

Effect of Mixing Ratio of Precursors on Structural and Optical Characteristics of Nanostructured Nickel Oxynitride Thin Films

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Abstract

In this work, the effect of mixing ratio of the precursors on the structural and optical characteristics of nickel oxynitride thin films has been determined and studied. Thin film samples were prepared using different mixing ratios of $\text{Ni}(\text{NO}_3)_2:\text{NiCl}_2$ precursors (1:1, 2:1, 3:1, 4:1, 5:1, and 6:1). The x-ray diffraction (XRD) patterns of the prepared samples were recorded and compared. A reasonable change in the crystalline structure was observed as the mixing ratio of the precursors was changed. As well, the surface roughness of the prepared samples were compared. The optical characteristics of the prepared films were compared and found very sensitive to the variation of the mixing ratio of the precursors.

Keywords: Nickel oxynitride; Chemical reduction; Structural characteristics; Optical characteristics

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1. Introduction

Nickel oxynitride (NiO_xN_y) is a unique compound formed by the incorporation of nitrogen into nickel oxide (NiO) [1,2]. It can be synthesized via methods such as reactive sputtering, thermal nitridation, or chemical vapor deposition [3]. The preparation conditions, including temperature and nitrogen concentration, influence its structural and electronic properties [4]. NiO_xN_y exhibits a mixed-phase structure, combining both oxide and nitride characteristics, which leads to improved electrical conductivity and catalytic properties compared to pure NiO [5,6]. These properties make it suitable for applications in electrochemical energy storage (batteries, supercapacitors), sensors, and catalysis, particularly in hydrogen production and environmental remediation [7].

Carrier injection significantly impacts the response characteristics of thin-film photodetectors by influencing their efficiency, speed, and sensitivity [8]. When carriers (electrons and holes) are injected into the photodetector material, they contribute to the photocurrent generated under illumination [9,10]. Effective carrier

injection improves the signal-to-noise ratio, enhancing the device's sensitivity to light [11,12]. However, excessive injection can lead to increased recombination rates, reducing the photodetector's quantum efficiency and slowing down the response time [13-15]. Optimizing carrier injection involves balancing injection efficiency and recombination processes, ensuring that the device can swiftly and accurately detect light while maintaining high performance [16-18].

In this work, the effect of mixing ratio of the precursors on the structural and optical characteristics of nickel oxynitride thin films has been determined and studied.

2. Experimental Part

The chemical reduction method for preparing nickel oxynitride (NiO_xN_y) nanostructures involves several key steps to achieve the incorporation of nitrogen into nickel oxide. The process typically begins by selecting a suitable nickel precursor, such as nickel nitrate ($\text{Ni}(\text{NO}_3)_2$) or nickel chloride (NiCl_2). The precursor is dissolved in a solvent, commonly water or ethanol, to form a solution. To introduce nitrogen into the structure, nitrogen-containing agents like

ammonia (NH_3) or urea (NH_2CONH_2) are added to the solution. Figure (1) show schematically the chemical reduction method used in this work to prepare nickel oxynitride thin films.

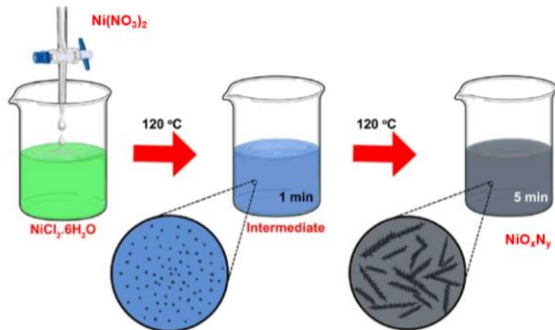


Fig. (1) Schematic diagram of the chemical reduction method used in this work to prepare NiO_xN_y thin films

The mixture is then heated in a reducing atmosphere, often using hydrogen (H_2) gas, which facilitates the reduction of nickel ions and promotes the incorporation of nitrogen into the nickel oxide matrix [19]. The heating temperature and time are crucial parameters; typically, a temperature range of $300\text{--}600^\circ\text{C}$ is used. This step leads to the formation of nickel oxynitride, with the nitrogen atoms substituting oxygen in the nickel oxide lattice, altering its electronic and structural properties [20]. Figure (2) shows the thin film samples prepared in this work.

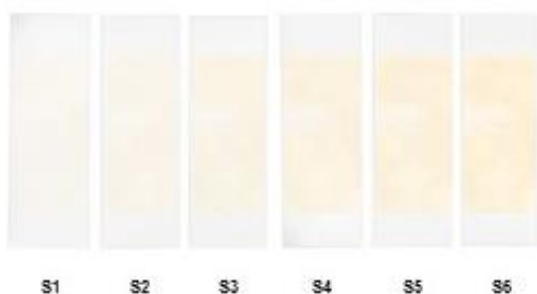


Fig. (2) Thin film samples prepared in this work at different mixing ratios of $\text{Ni}(\text{NO}_3)_2$: NiCl_2 precursors (S1) 1:1, (S2) 2:1, (S3) 3:1, (S4) 4:1, (S5) 5:1, (S6) 6:1

After the reduction process, the product is washed with deionized water to remove any residual reactants, followed by drying in an oven. The nanostructures are characterized using techniques such as x-ray diffraction (XRD), atomic force microscopy (AFM),

and UV-visible spectrophotometry to confirm the formation of nickel oxynitride nanostructures and assess their morphology and crystallinity.

This method allows for scalable production of NiO_xN_y with tailored properties for various applications in catalysis, energy storage, and sensing.

3. Results and Discussion

X-ray diffraction (XRD) patterns shown in Fig. (3) of nickel oxynitride films prepared by the chemical reduction method typically exhibit diffraction peaks corresponding to a mixed phase of nickel oxide (NiO) and nickel nitride (Ni_3N). The intensity and position of these peaks vary depending on nitrogen incorporation, reflecting changes in crystallinity and phase structure.

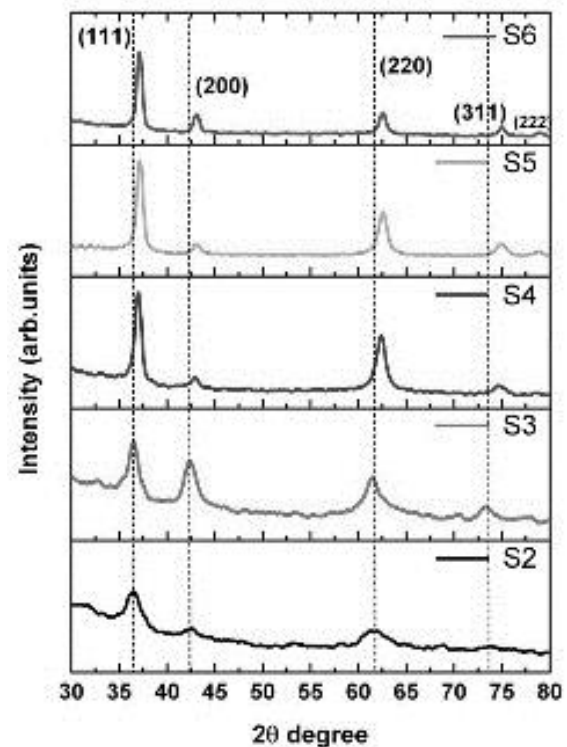


Fig. (3) XRD patterns of the prepared samples

Atomic force microscopy (AFM) images shown in Fig. (4) for nickel oxynitride (NiO_xN_y) films prepared by the chemical reduction method reveal crucial information about their surface morphology and roughness. These images typically show nanoscale features, including grains,

clusters, or uniform films, with surface roughness varying depending on synthesis parameters like temperature, nitrogen concentration, and precursor type [21,22].

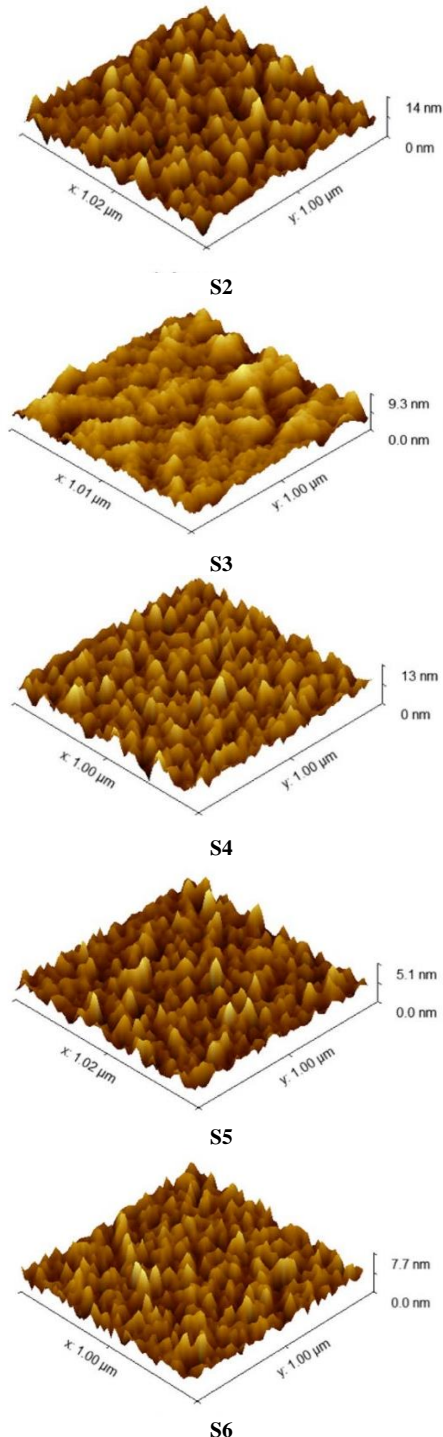


Fig. (4) AFM patterns of the prepared samples

AFM can provide quantitative measurements of surface roughness (RMS), highlighting the impact of processing conditions on film quality. The images may also display variations in height, reflecting

the formation of nanostructures, which influence the material's electronic properties and its potential applications in catalysis and sensing [23-25].

The transmission spectra shown in Fig. (5) for nickel oxynitride (NiO_xN_y) films prepared by the chemical reduction method typically exhibit distinct features due to the unique optical properties imparted by nitrogen incorporation. These films often show a broad absorption band in the ultraviolet (UV) to visible region, indicating increased optical absorption compared to pure nickel oxide (NiO). The nitrogen doping reduces the bandgap of NiO, allowing for enhanced light absorption in the visible range. Transmission spectra generally show a decrease in transmittance, especially in the UV region, with a shift in absorption peaks that corresponds to the formation of NiO_xN_y and its modified electronic structure.

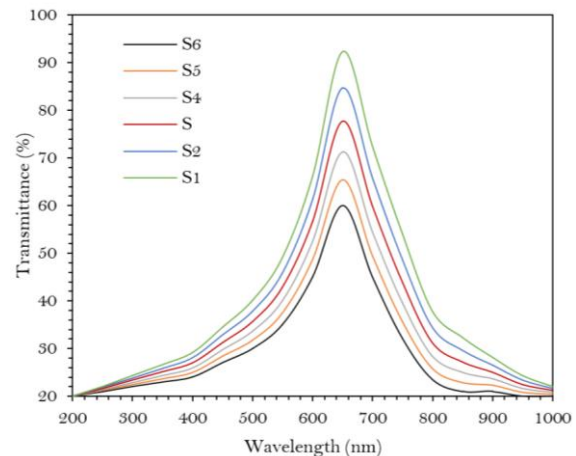


Fig. (5) Transmission spectra of the prepared samples

4. Conclusions

In conclusions, the effect of mixing ratio of the precursors used for the preparation of nickel oxynitride thin films has been studied and found to have reasonable controlling role on the structural and optical characteristics of the prepared thin films.

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