

Synthesis of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ Nanoparticles and Study of Their Optical Band Gap

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ABSTRACT— $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles have been synthesized by a simple co-precipitation method. Nanoparticles crystallize in lower temperature (350°C) and shorter time (2h) respect to other methods. The sample characterized by various standard techniques such as Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), Atomic absorption spectroscopy (AAS) and UV-Vis spectroscopy. The X-ray diffraction reveals that sample is pure rutile-type tetragonal phase, the crystalline size $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles is 27 nm. UV-Vis spectroscopy is revealed the optical band gap to be 3.98 eV for $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles that is higher than the bulk value of SnO (2.5–3 eV).

KEYWORDS: Nickel, tin monoxide, nanoparticles, optical band gap

I. INTRODUCTION

Semiconductors have become familiarly known as an important part of the modern world. Their device potential is immense, and only through careful study of physics have we been able to create devices which maintain life as we know it. Since many of these devices have been and will likely continue to utilize Tin monoxide.

Tin monoxide is a technologically important p type Semiconductor, Semiconductor nanoparticles have been extensively studied from both experimental and theoretical viewpoints, owing to their potential application in solar energy conservation, photo

catalysis and in the field of optoelectronics [1-3]. Preparation of these materials in the nanoscale size range is more interesting due to the increased surface-to-volume ratio that might affect the structural and most other physical properties.

In this work, we synthesize $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles by chemical co-precipitation method because this method has some advantages such as precise control over the stoichiometry, low temperature synthesis, high purity and high chemical homogeneity.

II. EXPERIMENTS

$\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nano-powders were successfully prepared by means of dissolving tin chloride (hydrous $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ (98% Merck)) and nickel chloride (hydrous $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (98% Merck)) in distilled water, this was followed by the addition of sufficient amount of Na_2CO_3 (2M) to the above solution which was then stirred for 2 h. The dropping rate must be well controlled for the chemical homogeneity. The resulting precipitate were collected, washed in distilled water, and then dried at 120°C for 15 hours. Heating treatment of the synthesized nanopowders was conducted in air for 2 h at 350°C.

Crystallinity, structure and particle size of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles were determined by X-ray diffraction (XRD) using Rigaku-Miniflex X-ray diffractometer with $\text{CuK}\alpha$ radiations ($\lambda=0.15406$ nm) in 2θ range from

20° to 70, FTIR spectrum was recorded in the range 400–4000 cm^{-1} on a FTIR 460-plus spectrophotometer using KBr pellets and UV-Vis absorption spectrum of the sample were recorded at room temperature by using PG instrument T80 Uv-Vis spectrophotometer.

III. RESULTS AND DISCUSSION

The powder X-ray diffractogram of sample calcined at 350°C is given in Fig. 1. As seen in Fig. 1, X-ray diffraction measurements reveal that the structure phase of the sample is tetragonal.

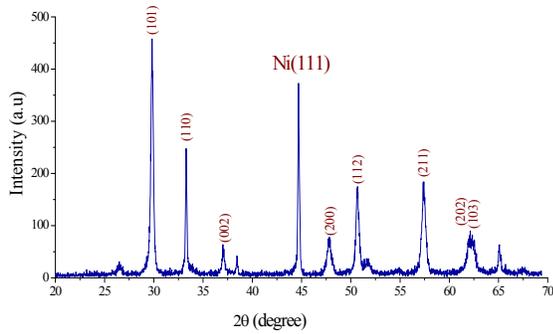


Fig. 1. XRD patterns of the $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles.

The crystalline size of sample was calculated using Scherer's formula,

$$D_{hkl} = \frac{0.9\lambda}{\beta_{hkl} \cos(\theta)} \quad (1)$$

where λ is the wavelength of $\text{CuK}\alpha$ radiation ($= 0.154056 \text{ nm}$), β_{hkl} is the full width at half maximum (FWHM) of the peak (101) at the diffracting angle $2\theta_{101} = 29.83$ [4]. The crystalline size of sample is found to be 27 nm by using Scherer's formula. For the tetragonal structure, the lattice constants can be calculated from,

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2} \quad (2)$$

and

$$2d_{hkl} \sin(\theta) = m\lambda \quad (3)$$

where h , k , and l are all integers, (hkl) is the lattice plane index, a and c are lattice constants. Where h , k , and l are all integers, (hkl) is the lattice plane index, a and c are lattice constants, d_{hkl} is distance between two consecutive planes ($m=1$) with lattice plane index (hkl) . The obtained lattice constants are presented in Table 1, in which a and c are calculated from XRD peaks (110) and (101), Δa and Δc are the differences between the measured lattice constant and that of the standard SnO for $a = 3.801 \text{ \AA}$ and $c = 4.835 \text{ \AA}$ respectively [5].

Table 1. Structural parameters of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles.

Sample	a (Å)	c (Å)	Δa	Δc	Volume of unit cell (Å^3)
$\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$	3.803	4.850	0.002	0.015	70.144
SnO	3.801	4.835	0	0	69.854

The FT-IR transmittance spectrum of sample is given in Fig. 2, in which the band located at 3398 cm^{-1} is owing to the vibration of O–H and the band located at 1636 cm^{-1} is due to the H–O–H vibrating mode of the absorbed water, while the broad band between 800 and 500 cm^{-1} was due to the vibrations of Sn–O [6, 7].

Figure 3. shows the UV–V is spectrum of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles. The absorbance is expected to depend on several factors, such as band gap, oxygen deficiency, surface roughness and impurity centers.

The size dependence of the band gap E^* can be represented by the following equation:

$$E^* = E_g + \frac{h^2}{8\mu R^2} - \frac{1.8e^2}{4\pi\epsilon_0\epsilon_\infty R} \quad (4)$$

where E_g is the band gap of the microcrystalline material, h is the Planck's constant, μ is the effective mass of the exciton, ϵ_∞ is the high frequency dielectric constant, and R is the radius of the particle [8], so theory predicts that optical band gap increase with decreasing of radius of the particle.

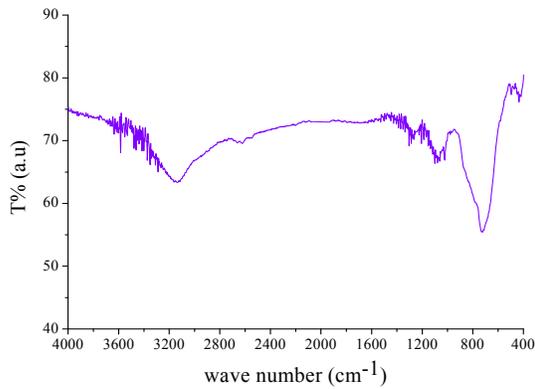


Fig. 2. FT-IR transmittance spectra of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles.

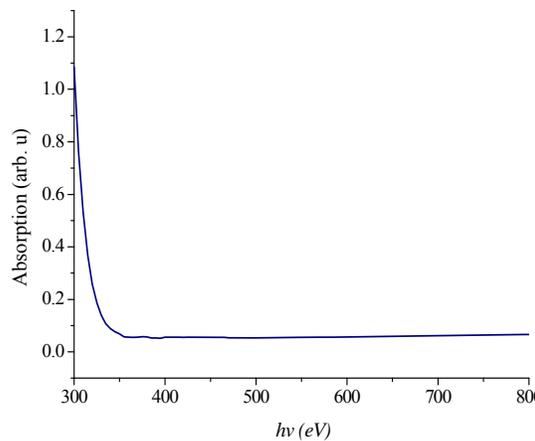


Fig. 3. UV-Vis spectrum of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles.

On the other hand, the doping elements (in this work, nickel) decrease particles size of host material [9, 10].

Therefore, we expect double increase in the optical band gap of bulk SnO because of, a) nanosize particles and b) nickel doping.

In order to calculate the direct band gap we used the Tauc relation,

$$\alpha h\nu = A(h\nu - E_g^*)^n \quad (5)$$

where α is the absorption coefficient, A is a constant, $n=1/2$ for direct transition. An extrapolation of the linear region of a plot of $(\alpha h\nu)^2$ vs. $h\nu$ gives the value of the optical band gap E_g (Fig. 4).

The measured band gap was found to be 3.98 eV for $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles, which is

higher than the reported value of the bulk SnO, i.e. 2.5–3 eV [11].

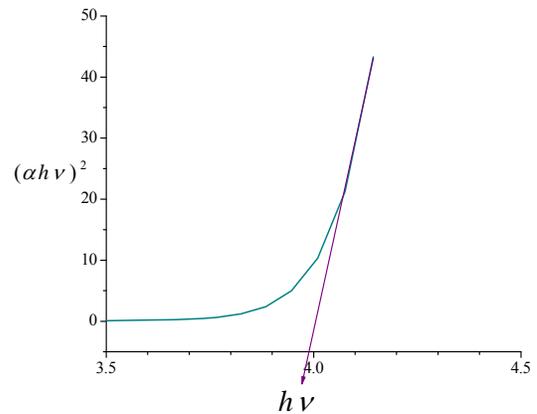


Fig. 4. Determination of optical band gap from the UV-Vis spectrum for the $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles.

IV. CONCLUSION

$\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles have been successfully synthesized using simple co-precipitation method. The crystalline size of sample is found to be 27 nm by using Scherer's formula, and nanoparticles have pure rutile structure. In addition, lattice constants of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles are lower than the lattice constants of bulk SnO. The FT-IR transmittance spectrum of $\text{Sn}_{0.986}\text{Ni}_{0.014}\text{O}$ nanoparticles confirms the formation of SnO. Absorption spectrum of sample shows that the optical band gap value of sample is higher than the bulk value of SnO; this is because of nanosize particles and nickel doping.

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