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STRUCTURAL AND OPTICAL PROPERTIES OF PURE AND COBALT DOPED TIN OXIDE NANOPARTICLES

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ABSTRACT

In this work, Tin Oxide (SnO2) nanoparticles doped with different concentrations of cobalt (0.2M and 0.5M) were synthesized by Microwave assisted method. The as-prepared samples were characterized by Powder X-ray diffraction (XRD), UV–visible spectroscopy, and Scanning Electron Microscopy (SEM). Powder XRD patterns of the samples are identified to be crystalline in nature having tetragonal structure. The UV – Visible Spectroscopy shows that the energy band gap increases with increase in the concentration of the dopant. The SEM images of pure and cobalt doped tin oxide nanoparticles clearly reveals the formation of nanoclusters which are predominantly quasi-spherical, uniform and nanodispersed.

KEY WORDS: *Metal oxides, Analytical Reagent grade, Ethylene glycol, Energy band gap and Topographical image*

1. INTRODUCTION

Nanoscience has been established recently as a new interdisciplinary science. Nanotechnology can be defined as a whole knowledge on fundamental properties of nano-size objects. Nanoparticles, generally considered as particles with a size up to 100 nm [1] and exhibit completely new properties or improved properties as compared to the bulk material that they are collected based on particular characteristics such as size, distribution and morphology. Recent developments in nanoscience and nanotechnology have brought potential building blocks for electronics, optoelectronics, medicines, solar cells and gas sensing property [2]. Nowadays, nanoparticles based on their electrical properties, optical properties [3], magnetic, chemical and mechanical properties are used in various areas, such as the medical sector for diagnosis, antimicrobial, drug delivery [4] and also used in the chemical sector for catalysis of environmental protection and energy conversion.

Metal oxide nanoparticles differ from their bulk analogs in chemical, thermal, optical, magnetic properties and are also widely used in catalysis, medicine, electronics etc., [5].

In the present study, pure and cobalt doped tin oxide nanoparticles have been prepared by simple microwave assisted method. Among the various semiconducting metal oxides, tin oxide has been the most popular gas sensing material. Tin oxide crystallizes in the tetragonal crystal system and is isostrucutral with rutile phase [6]. Magnetic properties of tin oxide nanoparticles are used in magnetic data storage and magnetic resonance imaging. They are used in energy-saving coatings and anti-static coatings as catalysts. As they have very good transparent mirror properties they are used as electrodes and anti-reflection coatings in solar cells [7]. They are used in the making of gas sensors, optoelectronic devices and resistors, transparent oven and liquid crystal displays. Tin alloy is used in superconducting magnets. Cobalt nanoparticles possess magnetic properties, which leads to applications in imaging, sensors and many other areas. Cobalt is very much useful in radio therapy. Cobalt doped tin oxide has a wide application in medical field.

2. OBJECTIVES

1. To synthesize the pure and cobalt doped tin oxide nanoparticles by a simple microwave assisted method.
2. To study the structural behavior of all the synthesized pure and cobalt doped tin oxide nanoparticles using PXRD.
3. To calculate the lattice parameters, crystallite size, lattice strain and dislocation energy of the prepared nanoparticles using PXRD data.
4. To analyze the optical transparency of the pure and cobalt doped tin oxide nanoparticles using the UV-Visible spectroscopy.
5. To identify the morphological of the pure and cobalt doped tin oxide nanopartcles using scanning electron microscope.
6. To determine the energy band gap of the pure and cobalt doped tin oxide nanoparticles by plotting Tauc plot.

3. METHOD OF PREPARATION

3.1Preparation of Pure Tin Oxide Nanoparticles:

Analytical Reagent (AR) grade of tin chloride, urea and ethylene glycol are used for the preparation of pure tin oxide nanoparticles. Tin chloride and urea in 1:3 molecular ratio are mixed and dissolved in 50ml of ethylene glycol. The solution is continuously stirred for 1 hour to make a homogeneous mixture. Then the solution is kept in microwave oven. Microwave irradiation is given to the solution till the solvent is evaporated completely. The colloidal precipitate thus formed is cooled at room temperature. Then the samples are dried in the atmospheric air and collected as the yield. Further the prepared samples are annealed at 500°C for 1 hour to improve the ordering.

3.2 Preparation of Cobalt doped Tin Oxide Nanoparticles:

The required amount of Analytical Reagent (AR) grade cobalt chloride is added separately to mixture of tin chloride and urea for the preparation of cobalt doped tin oxide nanoparticles. The dopant concentrations used in the present study are 0.2M, 0.5M. Thus these mixtures are also allowed for further steps as per the previous process [8]. The yield percentage was measured individually. The collected samples appeared in different colors were compared to pure tin oxide nanoparticles. All the prepared samples are kept in air tight bags for characterizations.

4. CHARACTERIZATION

The pure and cobalt doped tin oxide nanoparticles were examined using Powder XRD, UV-Visible spectroscopy and SEM.

4.1 Powder XRD:

The crystalline nature of the prepared pure and cobalt doped tin oxide nanoparticles were investigated by X-ray diffraction technique as shown in Fig. 1, 2 and 3. All the prominent peaks were indexed for the tetragonal structure of tin oxide. In the case of pure tin oxide nanoparticles the three predominant characteristic peaks were observed at 51.7389°, 26.5420° and 33.8770°. Pure tin oxide are indexed and compared with JCPDS [file no: (41-1445)] data [9]. In case of 0.2M cobalt doped tin oxide nanopartcles the characteristic peaks were observed at 51.9554°, 26.8516° and 34.1211° and in the case of

0.5M cobalt doped tin oxide nanoparticles the characteristic peaks were observed at 51.8225°, 26.7117° and 33.9306°. Table 1, 2 and 3 shows the indexed data of pure and cobalt doped tin oxide nanoparticles. The lattice parameters of pure and cobalt doped tin oxide nanoparticles are listed in the Table.4.

The average crystal size of the pure and cobalt doped tin oxide nanoparticles were calculated from the diffraction peaks using the Debye-Scherrer's formula [10], $D = \frac{K\lambda}{\beta \cos \theta}$ where D is the mean diameter of the grains, K (=0.9) is the size factor, β is the full width at half maximum (in radians), λ is the wavelength of the X-radiation used and is the Bragg diffraction angle. The lattice strain and the dislocation energy were also calculated using the relation $\Sigma = \beta \cos \theta$ and $\delta = \frac{15\,\Sigma}{aD}$. The calculated values are summarized in the Table.5.

4.2 UV – Visible Spectroscopy:

The optical absorption studies for pure and cobalt doped tin oxide nanoparticles were studied. All the prepared samples have maximum transmission in the entire visible region [11]. The lower cut off wavelength of pure, 0.2M and 0.5M cobalt doped tin oxide nanoparticles are at 400nm, 370nm and 340nm respectively. The lower cut off wavelength of cobalt doped tin oxide nanoparticles decreases when the concentration of impurity increases in the pure tin oxide nanoparticles[12].

The energy band gap of the samples were calculated using Tauc relation and are shown in the figures 7, 8 and 9 respectively.

$$\alpha h\nu = A\,(h\nu - E_g)^n$$

Where, $h\nu$ is photon energy, α is the absorption coefficient, E_g is the direct band gap energy, A is constant and the value of n depends on the type of transition. Table 6 shows that the plotting $(\alpha h\nu)^2$ versus (hυ) for all the samples, the energy band gap have been obtained[13].

4.3 SEM:

The morphology and topography of the samples were investigated using the imaging technique of Scanning Electron Microscope (SEM) as shown in figures 10, 11 and 12. It was understood that the tiny particles were joined together and forms an elongated spherical shape. From that, one can observe that the particle shapes changes at higher dopant concentration. This investigation shows that oxide particles have the tendency to form spherical agglomeration [14]. The rough and spongy surface morphology is evident which makes it difficult to estimate the crystalline size due to agglomeration of the particles. SEM shows doping process is often accompanied by major changes in morphology. From the images of pure and tin doped cobalt oxide nanoparticles, the shape of the nanoparticles is quasi-spherical but the actual size of the nanoparticles cannot be distinguished from the SEM image, since SEM shows only the topographical image [15].

5. CONCLUSION

Powder X-ray diffraction pattern of pure and cobalt doped tin oxide nanoparticles reveals that the synthesized nanoparticles have tetragonal structure. The lattice parameters of all the prepared samples have been calculated and it was found that the lattice volumes of the cobalt doped tin oxide nanoparticles are lower than the pure tin oxide nanoparticles. The sizes of the synthesized nanoparticles are in nanometer scale. The lower cut off wavelengths of all the prepared samples is measured and they are found to decrease with increasing dopant concentration. The energy band gap of pure and cobalt doped tin oxide nanoparticles are measured using Tauc Plot. It is inferred from Tauc plot, the energy band gap increases with increase in the concentration of the dopant. The SEM images of pure and cobalt doped tin oxide nanoparticles clearly depicts the formation of nanoclusters which are predominantly quasi-spherical, uniform and nanodispersed.

6. FIGURES AND TABLES

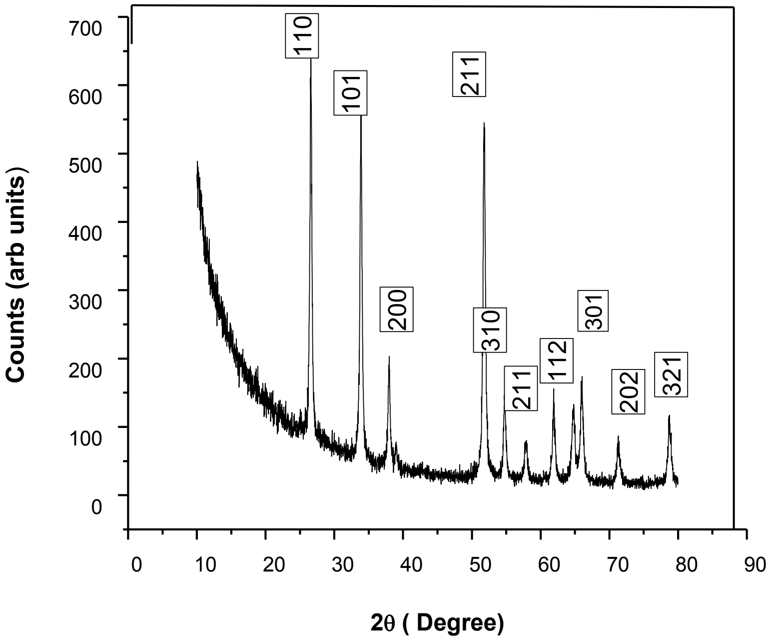

Figure 1. PXRD patterns of pure tin oxide nanoparticles

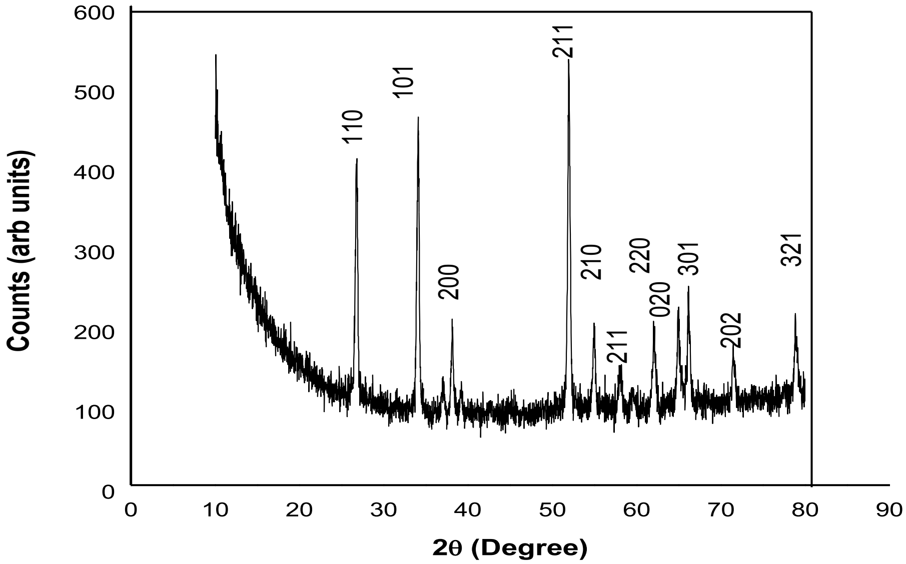

Figure 2. PXRD patterns of 0.2M cobalt doped tin oxide nanoparticles

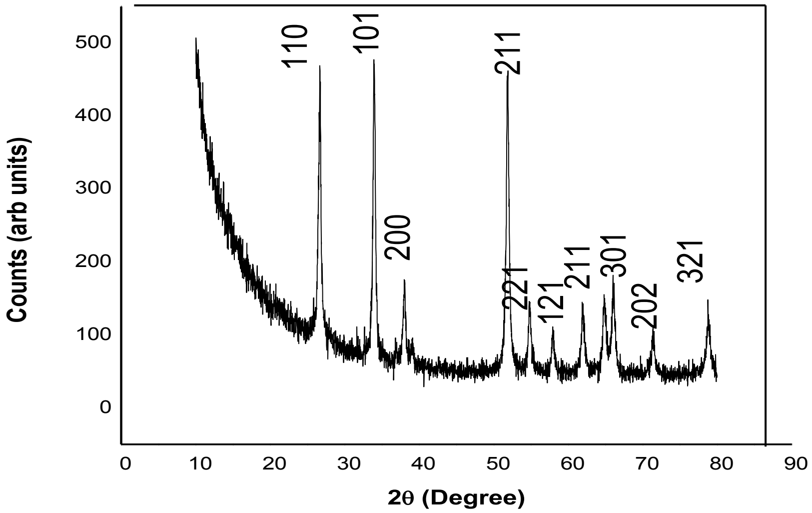

Figure 3. PXRD patterns of 0.5M cobalt doped tin oxide nanoparticles

S.No.	2θ (Deg)	d (Å)	h k l	Intensity (%)
1.	26.5420	3.35836	110	98.18
2.	33.8770	2.64613	101	98.57
3.	38.0055	2.36764	200	30.07
4.	38.9890	2.31016	111	6.32
5.	51.7389	1.76690	211	100.00
6.	54.7959	1.67534	220	23.58
7.	57.8894	1.59296	002	10.11
8.	61.9072	1.49887	310	22.65
9.	64.7653	1.43947	112	20.14
10.	65.8919	1.41756	301	25.59
11.	71.2684	1.32325	202	10.52
12.	78.6491	1.21553	321	17.66

Table 1. Indexed data of pure tin oxide nanoparticles

S.No.	2θ (Deg)	d (Å)	h k l	Intensity (%)
1.	26.8516	3.32035	110	78.01
2.	34.1211	2.62776	101	60.44
3.	37.0514	2.42639	200	9.01
4.	38.1414	2.35952	111	25.65
5.	39.2055	2.29790	210	6.40
6.	51.9554	1.76004	211	100.00
7.	55.0032	1.66951	220	21.85
8.	58.0758	1.58829	002	11.15
9.	59.4844	1.55400	310	4.55
10.	62.0995	1.49470	221	19.00
11.	64.9649	1.43553	112	26.75
12.	66.1823	1.41204	301	27.10

Table 2. Indexed data of 0.2M cobalt doped tin oxide nanoparticles

S.No	2θ (Deg)	d(Å)	h k l	Intensity (%)
1.	26.7117	3.33741	101	78.41
2.	33.9306	2.64207	110	99.21
3.	38.0454	2.36525	200	27.55
4.	39.0768	2.30517	111	6.60
5.	51.8225	1.76425	211	100.00
6.	54.8302	1.67437	220	21.19
7.	57.9794	1.59070	002	13.21
8.	61.9537	1.49786	221	21.46
9.	64.8645	1.43751	112	24.36
10.	66.0546	1.41446	301	28.85
11.	71.4347	1.32058	202	12.30
12.	78.7810	1.21383	321	18.84

Table 3. Indexed data of 0.5M cobalt doped tin oxide nanoparticles

Table 4. The lattice parameters of pure and cobalt doped tin oxide nanoparticles

Sample	Lattice constant			Lattice Volume
	a (Å)	b (Å)	c (Å)	V (Å)^3
Pure tin oxide nanoparticles	4.7494	4.7494	3.1736	71.59
0.2M Cobalt Doped Tin oxide nanoparticles	4.7198	4.7198	3.1969	71.21
0.5M Cobalt Doped Tin oxide nanoparticles	4.6957	4.6957	3.1893	70.32

Sample	Grain size D (nm)	Lattice Strain Σ (10^{-4}) m	Dislocation Energy (δ) (10^{14}) m^{-2}
Pure tin oxide nanoparticles	57.1543	6.3896	3.9340
0.2M cobalt doped tin oxide nanoparticles	29.1005	11.8005	12.9475
0.5M cobalt doped tin oxide nanoparticles	30.4571	11.6296	12.6781

Table 5. The grain size, lattice strain, and dislocation density of pure and cobalt doped tin oxide nanoparticles

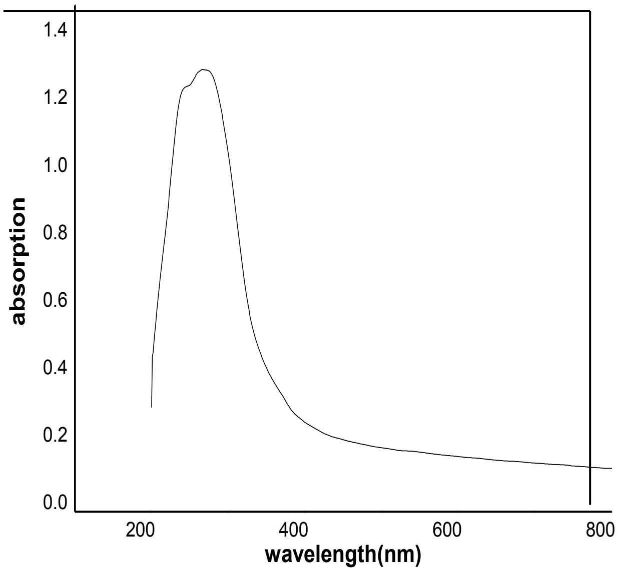

Figure 4. Absorption spectrum of pure tin oxide nanoparticles

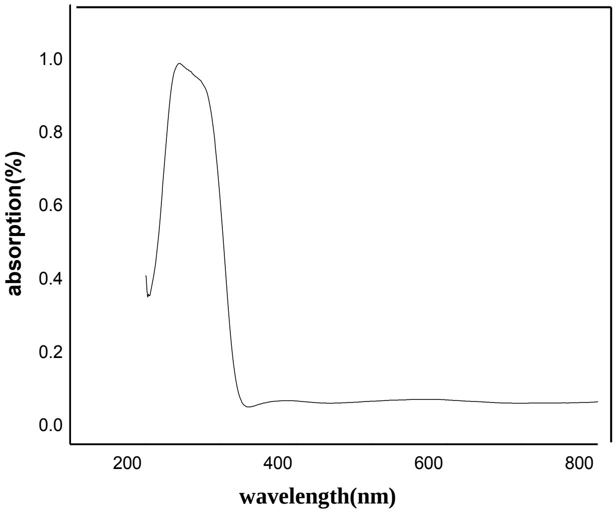

Figure 5. Absorption spectrum of 0.2M cobalt doped tin oxide nanoparticles

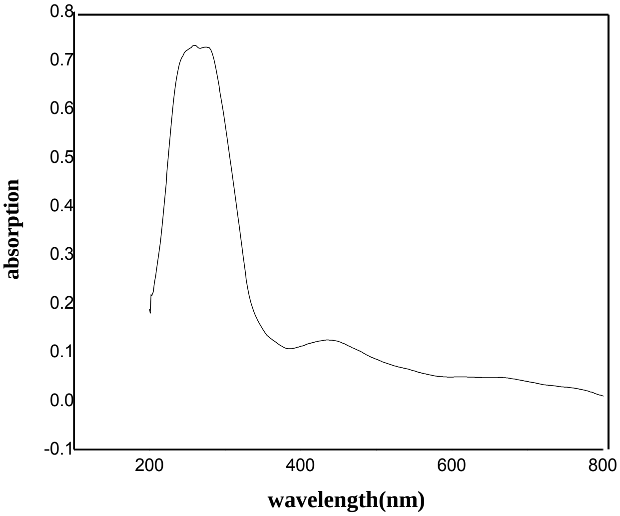

Figure 6. Absorption spectrum of 0.5M cobalt doped tin oxide nanoparticles

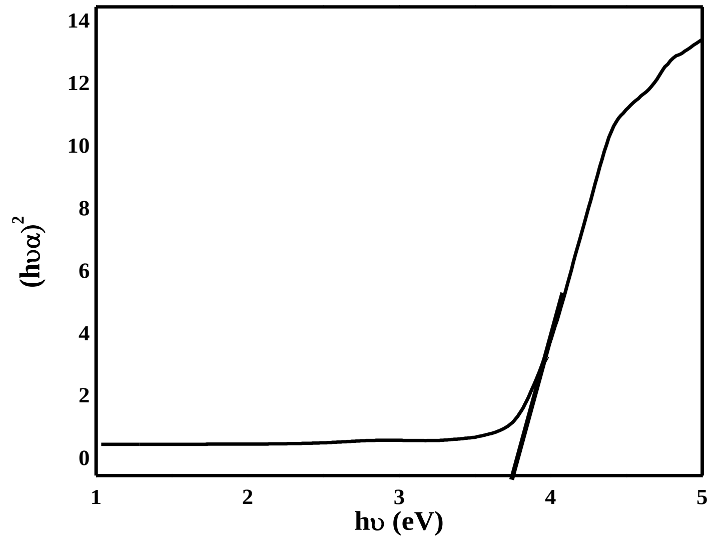

Figure 7. Tauc plot for pure tin oxide nanoparticles

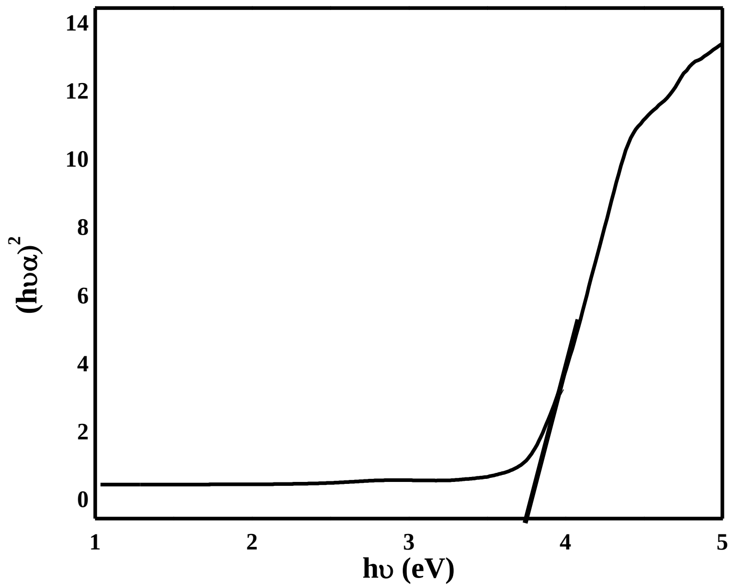

Figure 8. Tauc plot for 0.2M cobalt doped tin oxide nanaparticles

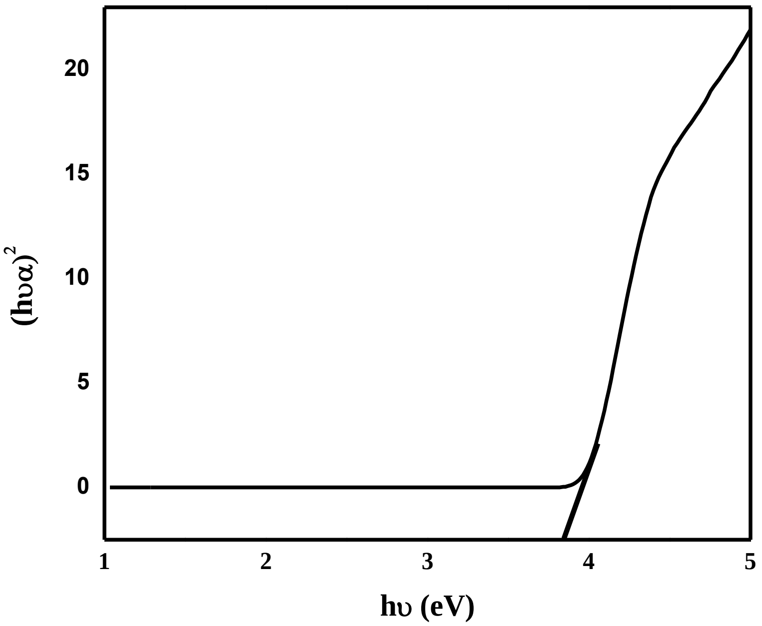

Figure 9. Tauc plot for 0.5M cobalt doped tin oxide nanaparticles

Prepared Samples	Energy Band gap (eV)
Pure Tin oxide nanoparticles	3.67
0.2M Cobalt doped Tin oxide nanoparticles	3.74
0.5M Cobalt doped Tin oxide nanoparticles	3.8

Table 6. The calculated energy band gap (E_g) for pure and cobalt doped tin oxide nanoparticles

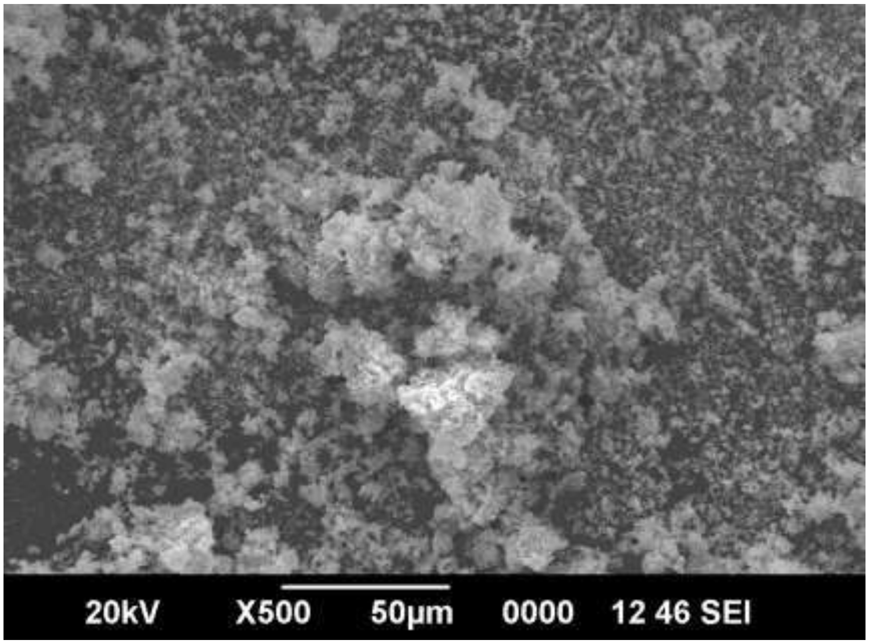

Figure 10. SEM image of pure tin oxide Nanoparticles

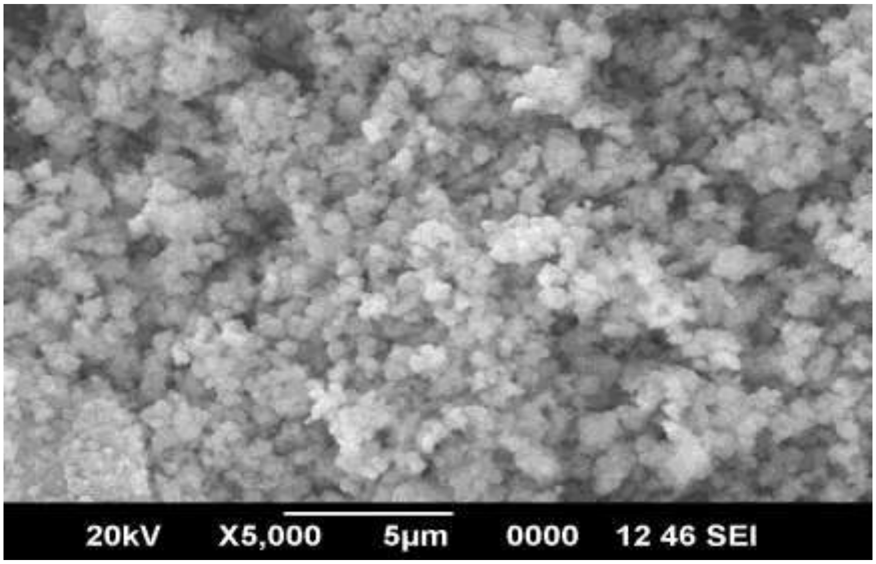

Figure 11. SEM images of 0.2M cobalt doped tin oxide nanoparticles

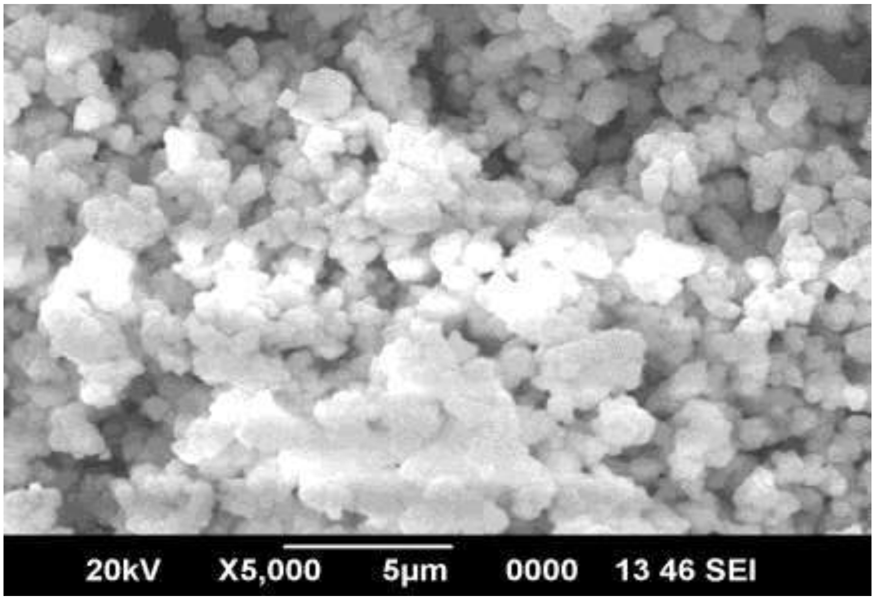

Figure 12. SEM images of 0.5M cobalt doped tin oxide nanoparticles

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