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The Effect of Fe Concentration on the Structure and Optical Properties of Zno Films by Using Pulsed Laser Deposition

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Abstract: *Pure ZnO and (3, 5,7wt. %) Fe doped ZnO thin films were deposited on glass substrate using pulse laser deposition (PLD) technique. The deposition was carried out using Q-switched Nd: YAG Laser(1064nm) as the light source. The structure and optical properties were characterized by X-ray diffraction (XRD), atomic force microscopy (AFM) and UV-Vis spectrometer measurements. XRD patterns show films have a polycrystalline wurtzite structure. It can be seen from AFM that the average grain size, roughness and RMS increased with increasing doping concentration of Fe .Optical properties investigation found that high transparent of thin films in the visible wavelength region. Band gap of pure ZnO the films has been found to be 3.02 eV and 2.52 eV for 7 wt. %Fe doped ZnO films. The refractive index (n) and extinction coefficient (K_e)is increased as the concentration of Fe increased.*

Keywords: *Pulse laser deposition, Zinc oxide, Thin film, Fe*

I. Introduction

Zinc oxide (ZnO) is a semiconductor compound of the II-VI family, with wide and direct band gap of (3.37 eV) and large exiton binding energy (60 meV) at room temperature in the ultraviolet (UV) range[1]. ZnO has a great potential for applications in short wavelength optoelectronics, laser, detectors , light- emitting diodes and solar cell . Moreover it has the potential to compete GaN, because of its properties such as higher chemical etching rate, larger exciton binding energy, and lower cost[2,3] which makes it more resistant to radiation, a high potential for room temperature light emission, and multifunction as it has piezoelectric, transparent, dielectric, semiconducting oxide and optoelectronic applications in UV-Blue spectral range. Lots of research groups carried out doping elements such as Cu,Mg,Ti, and Fe in order to improve crystallization quality or obtain better optical, electrical or ferromagnetic properties [4-7]. ZnO:Fe film could be an important multi-functional material. It has found that physical properties of ZnO depends on growth method, environmental conditions such as pressure, doping concentration, temperature and the crystal structure. ZnO thin films can be deposited using a number of different deposition techniques. One of these techniques is the PLD method. In this techniques environment parameters during the growth of the films affect the properties of the films[8]. In this paper we prepared Fe- doped ZnO thin films via PLD method on glass substrates and study the effect of Fe-doping concentration on the optical and structural properties.

II. Experimental Work

Pure ZnO and ZnO:Fe films were deposited by (PLD) technique as shown in figure (1). The deposition were carried out using a Q switched Nd:YAG Laser at wavelength of (λ=1064nm), the pulse repetition rate was set at (6)Hz, 900shot and laser fluencies 800mj/cm^2,The pressure kept at 10^{-2}mbar. The target to substrate distance maintained at (1.5)cm. The glass substrates were cleaned in methanol solutions in an ultrasonic bath for 30 minutes, then compress the mixture under 5 ton (hydraulic compressor) to get the final pellet 2.5 cm diameter of ZnO powder and ZnO doped Fe . Crystalline quality and crystal orientation of prepared thin films were investigated by XRD(Cu KαI, λ= 0.154 nm). The optical properties of the films were studied at room temperature by using UV-Vis spectrometer in the wavelength range of (200-1100nm) in order to determine the refractive index and energy gap value for each sample.

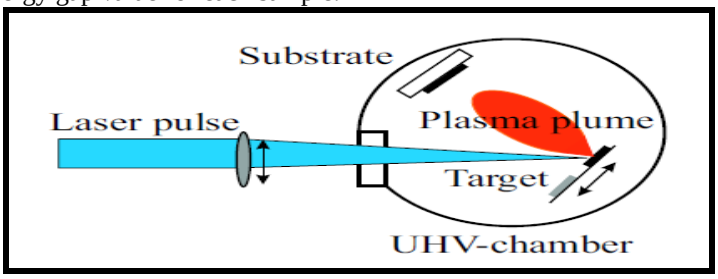


Figure.(1): Schematic diagram of the pulsed laser deposition system[9]

III. Results And Discussion

3.1 X-Ray Diffraction Analysis

Figure (2) shows the XRD analysis of pure ZnO and(3,5,7.wt%) Fe doped ZnO thin films grown on glass substrates at room temperature (RT). The main peaks of ZnO(100) and (101) have wartzite polycrystalline structure can be seen in all of the patterns. According to XRD analysis, it can be noticed that higher intensity of peaks as the Fe concentration increased due to the increase of the concentration of the film. Also XRD patterns indicate the percentage of %wt concentration of Iron does not change the polycrystalline structure of ZnO. From table (1) the grain size of thin films increased as the concentration of Fe increased. To Calculate average grain size, we used Scherre's relationship[10]:-

$D_{av}=K\lambda/\beta\cos\theta$ ……(1)

Where, λ is the wavelength of X-ray , β is the full width at half the maximum intensity (FWHM) of the peak, θ_β is the Bragg angle and K is the shape factor of the average crystallite which equal to 0.9.

Table.1.The structural parameters of pure ZnO andFe doped ZnO

Fe%	2 □ (Deg.)	FWHM (Deg.)	d_{hkl} Exp.(Å)	G.S (nm)	d_{hkl} Std.	hkl
Pure	31.7259	0.3807	2.8181	21.7	2.8137	(100)
ZnO	36.2183	0.4569	2.4782	18.3	2.4754	(101)
	31.5736	0.4569	2.8314	18.1	2.8137	(100)
3	34.1624	0.6137	2.6225	13.5	2.6035	(002)
	35.9898	0.3046	2.4934	27.4	2.4754	(101)
	56.3959	0.5330	1.6302	16.9	1.6245	(110)
	31.6211	0.3046	2.8272	27.1	2.8137	(100)
	34.2985	0.3807	2.6124	21.8	2.6035	(002)
5	36.1454	0.3046	2.4830	27.4	2.4754	(101)
	47.4873	0.3046	1.9131	28.5	1.9110	(012)
	56.4721	0.6853	1.6282	13.2	1.6245	(110)
	62.7157	0.5330	1.4803	17.5	1.4772	(013)
	67.8173	0.5330	1.3808	18.0	1.3782	(112)
	31.6497	0.2946	2.8247	28.0	2.8137	(100)
	34.3147	0.2946	2.6112	28.2	2.6035	(002)
7	36.1421	0.2284	2.4833	36.6	2.4754	(101)
	47.4112	0.3807	1.9160	22.8	1.9110	(012)
	56.5482	0.3807	1.6262	23.7	1.6245	(110)
	62.7919	0.3807	1.4786	24.4	1.4772	(013)

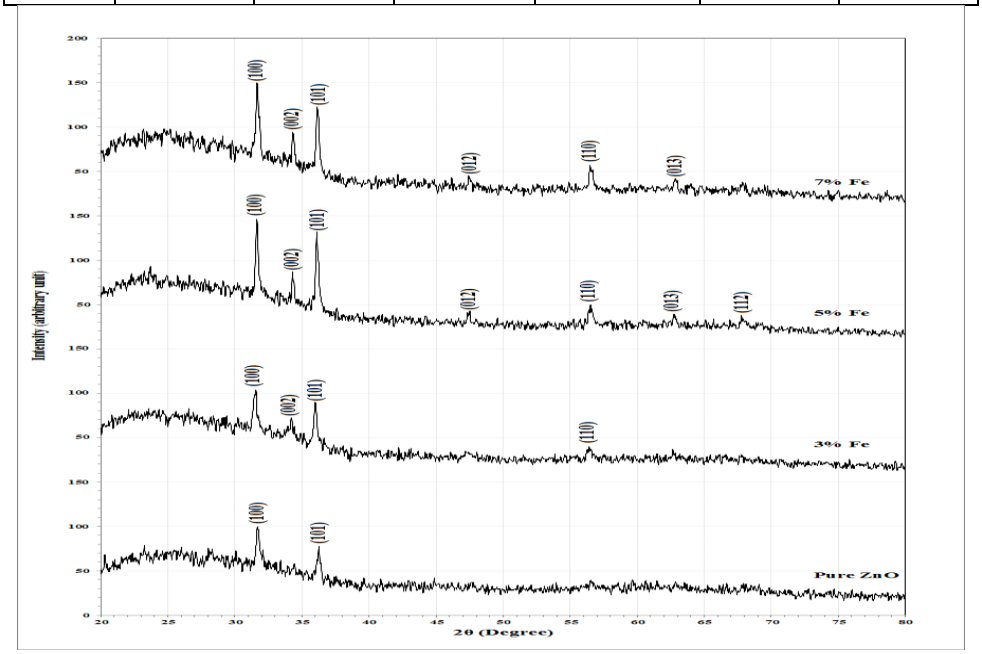


Figure (2) XRD analysis of pure ZnO and(3,5,7wt%) Fe doped thin films at room temperature3.2- AFM analysis

3.2- AFM analysis

The AFM images of pure ZnO and (3,5,7wt.%) Fe doped ZnO thin films on glass substratee were presented in Figure(3) the RMS roughness and the grain size have got correlation with the percentage of the doping concentrations of Fe(any increment in the percentage of doping there will be a relative increase value of the grain size). Moreover the surface roughness is increased from (3.84)nm to (7.35)nm with increasing doping concentration up to 7 wt% (shown in table 2). This increase of the surface roughness may be due to the increase of the grain size. The Cumulating Distribution report of pure ZnO and (3,5,7wt%) Fe doped ZnO thin films is shown in Figure(4)

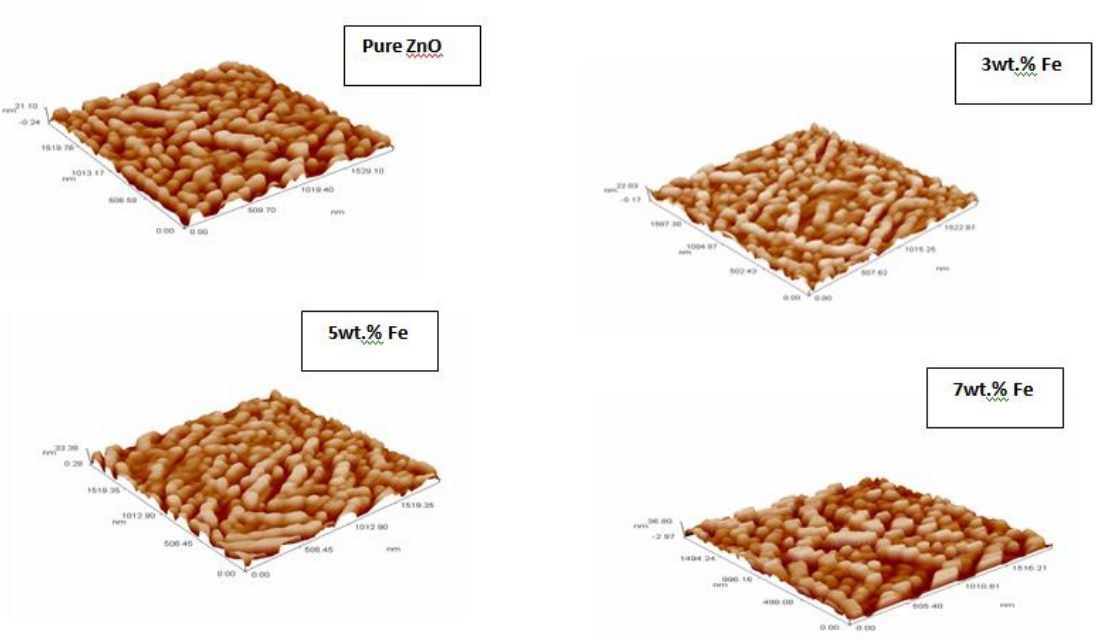
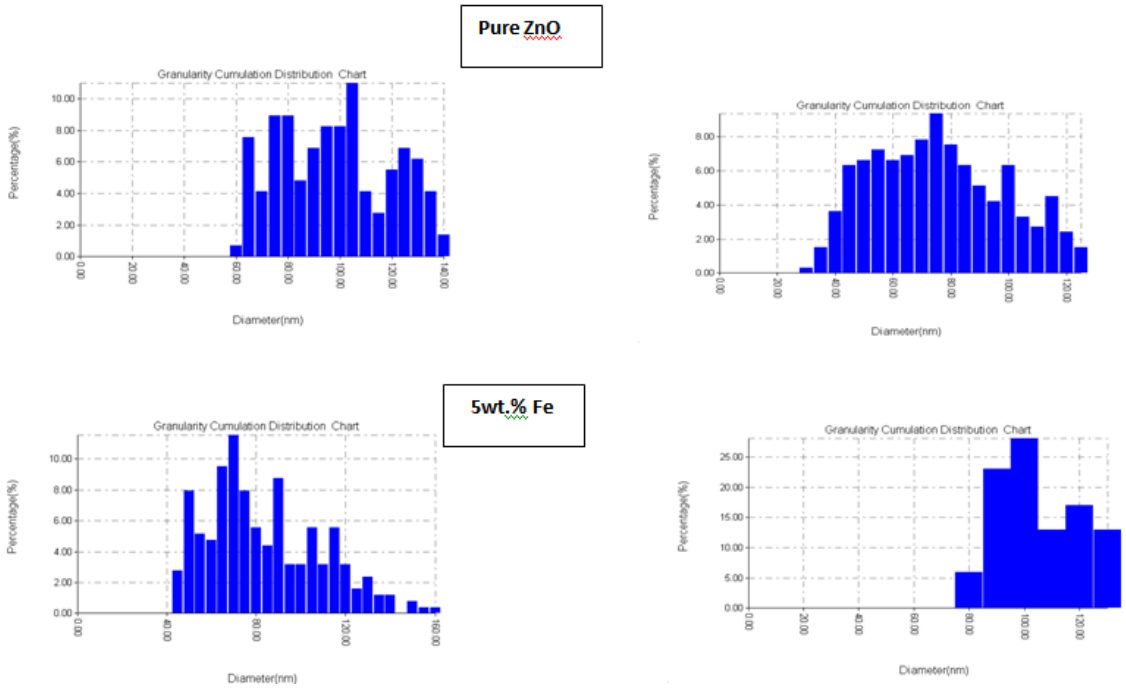


Figure (3): AFM image of pure ZnO and(3,5,7wt%) Fe doped ZnO thin films.

Table (2): Grain Size and Roughness of pure ZnO and doped Fe ZnO thin films

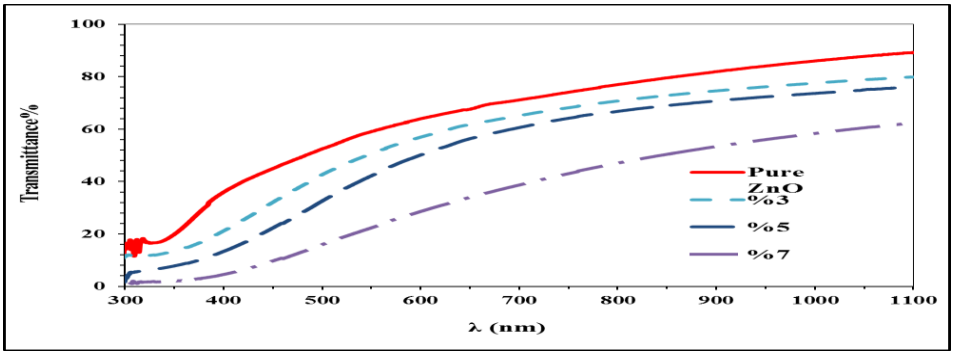
Sample	Average Diameter(nm)	sa(Roughness Average)(nm)	Sq(RMS)(nm)
ZnO:Fe(PURE)	95.59	3.59	4.15
ZnO:Fe (0.0)	73.30	3.29	3.84
ZnO:Fe(0.05)	81.21	4.99	5.8
ZnO:Fe(0.07)	100.75	7.35	8.55



Figure(4):Granularity Cumulating Distribution Report of pure ZnO and (3,5,7wt.%) Fe doped ZnO thin films

3.3 Optical Properties Of Thin Films

Figure(5) shows a series transmittance spectrum of Fe doped and pure ZnO films measured at room temperature . The variation of concentration of Fe doped ZnO thin films have significant effect on the optical properties. The average optical transmittance in the visible spectrum region of(300-1100)nm was decreased with increasing doping concentration. This is in consistent with the increasing of the surface roughness promoting the increase of the surface scattering of the light.



Figure(5): Transmittance spectrum of pure ZnO and (3,5,7wt.%)Fe doped ZnO thin films.

The absorption coefficient (α) was calculated from absorptance spectrum by using the following equation[11].

$\alpha = 2.303\ A/t$ ……..(2)

where(A)is absorbance

It is observed that the absorption coefficient (α) increased with increasing the concentration of Fe as shown in figure 6.

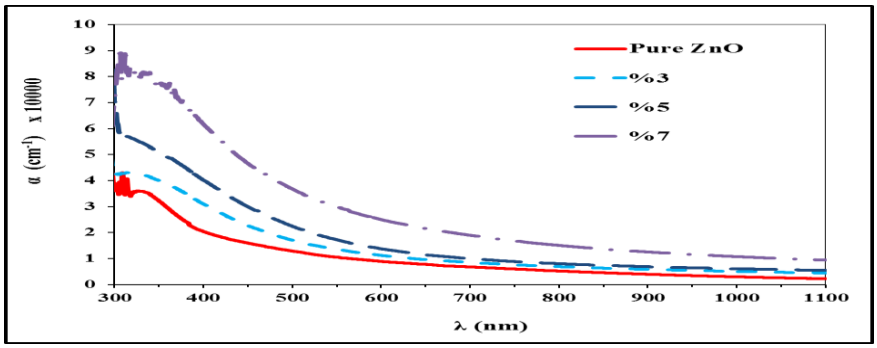


Figure (6): The absorption coefficient for ZnO thin films with different Fe concentrations doping

This is due concentration led to the composition of donor levels inside the energy gap near the conduction band worked to turn the absorption of photons with few energies and therefore a clear increase in the values of absorption coefficient, and the decrease in the optical energy gap. A plots of$(\alpha h\nu)^2$ verses photon energy (hυ) of the ZnO: Fe films at different concentration of Fe. The direct Eg_{opt} decreases from(3.o2)to(2.52)eV, when Fe concentration increases from (3% to 7%) as shown in the figure (7). And this due concentration led to the displacement of the absorption edge towards the few energies and this decrease can be explained that the impurities led to the formation of donor levels inside the energy gap and near the conduction band and therefore the absorption of photons with a few energy and increase in the transfer of electronic and then decrease in the optical energy gap values. This result is in agreement with[Alver.U et.al,2007][12]

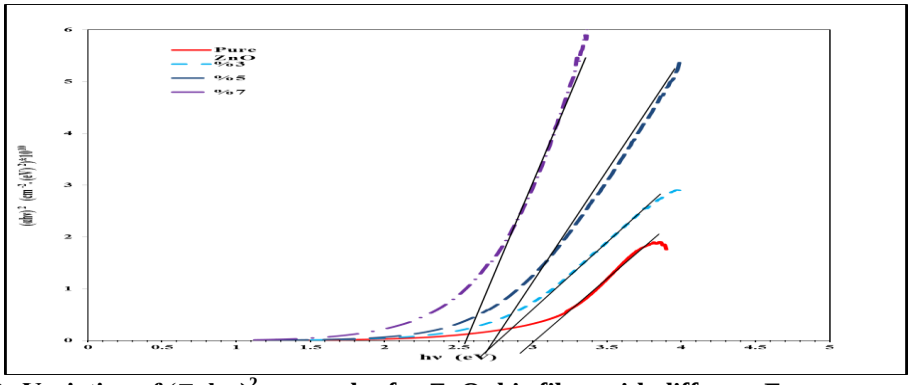


Figure. (7) :Variation of (□ hυ)^2 versus hυ for ZnO thin films with different Fe concentrations doping

The extinction coefficient, which is related to the exponential decay of the wave as it passes through the medium can be determined by using the following equation [11]:

$$k = \frac{\alpha\lambda}{4\pi} \quad \text{……..…….. (3)}$$

where λ: is the wavelength of the incident radiation.

We can observe from these figure(8)that the extinction coefficient, in general, increases with increasing of Fe content for all films. Increasing in k value can be ascribed to increasing topical donor levels formed within the ergy that led to increased extinction coefficient which shows the electronic transitions occur directly gap.

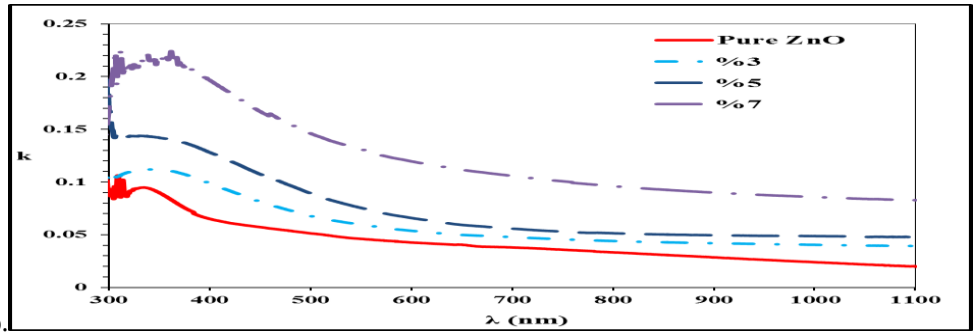


Figure (8) :The extinction coefficient versus wavelength for thin ZnO

We can notice the refractive index increases with increasing of concentrations doping as shown in the Figure(9).

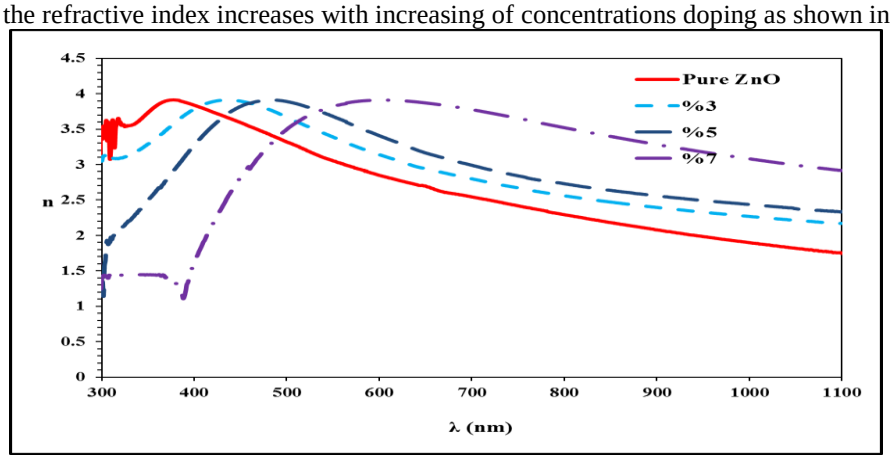


Figure (9): The refractive index versus wavelength for thin ZnO films with different Fe concentrations

This due to Increase the levels intensity of the energy in the optical energy that in turn serve as centers dispersion of rays falling gap thus increasing the reflectivity and thus increase the refractive index (n)[13].

$$n=\left[\frac{4R}{(R-1)^2}-k^2\right]^{1/2}-\frac{(R+1)}{(R-1)} \quad \text{--------} \quad (4)$$

where R is the reflectance and is given by the equation $R=\frac{(n-1)^2+K^2}{(n+1)^2+K^2}$……(5)

The complex dielectric constant is given by the following equation[14] :

$\varepsilon=\varepsilon_r+\varepsilon_i=(n+ik)^2$……(6) Where ε_r , and ε_i are the real and imaginary parts of ε and $(n+iK)^2$ is the complex refractive index. From equation (6) we obtain:

$\varepsilon r=n^2+k^2$ and $\varepsilon i=2nk$…..(7)

The real (ε_r) and imaginary (ε_i) parts of the dielectric constant values versus wavelength in the range (300-1100) nm for pure ZnO and doped with different Fe concentration as shown in figures (10),(11) the behavior of ε_r is similar to that of the refractive index because of the smaller value of k^2 compared with n^2 according to equation (7) while ε_i mainly depends on the k values equation(7) It is found that ε_r and ε_I, increase with increasing of Fe concentration. This behavior is in agreement with the results is shown by (S.Ilican .)[13]

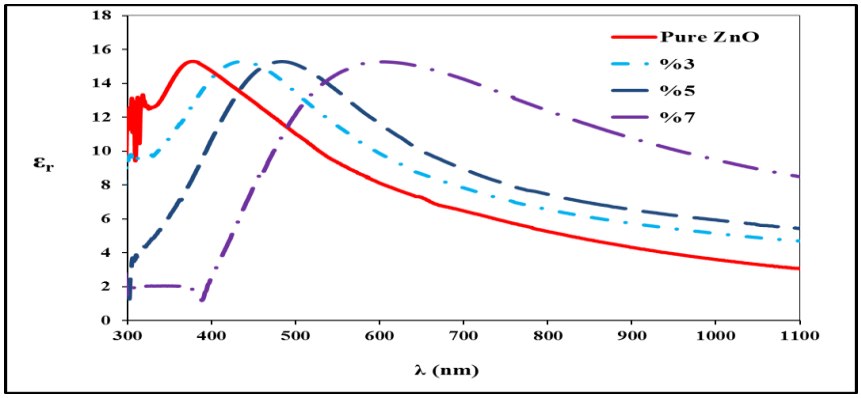
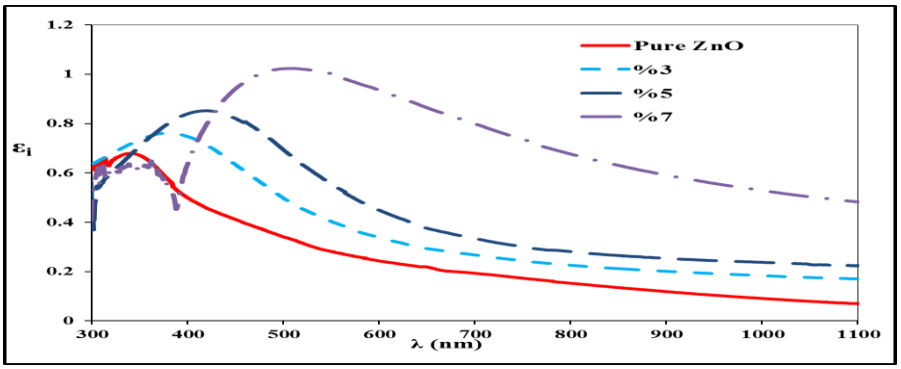


Figure (10): Real dielectric constant versus wavelength for thin ZnO films with different Fe concentrations



Figure(11): Imaginary dielectric constant versus wavelength for thin SnO_2 films with different Fe concentration

IV. Conclusions

ZnO and ZnO:Fe have been successfully prepared by puls laser deposition (PLD). X-ray diffraction results show that the structure of ZnO films is polycrystalline with hexagonal wurtzite structure preferential orientation in the (100) direction and intensity increased with doped by Fe. And doping concentration increases the grain size and root mean square, surface roughness was found increased. The optical transition in ZnO are direct and the optical energy gap decrease with increasing doping concentration.

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