Facile Synthesis and Characterization of Nickel (III) Oxide Nanoparticles for Smart window Device Application

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ABSTRACT

In the present work Nickel (III) oxide nanoparticles were synthesized by means of simple chemical precipitation method. Nickel chloride and Oxalic acid was used as a starting material and the aqueous solution potassium hydroxide solution was used for this synthesis. The prepared nanoparticles of metal oxide nanoparticles, nickel (III) oxide nanoparticles were characterized by using X-Ray Diffraction (XRD) and Ultra Violet-Visible (UV-Vis) spectroscopic techniques. The average particle size, crystalline structure, phase identification and dislocation densities were determined using XRD analysis. The optical characters such as position of band gap, valance band edge, conduction band edges were analyzed by using UV-Vis Technique.

Keywords: *Nickel Oxide, UV Spectroscopy, XRD.*

1. Introduction

When compared to their bulk counterparts, nanomaterials have dramatically improved properties such as mechanical, electrical, magnetic, thermal, catalytic, and optical capabilities, which have greatly stimulated the attention [1, 2]. Due to its huge surface areas, peculiar adsorptive qualities, surface flaws, and quick diffusivities, nanosized crystalline metal oxides have attracted more and more attention in recent years [3]. Numerous products, including electro chromic films, magnetic materials, p-type transparent conducting films, gas sensors, catalysts, alkaline battery cathodes, and solid oxide fuel cells anodes, can be manufactured using nickel oxide nanoparticles [4]. Crystalline oxide particles with nanoscale dimensions have been created using a variety of mechanical and chemical processes. The primary goal is to reduce the costs of chemical synthesis and to produce materials for technological applications [5].

In the present work, our aim is to the synthesis of nickel oxide nanoparticles by the simple chemical precipitation method. The novelty of the work is the aqueous solution potassium hydroxide is used in the first time for the synthesis process; it reduces the particle size of the synthesis nanoparticles below 10 nm. Further the structural and optical properties of the nanoparticles were analysed using the characterization techniques.

2. Materials and Methods

A facile chemical approach was used to synthesize nickel (III) oxide nanoparticles. Oxalic acid and nickel chloride are the starting materials used in the synthesis process. The temperature controlled magnetic stirrer was used to effectively mix 0.5 Mole of nickel chloride hexahydrate into 50 ml of deionized water. In a similar manner, 50 ml of distilled water was used to dissolve 0.5 M of oxalic acid. Until it dissolved, the solution was thoroughly agitated using a magnetic stirrer. Oxalic acid and the nickel chloride solution was gradually added together and thoroughly agitated for about 30 minutes.

An aqueous solution of potassium hydroxide was prepared by adding 4 Mole of potassium hydroxide into 50 ml of distilled water. The as prepared aqueous solution was added to the mixture of solution that contains the precursor's cations and anions. The ions in the aqueous solution precipitate as an insoluble nickel (III) oxide nanoparticles. The chemical reaction takes place during the preparation process is as follows:

$NiCl_2. 6(H_20) + C_2H_2O_4 + KOH \rightarrow NiO + KCl_2 + 7(H_20) + C_2H0_4$

The solution contains solid nickel (III) oxide nanoparticles and also the potassium chloride, water in the solution form. The sub products were removed by washed using distilled water three instances consistent with day, washing system repeated for 2 days. After washing, the solution was stored in hot air oven at 100° C to get dried. Then the dried sample was powdered using the mortar and then kept in muffle furnace for heating at 300° C and subsequently preferred nickel (III) oxide nanoparticles was obtained.

3. Results and Discussion

The X- Ray Diffraction pattern of the as prepared nickel (III) oxide nanoparticles was recorded using X- Ray Diffractometer interfaced 'X' pert software with Cu-K Alpha radiations of wavelength of 1.54060 Å. The XRD pattern obtained for the synthesized Nickel (III) Oxide nanoparticles is shown in fig. 1 and the computed structuralparameters such as angle 2θ, d-spacing, miller indices and relative intensity data's are tabulated in Table 1.

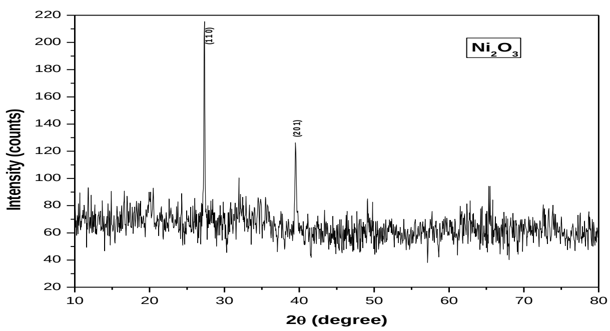

Fig 1. XRD pattern of Nickel (III) Oxide nanoparticles.

Table 1. Computed XRD parameters of Nickel (III) Oxide nanoparticles.

2θ (degree)	d-spacing (A°)	Miller Indices (h kl)	Relative Intensity (%)
27.3269	3.26366	110	100.00
39.5181	2.28044	201	41.33

From the XRD pattern, it was confirmed that the prepared nickel oxide nanoparticles show poor crystalline nature due to the reason that the samples were calcinated at low temperature as 300° C for an hour. Furthermore, the pattern indicates that the synthesized nickel (III) oxide nanoparticles belongs to hexagonal crystal system with preferred (1 0 0) orientation. The phase identifications were also carried out from the XRD and it was identifies the Ni_2O_3 phase which is highly agreed with the report of Kh M. Haroun et.al [6]. In order to know more about the particles nature, the average grain size or particle size and the dislocation densities were found out are shown in table 2. The average grain size of the as-synthesized nanoparticles is found out from the powder XRD pattern using Scherer's formula,

$$D = \frac{0.9\lambda}{\beta cos\theta} \text{ nm} \qquad (1)$$

Where λ is a wavelength (λ=1.5406 A°), β is full width at half maximum of the diffraction line and θ is the angle of diffraction. The Dislocation density of the prepared sample was determined using the relation;

$$\delta = \frac{1}{D^2} \text{ lines/m}^2 \qquad (2)$$

Table 2. Calculated Particle size and Dislocation density

Angle2θ (degree)	θ (degree)	β (radian)	Grain size (nm)	Dislocation density 10^{15} (lines / m^2)
27.3269°	13.66345°	0.1476°	9.669	0.001069
39.5181°	19.75905°	0.1968°	7.486	0.001784

The calculated average particle size and dislocation density values are 8.5775 nm and 0.001426× 10^{15} lines / m^2 respectively. The particle size calculation conforms that the prepared materials are nanomaterials. Thus from the structural analysis, it was concluded that the aqueous solution used potassium hydroxide reduces the particle size of the nickel (III) oxide nanoparticles below 10 nm.

UV-VIS-NIR spectrum of the nickel (III) oxide nanoparticles were recorded in the wavelength range between 190 to 1100 nm using UV-VIS-NIR spectrophotometer. The optical properties of the nickel (III) oxide nanoparticles were analysed with the aid of the recorded absorbance and reflectance spectrum shown in fig. 2 and 3.

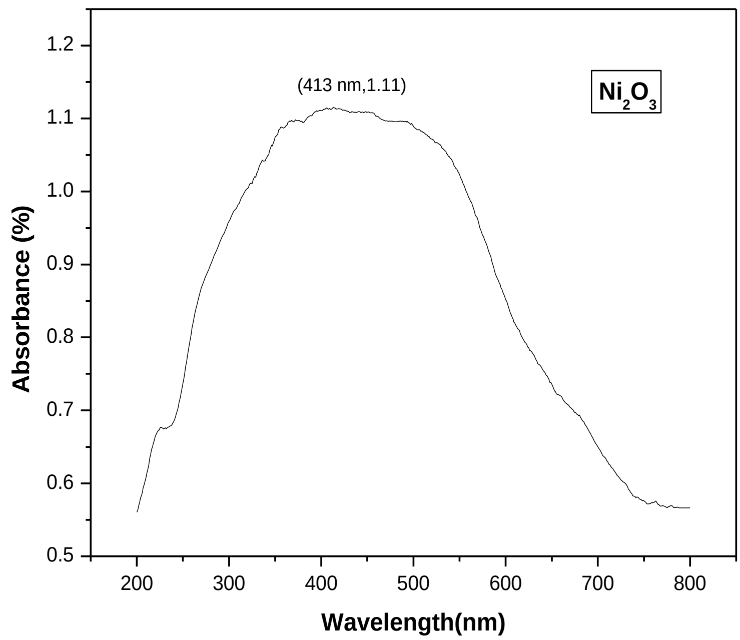

Fig 2. Optical absorbance spectrum

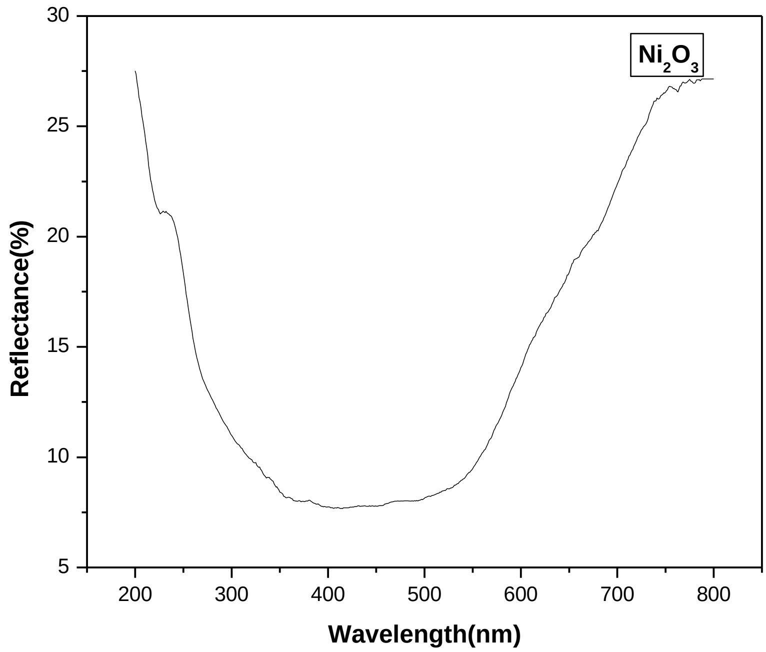

Fig 3. Optical Reflectance spectrum

According to Miessya et al [7], the characteristic absorbance peak at 413 nm wavelengthrange is due to the Ni_2O_3 nanoparticles. Nickel (III) oxide nanoparticles experience maximum absorbance of 1.1% at 413 nm wavelength. Reflectance spectrum confirms the maximum reflectance at the lower wavelength (200 nm) and higher wavelength (800 nm) of about 27.5 %. The lower reflectance of 7.5 % observed at the 413 nm wavelength. The optical band gap (E_g) value at the maximum absorbance wavelength (λ) is evaluated using the relation [8],

$$Eg = \frac{hc}{\lambda} \quad (3)$$

Where h and c are Plank's constant and velocity of light respectively. Furthermore, the position of the valance and conduction band [9] of the nickel oxide nanoparticles can be determined using the relations as follows;

$$E_{(CB)} = \chi - E^c - 0.5Eg \quad (4)$$

$$E_{(VB)} = E_{(CB)} + Eg \quad (5)$$

χ represents absolute electro negativity of the nickel oxide compound, calculated as the arithmetic mean of electron affinity and first ionization energy. E^c denotes the energy of free electrons on the hydrogen scale i.e. 4.5 eV. Where $E_{(CB)}$ is the band edge position of the valance band, $E_{(VB)}$ is the band edge position of the conduction band.

Table 3. Calculated optical parameters.

Optical Parameters	**Calculated Value**
Band Gap (eV)	3.00
Electro negativity	6.5
Position of valance Band (eV)	27.75
Position of conduction Band(eV)	30.7

The calculated optical parameters are tabulated in table 3. Wide band gap semiconductors are the semiconductor materials which have the optical band gap in the range above 1.5 eV. From the calculation it was known that the prepared nickel (III) oxide nanoparticles are wide band gap third generation semiconductor materials with electro negativity 6.5 value can be used as smart windows in power devices.

4. Conclusion

Nickel oxide nanoparticles of particle size 8.5775 nm were successfully synthesized by a simple chemical precipitation method. The preparation process is faster, cheaper and cost effective. From the structural characterization, it was confirmed that the synthesized nickel oxide nanoparticles belongs to hexagonal crystal system and Ni_2O_3 phase. It was also interesting to note that, the aqueous solution used potassium hydroxide is used in the synthesis process; it reduces the particle size of the nickel oxide nanoparticles below 10 nm. The optical properties of the prepared nanoparticles were analysed using UV-Vis spectrophotometer. The prepared nanoparticle shows lower absorbance percentage, which confirms that the nanoparticles have higher transmittance. Thus the third generation semiconductor materials nickel oxide with lower absorbance and higher transmittance percentage materials can be used as smart windows in power devices. The future scope is the work can be extended to analyse the materials morphological and magnetic properties.

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