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Effect of Lanthanum Doping on the Optical Properties of Hematite (α -Fe₂O₃) Thin Film

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Abstract

Hematite (α -Fe₂O₃) thin films are formed on the surface of the precursor solution. The effect of lanthanum (La) doping on the optical property and an effect of deposition conditions of the film morphology has been studied. The α -Fe₂O₃ films formed on the surface of solution were transferred to the glass substrate. XRD, SEM and UV-Vis spectroscopy techniques have been used for the structural, morphological and optical characterizations of the films. The as deposited films were observed crystalline as analyzed by XRD. Depending upon the deposition conditions the films have thickness 400 nm, and are optically transparent and smooth surface morphology. Also, a variation in the optical band gap with the La concentration in the film has been observed.

Keywords: Hematite thin films, Band gap, lanthanum

1. Introduction

Hematite (α -Fe₂O₃) is a thermodynamically stable iron oxide with corundum hexagonal closed packed crystal structure. It is a semiconducting material with an optical band gap around 2.0 eV [1]. The nanocrystalline α -Fe₂O₃ has attracted a great deal of attention over the past decade due to a wide range of applications in chemical industry as active catalytic, non linear optical material, as photo electrode and gas sensors to detect combustible gases like CH₄ and C₃H₈ [2]. Although, the physical preparation method such as chemical vapor deposition (CVD) and laser assisted CVD result into excellent thin films quality, they have some shortcoming from the point of view of wide usage for e.g. lack of flexibility and cost effectiveness [3].

Now a days, great attention has to be drawn to miniaturization of electronic devices. For this reason, surface and interfacial phenomena play an important role in the device performance. One of the main characteristics of the electronic state of the surface is the energy band gap. Thin film of α -Fe₂O₃ (with no added metal dopants) has been extensively studied with reported photo conversion efficiency of up to 2% for water splitting. So,

adding element such as B, Al, In and Ga, Mo, Cr, Si improve the range of solar radiation absorption and conductivity of α -Fe₂O₃ film [3-7]. In the present paper, the α -Fe₂O₃ film is doped with La and variation in the optical properties has been studied.

2. Experimental

Iron salts FeCl₂ and FeCl₃ each in with 24 mM were added in a flask containing 32 μ M solution of PVA. The solution was heated at 70°C for 30 minutes on magnetic stirrer and then transferred in a petri dish placed inside an argon (Ar) gas chamber with a volume of 2 litres. A measured volume (120 cm³) of the NH₃ vapor was poured deliberately inside the chamber containing solution filled petri dish. In this process, the NH₃ vapors react with the surface of the solution and a floating film was formed on the solution surface within 15 minutes after the NH₃ was poured. After the formation of film, it was transferred to the glass substrate and annealed at argon gas environment at 500°C temperature. The film was doped with 5% concentration of Lanthanum by adding Lanthanum (III) chloride heptahydrate in initial precursor solution. Thus formed film (α -Fe₂O₃) was characterized by Field Emission Electron Microscopy (FESEM), X-ray Diffractometer (XRD) and UV-Vis-NIR spectrophotometer.

3. Result and Discussion

Figure 1 shows the XRD patterns of α -Fe₂O₃ and La-doped α -Fe₂O₃ thin films annealed at 500°C temperature. All the peaks in the figure 1 matched the standard data for α -Fe₂O₃ (JCPDS 33-664). The XRD pattern shows no phase change with the lanthanum doping although the peak become sharper with La doping. The increase in the peak intensity with lanthanum doping shows increase in crystallinity and grain size within the thin film due to La doping.

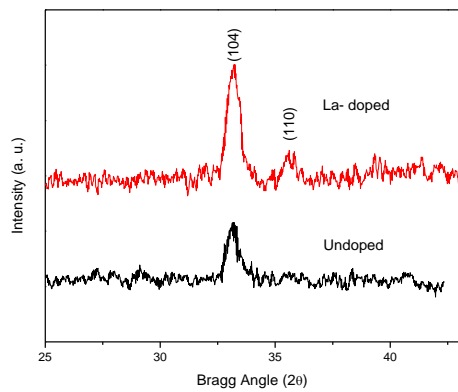


Figure 1 XRD patterns of the α -Fe₂O₃ and La doped α -Fe₂O₃ thin film.

Figure 2(a) & (b) shows the SEM micrograph of the α -Fe₂O₃ and La-doped α -Fe₂O₃ thin film deposited on the glass substrate and annealed at 500 °C temperature respectively. Figure 2(a) is the SEM image of the α -Fe₂O₃ thin film which shows very small grain of the particles with smooth surface. Figure 2b is the La doped α -Fe₂O₃ film shows increase in the grain size and clustering of the particles with La doping in α -Fe₂O₃ thin film

The thickness of the all film is measured with the profillometer and found to be 400 nm. The optical property of the α -Fe₂O₃ film deposited on the glass substrate and annealed at 500°C temperature has been studied by the UV-Vis-NIR spectrophotometer. With the doping of La in α -Fe₂O₃ thin film a red shift is observed.

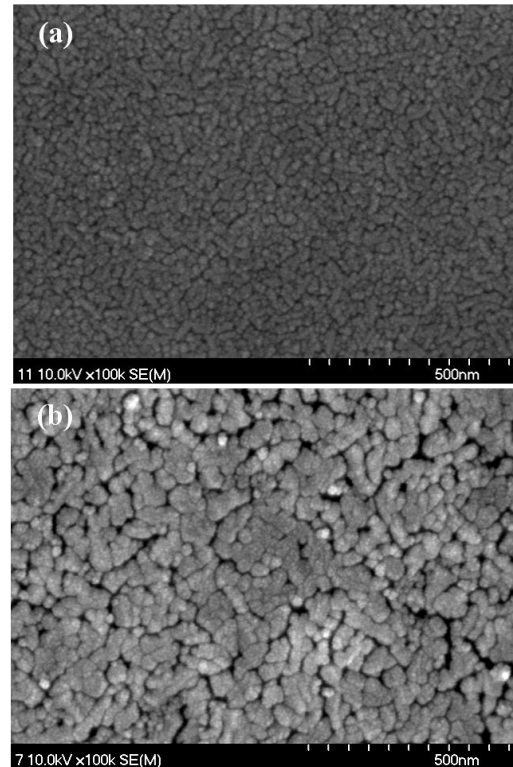


Figure 2 (a) SEM images of the undoped α -Fe₂O₃ thin film and (b) the α -Fe₂O₃ film doped with 5% La.

Figure 3(a) shows the transmission spectra of α -Fe₂O₃ and La doped α -Fe₂O₃ thin film and all the samples have high transmission in the visible and IR region. The results shows a decrease in transmission with La doping this is due to large absorption resulting from the large grain size in La doped thin film.

The optical absorption coefficient α can be calculated as

$$\alpha = (1/t) \ln (1/T) \quad (1)$$

Where T is the transmission & t is the thickness of the film. Further, the optical band gap (E_g) was determined using the following “Tauc,s relation”[8]:

$$ahv = C_1 (hv - E_g)^n \quad (2)$$

Where h is Planck’s constant, C_1 is a constant and prefix n has values 0.5 and 2, respectively for a direct and indirect band gap transitions.

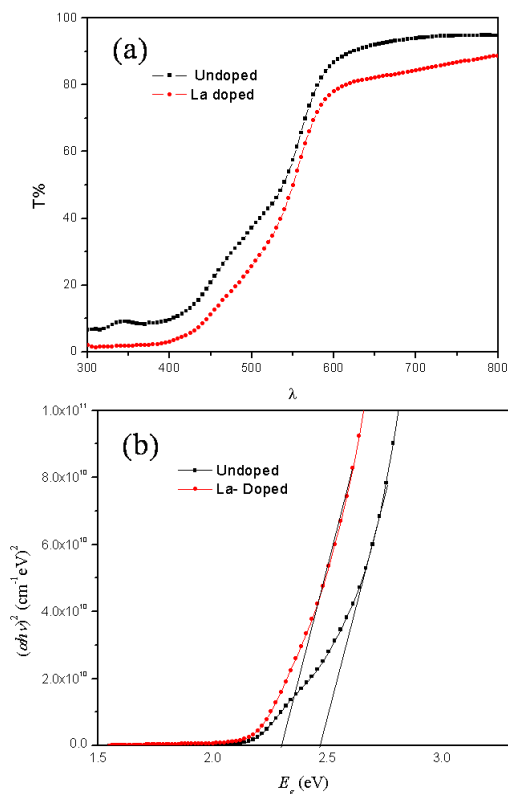


Figure 3(a) Transmission spectra, (b) band gap (E_g) of the α - Fe_2O_3 and La-doped α - Fe_2O_3 thin films.

The direct band gap values (Fig 3b.) of the undoped and La doped α - Fe_2O_3 films are 2.47 and 2.30 eV, respectively. This indicates that the optical band gap decreases with the La doping in α - Fe_2O_3 thin film. The decrease in the band gap with La doping can be explained on the basis of increase in particle size of the thin film with La doping as seen in the SEM images. Further, as observed from the XRD and SEM results, the size of particles and crystalline inside the film is changed with La doping.

4. Conclusion

Doped and undoped α - Fe_2O_3 thin film are prepared by using simple chemical method. The band gap variation is found with the La doping in α - Fe_2O_3 thin film. The band gap measured from optical properties shows variation in values which are found to be related to size of the nanoparticles inside the film. In this study the size of α - Fe_2O_3 grain also increase with the La doping. The band gap tunability and strong optical absorption with high chemical stability make this material a

potential candidate for many nanotechnology based application.

5. Acknowledgements

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6. References

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