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Investigation of the effect of Ni Doping on the Structural, Luminescence, Optical and Electronic Properties of ZnO Nanopowders

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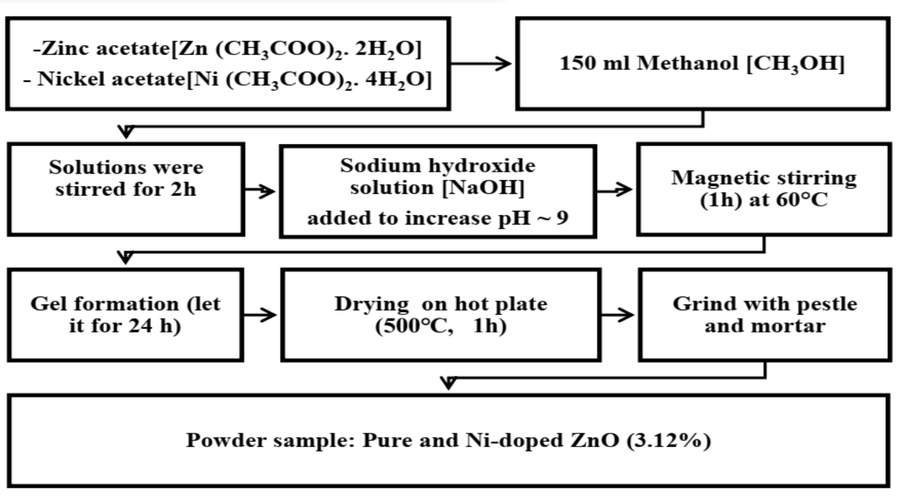
Abstract: In this Study, pure and Ni-doped ZnO nanoparticles (NPs) with concentration of Ni (3.12%) were successfully prepared by using co-precipitation method [1]. Among TM, nickel is very significant element which has a similar ionic radius as that of Zn. Literature studies show that Ni doping into ZnO matrix can enhance its various properties [2, 3]. Zinc acetate dihydrate [Zn (CH3COO)2 2H2O], nickel acetate dihydrate [Ni (CH3COO)2 2H2O] and sodium hydroxide solution [NaOH] were used as precursors. For getting homogeneous solution, stoichiometric amount of zinc and nickel acetate were dissolved in methanol, after stirred continuously on a magnetic stirrer at room temperature. For raising the pH of the obtained solution to ~9, small amount of sodium hydroxide solution [NaOH] was added drop by drop. The precursor solution is then stirred again until the liquid solution turns into a gel. After gel formation, the beaker was transferred on the hot plate at 500°C for 1h. The obtained sample yield in the form of loose powder was then finely grounded by agate mortar and pestle. The prepared samples in powder form were characterized by X-ray diffraction spectroscopy (XRD), Scanning Electron Microscopy (SEM), Ultraviolet–visible spectroscopy (UV-Vis), Photoluminescence (PL) and Fourier transform infrared spectroscopy (FTIR). The obtained results have been discussed and compared with those from other sources whatever possible.

Experimental Details



Flowchart for the synthesis of pure ZnO and NZO NPs by co-precipitation method.

Structural Properties

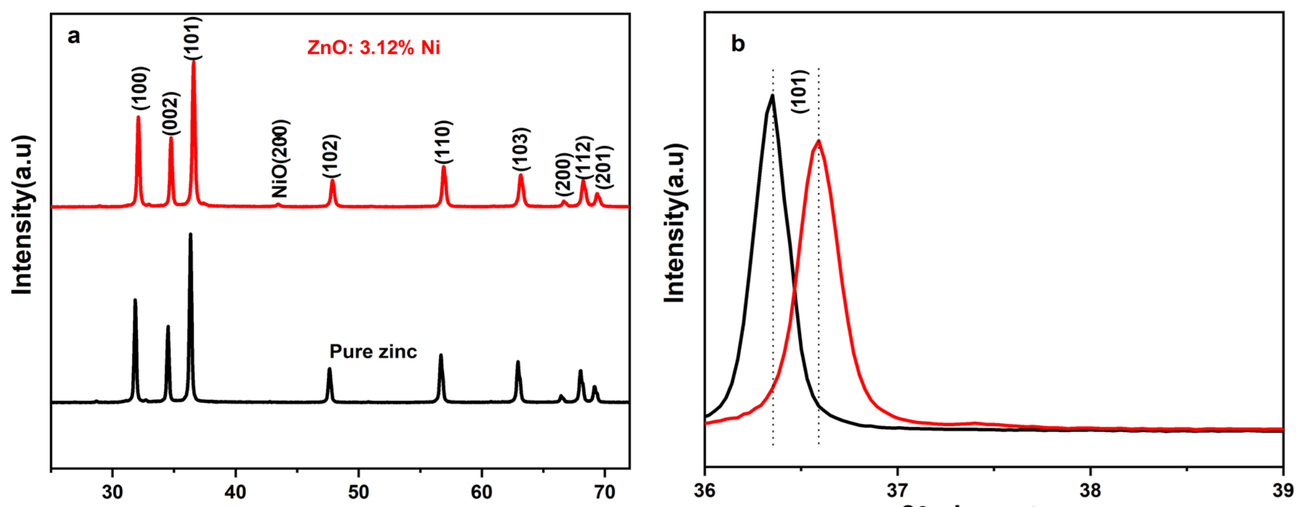


Fig 1: **(a)** XRD patterns, and **(b)** shift of main peak (101) of pure ZnO and NZO NPs (x = 3.12%).

	Structural parameter x(%)		Ref.
a (Å)	3.241, 0% 3.278, 0%	3.214, 3.12% 3.266, 3%	Present [1]
c (Å)	5.195, 0% 5.223, 0%	5.176, 3.12% 5.228, 5%	Present [1]
D (nm)	36.61 0%	29.17 6.25%	Present
ε x10^{-2}(%)	30.42, 0%	31.74, 3.12%	Present
δ x10^{-5}(nm^{-2})	74.61, 0%	99., 3.12%	Present

[1]: R. Gopalakrishnan et al

Table:Summary of the lattice parameters (a and b) calculated from the XRD pattern and those reported from literature for pure ZnO and NZO NPs. crystallite size (D), Strain (ε) and dislocation density (δ) are also included.

Morphological

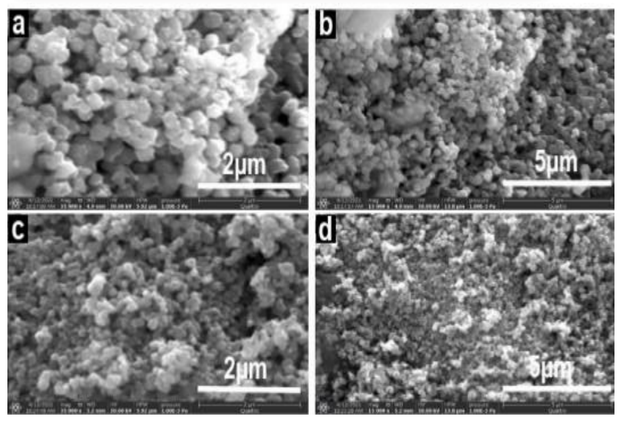


Fig 2: SEM images of pure ZnO and NZO NPS at two magnifications 35k and 15k; (a) 0% (35k), (b) 0% (15k), (c) 3.12% (35k), (d) 3.12% .

FTIR

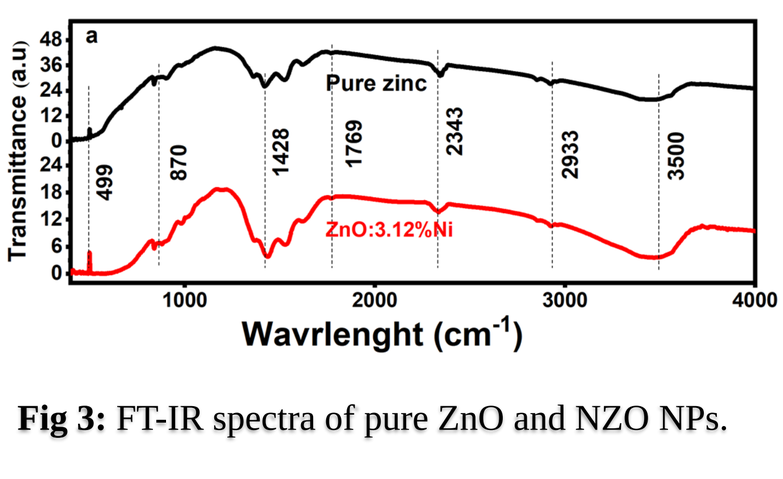


Fig 3: FT-IR spectra of pure ZnO and NZO NPs.

Optical Properties

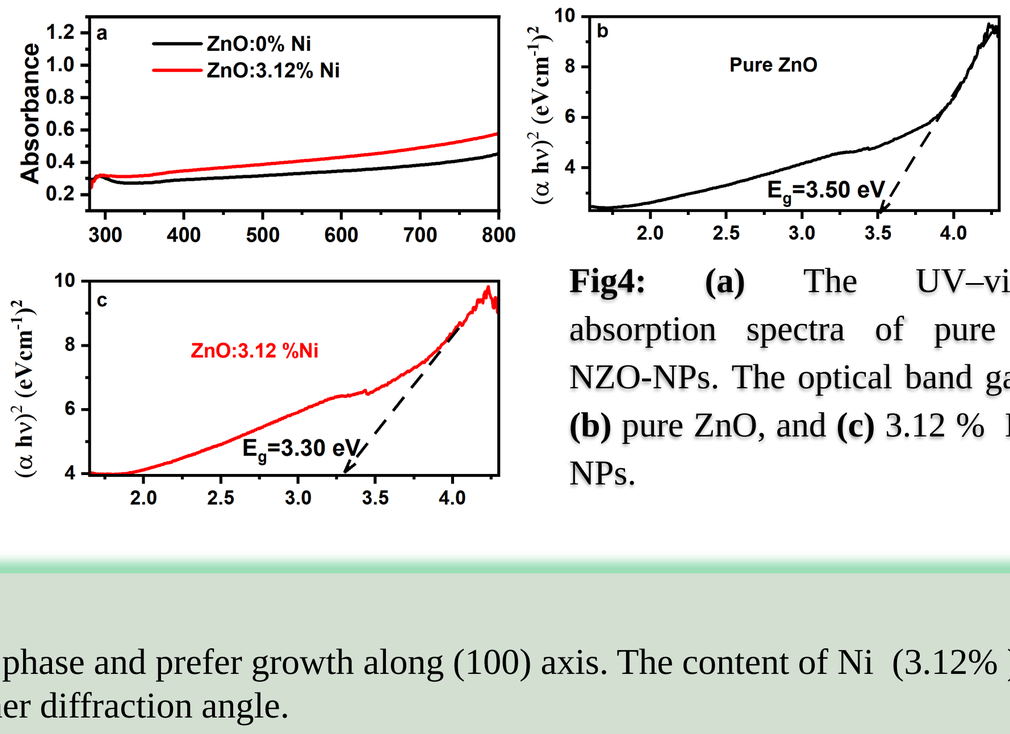


Fig4: (a) The UV–visible absorption spectra of pure and NZO-NPs. The optical band gap of **(b)** pure ZnO, and **(c)** 3.12 % NZO NPs.

Photoluminescence

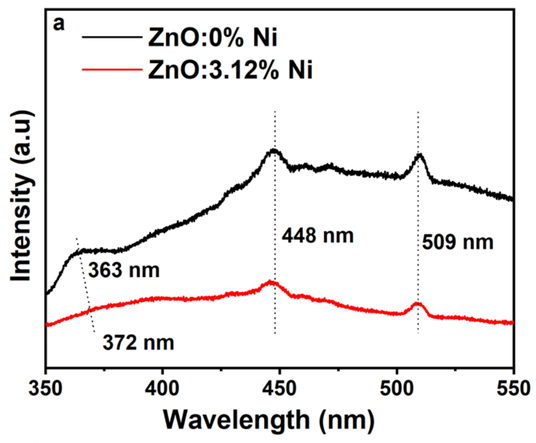


Fig 5:PL spectrum of pure ZnO and 3.12% NZO NPs.

Conclusion

✓All nanopowder samples exhibit a hexagonal wurtzite phase and prefer growth along (100) axis. The content of Ni (3.12%) leads to the formation of NiO secondary phase and the shifting of characteristic peak toward higher diffraction angle.

✓The crystallite size exhibits an inverse trend to that of the strain and dislocation density for NZO NPs (3.12%) Compared to Pure ZnO. Densely packed spherical-like-shaped structures with the agglomeration of nanoparticles are observed for Pure ZnO some nanorod-like-shaped structures start to appear when doped by Ni.

✓The absorption edge shifts to higher wavelengths (red shift) implying a decrease in the optical band gap from 3.50 eV to 3.30 eV by increasing of Ni defects in ZnO NPs. This leads to the stretching vibration of the Zn-O bond (497 cm-1).