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Structural properties of Sb, Al, Mg and Cd doped ZnO

Physics

KEYWORDS:XRD, Raman spectroscopy, PLD

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ABSTRACT

Raman and X-ray diffraction spectroscopy were used to study the structural and vibrational properties of Sb, Al, Mg and Cd doped ZnO pallets prepared by solid state reaction route. Sb and Al doping were used to form p-type and n-type ZnO pallets, respectively. Whereas Cd and Mg doping was used to decrease and increase the optical band gap energy of ZnO. Raman spectra reveled that A1, B1, E1 and E2 modes were obtained in all pallets, whereas shift in peak positions and intensity was observed with various doping. Full width half maxima of X-Ray Diffraction (XRD) peaks also explains wurtzite crystalline symmetry.

INTRODUCTION

III-Nitride materials have been commonly used by researchers, due to its high mobility, wide and direct band gap and high electron saturation velocity [1-2]. GaN based quantum well devices are high reliable, stable and energy efficient [3]. Auger recombination, polarization charges/field (lattice mismatch), non uniform distribution of hole in quantum well, junction heating and electron overflow over active layers are some problems faced by researchers in InGaN/GaN quantum well devices [4]. The major problem, which limits the InGaN/GaN quantum well devices are, growth conditions and cost effective, so an alternate semiconductor is required. ZnO can be used as an alternative due to its large and wide band gap, good transparency, high electron mobility, strong room-temperature luminescence, non toxicity, easy to grow, similar hexagonal wurtzite crystal structure as that of GaN [5]. For material science applications, zinc oxide has high refractive index, binding, high thermal conductivity, UV-protection properties, high exciton binding energy (~ 60 meV) than GaN (~25 meV) at room temperature which makes it suitable candidate for quantum well devices like solar cells, transparent conducting films, varistors, chemical sensors, laser diodes, light-emitting diodes etc [6-7]. ZnO shows n-type behavior due to oxygen vacancies or zinc interstitials. Now, we focus our attention on the requirement of optoelectronic device; quantum well, p-type behavior and n-type behavior of ZnO. Quantum wells are fabricated from Cd doping in ZnO, Sb doping can be used to check p-type behavior and Al doping can be used as n-type doping. Mg doped ZnO layer can be used as electron blocking layer to reduce electron overflow at higher current density [8-11]. For the same, we have used Cd, Mg, Al and Sb doping in ZnO and study the structural properties by XRD and Raman spectroscopy

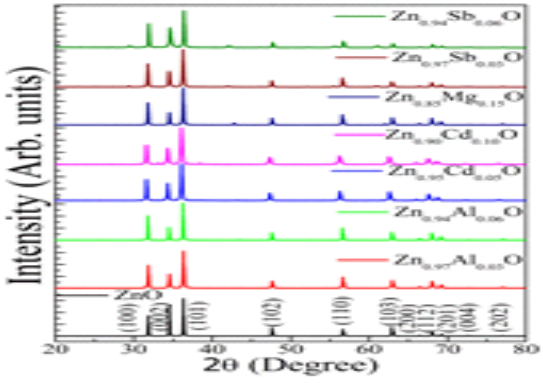


Figure 1: X-Ray Diffraction Pattern of undoped and doped samples

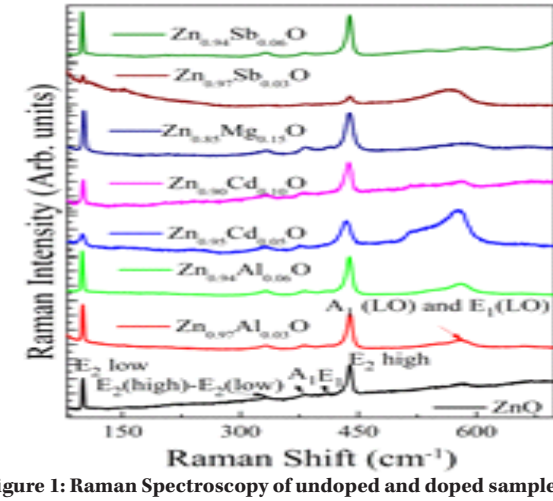


Figure 1: Raman Spectroscopy of undoped and doped samples

TABLE – 1 Lattice Parameter 'a' and 'c' of doped and undoped samples.

GENERAL DETAILS

Sample	a	c
ZnO	3.578	5.755
Cd 5	3.599	5.782
Cd 10	3.602	5.782
Al 3	3.579	5.749
Al 6	3.582	5.762
Sb 3	3.579	5.755
Sb 6	3.574	5.733
Mg 15	3.580	5.752

EXPERIMENTAL

Pallets of pure ZnO, 3 and 6 wt. % Sb doped ZnO, 3 and 6 wt. % Al doped ZnO, 5 and 10 wt. % Cd doped ZnO, 15 wt. % Mg doped ZnO were prepared by solid state reaction route. For the preparation of these pallets, first stoichiometric amount of powders were mixed and grinded for 2 hours. Initially the powder was heated at 500^{0}C for 12 hours (Calcination). Then the heated powder was grinded and mixed. After grinding and mixing, hydraulic pressure (1Tonn) was given for

preparation of pallets. Again pallets were heated at 1000^{o}C (sintering) for 24 hours, to remove the impurities. Diameter of pallets were 20 mm.

RESULT AND DISCUSSION

Structural analysis was performed by Bruker D8 Advance X-Ray diffractometer using -2 geometry with CuK radiation having wavelength 1.5406 A$^{\circ}$. XRD pattern of of pure ZnO, $Al_{0.03}Zn_{0.97}O$, $Al_{0.06}Zn_{0.94}O$, $Cd_{0.05}Zn_{0.95}O$, $Cd_{0.10}Zn_{0.90}O$, $Mg_{0.15}Zn_{0.85}O$, $Sb_{0.03}Zn_{0.97}O$ and $Sb_{0.06}Zn_{0.94}O$ pallets are shown in Fig. 1. From the XRD pattern peaks related to (100), (002), (101), (102), (110), (103), (112) and (201) planes are observed which indicate that the pallets are polycrystalline in nature. No peaks were observed as phases of aluminum, cadmium, magnesium and antimony clusters and impurities, which indicates that all the pallets are in single phase. Lattice parameter 'a' and 'c' are calculated using Bragg's law. Calculated value of lattice parameter 'a' and 'c' are listed in Table 1.

Micro-Raman scattering experiment was performed to study the vibrational properties of Cd, Mg, Al, Sb doped and undoped ZnO pallets. He-Ne laser was used for Raman scattering with spectral resolution of 4 cm^{-1} in wave-number range from 98 cm^{-1} to 800 cm^{-1}. The optical symmetry modes of

$$\Gamma = 1A_1\ (z,\ z^2,\ x^2+y^2) + 2B_1 + 1E_1\ (x,\ y,\ xz,\ yz) + 2E_2\ (x^2-y^2,\ xy) \quad (1)$$

where polar modes A_1 and E_1 are split into transverse optical phonon and longitudinal optical phonon. A_1 and E_1 are Raman and Infrared active modes [14]. In B_1 mode Raman and Infrared both are silent. E_2 modes are non-polar and Raman active modes. E_2 modes splits into E_2^{Low} and E_2^{High} [15]. Fig. 2 shows Raman spectra of pure ZnO, $Al_{0.03}Zn_{0.97}O$, $Al_{0.06}Zn_{0.94}O$, $Cd_{0.05}Zn_{0.95}O$, $Cd_{0.10}Zn_{0.90}O$, $Mg_{0.15}Zn_{0.85}O$, $Sb_{0.03}Zn_{0.97}O$ and $Sb_{0.06}Zn_{0.94}O$ pallets. E_2^{Low} mode at 99 cm^{-1} corresponds to vibration of the heavy Zn sub-lattice, whereas into E_2^{Low} and E_2^{High} mode were present in all pallets but intensity varies with various doping. 3% Sb doping and 5% Cd doping in ZnO reduces the intensity of ZnO. A second order frequency E_2^{High}-E_2^{Low} mode occurs at ~335 cm^{-1} in all pallets. Features at ~380 and ~415 cm^{-1} frequency represents A1 (TO) and E1 (TO) modes, respectively [17]. A1-LO mode and E1-LO vibration modes occurs at 574 cm^{-1} frequency and this is mainly due to crystal disorder when peaks were shifted at different frequency in all pallets. These peaks are usually present due to the structural or doping induced disorder in the ZnO substrate. Fig. 2 explains that with $Cd_{0.05}Zn_{0.95}O$, $Cd_{0.10}Zn_{0.90}O$, $Al_{0.03}Zn_{0.97}O$, $Sb_{0.03}Zn_{0.97}O$ and $Mg_{0.15}Zn_{0.85}O$ doping in pure ZnO, wurtzite crystalline symmetry was maintained and no structural deformation occurs.

CONCLUSIONS

In summary, we have studied the structural properties of undoped and doped ZnO pallets using XRD and Raman spectroscopy. XRD pattern explains polycrystalline nature of undoped and doped pallets. Lattice parameter 'a' and 'c' shifts with various doping, but shift is very small. All samples are in single phase. Shift in Raman modes has been observed with various doping in ZnO, but shift is very small and wurtzite crystalline symmetry was maintained.

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