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Effect of Magnesium Doping on the Structural, Morphology and Optical Properties of Nanostructured Fe_2O_3 Thin Films Prepared by CSP

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Abstract.

Nanocrystalline Fe_2O_3 and Fe_2O_3: Mg thin films are grown CSP technique. XRD is shown that grown films were polycrystalline with a predominant peak along (116) . values of the crystallite size were found to increase upon doping magnesium. AFM images confirm the appearance of nanostructure. Average Particle size and rms values of the deposited films were (80.86, 69.47 and 54.03) nm and 9.74, 6.69 and 4.74) nm for Fe_2O_3 Fe_2O_3: 2% Mg and Fe_2O_3: 4% Mg respectively. The optical constants including transmittance , absorption coefficient, extinction coefficient and refractive index , It was found that all these constants were affected by upon doping magnesium. The direct energy gap was decreased with the increase of Mg content from 2.24 eV for as deposited Undoped Fe_2O_3 thin film to 2.10 eV for Fe_2O_3: 4%Mg thin film.

Keywords: Fe_2O_3, Mg doping, chemical spray pyrolysis, XRD, AFM, optical properties.

Introduction

Metal oxides is an appropriate materials for solar cell, photoelectron [1]. Fe2O3 have bandgap of 2.2 eV. It draw an inclusive notice due to its pretty physical and chemical properties,[2]. It can be used in tunneling magneto resistance (TMR) devices[3–5]. Besides it can be deposited on Si wafer [6-7]. Many authors utilizing various methods for prepared Fe_2O_3 such as; colloidal chemistry method [8], sol-gel [9], usual ceramic technique [10], spin coating [11,44-64], sputtering [12], PLD [13], MBE [14] and spray pyrolytic method [15-22], In this work spray Fe_2O_3 thin films had been Synthesized by CSP, to study the physical properties of Fe_2O_3 and Fe_2O_3: Mg thin films.

Experimental

Thin films of iron oxide (Undoped Fe_2O_3 and Fe_2O_3: Mg) is grown via SPT. These films were grown od on glass bases prserved at (400 °C). The solution was done by mixing (1.6221 g) of (FeCl3·6H2O) with 100 ml of deionized water D_w. (MgCl2·6H2O) to get Mg on 100 ml of D_w. The optimized conditions are achevied via these parameters, spraying period (8 sec), go on by 120 S to prevent too much cooling, grown rate (10 ml/min), space between spout and base was 29 and the transporter gas (filtered air) is preserved at a pressure of 5 bar. Specimen Thickness is obtained employing gravimetric method to be 300 ± 25 nm. transmittance were recorded employing UV-Visible spectrophotometer. AFM is employed to obtain surfacetopography. The XRD was employed to get film structure.

Results and discussion

The structure of undoped Fe_2O_3 and Fe_2O_3: Mg films are tested by XRD are shown in Fig. 1. We can observe that XRD patterns of the grown Undoped Undoped Fe_2O_3 and Fe_2O_3: Mg thin film is 24,37°, 33.71°, 37.84°, 53.82° and 63.41° correspond to anatase (017),(116), (119), (300) and (223) planes, respectively. High peak at (116) was seen that fit with ICDD card no 40-1139.

to investigate the effect of the magnesium doped Fe_2O_3 thin films on the average crystallite size D and β (FWHM) that calculated fromthe Scherer formula [23-25]:

$$D = \frac{k\,\lambda}{\beta cos\theta} \qquad (1)$$

Where λ is the x-ray wavelength used, k = 0.9 and θ is Bragg's angle.

The acquired data are given in Table 1. It shown that the crystallite sizes were increased from 9.77 nm to 11.68 nm as in XRD. and dislocation density (δ) in the films was determined by [26-28]:

$$\delta = \frac{1}{D^2} \qquad (2)$$

Table 1. It shown that dislocation density (δ) decreased from 10.47 to 7.33 and strain (ε) in the films was determined by [29-31]:

$$\varepsilon = \frac{\beta cos\theta}{4} \qquad (3)$$

Table 1. It shown that strain (ε) decreased from 3.54 to 2.96.

Structural parameters S_p were shown in Figure (2).

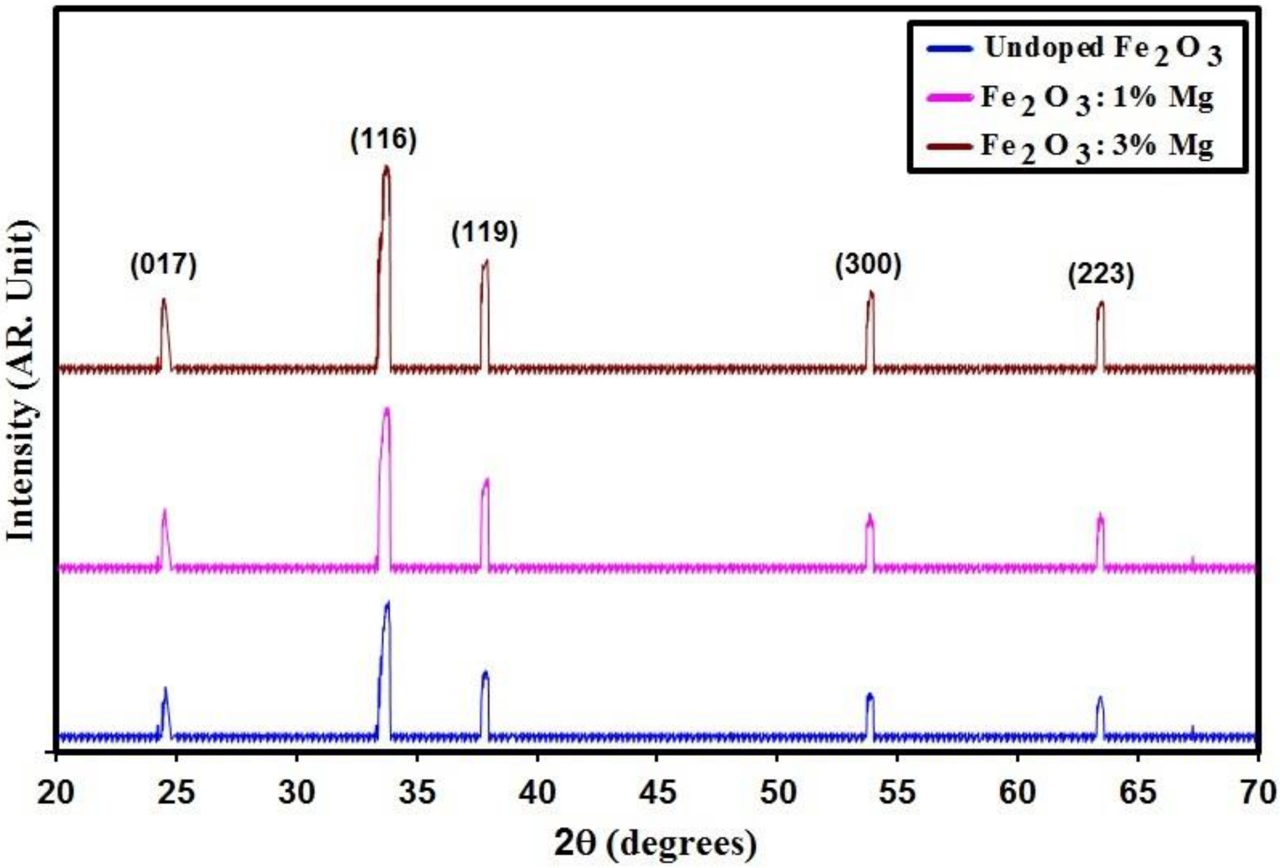

Fig.1. XRD styles of deposit films.

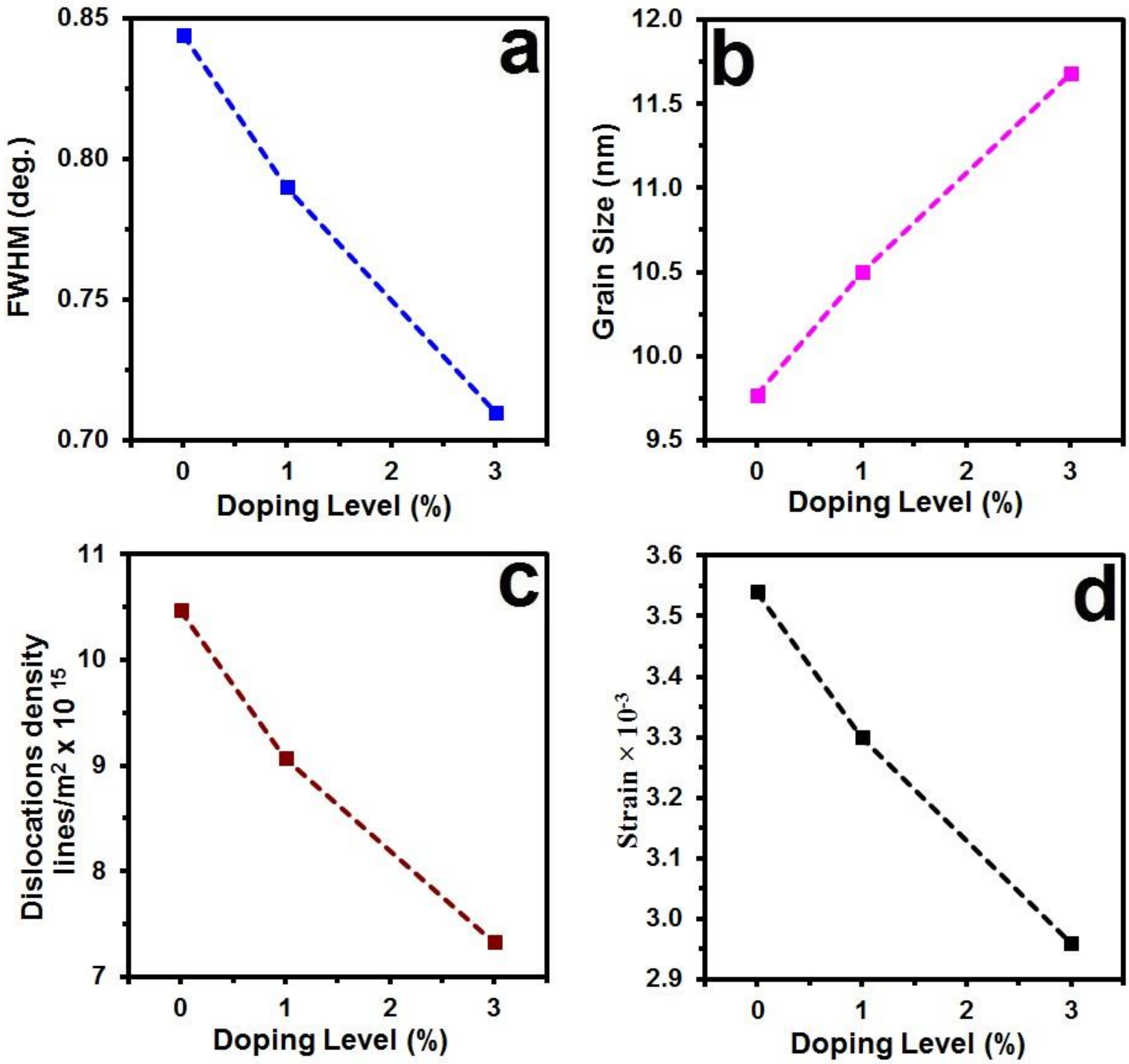

Fig.2. FWHM (a) *D* (b) δ (c) ε (d) of deposit films.

Table 1. *D*, E_g and S_p of intended films.

Samples	**(hkl) Plane**	**2 □ (º)**	**FWHM (º)**	**Grain size (nm)**	**Optical bandgap (eV)**	**Dislocations density ($\times 10^{15}$)(lines/m^2)**	**Strain $\times 10^{-3}$**
Undoped Fe_2O_3	116	33.71	0.84	9.77	2.24	10.47	3.54
Fe_2O_3: 1% Mg	116	3.48	0.79	10.50	2.18	9.07	3.30
Fe_2O_3: 3% Mg	116	33.43	0.71	11.68	2.10	7.33	2.96

AFM images with (4µm x 4µm) was used. Fig. 3 shows the AFM micrograph of the intended films. The Average Particle size P_{av} decreased from 9.77 nm to 11.68 nm by increasing the for Fe_2O_3 and Fe_2O_3: 3%Mg. From Figure 3 (a_3, b_3 and c_3). The surface roughness and rms values were (10.47, 9.07 and 7.33) nm and 3.45,3.30, and 2.96) nm for Fe_2O_3 , Fe_2O_3:1% Mg and Fe_2O_3:3% Mg respectively.

Table (2) offers AFM parameters A_P.

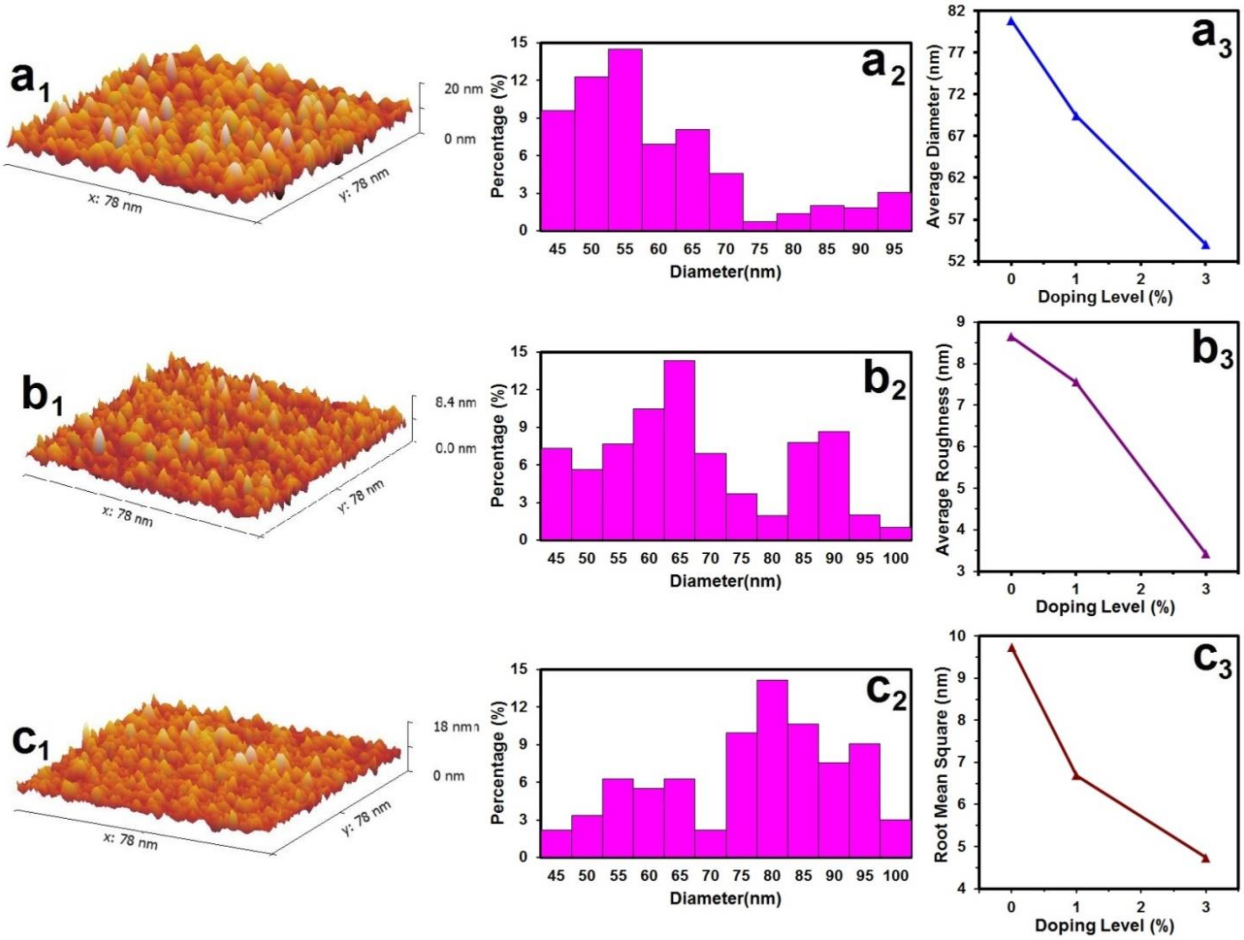

Fig.3. AFM information

Table 2. A_P of the intended films.

Samples	P_{av} nm	Ra (nm)	rms (nm)
Fe_2O_3	80.86	8.65	9.74
Fe_2O_3: 1% Mg	69.47	7.56	6.69
Fe_2O_3: 3% Mg	54.03	3.42	4.74

The transmittance T spectra of Fe_2O_3 and Fe_2O_3: Mg thin films are displayed in Fig. 4. T of undoped Fe_2O_3 and Fe_2O_3: Mg thin films decreases from 95% to 85% as Mg content increases from 0 to 4 at%.
The absorption coefficient (α) is obtained from [3234]:

$$\alpha = \ln(1/T)/d \qquad (4)$$

Where, d is film thickness.

Fig.5 displays α decreased with an increase at 1% or 3 % magnesium doping.

The optical band gap was obtained by Tauc model [35-37]:

$$(\alpha h\nu) = A\left(h\nu - E_g\right)^{\frac{1}{2}} \qquad (5)$$

Where A is the constant,, $(\alpha h\nu)^2$ against incident photon energy ($h\nu$), plots were gained.
as shown in Fig. (6) The direct bangap show a decrement with the of Mg-doping from 2.24 eV for as deposited undoped Fe_2O_3 thin film to 2.10 eV for Fe_2O_3: 4%Mg thin film.
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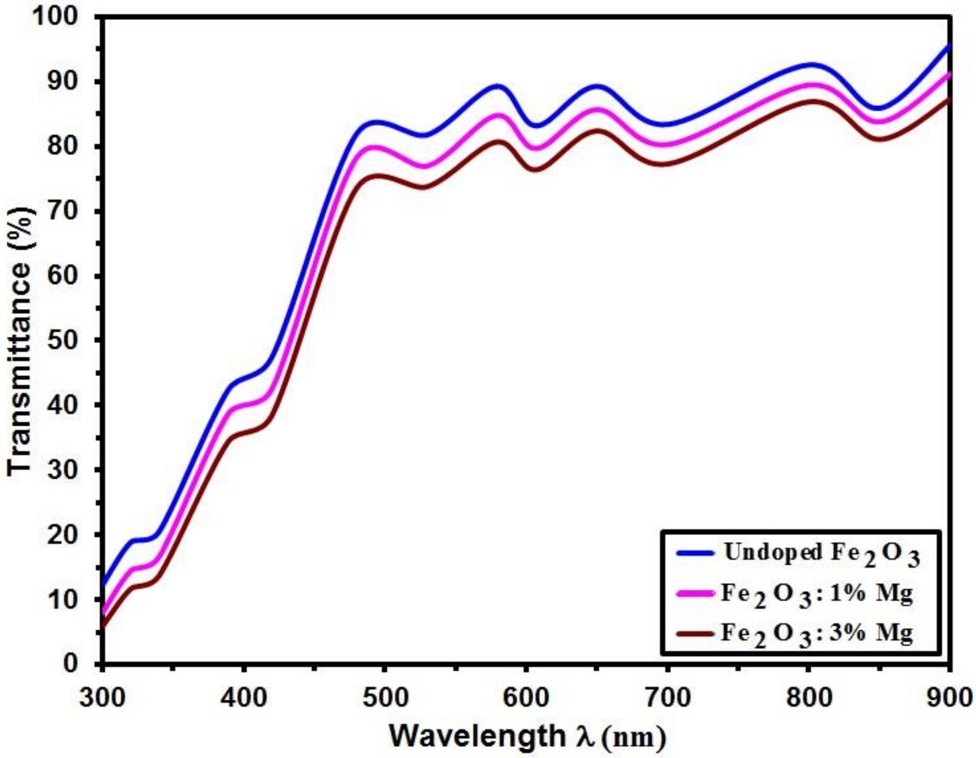

Fig. 4. T of the deposit films.

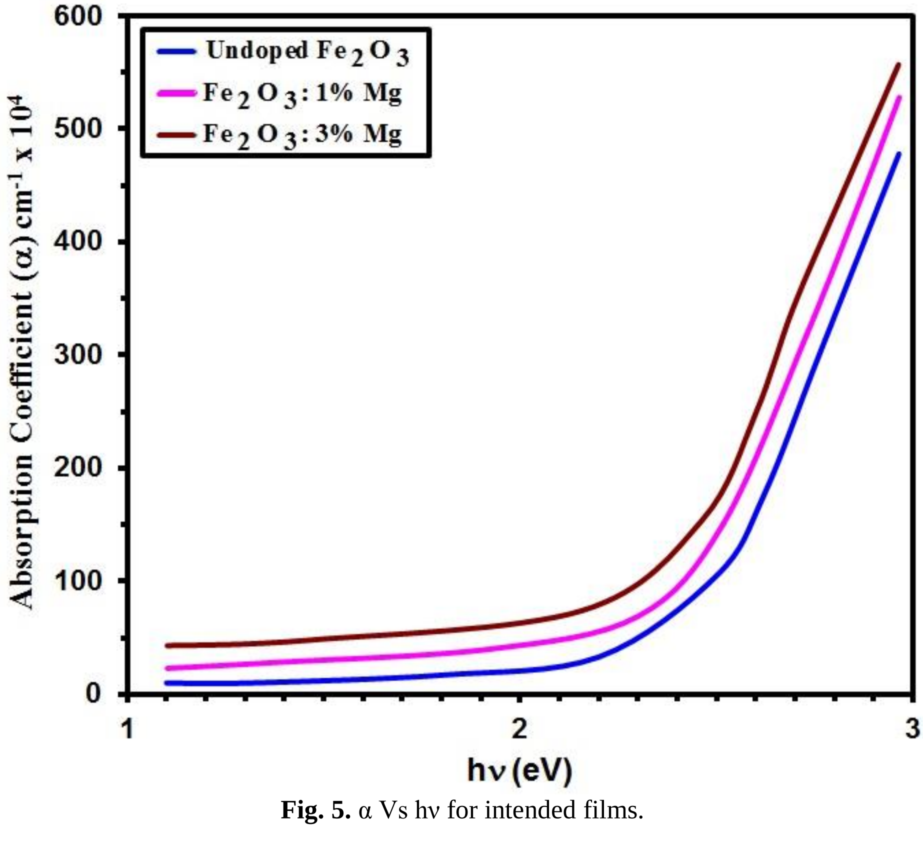

Fig. 5. α Vs hν for intended films.

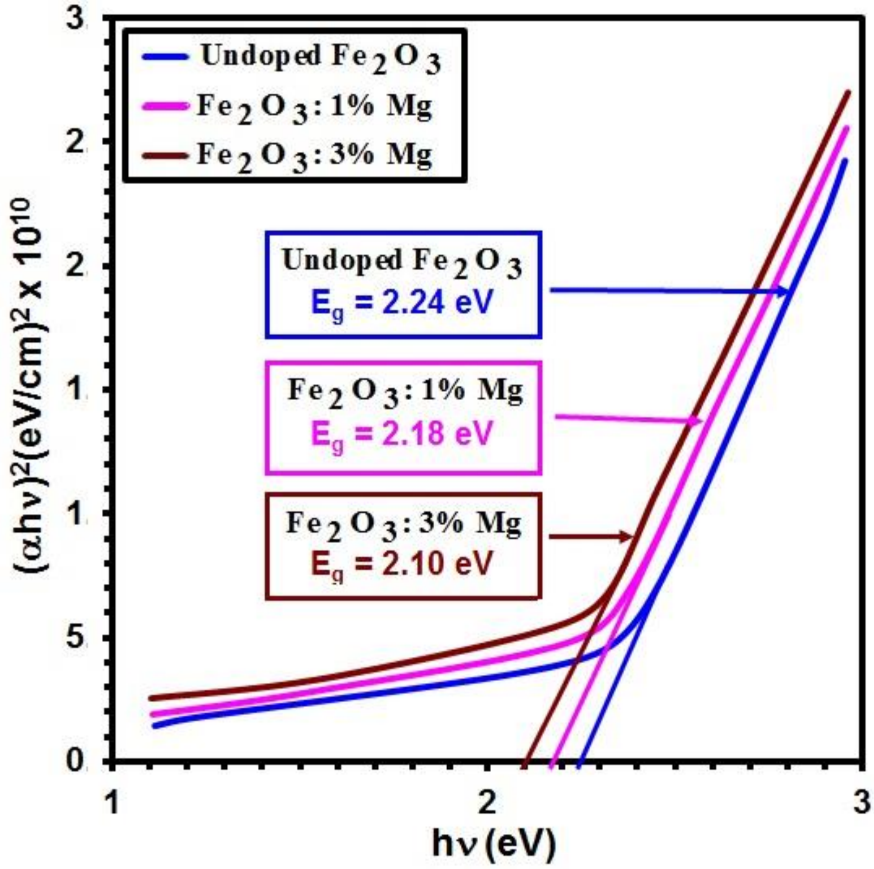

Fig. 6. $(\alpha h\nu)^2$ Vs hν of deposit films.

The extinction coefficient (K) is gained by employing relation [38-40]:

$k = \frac{\alpha\lambda}{4\pi}$ -----(6)

Fig. 7 displays the variance of K with the wavelength. Analogous k variation belong to wavelength of polarized light, and there is slightly decrease in the extinction coefficient after magnesium doping. K is immediately recarding its absorption characteristic. The refractive index *n* was evaluated employing Eq. (7) [41-43]:

$$n = (\frac{1+R}{1-R}) + \sqrt{\frac{4R}{(1-R)^2} - k^2} \quad \text{----- (7)}$$

Where R is the reflectance

and the distinction of n via wavelength is offered in Fig. 8. Anologus manner in n spectra was seen. There is a little decrease in n via magnesium doping.

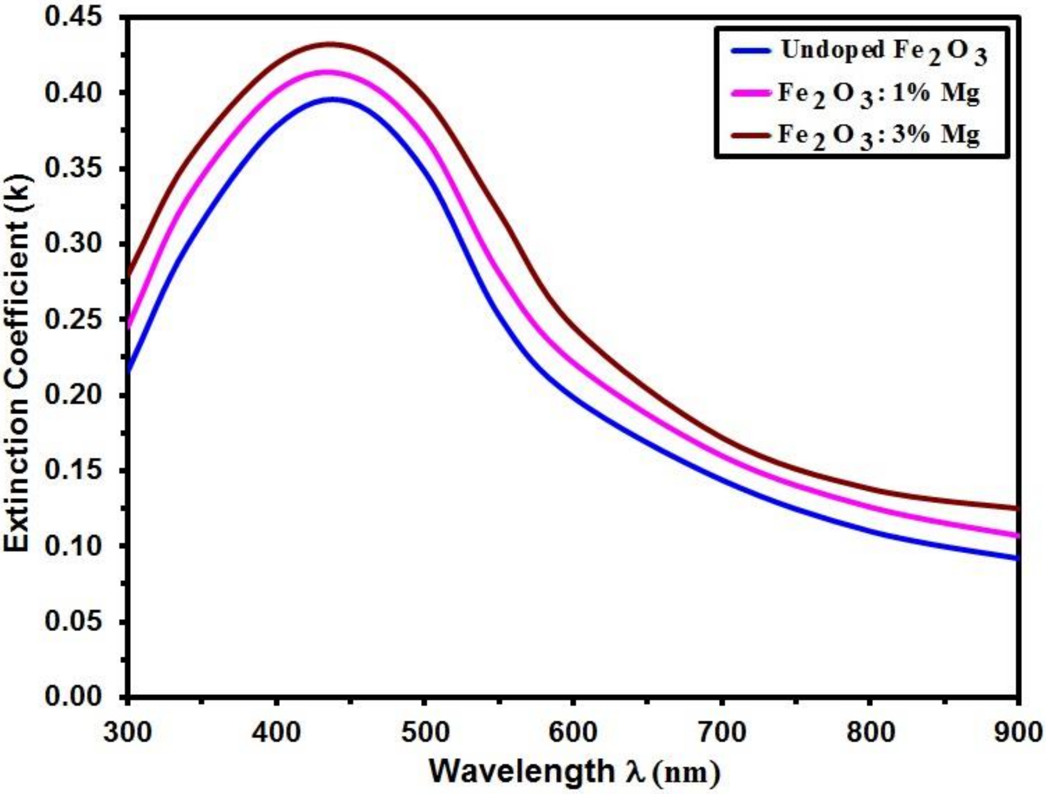

Fig. 7: k of the deposit films.

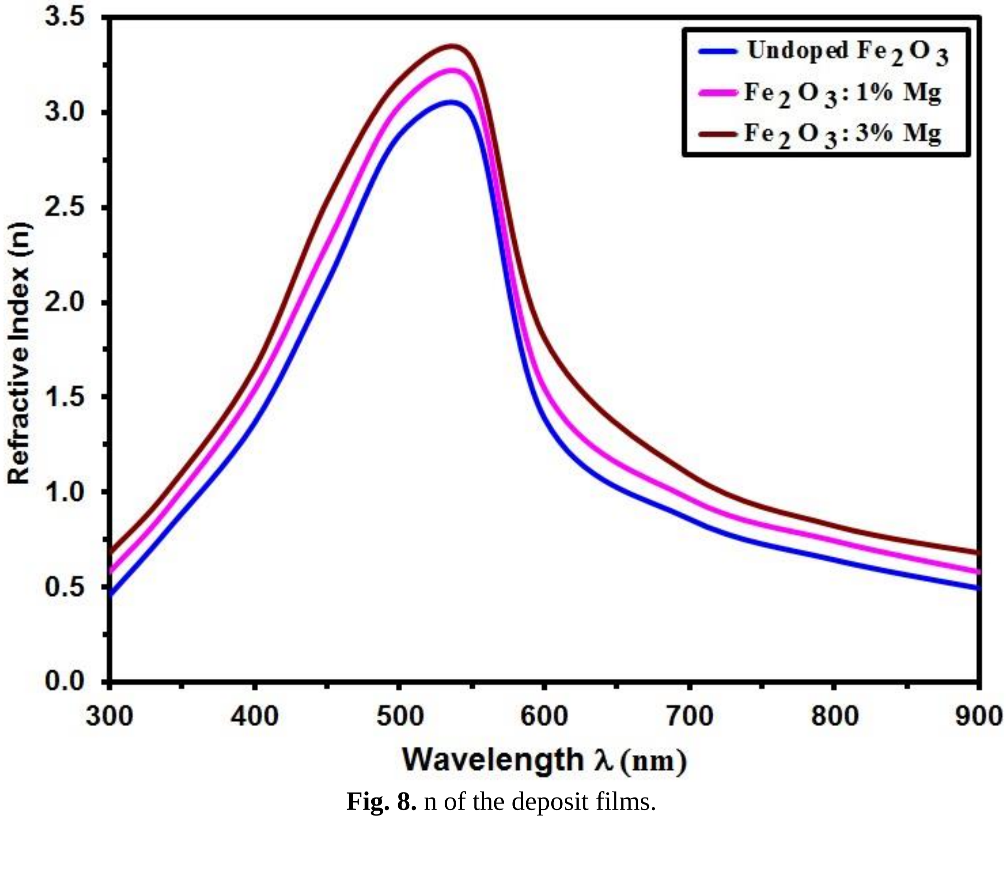

Fig. 8. n of the deposit films.

Conclusion

The preparation of Fe_2O_3 and Fe_2O_3: Mg thin films was done by CSP method. XRD study offer a polycrystalline with predominant peak toward (116) were increased with Mg doping and reveal new peak. the crystallite sizes were increased from 9.77 nm to 11.68 nm, whilst dislocation density (δ) decreased from 10.47 to 7.33, whilst strain (ε) decreased from 3.54 to 2.96, AFM image showed that R_a and rms were decreased with the increasing Mg-doping, while the crystallite size was increased. transmittance of Undoped Undoped Fe_2O_3 and Fe_2O_3: Mg films decreases from 95% to 85% as Mg content increases from 0 to 4 at%. α increases with increment of Mg content , E_g shows a decrement in their values from (2.24 to 2.10) eV by Mg doping. K and n are increasing with increasing with Mg content.

Acknowledgments

This paper is backup via Mustansiriyah University (www. uomustansiriyah.edu.iq).

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