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Study of Structural and Optical Properties of Fe^{2+} Doped Tin Oxide Nanoparticles

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Abstract: Tin dioxide nanoparticles (SnO_2) were synthesized by a sol-gel method. And tin tetra chloride ($SnCl_4$) and ammonium hydroxide (NH_4OH) were used as the precursor. NH_4OH maintain the homogeneity and stoichiometry of solution through pH. The obtained powder subjected to calcination about 110ºC. The obtained samples are characterized by X-ray diffraction, Scanning electron microscope, Fourier transform infrared spectroscope and UV-Visible spectroscopy. From the characterizations it is confirmed that the tetragonal structure and the particles are small and nanosizes, The O-H stretching and C=C bending stretching with chemical compositions are analyzed. The improved conduction properties through lower bandgap and the results are further interpreted and discussed.
Keywords: Tin oxide; Fe^{2+}; Sol-gel techniques; Electrical; Optical.

1. Introduction

In recent years the need of semiconductor are very important for functional and active devices. The active devices such as diode, triode and thin film for mass saving purpose are the demand in few decades. Tin oxide semiconductor possess the transparent, highly stable even upto 500ºC in air, physical, chemical and good absorber etc., SnO2 is an IV-VI groups of semiconductor with n-type, the range of band gap from 3.6 to 3.8 eV [1-3]. It is a potential candidate for gas sensing materials such as CO and O_2 for better environment. For this low bandgap and active nature, it can be widely used in many active materials such as semiconductor devices, electrochemical devices such capacitors, condenser, charge storage devices such as batteries and it act as better catalysis rather than other metal oxides [4-6]. It is an ideal candidate used for oxidizing agent for CO, propane, and sometimes used as oxidation reduction in NO, NO_2 to N_2, esterification, hydrogenation and etc., it is a good catalyst especially for organic compounds [7-9].

Materials (SnO2) with large surface area lead to large number of contacts with active groups, and they have large chance to produce various active groups CTAB, AOT and etc. The researcher encounter a problem with removal of surfactant from the sample, ie sample free from surfactant, goods and products. SnO2 can be synthesized by many methods such as combustion, co-precipitations, sol-gel techniques, slow-evaporation, hydrothermal, polymerization and precipitations and etc [10-12].

In this present work the authors adopted a sol-gel method for control over particle size, uniformity, pure and cost effective for synthesis SnO_2 with Fe2+ dopant.

2. Sample preparations

The mixture of tin-tetrachloride-pentahydrate and ammonia water of their purity is 99 %. In order to maintain the tin-oxide nanoparticles through NaOH, and from their pH through maintain homogenity and stoichiometry of the solutions. Initially 2.94 g of tin tetrachloride was added to 50 ml water stirring and added with Ferrous oxide is added to the above mixture and again stirred till its forms the clear solution form a gel phase. The surfactant NaOH is added to the above sol slowly drop wise while stirring about 30 minutes to form a gel. In this process,

the additional ammonia conert tin chloride into tin hydroxide. After thorough washing the precipitation with deionized water removed the other products. Finally the sample collected through the normal procedure [13, 14].

3. Characterization techniques

The structural and phase identifications of a samples analysis through powder X-ray diffraction technique [14]. The surface features and composition analysis carried out through scanning electron microscope [15]. Type of chemicals, stretching and vibration identified through Fourier transform infrared (FTIR) spectroscopy [16, 17]. The optical absorption study performed through UV-Visible absorption spectroscopy [16].

4. Results and discussions

The crystallographic data of SnO_2 powders were collected by using XRD data which is shown in Figure.1. From the observation the (hkl) planes depicts the sample is SnO2 with tetragonal structure and it matches well with standard reference (JCPDS card no. 41–1445). The XRD pattern of the sample exhibit the characteristic peak at 2θ = 26.6°. The peak at this angle causes more broadened, it meant for nanosized particles. The size of the particles are computed from the XRD observation through the known Scherer formula

$$D = \lambda k/\beta cos\theta \quad (1)$$

where, D is the average particle size, λ – wavelength of X-ray source, k - constant (0.9) and β – full width half maximum (FWHM) in radians for the diffraction angle (2θ). The diffractions angles with hkl values are given in Table.1 is 26.6, 33.8, 37.9, 51.8, 54.7, 61.9, 65.9 and 78.4 with 100, 101, 200, 211, 220, 310, 301 and 321 respectively. The average particle sizes determined at the intense peaks of (110) at 26.6 degree (2θ). By this sol-gel method the growned particle is 63.68 nm [17].

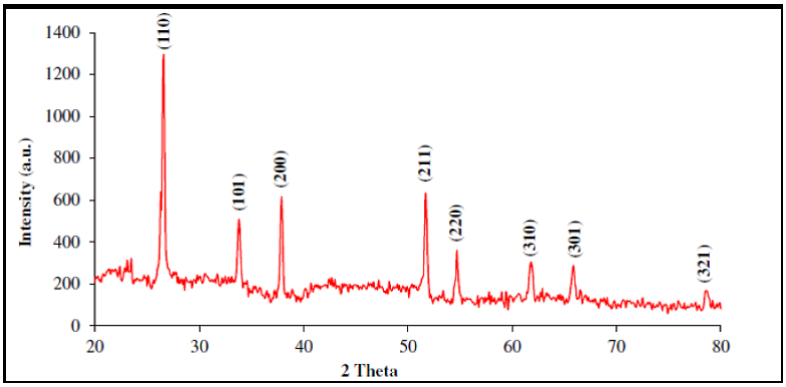

Figure.1. X-ray diffraction pattern of Fe doped tin oxide powder prepared by sol-gel method

Table.1. Diffraction angles and respective (hkl) values,

Peaks (2θ)	hkl
26.6	110
33.8	101
37.9	200
51.8	211
54.7	220
61.9	310
65.9	301
78.4	321

The SEM micrographs of SnO_2 nanoparticles at various magnifications are shown in Fig. 2. (a) and (b) of 500nm and 2μm magnification respectively. From the figures it can be observed that the particles are fine, finer and forms large clusters. The mean size of particles from this SEM analysis 69 nm, and it is slightly greater than XRD analysis [12]. These marginal changes in sizes may due to different shape of molecules and texture. Even though, both these experimental observations confirmed that the synthesized particles are in nano phase.

The FTIR spectrum of Fe doped SnO_2 nanosized particles in the range of 400- 4000 cm-1, are shown in Figure 3. From the same Figure.3, the O-H stretching at observed at 3389.86 cm-1, aromatic C=C bending stretching at 1631.56 cm-1, alkyl methyl at 1400.75 cm-1, alkenes at 899.69 cm-1, chloroalkanes at 561.61 cm-1, and Iodoalkanes at 482.16 cm-1 and 428.20 cm-1 wavelengths. These characteristics absorption peaks and their functional groups also presented in Table.2.

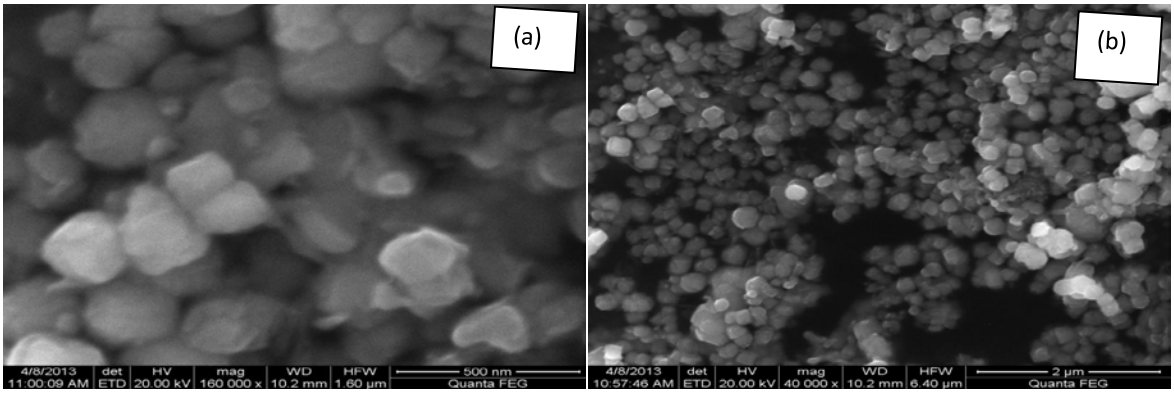

Figure.2. SEM image of Fe doped SnO2 sample for (a) (500 nm) and (b) (2 µm).

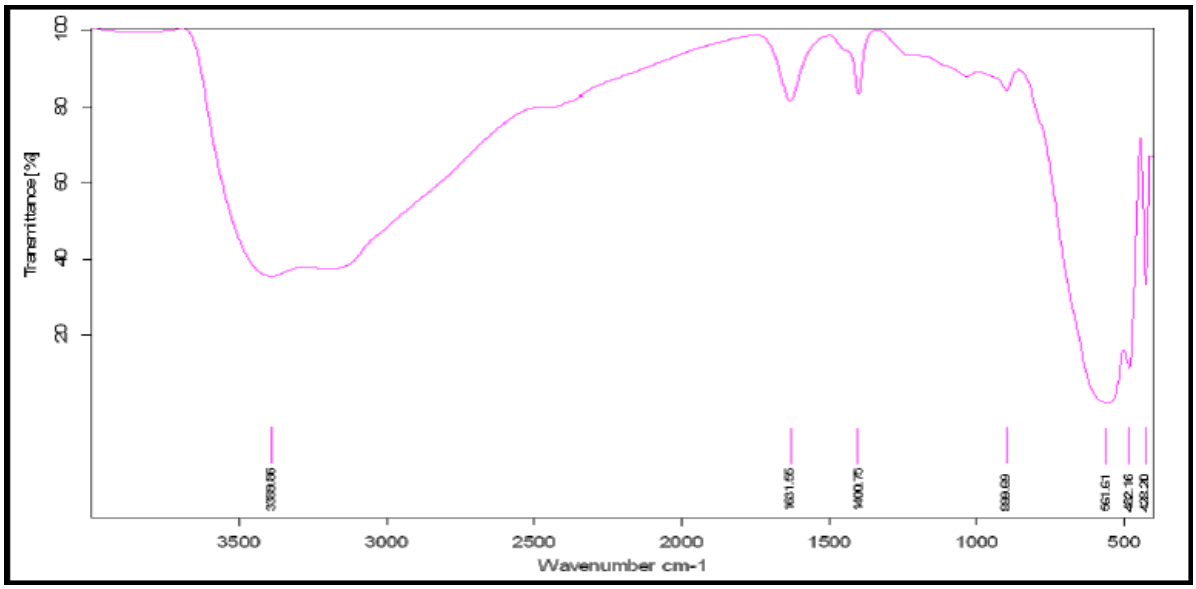

Figure.3. FTIR Spectra of Fe doped SnO_2 nanoparticles.

Table.2. FTIR spectral Data

Name	Functional group	Adsorption
Tin Oxide	Alcohol/Phenol O-H stretch	3389.86
	Aromatic C=C bending	1631.56
	Alkyl methyl	1400.75
	Monosubstituted alkenes	899.69
	Chloroalkanes	561.61
	Iodoalkanes	482.16
	Iodoalkanes	428.20

The size of particles such as spherical and different sizes like clusters are may be influenced the additional parameters of IR bands, the position, and their relative intensity. Ie, different size of particle is due to different nature of agglomeration [11, 15].

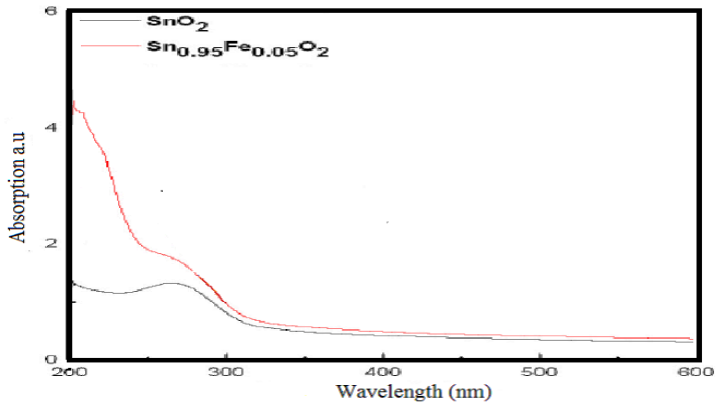

Fig.4. UV-Visible absorption spectra of SnO_2, $Sn_{0.95}Fe_{0.05}O_2$

UV- Vis Spectroscopy: In order to analyze the optical behavior of pure and Fe doped SnO2, the UV - Visible absorption spectra are recorded in the range of 200 nm to 600 nm is shown in Figure 4. The estimation of bandgap values for pure SnO_2 is 4.1 eV, but for doped with Fe ions the bandgap values is 3.87 eV. So, the decreasing band gap value is due to the more accumulation of donor energy levels of TM ions by Fe than the band gap of Sn. And this is evident that the Fe ions enhancing the conduction behavior and also having more absorption further indicating the more optical response [16-17].

5. Conclusions

Fe doped SnO_2 nanoparticles were synthesized by using sol-gel method. The tetragonal structure identified through XRD analysis. From Scherrer method using XRD datas and the SEM micrographs confirmed the particles are in nanophase. The FTIR spectra of SnO_2 show different peaks at different wave number. The presence of Fe ions enhancing the optical behavior and decreasing band gap is suitable for functional/active devices.

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