Preparation and Characterization of NiS Thin film on ITO coated Glass substrate for Solar cell Applications

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Abstract— Thin films of NiS have been deposited on indium doped tin oxide coated conducting glass substrates using chemical bath deposition technique. The X-ray diffraction was used to obtain structural characterization. Structural parameters such as crystallite size, strain and dislocation density are calculated for films with different thickness values obtained. Optical absorption analysis showed that the deposited films possess band gap value around 0.7 eV. The film composition and surface morphology have been analyzed using scanning electron microscopy and energy dispersive analysis by X-rays.

Keywords— NiS, Thin film, CBD, SEM

I. INTRODUCTION

In the last few decades, there has been a significant interest in the deposition of metal sulfide thin films due to potential application in the field of electronics industry or photovoltaic [1]. Chemically deposited Ni Sulfide (NiS) thin films are of particular interest for the fabrication of solar selective coatings, IR detectors and a storage electrode in photo-electrochemical storage devices [2,3]. Kim et al reported Ni sulfide films deposited on Ti–Ni substrate as a promising active material for flexible secondary battery [4]. The bandgap of Nickel sulfide was found to be 0.45eV by Sartale et al (2001) [5]. Cheon et al. have reported deposition of stoichiometric NiS from both a thermal and photochemical CVD routes using Ni(S2COCHMe)2[6]. The deposition of NiS on Si by low pressure metal-organic chemical vapour deposition was reported by Nomura and Hayata [7]. Lee et al deposited NiS thin film on Si and Al2O3 substrates by pulsed laser ablation of nickel sulfur targets [8]. NiS has been deposited by successive ionic layer adsorption and reaction technique using solutions of nickel sulfate and sodium sulfide at alkaline pH [9]. Nickel sulfide thin films were also prepared from solutions of nickel sulfate and thioacetamide in an alkaline medium [9] and from acidic solutions of sodium thiosulfate [10]. In a recent study, films and powders of various phases of nickel sulfides include solid-state reaction [12, 13] and precipitation from aqueous [14] and organic solutions [15]. For the present work, Chemical bath deposition (CBD) technique has been used to prepare NiS thin films on indium doped tin oxide (ITO) coated conducting glass substrates due to its simplicity, cost effectiveness and suitability in an industrial scale.

II. EXPERIMENTAL

The NiS film was prepared from an acidic bath containing aqueous solutions of 25ml of 0.1M Nickel sulphate, 25ml of 0.1M Sodium Thiosulphate and 3ml of Triethanolamine. The pH was adjusted to 2.5 by using Hydrochloric acid. The cleaned
ITO glass plate was immersed vertically into the beaker which was maintained at 308K. After three hours the slide was removed and washed with distilled water dried in desiccators an good quality NiS film on ITO glass substrate was obtained.

X-ray powder diffraction (XRD) pattern of the product was obtained on a X-ray diffractometer equipped with graphite monochromatized Cu Ka radiation (\(k = 0.154178\) nm). UV-Visible absorption spectrum was recorded in the spectral range 300-1100 nm by using Varian Cary 5000 spectrophotometer. Scanning electron microscopy (SEM) images and energy dispersion X-ray (EDX) analysis were recorded on a scanning electron microscope, Hitachi, X650/EDAX, PV9100.

### III. RESULT AND DISCUSSION

#### A. X-Ray Diffraction Analysis

The crystalline quality of the film were examined by X-ray diffraction (XRD) analysis and the structural parameters such as crystallite size, micro strain, dislocation density and number of observed crystallites were also calculated by a well-known Scherrer’s formula. The recorded X-Ray diffraction pattern on deposited thin film was shown in Fig. 1. The observed peak at \(2\theta = 30.19^\circ, 34.69^\circ, 45.91^\circ\) and position correspond to (100), (101) and (102) planes were compared with standard JCPDS Reference Code: 65-3419 confirmed the NiS thin film structure.

The crystallite size (D), microstrain (\(\varepsilon\)) and dislocation density (\(\rho\)) were calculated by using the reported Scherrer’s formula.

\[
\text{Crystallite Size} = \frac{0.94 \lambda}{\beta \cos \theta}
\]

Where, \(\lambda\) is the wavelength of the X-ray source ie 1.54178 Å, 
\(\beta = \text{FWHM/180}\) 
\(\theta\) is the observed diffraction angle 
microstrain (\(\varepsilon\)) = \(\beta \cos \theta / 4\) 
Dislocation density (\(\rho\)) = \(1 / (D^2)\)

The calculated crystallite size \(D\) was 68.43nm, microstrain (\(\varepsilon\)) was .0054 and dislocation density (\(\rho\)) was \(2.16 \times 10^{14}\). The calculated crystallite size, strain and dislocation density was shown in the Table. 1 for all obtained peaks. All the obtained peaks belong to the crystallite size in the range of less than 70 nm.
TABLE I

THE CALCULATED CRYSTALLINE PARAMETER OF NiS THIN FILM ON ITO GLASS

<table>
<thead>
<tr>
<th>2θ</th>
<th>FWHM</th>
<th>Crystallite Size (D) nm</th>
<th>Microstrain (ε)</th>
<th>Dislocation Density(ρ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.19</td>
<td>0.13(8)</td>
<td>63.54</td>
<td>5.4 X 10^-4</td>
<td>2.476 X 10^14</td>
</tr>
<tr>
<td>34.69</td>
<td>0.11(7)</td>
<td>66.08</td>
<td>4.5 X 10^-4</td>
<td>2.290 X 10^14</td>
</tr>
<tr>
<td>45.91</td>
<td>0.16(9)</td>
<td>75.69</td>
<td>6.42 X 10^-4</td>
<td>1.74 X 10^14</td>
</tr>
</tbody>
</table>

B. UV Analysis

The optical absorption studies provide an easy method for the investigation of optically induced electronic transitions and furnish ideas about the band structure as well as the energy gap in crystalline and non-crystalline materials. In this work, the optical absorption are examined between 200 nm to 1100 nm and absorption spectrum of NiS thin film coated on ITO substrate as shown in Fig. 2. It reveals that the absorbance is very less in the visible region. The band gap was estimated using the Tauc’s relationship [17] between absorption coefficient $\alpha$ and the photon energy $\hbar \nu$

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

Where, ‘$\nu$’ is the frequency, ‘$h$’ is the Planck’s constant $E_g$ is the band gap energy, ‘$A$’ and ‘$n$’ are constants. For allowed direct transitions, $n = 1/2$ and for allowed indirect transitions, $n = 2$. The plot of $(\alpha h \nu)^2$ vs $h \nu$ is shown in Fig. 3 for NiS films. The band gap energy ‘$E_g$’ was determined by extrapolating the straight line portion to the ‘$h \nu$’ axis. The optical band gap energy was found to be 0.72 eV for the as-deposited NiS film.

![Fig. 2 UV absorbance spectrum of NiS on ITO coated glass](image1)

![Fig. 3 Plot of (hν) versus (αhν)^2 for NiS thin films on ITO coated glass](image2)
C. Scanning Electron Microscope Analysis

The scanning electron microscopy (SEM) analysis was conducted to investigate the surface micro morphology of the NiS thin films on ITO glass. The observed surface morphology of the deposited NiS thin film on ITO glass under different magnification were shown in the Fig. 4. The observed surface features reveal the film evenness and having free smooth surface morphology.

Fig. 4(a,b,c,d) SEM image of NiS on ITO glass with different magnification
D. EDX Analysis

The energy dispersive X-Ray spectrum of deposited NiS on ITO glass was shown in Fig 5. The elements on the deposited film were confirmed and results shown that the film contain Ni, S, Si, In, Fe and O. EDX analysis of the product proves the existence of NiS. In Fig. 5, the two peaks in the range from 1 to 3 keV are ascribed to Ni and S. The other elements such as Si, In, Fe and O most likely from ITO glass substrate and holder.

IV. CONCLUSIONS

Nanocrystalline NiS semiconductor thin films were fabricated on ITO coated glass substrate using chemical bath deposition technique. The X-ray measurements reveal that the deposited films exhibit cubic crystal structure. UV-Visible absorption studies shows that the deposited NiS thin film has less absorbance and more transmittance. The nano size nature of the deposited films was examined by scanning electron microscopy and found that NiS deposited uniformly on ITO glass substrate. EDX analysis confirmed that the presence of functional elements. The deposited NiS thin films are technologically important in optoelectronic and solar cell device fabrication where the large area is required.

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REFERENCES
