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Influence of pH on particle size and optical band gap of SnO_2 Nanomaterials

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Abstract: In this work SnO_2 nano particles were synthesized by Microwave assisted technique. The pH of the solution varied from 7 to 9 in step of 0.2. The particle size was calculated using Scherrer formula, it varies from 57 to 66 nm for different pH values. The functional groups were confirmed by FTIR spectra. The absorption spectrum was recorded from 1100 nm to 190 nm, and the optical band gap was calculated using Touc plot. The band gap value varies from 1.6eV to 5.5eV. From the above studies the optimum pH value was found from for good optical SnO_2 nano particles.

Introduction

Tin oxide (SnO_2), an n-type semiconductor with a wide band gap (E_g =3.62eV), is a key functional material that has attracted interests a candidate for optoelectronic devices, gas sensors, transparent conducting electrodes and catalyst supports SnO_2 nanostructures arises due to their high surface to volume ratio, large band gap, high exciton binding energy of 130 meV[1,2] at room temperature (300 K), remarkable resistivity variation in gaseous environment, mechanical, thermal and chemical stability etc. Optoelectronic properties[3] of SnO_2 depend on the presence of impurities and its with respect to oxygen. Recently various SnO_2 based nanoscale devices have been fabricated from zero to three dimensional SnO_2 building blocks, e.g., nanosheets, nanowires, nanoribbons, nanoparticles, nanowhiskers, nanobelts, nanotubes etc. using different synthesis techniques like spray pyrolysis , decomposition, sol-gel method laser ablation, chemical vapour deposition, solid state reaction etc[4,5,6,7].

In this paper, the SnO_2 nano particles a nanostructure and consist of lot of tiny nanocrystalline was successfully synthesized by microwave assisted technique. The structure and morphology information of the products was characterized by means X-ray powder diffraction (XRD), Optical properties of the products were carried out UV-vis and Photoluminescence (PL)

Experimental

0.1 M solution of Tin (II) chloride in deionized water was prepared. The pH solution was maintained 8 using liquid ammonia diluted with water. The resulting precipitate was washed with water more than ten times until no chlorine ions are detected (silver nitrate test). The precipitate was washed ethanol to remove ethanol to remove NH^+_4 ions. The resulting precipitate was irradiated with house hold microwave oven for 10 min. The radiation frequency was 2.45 GHz and its power up to 1kw.

The crystal structure and size of the resulting products was characterized by X-ray powder diffraction (XRD, JSO-DEBYEFLEX 2002 X-ray diffraction meter with Cu-Kα radiation, λ=0.1540nm). Optical properties of the products were carried out by Ultra-violet and Photoluminescence. The SnO_2 Nanostructures Synthesized via microwave assisted Technique.

Result and discussion

XRD analysis

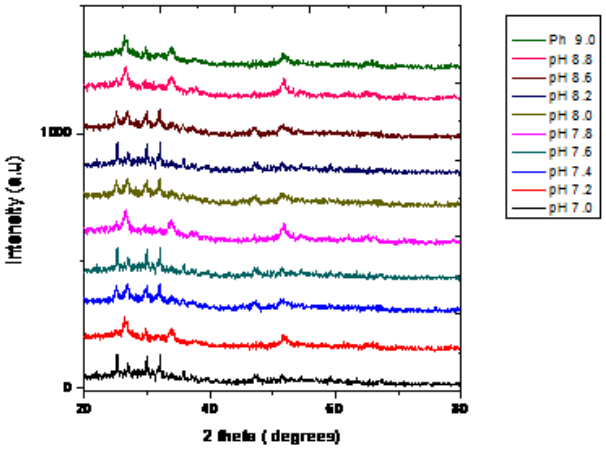

Fig. 1 XRD pattern of SnO_2 nano particles

The XRD pattern of the product is shown in Figure 1. The peaks at 2θvalues of 26.6°, 29.8°, 31.9°, 34.8°, 36.7° and 51.9°[1,13,15,19]. A matching of the observed and standard (hkl) planes confirmed that the product is of SnO_2 having a tetragonal Structure. The average particle size (D) was estimated using the Scherrer equation[9,10]:

$D=k\lambda/\beta\cos\theta$

where D is the crystallite size, λ is the X-ray wavelength, β is the full width at half maximum of the diffraction peak, and θ is the Bragg diffraction angle of the diffraction peaks. The average particle size was found to be 56 to 66 nm the values are given in table -1

Table -1

S.No	pH Range	Average particle size (nm)
1.	7.0	66
2.	7.2	64
3.	7.4	66
4.	7.6	62
5.	7.8	62
6.	8.0	66
7.	8.2	62
8.	8.4	66
9.	8.6	56
10.	8.8	57
11.	9.0	57

UV-vis absorption spectrum

The absorption spectrum was recorded from 1100 nm to 190 nm the optical absorbance of the SnO_2 nanocrystalline. For semiconductor materials, the quantum confinement effect is expect different the

semiconductor dimension become smaller than the Bohr radius (2.7nm) of the exciton, and the absorption edge will be shifted to a higher energy. The absorption spectrum of as-synthesized SnO_2 nanostructure shows in Fig. 2.[11].The intercept of the tangent to the plot will give a good approximation of the band gap energy for this direct band gap material (shown in Fig. 3)[3,8,11,12]. The band gap of the as-prepared SnO_2 nanocrystalline calculated to be 1.5eV to 5.5 eV is larger than the value of 3.62 eV for the bulk SnO_2 due to the contribution of quantum size effect of the present SnO_2 nano particles.

$(\alpha h\nu)^2=A(h\nu-E_g)$

where α is the absorption coefficient, A is a constant, E_g is the band gap and n is equal to 1 for a direct transition. The band gap can be estimated from a plot of (αhν) versus photon energy (hν)[9,10,13]. The band gap of SnO_2 annealed at different in the range 7 to 9 pH was found to be 1.5–5.5 eV the calculated band gab values are tabulated in table 2. The effective mass model is commonly used to study the size dependence of optical properties of quantum systems.

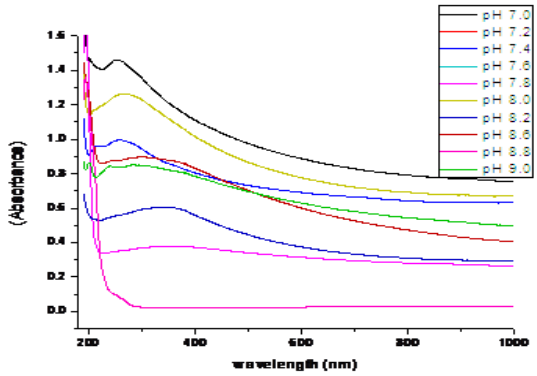

Fig 2. UV absorption spectrum of SnO_2 nano particles

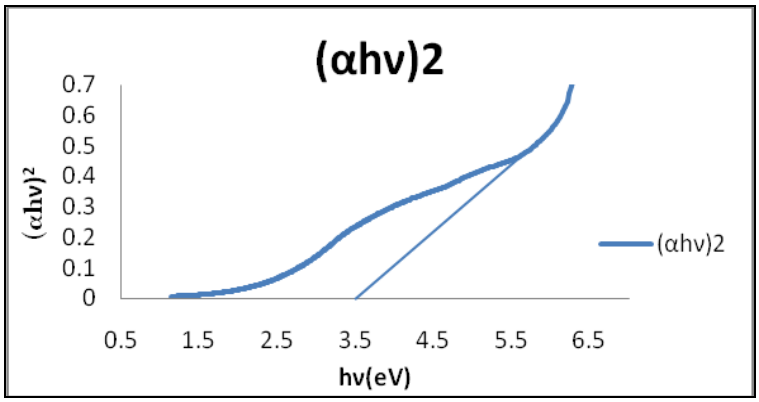

Fig 3 .optical band gap of SnO_2 Nano particles

Table -2

S.No	pH Range	Band gab (eV)
1.	7.0	1.6
2.	7.2	1.7
3.	7.4	1.7
4.	7.6	1.9
5.	7.8	4.5
6.	8.0	1.7
7.	8.2	3.5
8.	8.4	2.5
9.	8.6	2.0
10.	8.8	5.5
11.	9.0	5.25

FT-IR spectrum

Figure 4 shows the FTIR spectrum of tin oxide nano particles thermally treated at different pH range 7 to 9 in steps of 0.2. The absorption band at 539 cm^{-1} [13,14,15] the presence of the hydroxyl group $V_{(Sn\text{-}OH)}$. The peak at 1628 cm^{-1} was ascribed the vibration of NO^{-}_{3} ions. The absorption band at 3306 cm^{-1} was mainly due to V_{OH} stretching vibration of surface hydroxyl group or adsorbed water which has been observed due to readsorption of water molecules from ambinent atmosphere.

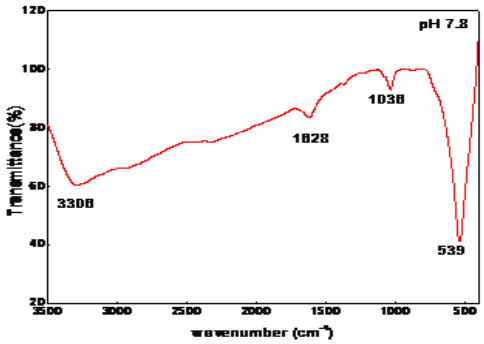

Fig.4 FT-IR spectrum of SnO_2 nano particles

Photoluminescence spectra

The figure 5 shows the room temperature photoluminescence spectra of the synthesised nanocrystalline SnO_2 nano particles. The PL spectra consists of the strong emission band located at 485, 486, 488,and 490 nm. Since the energy band gap of the SnO_2 bulk is 3.62[10,15] eV. The 485 to 490 nm is possibly to attributed the electron transition mediated by defect levels such as oxygen vacancies[18,19] in the band gap the blue emission was eventually dominated in the PL spectrum. It suggested that there was a high concentration of defects (oxygen vacancies) in the SnO_2nanoparticles likely due to the evaporation of [4,7,15]O. This behaviour should be due to the competition between the O atoms getting into the lattice and those evaporating out of the SnO_2 lattice in O_2 atmosphere. The kinetic energy of the surface atoms was large, resulting in a larger escaping rate of O atoms than the adsorption rate to make more O vacancies[7,13,15]

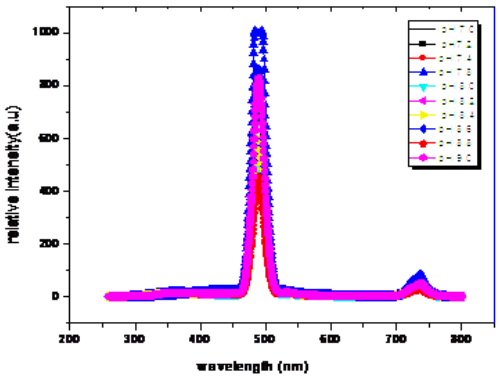

Fig 5 Photoluminescence spectrum of SnO_2 nano particles

Conclusion

The tin dioxide nano particles were synthesized by microwave-assisted technique. The formation of single crystalline tin dioxide nano particles are confirmed by the XRD spectrum. The samplewere further characterized by FT-IR, UV and PL. The optical band gap was found from UV–Vis spectrum. The PL spectrum of the SnO_2 nanomaterials was discussed in detail, and the 485 nm peak suggested that the synthesized material was free from defects or oxygen vacancies.

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