Scientific Journal of Impact Factor (SJIF): 4.72

e-ISSN : 2348-4470
p-ISSN : 2348-6406

International Journal of Advance Engineering and Research Development

National Conference On Nanomaterials, (NCN-2017)

Volume 4, Special Issue 6, Dec.-2017 (UGC Approved)

Structural and Dielectric properties of Ti doped $Zn_{0.94}Cd_{0.06}O$

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Abstract: *$Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3) nanoparticles were prepared by low temperature sol-gel auto combustion method. XRD analysis reveals that the samples prepared are polycrystalline hexagonal wurtzite structure (with space group $P6_3mc$). Slight variation in the lattice parameter of 3% Ti doped $Zn_{0.96}Cd_{0.06}O$ has been observed due to the difference in ionic radii of cations. The Raman spectra revel the seven active phonon modes. The phonon modes shift towards higher wave number (blue shift) as Ti doped at Cd site, it might be due to the bond distribution in the samples. The dielectric constant and loss shows decreasing trend and becomes constant at higher frequencies. The values of ε' and tan δ is high (~13.8 and 27.5, respectively) at low-frequency region for $Zn_{0.94}Cd_{0.03}Ti_{0.03}O$ as compare to $Zn_{0.94}Cd_{0.06}O$.*

Keywords: *Metal oxide, X-ray diffraction, Raman spectroscopy, Dielectric properties.*

1 Introduction

Zinc oxide (ZnO) is II–VI semiconductor with a direct wide band gap (3.37 eV at 300 K). It has high optoelectronic efficiencies as compared to indirect band gap semiconductor [1]. Whereas cadmium oxide is II–VI semiconductor with rock salt structure and low direct optical bandgap (2.2 - 2.7 eV). CdO nanoparticles have variety of applications in the fields of photo transistors, solar cells, transparent electrodes and sensors [2]. $Zn_{0.94}Cd_{0.06}O$ has a band gap of 3.08 eV at room temperature. Due to the small direct band gap of CdO, incorporation of Cd in ZnO is caused a reduction in the band-edge of $Zn_{0.94}Cd_{0.06}O$ nanoparticles as compared with ZnO nanoparticles [3]. Cd doped ZnO is difficult to fabricate because rocksalt CdO, in wurtzite ZnO has the strong solubility limits. The greatest challenge for Optoelectronic applications remains the fabrication of efficient and reliable p-type ZnO because Optoelectronic devices required for the p-n junction.

The present study is aimed at studying the structural and dielectric properties of transition metal doped $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3).

2 Experimental Details

The pristine and doped $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3) were prepared by sol-gel method using high purity zinc nitrate [Zn $(NO_3)_2 \cdot 6H_2O$] and cadmium nitrate [Cd $(NO_3)_2 \cdot 4H_2O$]. The calculated amount of citric acid was added for making a reaction. 1 ml of ethylene glycol was dropped for difreezing the solution and ammonia were added to maintain the pH level up to 10. The neutralised solution was stir using a magnetic stirrer at 80°C until it becomes viscous and finally formed a very viscous gel. A white gel formation was obtained and burned till black powder was obtained. This sample was calcined at 600°C for 4h and obtained a pure white coloured sample. The powders were pressed into pellets of size 10×1 mm by applying a pressure up to 8 Tons and then sintered at 650°C for 5 h.

The crystal structure of the samples $Zn_{0.94}Cd_{0.06}O$ and $Zn_{0.94}Cd_{0.03}Ti_{0.03}O$ were identified by means of x- ray diffraction (XRD) technique at room temperature using Bruker D8 Advance X-ray diffractometer with Cu $K\alpha_1$ (1.5406 Å) radiation. The Raman measurements on as synthesized samples were carried out on LABRAM HR800 spectrometer. The spectrometer comprises of He-Ne laser: Wavelength: 632.81nm (1.95 eV) excitation source. The Wayne Kerr impedance analyzer 6500B is used in the frequency range of 20 Hz to 120 MHz, ac voltage range from 10 mV to 1 V and temperature range varies up to 1000°C. For dielectric measurement high purity conducting silver paste was coated on pellets.

3 Results and Discussion

The XRD patterns of $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3) samples are depicted in Figure 1. All the diffraction peaks for $Zn_{0.94}Cd_{0.06}O$ and $Zn_{0.96}Cd_{0.03}Ti_{0.03}O$ nanoparticles are attributed to wurtzite structure. The XRD pattern confirms that there is no structural change. The analysis confirms that both samples have wurtzite structure with $P6_3mc$ space group (JCPDS card No. 36-1451) [4], without having any impurity phase. The slight variation in lattice parameter of $Zn_{0.96}Cd_{0.06}O$ ($a = b$ = 3.245 Å, c = 5.199 Å) and $Zn_{0.96}Cd_{0.03}Ti_{0.03}O$ ($a = b$ = 3.248 Å, c = 5.201 Å) were obtained, suggesting that Cd^{2+} / Ti^{4+} ions would uniformly substitute into the Zn^{2+} sites in ZnO lattice [5].

Figure 2 shows the Raman spectra of $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3) in the frequency range of 200-900 cm^{-1} at 300 K. Lorentzian line shape function is used to fit the Raman spectra. ZnO has Wurtzite crystal structure belongs to C_{6v} point group and $P6_3mc$ space group with two formula units per primitive cell. The Raman active modes of the structure

can be summarized as: Γ_{opt}= $1A_1$+ $2B_1$+ $1E_1$+ $2E_2$ [6, 7]. Here, the B_1 modes are Raman inactive (silent) mode. The spectrum represents seven optical phonon modes at 269, 332, 437, 501, 582, 682, 867 cm^{-1} for $Zn_{0.96}Cd_{0.06}O$. The modes shifted towards higher wave number (blue shift) as Ti doped at Cd site, it might be due to the bond distribution in the samples. The obtained phonon modes are the indicative of high quality hexagonal crystal structure of ZnO nanoparticles in agreement with XRD results [8].

Variation of the real part of the dielectric constant (ε') with applied frequency is shown in the inset of Figure 3. It is clear that prepared nanomaterials exhibit dielectric response where the value of real part of dielectric constant (ε') decreases with enhancing the frequency of the applied field. The data reveal that none of the nanomaterials exhibit any anomalous dispersion or peaking behaviour. The observed dielectric response can be explained in the light of space charge polarisation and hopping of charge carriers. Polarisation is also influenced by a component such as structural homogeneity, stoichiometry, grain size, density and porosity of the metal oxides. Maxwell-Wagner confirms the larger value of dielectric constant (ε') at lower frequency region due to a dielectric inhomogeneous structure which is good approving with Koops Phenomenological theory [9].

Dielectric loss tangent ($\tan\delta$) decreasing with frequency increasing up to 10^7 Hz at 300 K as shown in Figure 3. The dielectric loss decline with the rising frequency which is a normal behaviour of any material. Dielectric loss decreases immediately in the low-frequency region (50 Hz – 10 kHz), while the rate of decrease is gradual in the high-frequency region (10 kHz – 10 MHz), and it shows an almost frequency independent response in the high-frequency region. The low loss value (~ 0.5) at high frequency 10 MHz show the potential applications of these metal oxides samples in high-frequency microwave devices.

4 Conclusions

$Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3) was successfully prepared by sol-gel auto combustion method and was further investigated by x-ray diffraction, Raman scattering and frequency dependent dielectric measurements. X-ray powder diffraction confirms the wurtzite structure with $P6_3mc$ space group. The observed Raman active phonon modes were indicative of the hexagonal crystal structure of $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3) nanoparticles in agreement with the XRD results. Further, the dielectric constant decreases with an increase in frequency and becomes constant at a higher frequency, which signifying the presence of relaxation in the sample.

Acknowledgments

UGC-DAE-CSR, as an institute is acknowledged for extending its facilities. The authors acknowledge Dr. M. Gupta, Dr. V. G. Sathe, and Dr. V. Ganesan of UGC-DAE CSR, Indore for fruitful discussions. Financial support from UGC-DAE CSR, Indore is gratefully acknowledged.

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Figure captions

Figure 1X-ray diffraction (XRD) pattern of $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3).

Figure 2 Room temperature Raman spectra of $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3).

Figure 3 Dielectric loss and dielectric constant (ε') [inset view] as a function of frequency for $Zn_{0.96}Cd_{0.06-x}Ti_xO$ (x = 0.0, 0.3).

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Figure 1 (Color)

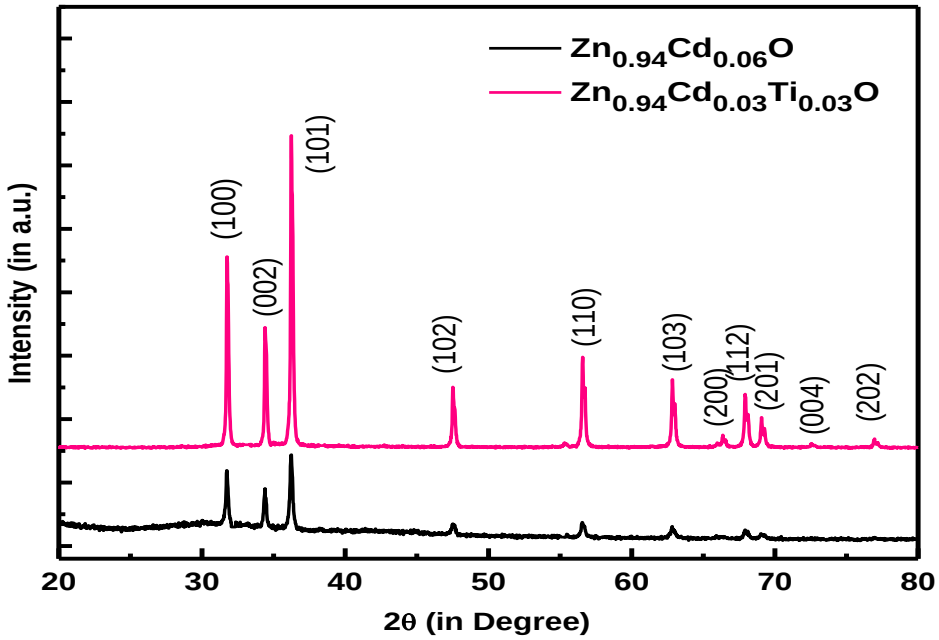

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Figure 2 (Color)

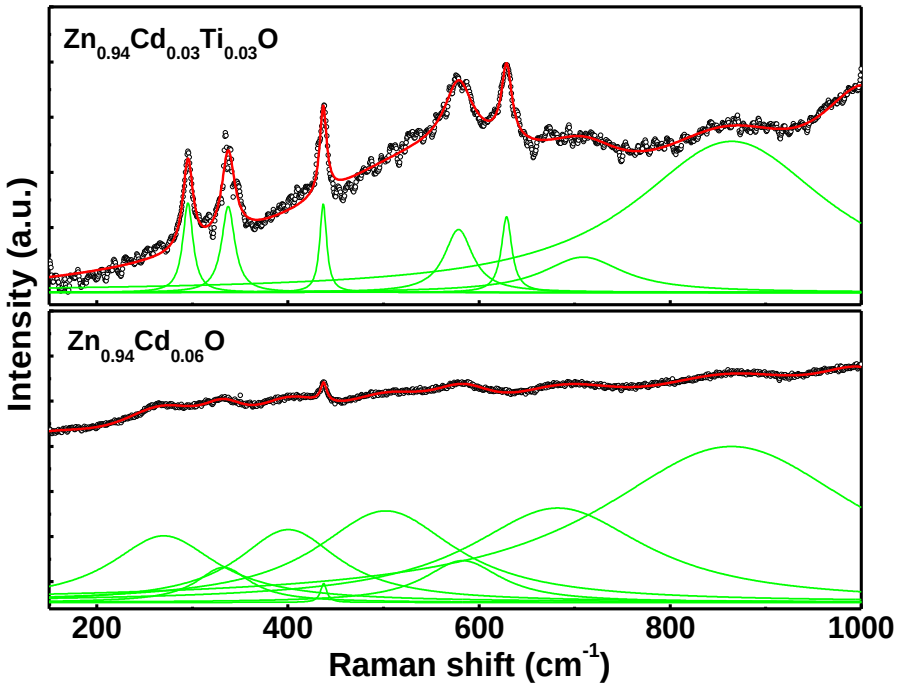

Figure 3 (Color)