesized by *Psidium guajava* leaf extract. The X-ray diffraction study confirmed that the prepared ZnO and Mg doped ZnO NPs were of the hexagonal wurtize structure. The line broadening analysis of ZnO and Mg doped ZnO NPs were done by W-H method. The results showed that lattice strain inversely proportional to the crystallite size.

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