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Impact of Nickel Concentration on Structural, Morphological and Optical Properties of Jet Nebulizer Spray pyrolysis Coated Ni-MoO₃ Thin Films: Evaluation of n-Ni-MoO₃/p-Si Junction Didoes

G.Lavanya 1*, N.Sivanandan 2

¹ Research Scholar, Department of Electronics, PSG College of Arts and Science, Coimbatore, India

^{*}Corresponding Author E-mail: lavanya.gnanavelk@gmail.com

Article History	Abstract
Received: 08 Sept 2023 Revised: 29 Oct 2023 Accepted: 05 Nov 2023	Monoclinic structured MoO_3 thin films were prepared on a glass substrate. The Ni doped materials to add the MoO_3 in different concentrations (1%, 3%, 5%) at Wt% with MoO_3 precursor and synthesis was done using the spray pyrolysis method. X-ray diffraction revealed the incorporation of Ni in the MoO_3 Monoclinic structure. FE-SEM images showed more dispersive and rod shapes than Ni-doped MoO_3 and pure MoO_3 respectively. The ideality factor, barrier height, and saturation current were measured for two samples
CC License CC-BY-NC-SA 4.0	pure MoO ₃ and Ni-doped MoO ₃ at 5% doping level. The ideality factor was calculated using electrical measurements, while the barrier height and saturation current were determined through analysis of the current-voltage (I-V) characteristics. Keywords: Monoclinic, MoO3 thin film, spray pyrolysis, junction diode.

1. INTRODUCTION

Transition metal oxide, remarkably MoO₃ due to its physical and chemical properties had a wide attention in research. Since last few years MoO₃ possess good structural, electronic and optical characteristics that finds its application in gas sensors, catalysts and opto electronic field [1-5]. The n-type MoO₃ films shows good results in photovoltaic applications. Among the various preparation methods available spray pyrolysis techniques is found to be the simplest and low cost method [6-8]. Which has economically attractive setups. The MoO₃ has a wide ban gap n-type material which possess good structural and electronic characteristic that can be used in many industrial applications [9-10]. The fabrication of p-Si junction diode using spray pyrolysis technique is a simple, low cost and low temperature process which has a remarkable opening for the making of photonic and nano electronic devices [11, 12]. This report presents an analysis of the ideality factor (n), barrier height (ΦB), and saturation current (Io) for two different samples: pure MoO₃ and Ni-doped MoO₃ at a 5% doping level. These parameters play a crucial role in understanding the electrical behavior of semiconductor materials. The ideality factor reflects the degree of deviation from the ideal diode behavior, the barrier height represents the energy barrier that charge carriers must overcome, and the saturation current provides insights into the leakage current across the material.

2. RESULTS AND DISCUSSION

XRD Analysis:

Figure 1 shows the XRD pattern of prepared samples of pure and Ni doped MoO₃ thin films using the jet nebulizer spray pyrolysis technique at 450° C. Figure 1 shows XRD all detectable peaks (0 0 1, 1 0 0, 0 0 2, 0 1 1, 1 1 0, 0 1 2, 1 0 2, 2 0 1, 0 2 0, 1 2 0, 2 1 1) can be indexed to Pure MoO₃ monoclinic structure with JCPDS card no. 85-2405. The monoclinic lattice parameter, the values of d, the distance between the crystal planes, were calculated from Bragg Law, λ =2d sinθ. Table 1 shows the Structural parameter of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%). The (2 2 1) (h k l) plane was selected to calculated the structural parameters of the prepared the samples [13-17].

² Assistant Professor, Department of Electronics, PSG College of Arts and Science, Coimbatore, India

¹lavanya.gnanavelk@gmail.com, ² sivanandan@psgcas.ac.in

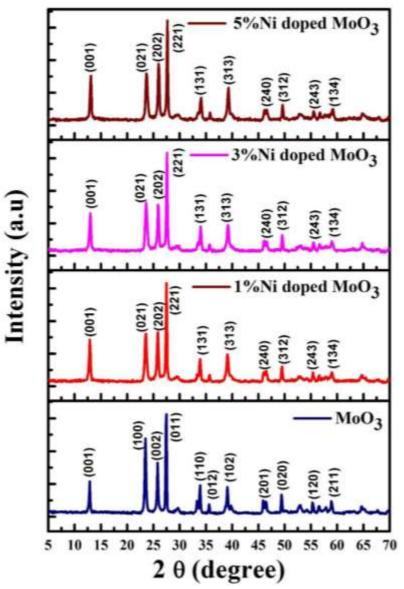


Figure 1. XRD pattern of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%)

Table 1. Structural parameter of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%)

Material	Diffraction Angle 20	(221) Inter planar distance Å	FWHM (Radians)	Crystallite size (D)	Micro strain (ε) (× 10 -3 lines- 2 m-4)	Dislocation density (×1014 lines/m2)	Stacking fault × 10– 2
Pure MoO ₃	27.4330	3.24859	0.27250	52.41	3.639	0.0661	0.14915
1% Ni doped MoO ₃	27.4848	3.24259	0.28080	50.87	3.863	0.0681	0.15386
3% Ni doped MoO ₃	27.5702	3.23274	0.28820	49.57	4.068	0.0699	0.15820
5% Ni doped MoO ₃	27.6417	3.22454	0.29520	48.40	4.267	0.07166	0.16229

FE-SEM Analysis:

Figure 2 displays the analyzed MoO₃ films as well as the thin film samples of Ni-doped MoO₃ at concentrations of 1%, 3%, and 5%. These samples underwent examination using low magnification (2μm) via FE-SEM analysis. In Figure 2a, visuals of multidispersive and unevenly sized rods are apparent. Upon introducing 1%, 3%, and 5% Ni doping into the MoO₃ samples, the images reveal a higher degree of dispersion and rod-like formations compared to pure MoO₃. The imagery illustrates a notable alteration in the shapes of the prepared samples, coinciding with an increase in doping concentration, which in turn contributes to a more loosely defined surface tension.

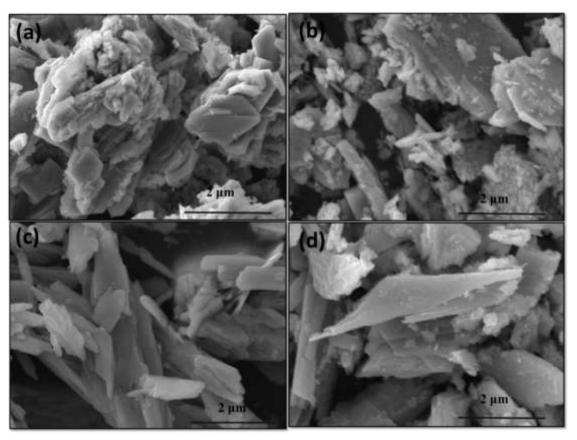
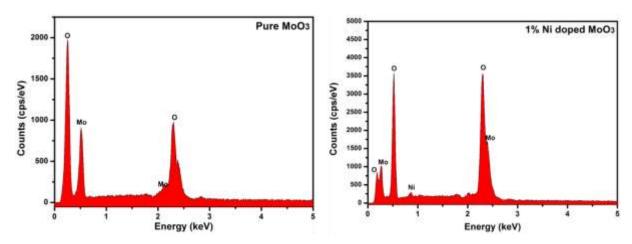


Figure 2. FE-SEM images of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%)

Elemental Analysis

Figure 3 shows the EDAX spectrum of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%). According to the data presented in Table 2 (a), the elemental analysis spectrum for pure MoO₃ unequivocally demonstrates the presence of Mo and O elements in the prepared samples, with no detectable indication of other elements [18, 19]. In Table 2 (b-d), the elemental analysis spectrum for Ni-doped MoO₃ illustrates the existence of Ni, Mo, and O elements within the samples that were prepared.



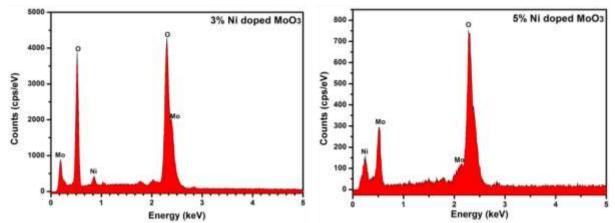


Figure 3. EDAX of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%)

Table 2. Elemental analysis of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%)

(a)	Elements	Weight %	Atomic %
	O k	35.68	75.82
	Mo L	64.32	24.18

b)	Elements	Weight %	Atomic %
	Ok	28.57	72.01
	Ni L	1.98	1.28
	Mo L	69.45	26.71

(c)	Elements	Weight %	Atomic %
	Ok	29.82	70.63
	Ni L	2.83	2.42
	Mo L	67.35	26.95

Elements	Weight %	Atomic %
Ok	26.92	69.32
NiL	3.24	3.01
Mo L	69.84	27.67

UV-Vis Analysis

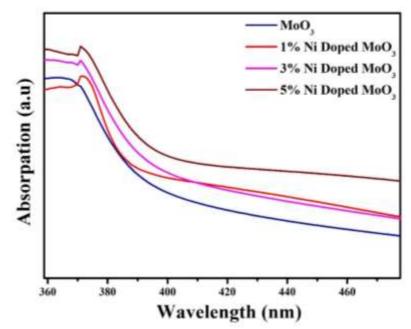


Figure 4. UV-Vis analysis of MoO₃ and Ni doped MoO₃ (1%, 3% and 5%)

Figure 4 shows the UV-Vis analysis spectrum of Pure and doped MoO₃. Compared with Pure MoO₃, 1%, 3%, and 5% Ni doped MoO₃ were peak observed 363 nm, 370 nm, 372 nm, 375 nm respectively.

I-V characteristics of n-Ni doped MoO₃/p-Si diodes

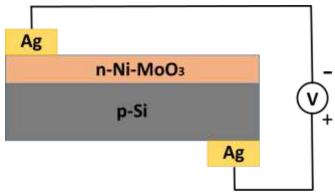


Fig. 5(a) The device structure of back contact

Fig.5 (a) shows represents the schematic of n-MoO₃/p-Si device structure the current voltage characteristics of undoped and Ni (wt.5%) doped n-MoO₃/p-Si diode.

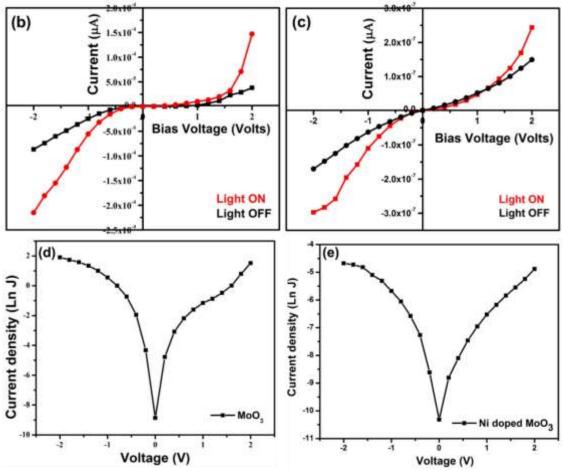


Fig. 5. (b - d). I-V curve of (b) n-MoO₃/p-Si, (d) n-Ni MoO₃/p-Si diodes, I-V curve of (c, e) current density (J)-voltage (V) plots of pure MoO₃ and n-Ni MoO₃/p-Si diodes

Figure 5 depicts the I-V curve of n-MoO3/p-Si, (d) n-Ni MoO3/p-Si diodes and current density (J)-voltage (V) plots of pure MoO3 and n-Ni MoO3/p-Si diodes.

For pure MoO₃, the ideality factor (n) was measured to be approximately 1.5744. In the case of Ni-doped MoO₃ at 5% doping, the ideality factor increased significantly to around 4.1864. The increase in the ideality factor for the doped sample suggests the presence of additional recombination centers or defects in the material. This deviation from the ideal value of 1 indicates a less ideal diode behavior, potentially due to the incorporation of Ni impurities. The barrier height (ΦB) represents the energy difference between the conduction band edge and

the Fermi level, indicating the ease with which charge carriers can move across the semiconductor junction [20, 21]. For pure MoO₃, the barrier height was calculated to be approximately 0.41702 eV. With Ni doping at 5%, the barrier height increased to around 0.58584 eV. The increase in barrier height with doping could be attributed to changes in the electronic structure of the material due to Ni incorporation, affecting charge carrier transport. Saturation current (Io) signifies the leakage current when the diode is in the reverse-biased condition and provides information about the material's quality and purity. Pure MoO_3 exhibited a saturation current of 5.42×10^{-5} A. Ni-doped MoO_3 at 5% doping showed a significantly lower saturation current of 8.96×10^{-8} A. The lower saturation current in the doped sample suggests improved material quality, possibly due to the reduction in defects or impurities at the semiconductor interface [22].

3. CONCLUSION

Pure MoO₃ and Ni-doped MoO₃ thin films were made coated successfully and characterized using simple and rapid synthesized method. The analysis of ideality factor, barrier height, and saturation current for pure MoO₃ and Ni-doped MoO₃ (5% doping) revealed distinct differences in the electrical behavior of the two samples. The increased ideality factor, higher barrier height, and lower saturation current observed in the doped sample suggest the influence of Ni doping on the electronic properties of MoO₃. Further investigations into the role of doping and its impact on the semiconductor behavior are warranted to gain a comprehensive understanding of the material's electrical characteristics.

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