

Temperature deposition impact on structure and optical properties of NiO: CdO nanostructure thin films

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Nickel and cadmium thin films were spray pyrolysed on glass substrates at temperatures between 200°C and 400°C. The impact of these temperatures on the films' growth mechanism and physical characteristics was investigated with a view to their potential use in optical applications. Irrespective of the substrate temperature, the films were characterized as having a polycrystalline structure with a cubic orientation predominantly at the (1 1 1) plane. With higher substrate temperatures, there was a notable increase in film transparency. Furthermore, as the substrate temperature increased, the optical band gap decreased between 3.45 eV and 2.48 eV. The results of the study demonstrated the potential for using these films in modern applications such as solar cells.

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1. Introduction

The potential use of low-resistance, transparent conductive films of metal oxides, including zinc oxide, metal-doped carbon oxides, metal-doped carbon oxides, and nickel oxide, in chemical sensors and other optoelectronic devices has been the subject of recent research. Metal oxide films comprise fundamental technologies such as optical reaching in the visible range and electrical contact [1,2]. For example, NiO is a significant antiferromagnetic p-type semiconductor that has been extensively researched for use in heterogeneous catalysts, solid-state sensors, electrochromic devices, and lithium batteries [3,4].

Furthermore, NiO displays unparalleled capabilities in gas sensing, catalysis, and electrochemistry. A multitude of techniques have been employed to generate nickel oxide thin films, including thermal evaporation [5], spray pyrolysis [6], and chemical vapor deposition. [7]. A p-type transparent semiconductor with a large band gap energy of 3.6–4.0 eV is a NiO compound that belongs to the binary oxides family. It is established that this substance is characterized by a cation deficiency. Moreover, this oxide exhibits both cubic and rhombohedral forms, with the cubic structure being the most prominent. Thin films of this binary oxide are the subject of significant interest and research over the past two decades due to their clear suitability for use in heterojunction solar cells and electronic devices. Moreover, it has been demonstrated that NiO thin films exhibit high sensitivity to a diverse array of gases, encompassing both reducing and oxidizing species [10].

NiO nanoparticles are highly chemically stable, exhibit exceptional electron transfer capacity and have anti-inflammatory properties. Due to their distinctive characteristics, including surface area, metal ion release, and adsorbing capacity, they have the potential to exert cytotoxic effects [11]. Nevertheless, the majority of NiO's applications are constrained by its elevated electrical resistivity ($10^{13} \Omega \text{ cm}$). The formation of nickel vacancies and interstitial oxygen atoms may result in a notable reduction in the high electrical resistivity of NiO. Recently, NiO has been utilised as a sensing material for the detection of acetone gas. Indeed, the hydrothermal method was employed by Lu et al. [12] to create porous NiO microstructures that resemble cacti. The shape of these microstructures, which are produced by selecting the optimal time, has been found to enhance the gas-sensing property. Consequently, the reaction to 100 ppm of acetone at an operating temperature of 260 °C is approximately 13.51, which indicates high gas sensitivity.

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Furthermore, the researchers determined that the samples exhibited reaction and recovery times of approximately 24 and 39 seconds, respectively. Nevertheless, certain studies have investigated the doping of nickel oxide samples with other elements, including iron and lithium (13).

CdO film can be used as a transparent conducting material. CdO film is undoubtedly one of the most intriguing transparent conducting films of metal oxides, as evidenced by experimental data. Its low resistivity, resulting from oxygen defects and cadmium interstitials, makes it a highly promising material. Due to its narrow energy band gap, excellent electrical conductivity in both doped and undoped films [14, 15], and optical transmittance value in the visible region of the electromagnetic spectrum, CdO has significant potential for a range of applications. The electrical characteristics of NiO can be enhanced through doping with metal ions, the creation of NiO nanostructures with unique morphologies, or the formation of composites with low-resistivity materials. The n-type direct band gap metal oxide II-VI group semiconductor cadmium oxide (CdO) has an indirect band gap of 1.36–1.98 eV and a direct band gap of 2.2–2.5 eV, respectively (17). CdO exhibits a remarkably low electrical resistivity ($10^{-4} \Omega \text{ cm}$), which, when coupled with its ionic properties and high optical transmission in the visible region, renders it a promising candidate for a range of technological applications, including transparent conductors. Due to the small direct band gap between the minimum of the Cd 5s conduction band and the O 2p-based valence band, CdO exhibits photoactivity. In light of these characteristics, a straightforward soft chemical method has been employed in this study to create a composite comprising NiO and CdO. The combination of these oxides may result in the formation of a single entity that could significantly enhance the electrical characteristics of NiO. The cohabitation of NiO and CdO in a single organism presents numerous potential avenues for the manipulation of their characteristics, to develop new specialized applications in physics, chemistry, and biology [18]. The straightforward soft chemical approach employed in this study offers a number of benefits over other nanocomposite synthesis techniques, including low cost, ease of use, and low processing temperature [19].

In this study, the chemical spray pyrolysis method is employed as a cost-effective technique for the production of large-area NiO thin films. A review of the literature reveals a paucity of research on cadmium-doped NiO films. This research presents a number of physical studies on thin films sprayed with Cd-doped NiO. The sensitivity of Cd-doped NiO thin films to different work temperatures (200°C, 250°C, 300°C, 350°C, 400°C) is a particular focus of the study.

2. Experimental part

Nickel and cadmium thin films were deposited through the spray pyrolysis technique using an aqueous solution of nickel nitrate $\text{Ni}(\text{NO}_3)_2$ and cadmium nitrate $\text{Cd}(\text{NO}_3)_2$ of 0.1 M for each solution at 200 °C, 250°C, 300°C, 350°C, and 400 °C substrate temperatures. For thirty minutes, the mixed solutions were magnetically stirred. The resulting precipitates were prepared. The substrate was cleaned with an ultrasonic cleaner. The solution was prepared using air as a carrier gas and sprayed onto the samples every two minutes for eight seconds. The distance between substrate- to- nozzle had kept around 29 cm. Surface morphology was determined using a FESEM, while the structure and optical characteristics were examined using XRD and UV-Vis, respectively.

3. Results and discussion

XRD testing of thin films is performed to determine the crystal structure of these films and to determine the crystal patterns and crystal orientations in them. The structure properties of cadmium-doped nickel oxide (NiO) films coated at varying substrate temperatures are identify via XRD patterns (Fig.1). The films were produced through the spray pyrolysis process, with the initial deposition temperature ranging from 200°C to 400°C with increasing 50°C. The XRD pattern corroborates the presence of numerous crystals arranged in a cubic configuration. The

principal peaks at $2\theta \sim 33^\circ$ and 38° are indicative of the crystal planes (111) and (200), respectively. Additionally, weaker peaks are observed at $2\theta \sim 55^\circ$, 65.9° , and 69° , which correspond to the crystal planes (220), (311), and (222), respectively [19]. These findings are in accordance with the data presented in the International Center for Diffraction Data (ICDD) card number 75-0592 [20]. Furthermore, Figure 1 provides additional evidence to support this observation. As the temperature increase, the diffraction peak intensity had increased, and at half-maximum, the full width had decreased, thereby rendering the peak more distinct.

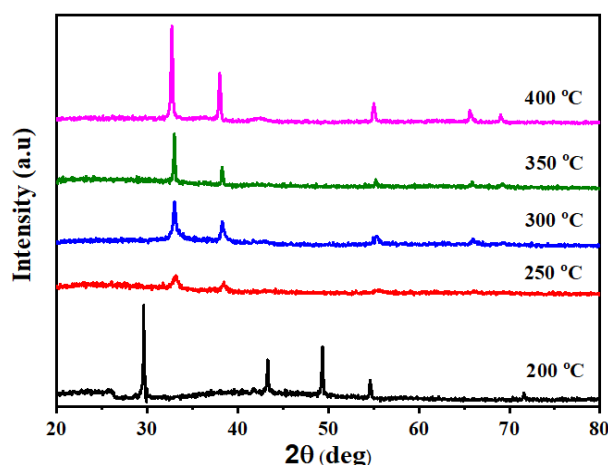


Fig. 1. Structure of XRD for cadmium-doped nickel oxide (NiO) films coated at different temperatures.

FE-SEM analysis of thin films provides high-resolution images of the surface of films, allowing the study of the surface composition and chemical distribution of materials on a very small scale. It can also be used to measure the thickness of films and analyze their nanostructures. The structure properties of cadmium-doped nickel oxide (NiO) films coated at varying substrate temperatures (200°C and 400°C) (Fig. 2a, b) are investigated. The FE-SEM images identify the substantial impact of temperature substrate on the morphological characteristic of cadmium-doped nickel oxide (NiO) films. It is noteworthy that well-crystallised grains in an irregular pattern, with a thickness of 315.58 nm at 200°C, are examined in (Fig. 2a) [19]. Upon increasing the substrate temperature to 400°C, the film's thickness reaches 342.51 nm, and the film surface becomes densely populated with spherical nanostructures (Fig. 2b)), indicating enhanced crystallinity of the film [22,23].

UV-Visible analysis of thin films is used to measure the absorption of ultraviolet and visible light by films. This analysis provides information about the optical properties of films such as light absorption and transmittance, which helps in understanding how films interact with light and determining their optical properties. The optical transmission and reflectance spectra of the CdO-doped NiO films are pointed in (Fig. 3). The results indicate that the films transparency is increased when the substrate temperature rising. The non-stoichiometric nature of the film is responsible for the reduced transmission observed for the film coated at 200°C, it was similar to the result of a surplus of unreacted metallic cadmium and ions. As the substrate temperature increases, the film's stoichiometry improves due to the reduction in the defect centre density. However, when the defect centre density decreases, light loss due to scattering is reduced, thereby increasing the transparency of the films. [24]. The data presented in (Fig. 3) indicates that the films exhibit minimal specular reflectance overall. The combination of high transmittance and low reflectance renders these films ideal for applications requiring anti-reflection coatings, particularly in solar cell technologies.

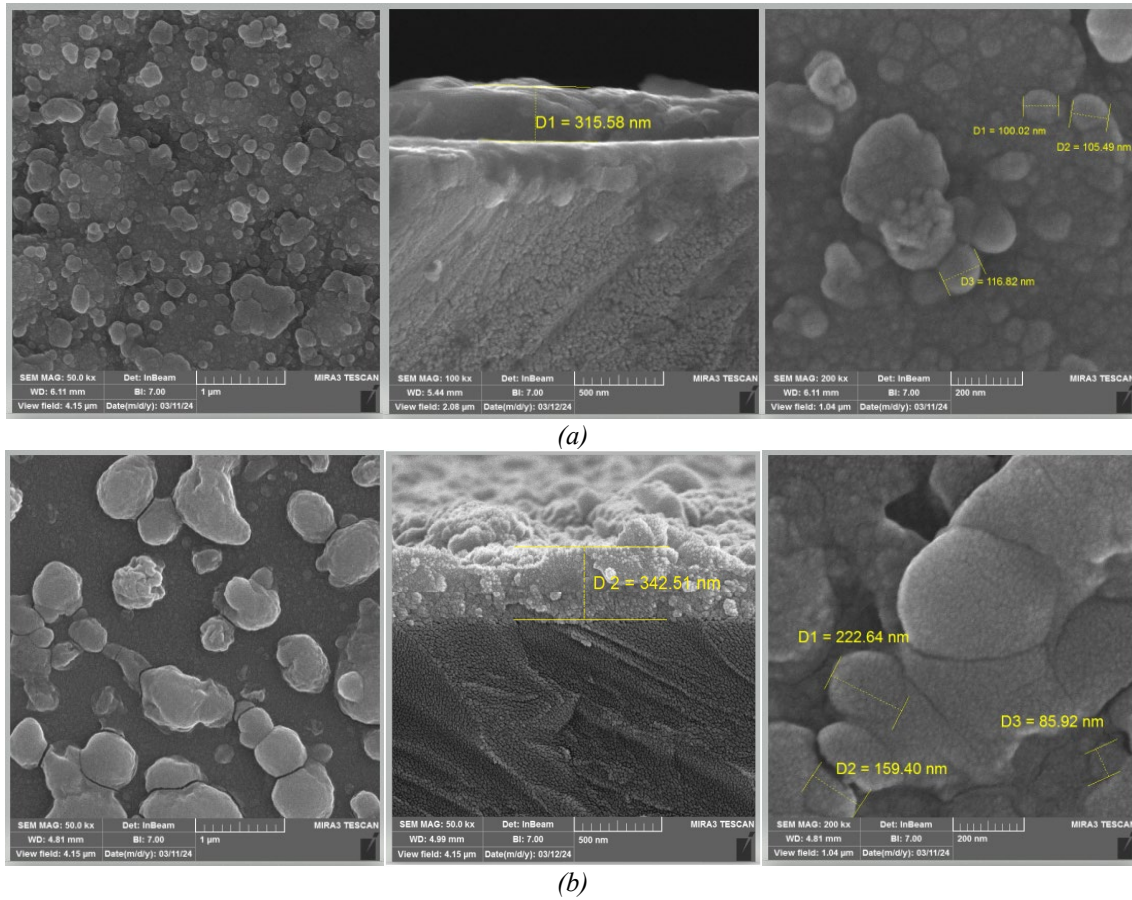


Fig. 2. FE-SEM Images of cadmium-doped nickel oxide (NiO) films (a) at 200°C (b) at 450°C.

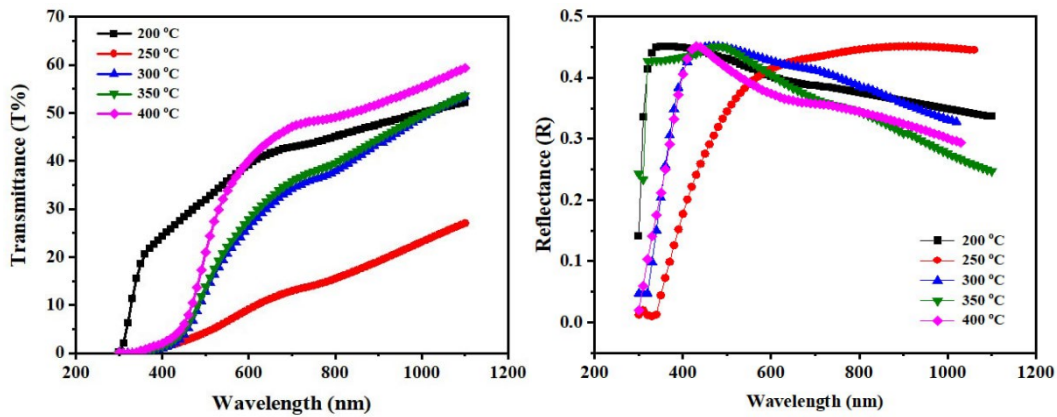


Fig. 3. ($T\%$) & (R) for Cadmium-doped nickel oxide (NiO) films coated at different temperatures.

The energy band gap for thin films is investigated (Fig.4). The study pointed that the values of energy gap decrease as the as-deposited temperature increasing from 200°C to 400°C. Specifically, the direct band gap decreased from 3.45 eV to 2.48 eV. This reduction is linked to the heightened absorption coefficient resulting from larger crystallite and particle sizes. Generally, an augmentation in both particle and crystallite sizes results in a decline in the optical energy gap [26-28].

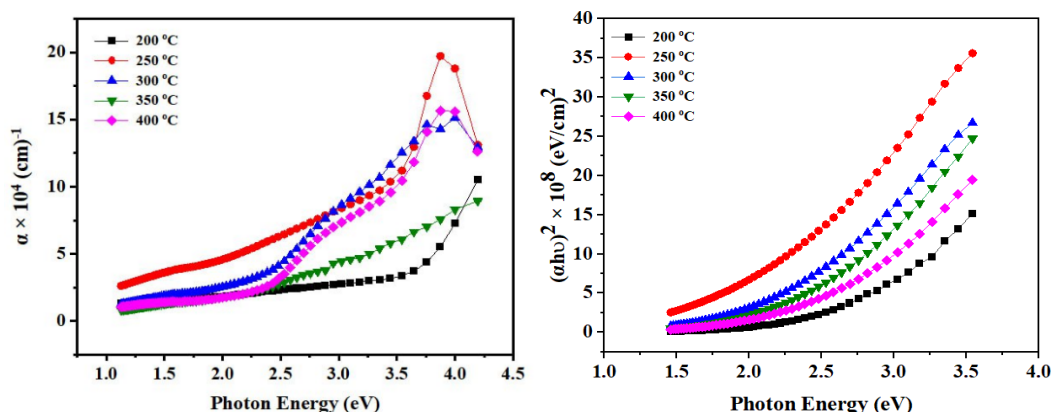


Fig. 4. (α) and (E_g) for Cadmium-doped nickel oxide (NiO) films coated at different temperatures.

The connection of the wavelength and refractive index (n) are examined (Fig. 5). The data demonstrates a decline in the refractive index as the wavelength increased, indicative of refractive index dispersion (29). Additionally, there is a gradual increase in the extinction coefficient value as the energy of the incident photons rises. This is attributed to the growth in the absorption coefficient, which subsequently results in higher absorption coefficient values. Moreover, the extinction coefficient values undergo a change, with the peaks shifting towards higher photon energies as the temperature increase [30].

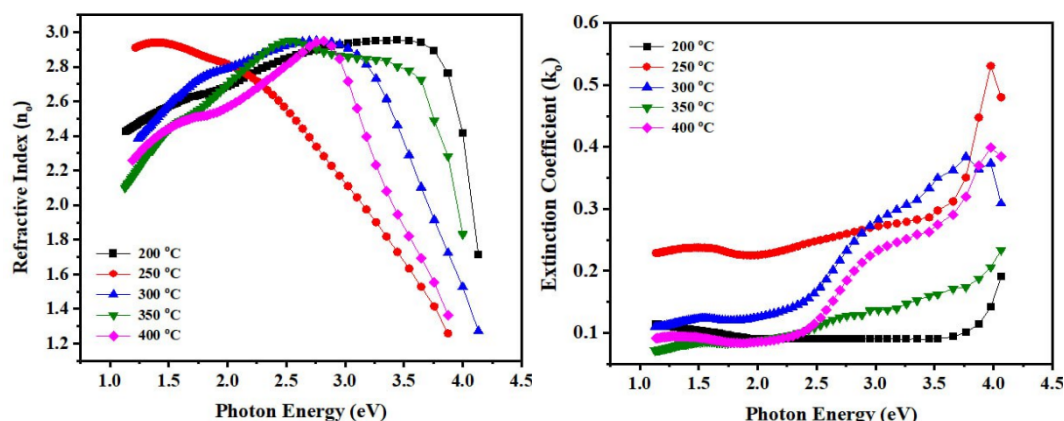


Fig. 5. (n_o) & (k_o) for Cadmium-doped nickel oxide (NiO) films coated at different temperatures.

4. Conclusion

The study contributed our understanding of the structure and optical properties for CdO-doped NiO films, the main findings are as follows:

The spray pyrolysis method was significant for synthesizing CuO-doped NiO films with various substrate temperatures.

X-ray diffraction (XRD) analyses indicated that the films exhibited a polycrystalline nature with a cubic crystal structure, regardless of the substrate temperature, there is a preferred orientation along the (1 1 1) plane.

Optical results indicated a rise in optical transparency and a decrease in the band gap value from 3.45 eV to 2.48 eV as the substrate temperature increased. The results of this study are important for the field of modern technology in several ways, for example, these CdO-NiO doped thin films can be applied in the solar panel industry to increase the light absorption efficiency and

improve the performance of solar panels. These films can also be used in the development of high-definition displays and thin-film electronic displays due to their improved optical properties.

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