Effect of Boron on Structural, Optical Characterization of Nanostructured Fe_2O_3 thin Films

Nagham Yassin Ahmed[1], Ban A. Bader[2], Muna Y. Slewa[2], Nadir Fadhil Habubi[3], Sami Salman Chiad[3*]

Abstract

Fe_2O_3 thin films were deposited on glass substrate by chemical spray pyrolysis (CSP) technique at a temperature of 450°C.X-Ray diffraction indicates that the films were polycrystalline with a dominant peak along (100). Surface morphology was studied using atomic force microscope (AFM). The grain size values were observed in the zone of (72.46), (71.53) and (59.87) nm for the (Fe_2O_3, Fe_2O_3:1% B, Fe_2O_3:3% B) respectively. Transmittance spectra were recorded to obtain the optical characterizations like absorption edges, which was shifted toward long wavelength. The optical bandgap shows a decrement in their values from (2.65 to 2.45) eV byB doping.

Key Words: Fe_2O_3: B, Spray Pyrolysis, XRD, AFM, Bandgap.

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Introduction

Metal oxides have entered many applications like solar cell; photoelectron and electrical devices[1-7]. Iron oxides have diverse shapes like wustite (FeO), magnetite (Fe_3O_4), hematite (α-Fe_2O_3), and maghemite (γ-Fe_2O_3) [8, 9]. Hematite (α-Fe_2O_3) is a material with a bandgap of about 2-2.2 eV allowing the absorption of ~40% solar energy via its visible area, due to this factor Fe_2O_3 is believed as a favorable material for solar energy application [10]. Iron oxide is one of the most famous magnetic materials. Magnetic properties of ferromagnetic and ferrite films were investigated by using the modified second and third order perturbed, gas sensitivity of many materials has been investigated in diverse gases [11-13]. As a sensor, the α-Fe_2O_3 nanostructures are capable to reveal different gases and vapors likeNO_2, NH_3, CO, andH_2S [14-15]. The high melting point of the metal oxide made the chemical spray pyrolysis technique is suitable method for preparing the metal oxide films [16-19].This work aims to prepare Fe_2O_3 and study the impact of B dopant on some physical characterization.

Experimental

Ferric oxide Fe_2O_3 thin films were prepared by chemical spray pyrolysis (CSP) methodFe_2O_3films are deposited from 0.1 M of ($Fe_2O_3Cl_2$) dissolved in redistilled water. The doped material was Borontrichloride (BCl_3) dissolved in redistilled water, HCl was added as drops to maintain clear solution.

Corresponding author: Sami Salman Chiad
Address: [1]Department of Medical Instrumentation Techniques Engineering, Electrical Engineering Technical College, Middle Technical University, Iraq; [2]Laser and Photonics Research Center, University of Al- hamdaniya, Nineveh, Iraq; [3]Department of Physics, College of Education, Mustansiriyah University, Iraq.
*E-mail: dr.sami@uomustansiriyah.edu.iq
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The optimal conditions of the deposition was : Glass substrate temperature 450°C, space between nozzle and substrate was 29 cm, spraying period 8 s held by 60 s to prevent cooling, spray average was 4ml/min, and the transporter gas was nitrogen. The structural properties of Fe_2O_3: B thin films were carried out employing X-ray diffractometer in 2θ range from 20 to 60. Surface topography of the as deposited films was evaluated by AFM. The UV–Vis spectrophotometer (SHIMADZU Japan) was utilized to gain optical properties.

Results and Discussion

Fig. 1 offers XRD pattern of the prepared films. (XRD) show that Fe_2O_3 and doping with 1% and 3% Fe_2O_3: B were polycrystalline with a rhombohedral structure and a dominant peak along (100) direction. These results in agreement with the standard Fe_2O_3 X-ray diffraction data file [No. 40-1139 JCPDS prevalent].

The average Grain size(D) was obtained from highest intensity peaks utilizing Scherrer's equation [20, 21,22]:

$$D = \frac{0.9\lambda}{\beta cos\theta} \quad (1)$$

Where λ is the wavelength of the X-rays (0.1541 nm), β and θ are (FWHM) and the diffraction angle respectively. The Grain size has been found to vary from 13.30 to 15 nm whereas the strain (%) parameter increased from 26.0 to 23.1, with Au concentration as listed in Table. 1

Other structural parameters such as dislocation density (δ) and strain (ε) are also evaluated. The δ gives number of defects in the films, the values of(δ) and(ε) listed in Table. 1 shows the structural parameters estimated from [23, 24, 25]:

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

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

Figure (2) displays the values of FWHM, D, δ and ε via doping content.

Table 1. Grain size, optical bandgap and structural parameters of the prepared films

Samples	(hkl) Plane	2 θ (°)	FWHM (°)	Grain size (nm)	Optical bandgap (eV)	Dislocations density (× 10^{14})(lines/m²)	Strain × 10^{-4}
Fe_2O_3 pure	111	31.13	0.62	13.30	2.65	56.5	26.0
Fe_2O_3: 1% B	111	30.80	0.58	14.21	2.55	49.5	24.3
Fe_2O_3: 3% B	111	30.28	0.55	15.00	2.45	44.4	23.1

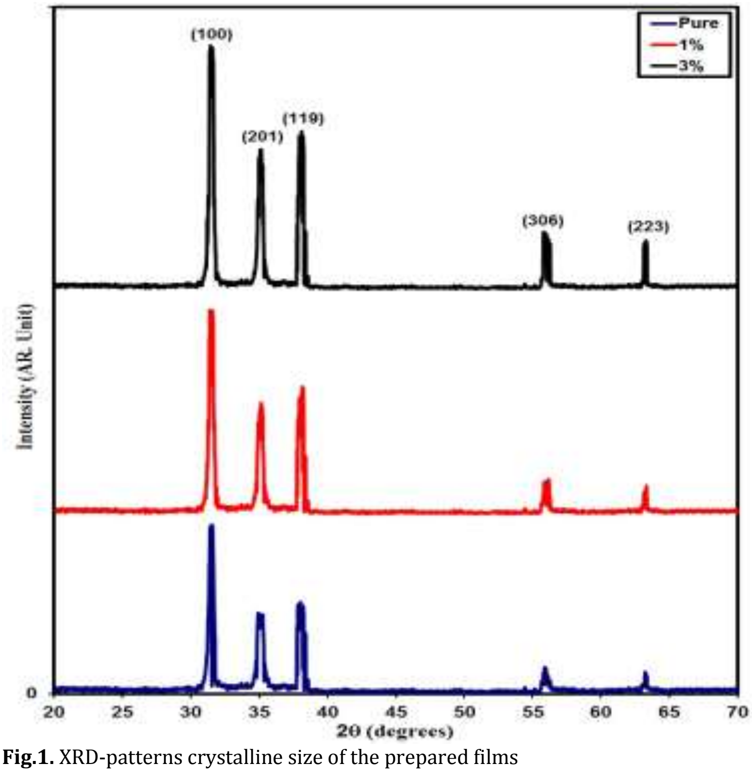

Fig.1. XRD-patterns crystalline size of the prepared films

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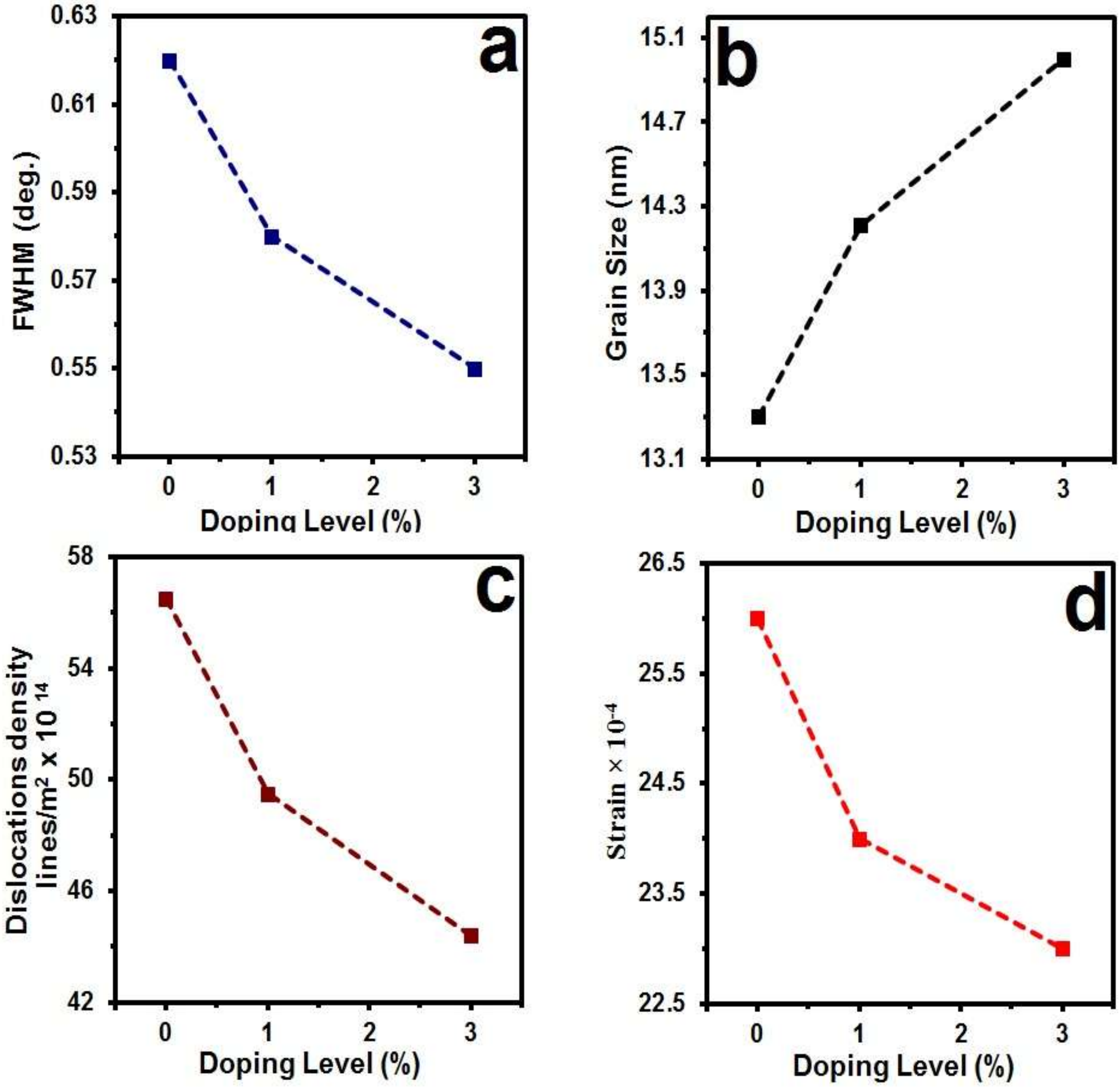

Fig.2. FWHM (a) Grain size (b) Dislocation (c) Strain (d) of the prepared films

Fig. (3) shows AFM image of three dimensional surface topography of the Fe_2O_3 films prepared by SPM. The root mean square roughness (R_{rms}) and average roughness (R_a) of prepared films are shown in Table 1. As can be seen, the R_{rms} and R_a follow the doping. The grain size values was in the range of (72.46), (71.53) and (59.87) nm for the (Fe_2O_3, Fe_2O_3 :1% B, Fe_2O_3 :3% B) respectively, The R_{rms} value of 11.9 nm for as deposited Fe_2O_3 thin films decreased to 4.43 nm by decreased of doping, R_a roughness parameters versus dopant content was given in Fig. 3 (a_3, b_3,and c_3) respectively. Table (2) represents the values of AFM parameters.

Table 2. AFM parameters of the deposited films

Samples	Average Particle size nm	Roughness Average (nm)	R_{rms} (nm)
Fe_2O_3	72.46	10.2	11.9
Fe_2O_3: 1% B	71.53	4.40	5.24
Fe_2O_3: 1% B	59.87	3.75	4.43

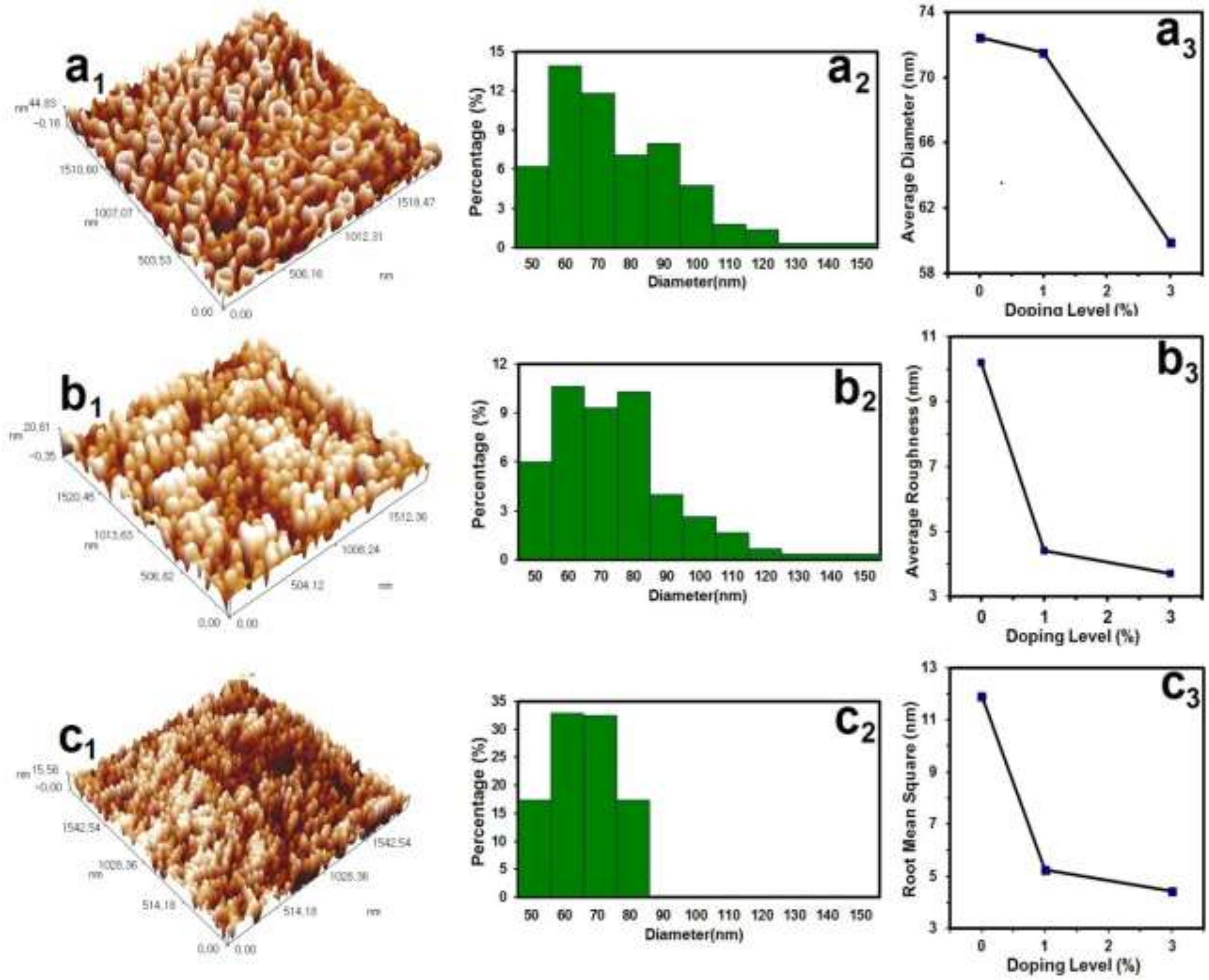

Fig. 3. AFM images of the prepared films (a_1, b_1 and c_1), granularly distributed (a_2, b_2 and c_2) and variation of AFM parameters via doping (a_3, b_3 and c_3)

Figure (4) displays transmittance spectra of pure Fe_2O_3 films for (Fe_2O_3:1% B, Fe_2O_3:3% B). It is seen that maximum transmittance was75% forFe_2O_3.

Fig.5 shows the absorption coefficient(α) decreased with an increase at 1% or 3%doping.

The bandgap energy Eg was estimated from the relation below[26,27]:

$$(\alpha h\nu) = A\left(h\nu - E_g\right)^{\frac{1}{2}} \quad (4)$$

Where A is the constant, $h\nu$ is the photon energy. Figure 6 shows relationof $(\alpha h\nu)^2$ vs. $h\nu$. The bandgap of Fe_2O_3 film for the three films is 2.65, 3.0 and 2.45 eV, respectively. It is clearly observed that with decrease of films, the optical bandgap was found to be decreased with doping content

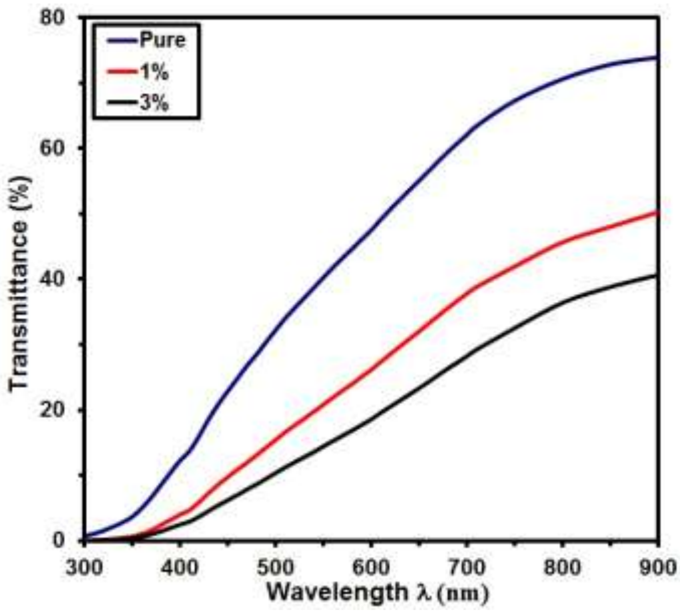

Fig.4. Transmittance for the prepared films.

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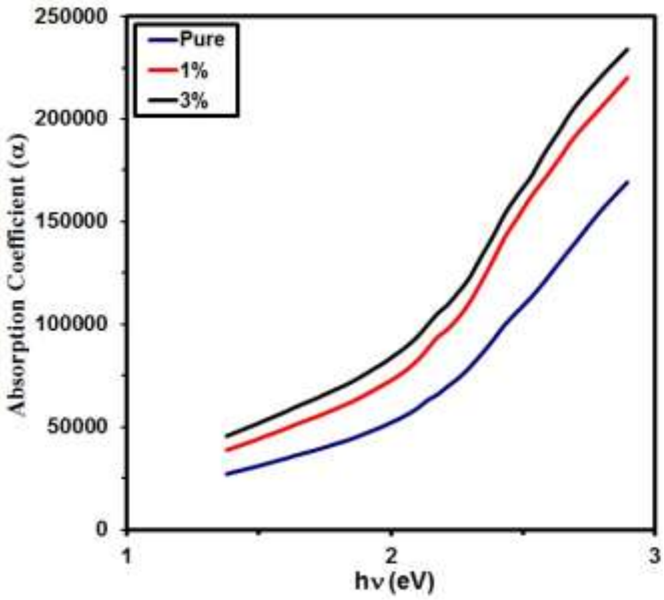

Fig. 5. α Vshν of the prepared thin films

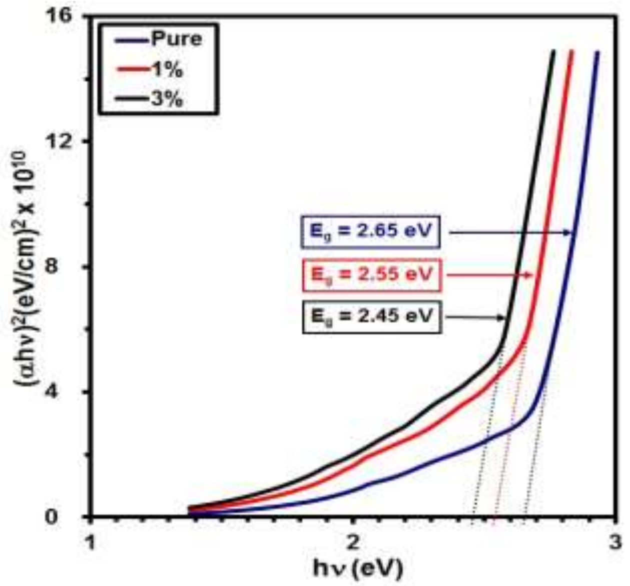

Fig. 6. $(\alpha h\nu)^2$Vshν of the prepared thin films

Conclusion

Fe_2O_3 films are prepared under various B dopants, The structure was rhombohedral with a preferred peak in (100). Surface morphology of the prepared films was studied using atomic force microscope (AFM). The grain size was in the zone of (72.46), (71.53) and (59.87) nm for the (Fe_2O_3, Fe_2O_3:1% B, Fe_2O_3 :3% B) respectively.

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