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Structural and Optical properties of Nickel Sulphide(NiS) nanoparticles

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Abstract

Due to their properties and applications in various fields nanomaterials gain a lot of importance. In the present paper we report the synthesis of NiS nanoparticle by co-precipitation method and characterization of NiS nanoparticle. Nickel acetate was used as a precursor to prepare pure NiS nanoparticle. Sodium sulphide and Sodium hydroxide is added to this solution. On calcinating the sample at 500^0C and 1000^0C for 1 hour, β-NiS nanoparticle was obtained. The prepared sample has been characterized by powder XRD and UV-VIS Spectroscopy. The average grain size was obtained through powder XRD. UV-VIS spectroscopy was used to determine the band gap of these nanoparticles. The band gap of NiS nanoparticles of 500^0C and 1000^0C was found to be 4.8eV and 2.8eV.

Keywords : Nanoparticles, nickel sulphide, XRD, UV-VIS spectroscopy

1. INTRODUCTION

Transition metal (TM) sulfides exhibit interesting optical, electronic, thermoelectric and photoelectric properties [1-4]. Nickel sulfide (NiS) an important member of this large family of TM sulfides, finds use as a potential cathode material for the rechargeable lithium battery, as a catalyst in the degradation of organic dyes and in magnetic devices[5,6].

Different synthesis routes have been tried for the synthesis of nanoparticles of NiS.The chemical precipitation method is one of the important methods for the synthesis of nanoparticles.

In this paper, β-NiS nanoparticles have prepared by Co-precipitation method.[7]The structure, average grain size of as-prepared sample is characterized by XRD and its optical properties is studied by UV Spectroscopy.

2. MATERIALS AND METHODS

Nickel acetate was used as a precursor to prepare pure NiS nanoparticle. For this 0.5M of nickel acetate was taken and was dissolved in 100ml distilled water and stirred it for half an hour. To this solution, 0.5M of sodium sulphide was added drop wise and a pH of 7 was observed. NiS precipitate was washed with water three times to remove the unwanted residues. It was also washed with ethanol two times to remove the impurities. At 100^{o}C, the solution was heated in hot air oven for 24 hours. NiS nanopowder thus formed was black in colour. The above mentioned method was repeated and a pH of 14 was maintained by adding 0.5 molar of sodium hydroxide. Then it was calcined at 500^{o}C for 1 hour (the obtained nanopowder was black in colour) and 1000^{o}C for 1 hour (the obtained nanopowder was pale green in colour).

3. RESULT AND DISCUSSION

3.1. STRUCTURAL STUDIES (XRD)

The Structure and lattice parameters of NiS nanoparticle were determined from the X-ray diffraction pattern. The Powder – XRD pattern of the prepared nickel sulphide samples for pH-14 is given in the Fig.1

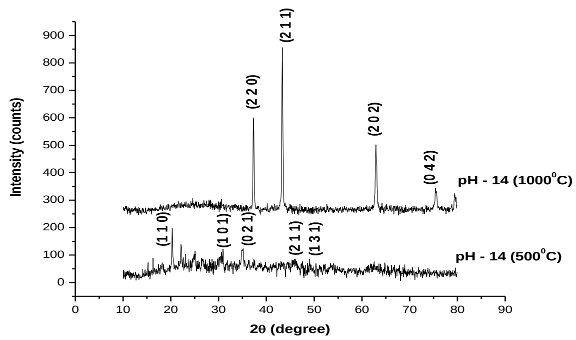

Fig 1. *XRD pattern of nickel sulphide nanoparticles at calcined at 500^{0}C and 1000^{0}C*

The XRD peak value are in agreement with the **JCPDS file No. 86 – 2281** (a=b=9.619 Å; c=3.1499 Å). Thus all the samples exhibit rhombohedral structure. When the NiS sample is calcined at 500^{0}C, it is amorphous in nature. Further, when it is heated at 1000^{0}C, the peaks are very sharp revealing its nanocrystalline nature.

The average grain size is calculated using the Debye – Scherrer formula[8]

$$\mathbf{D} = \frac{0.9\lambda}{\beta\cos\theta} \text{ nm}$$

The dislocation density δ have been calculated by the following relationship[9]

$$\boldsymbol{\delta = 1/D^2}$$

Where,

D = crystallite size

NiS nanoparticles calcinied at	**Average grain Size (nm)**	**Dislocation Density $\delta \times 10^{15}$lines/meter^2**
500^0C	30.51965	51.418123
1000^0C	42.092656	57.7744733

Average grain size and dislocation density of NiS nanoparticles

When the calcination temperature is increased, there is a increase in average grain size and dislocation density. This is due to the nanocrystalline nature of the sample calcined at 1000^0C.

3.2.OPTICAL STUDIES (UV-VIS-NIR SPECTROSCOPY)

UV-VIS-NIR spectra of the sample is taken in the wavelength between 200nm to 1200nm.The absorbance spectra of the NiS nanoparticles calcined at 500^0C and 1000^0C are shown in Fig.2-3

The band gap energy is estimated by Tauc plot[10] relation $\alpha = k\,(h\nu\text{-}E_g)\,^n/h\nu$

Where,

ν is the frequency ,

h is the Planck's constant,

K and n are constants.

For NiS, the value of n is 2.

The plots of $(\alpha h\nu)^{1/2}$ vs $h\nu$ for NiS nanoparticles calcined at 500^0C and 1000^0C are shown in Figure.4 and 5 respectively.

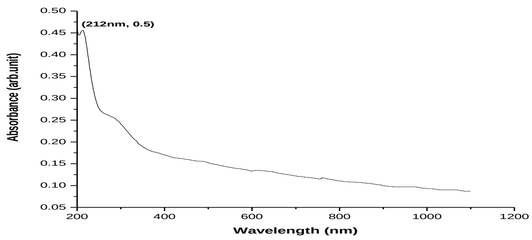

Fig 2. *Absorbance spectra for NiS nanoparticles(calcined at 500^0C)*

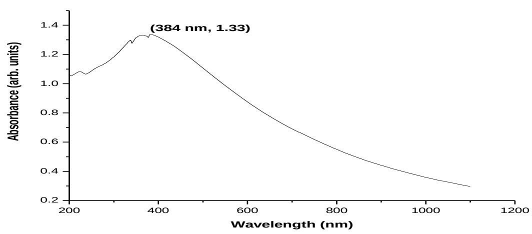

Fig 3. *Absorbance spectra for NiS nanoparticles (calcined at 1000^0C)*

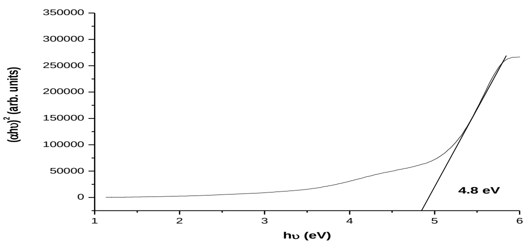

Fig 4. *Tauc plot for NiS nanoparticles (calcined at 500^{0}C)*

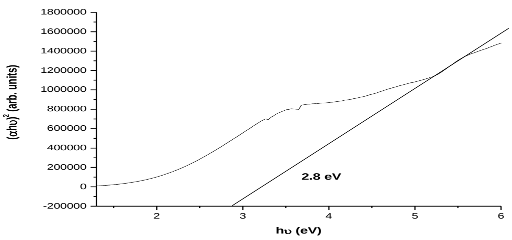

Fig 5. *Tauc plot for NiS nanoparticles (calcined at 1000^{0}C)*

The optical band gap of NiS calcined at 500^{0}C is 4.8 eV and for NiS calcined at 1000^{0}C is 2.8 eV. As the calcination temperature is increased, the optical band gap decreases. Both the samples show good transmittance. There is a blue shift observed in the samples.

4. CONCLUSIONS

Nickel Sulphide nanoparticles are prepared by co-precipitation method. The samples are calcined at two different temperatures. From the XRD analysis, it is found that the NiS nanoparticle possesses rhombohedral structure. The particle size and the dislocation density of the nanoparticles are found out. When the calcination temperature is increased, there is a increase in average grain size and dislocation density. This is due to the nanocrystalline nature of the sample calcined at 1000^{0}C. From UV characterization, it is observed that band gap is high for the sample which is annealed at low temperature. As size increases the bandgap decreases. Blue shift is also observed from the absorption peaks which reveal that the samples are in the nanoscale. Thus these NiS nanoparticles can be used in photocatalytic applications.

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