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STRUCTURAL AND OPTICAL ANALYSIS OF $Mg_{0.625}Zn_{0.375}Fe_2O_4$

Physics

KEYWORDS: co-precipitation, absorbance, spinel, band gap, stokes shift

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ABSTRACT

Magnesium zinc ferrite is one of the known soft ferrite. Magnesium zinc ferrite has useful magnetic and dielectric properties. $Mg_{0.625}Zn_{0.375}Fe_2O_4$ has been prepared by co-precipitation method. The investigation for structural parameters and optical properties has been carried with the help of X-ray diffraction, UV-Visible spectrophotometer and photoluminescence (PL) spectrometry. The X-ray diffraction studies reveal the formation of spinel phase structure. The crystallite size has been calculated with the help of Scherrer formula. The band gap calculated with the help of Tauc,s plot comes out to be 3.03 eV. There is stokes shift in the ferrite sample, which may be due to some electron-phonon interactions and lattice defects.

INTRODUCTION

Magnesium zinc compound is one of the known ferromagnetic oxide or also called as ferrite. The formula for these oxides is M Fe_2O_4 where M is divalent metal ion such as Mg^{2+}, Zn^{2+}, Ni^{2+} etc [1]. Magnesium Zinc ferrite is a soft ferrite. Magnesium zinc ferrite has useful dielectric and magnetic properties. Due to higher value of electrical resistivity, high curie temperature and low cost, magnesium zinc ferrite is useful for high frequency range applications [2]. Magnesium zinc ferrite has useful dielectric properties over wide frequency range [3]. Magnesium Zinc ferrite is beneficial as low hysteresis loss material, high density media storage, recoding and as sensor device [4]. Magnesium zinc ferrites have inverse spinel structure in which divalent magnesium occupy the octahedral site while Zinc occupies tetrahedral sites. Both magnesium and zinc divalent ions are diamagnetic in nature but their distribution in lattice sites affects the properties of ferrites very much [3]. The synthesis of magnesium zinc ferrite has been reported by various chemical and solid state reaction methods. For obtaining high purity magnesium zinc ferrites co-precipitation method has been used [5]. Co-precipitation route is less toxic, environment friendly and economic [4]. In this paper, we report the $Mg^{0.625}Zn_{0.375}Fe_2O_4$ sample prepared by co-precipitation route and characterized for structural and optical parameters.

EXPERIMENTAL

$Mg_{0.625}Zn_{0.375}Fe_{2O4}$ has been synthesized by co-precipitation route. The $FeCl_36H_2o$, $MgCl_26H_2o$ $ZnCl_2$ and NaOH chemicals are of AR Grade. The sodium hydroxide is used as precipitating agent. Magnesium, Zinc and Iron chlorides have been added in the 100 ml de-ionized water in stoichiometric amount. The chloride salts solution have been put drop wise in the 100 ml sodium hydroxide solution and solution has been kept on magnetic stirrer for mixing and heating. The reaction temperature has been kept at 358 K for one hour and continuously stirred till the reaction completes. The pH during the reaction has been maintained between 11 and 12. After the process completes, all the precipitates have been formed and settle down. The precipitates have been washed several times with distilled water. The washed ferrite precipitates have been dried at 373 K for 12 hours. After drying, the powder has been crushed with granite mortar pestle. The dark brown coloured powder has been obtained. After crushing, the powder has been subjected to sintering at 1173 K for three hours. The X-ray diffraction study of the sintered ferrite powder has been carried out using Rigaku Mini Flex II Diffractometer equipped with Cu Kα radiation (λ = 1.5418 Å). UV-Visible absorption spectrum has been taken in the wavelength range from 200 nm to 400nm, using Perkin Elmer UV-Vis-NIR spectrophotometer at room temperature. The Perkin Elmer LS-55 has been used to take the fluorescence spectrum.

RESULTS AND DISCUSSION

(a) X-ray diffraction (XRD) analysis..

The structural analysis of samples has been investigated by the X-ray diffraction peaks of powdered sample. Figure 1 shows the XRD pattern of Magnesium Zinc ferrite sample. All the obtained reflections signify the single phase spinel structure. The peaks are indexed as (220), (620), (311), (222), (400), (331), (422), and (511). All these peaks are the signature of single phase spinel structure (JCPDS card no 73-2410, 22-1012 and 02-1044)

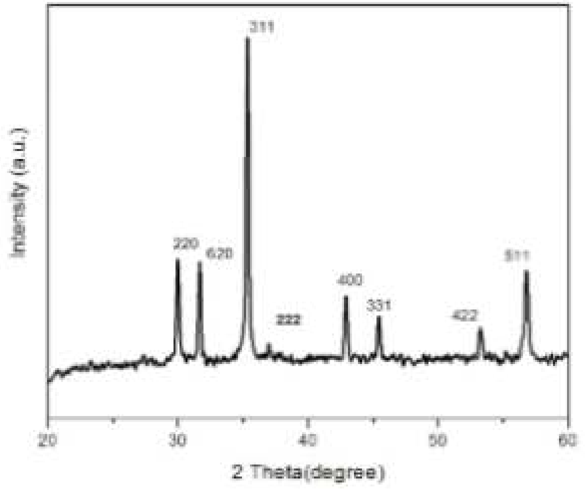


Fig 1: XRD pattern of $Mg_{0.625}Zn_{0.375}Fe_2O_4$

The crystallite size of the powdered sample has been calculated according to Scherrer formula [6]

$$D = 0.89\,\lambda / \beta \cos\theta$$

Here D is the average crystallite size, λ is the X-ray wavelength, β the full width at the half maximum and θ is the Bragg angle. The lattice constant (a) is calculated with the help of following equation [7]

$$a = d\,(h^2 + k^2 + l^2)^{1/2}$$

where h, k, l are the miller indices of the indexed diffraction peak and d is inter planar spacing. The strain εstr has been calculated by utilizing the Stokes Wilson relation [8],

$$\varepsilon_{str} = \beta / 4\tan\theta$$

By using the size of the crystallites (D), the dislocation density (δ), has been calculated using the relation [9]

$$\delta = 15\varepsilon / aD$$

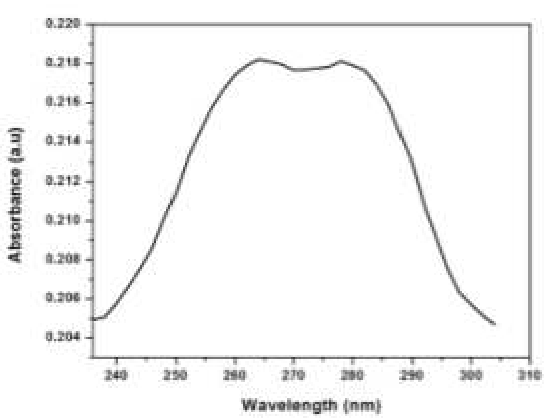
The packing factor (P) has been calculated using the equation [10].

$$P = D/d$$

These parameters have been calculated using diffraction peak indexed as (311), in the XRD profile. The crystallite size calculated from the XRD diffraction is 33.1 nm. The lattice constant of the synthesized ferrite is found to be 8.36 Ao. The lattice constant remains almost close to the values reported in the literature [2]. The packing factor for the synthesized ferrite has been calculated as 130.9. Strain, dislocation density and inter-planar spacing calculated for the synthesized ferrite comes out to be 0.003, 0.0162 x10-3 Å-2 and 2.53 Å respectively.

(b) UV-Visible absorption and Photo -luminescence studies.

UV-Visible absorption spectrum of Mg0.625Zn0.375Fe2O4 has been taken in the wavelength range from 200 nm to 400 nm. The UV-Visible absorption spectrum is due to the electronic transitions in the molecule [12]. By absorbing the photon energy, electron jumps from the lower energy band to higher energy band. The UV-Visible spectrum shows the maximum absorption peaks at 264.15 and 278.15 nm [11]. The figure 2 shows the UV-Visible absorbance spectrum.



Mg0.625Zn0.375Fe2O4.

The measured absorbance (A) has been used to calculate the absorption coefficient (α) using the formula [13].

$$\alpha = 2.303 \log (A) / t$$

where A is the absorbance and t is the thickness of the sample.
The optical band gap Eg has been calculated from optical absorption coefficient (α) near the absorption edge.

$$(\alpha h\upsilon)^m = C(E_g - h\upsilon)$$

where C is a constant, Eg is optical band gap, h is Plank's constant, υ is the frequency of incident photon, m is power coefficient and its value depend on the possible electronic transitions. i.e (m=1/2 for direct band materials and m=2 for indirect band materials.

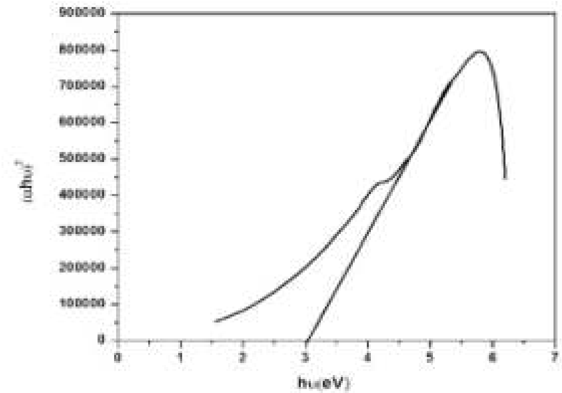


Figure 3: Tauc's plot- $(\alpha h\upsilon)^2$ v/s hυ for $Mg_{0.625}Zn_{0.375}Fe_2O_4$

The optical band gap has been obtained by plotting (α hυ)^2 vs. h as shown in the Figure 3 by extrapolating the linear portion of absorption edge in the photon energy axis which gives optical band gap[12,13]. The value of the calculated optical band gap is 3.03 eV. For the magnesium ferrite the reported values for the band gap is from 2.15 to 1.42 eV for different method [6]. The value of the band gap decreases with increase in magnesium content [6].

The Perkin Elmer LS-55 has been used to take the fluorescence spectra of $Mg_{0.625}Zn_{0.375}Fe_{2O4}$. In photoluminescence the emission of light takes place from a material when it is under optical excitation. Absorption of photons leads to electronic excitation. These excitations then relax and electron returns to ground state. PL takes place with radiative relaxation [14].The fluorescence spectrum show broad band emission around 333 nm and 345 nm. There is difference between the peaks of absorbance and photoluminescence. The energy difference between absorbance and PL emission peaks is termed as stokes shift [15,16]

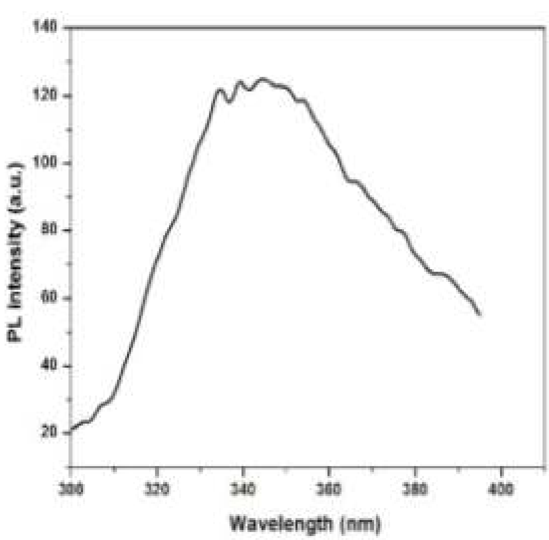


Figure 4: PL spectrum for $Mg_{0.625}$ $Zn_{0.375}Fe_{2O4}$ at room temperature

CONCLUSION

$Mg_{0.625}Zn_{0.375}Fe_2O_4$ has been prepared by co-precipitation method. The formation of single phase spinel structure has been confirmed by the X-Ray diffraction pattern. The crystallite size comes out to be 33.1nm.The maximum absorbance peaks are at 264.14 and 278.15 nm, as shown by the UV-Visible study. The value optical band gap calculated with taucs, plot is 3.03 eV. The PL maximum peak is at 344 nm. There is stokes shift of 80 nm.

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