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Gas Sensing Properties of CdO-MgO Nanocomposites: A Comprehensive Study

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Abstract: ***This study investigates the structural and gas sensing properties of CdO-MgO nanocomposites, offering a comprehensive analysis of their morphology, crystalline structure, and sensing performance. The nanocomposites were synthesized using a cost-effective sol-gel method, followed by detailed structural characterization. XRD analysis confirmed the successful incorporation of MgO into the CdO lattice, leading to enhanced structural stability and reduced crystallite size. FESEM images revealed uniform dispersion of nanoparticles with controlled morphology, while FTIR spectra validated the presence of functional groups essential for gas sensing applications. Gas sensing performance was evaluated against various target gases, including ammonia (NH_3), hydrogen sulfide (H_2S), and nitrogen dioxide (NO_2), under different operating temperatures. The results demonstrated that the CdO-MgO nanocomposites exhibit high sensitivity, fast response-recovery times, and excellent selectivity towards NH_3 at an optimized temperature. The improved sensing behavior is attributed to the synergistic effect between CdO and MgO, which enhances charge carrier mobility and increases surface oxygen vacancies. This study highlights the potential of CdO-MgO nanocomposites as promising materials for high-performance gas sensors in environmental and industrial applications. Further research on tuning the composition and doping strategies may lead to the development of highly efficient and selective gas sensors for real-world applications.***

Keywords: CdO-MgO nanocomposites, gas sensing, structural properties, sol-gel synthesis, ammonia detection

1. Introduction

The development of highly efficient gas sensors is crucial for environmental monitoring, industrial safety, and healthcare applications. Among various metal oxide semiconductors (MOS), cadmium oxide (CdO) has garnered significant attention due to its high electrical conductivity, low resistivity, and promising gas sensing properties [1,2]. However, pristine CdO suffers from limitations such as poor selectivity, high operating temperature, and moderate response stability, restricting its practical applications. To overcome these challenges, researchers have explored composite strategies by incorporating wide-bandgap metal oxides such as magnesium oxide (MgO) to enhance the sensing performance of CdO-based materials [3–5]. MgO is an insulator with a wide bandgap (~7.8 eV), which, when introduced into CdO (bandgap ~2.3 eV), leads to significant bandgap tuning effects, enhancing selectivity for target gases [6,7]. Additionally, CdO-MgO composites exhibit excellent thermal and chemical stability, making them ideal for applications in harsh environments such as industrial emissions monitoring and automotive exhaust sensing [8,9].

Another critical advantage of incorporating MgO into CdO is the enhancement of oxygen vacancies and surface reactions, which play a pivotal role in gas adsorption and sensor response kinetics. The increased number of oxygen vacancies in CdO-MgO nanocomposites promotes a higher concentration of adsorbed oxygen species, leading to improved sensitivity toward oxidizing gases such as NO_2 and CO_2 [10–12]. Furthermore, the large surface area and porous morphology of CdO-MgO structures facilitate rapid gas diffusion, ensuring faster response and recovery times [13–15]. Recent studies have demonstrated that CdO-MgO nanocomposites exhibit superior selectivity, high response magnitude, and long-term stability compared to individual metal oxides [16–18]. Therefore, the strategic integration of MgO into CdO presents a promising approach for developing next-generation gas sensors with enhanced performance and reliability.

2. Materials and Methods

2.1 Materials

For the synthesis of CdO-MgO nanocomposites, high-purity reagents were utilized to ensure accuracy and reproducibility. Cadmium nitrate tetrahydrate ($Cd(NO_2)_3{\cdot}4H_2O$) was obtained from SD Fine Chemicals with Analytical Reagent (AR) grade and a purity of ≥98%, serving as the cadmium precursor. Magnesium nitrate hexahydrate ($Mg\ (NO_2)_3{\cdot}6H_2O$) was sourced from Merck with Emplura grade and a purity of ≥97%, acting as the magnesium source. Polyvinyl alcohol (PVA), with a molecular weight range of 89,000–98,000 g/mol, was procured from Sigma Aldrich and functioned as a binder and stabilizer during the synthesis process.

2.2 Thick Film Synthesis

The CdO-MgO nanocomposites were synthesized via the sol-gel method with weight ratios of 90:10, 80:20, 70:30, 60:40, and 50:50 and pure CdO. as explained and published earlier [19]. The synthesis of CdO-MgO nanocomposite thick films using the screen-printing method involves several key steps. Initially, the nanocomposite powders were synthesized and blended with ethyl cellulose and a mixture of organic solvents such as butyl carbitol acetate, butyl cellulose, and terpineol to create a thixotropic paste. This paste was then screen-printed onto glass substrates to ensure uniform film deposition. The printed films were subsequently dried in ambient conditions to eliminate residual solvents. Finally, the dried films were subjected to a firing process at 500^0C for 9 minutes in a muffle furnace to

enhance their structural integrity and chemical stability [20-22].

3. Results and Discussion

The XRD, FESEM, EDS, and FTIR analyses have been previously explained and published. These studies confirm that the material has been properly synthesized. The findings validate the accuracy of the synthesis process.

3.1 Gas Sensing performance of the CdO-MgO nanocomposites

The measurement of gas response, selectivity, and response/recovery time involves defining the relative response to a target gas as the ratio of the change in the sample's conductance when exposed to the gas to its original conductance in air. The gas response can be expressed as:

$$\text{Gas Response} = \frac{G_g - G_a}{G_a} = \frac{\Delta G}{G_a}$$

Where G_a represents the conductance in air and G_g denotes the conductance in the target gas. Selectivity, or specificity, refers to the sensor's ability to detect a particular gas amidst the presence of other gases [23].

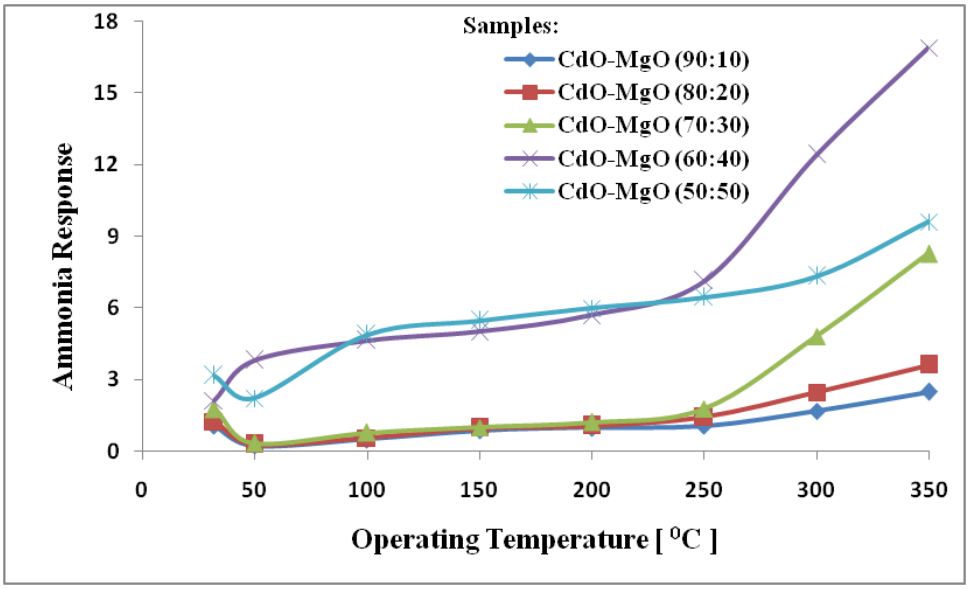


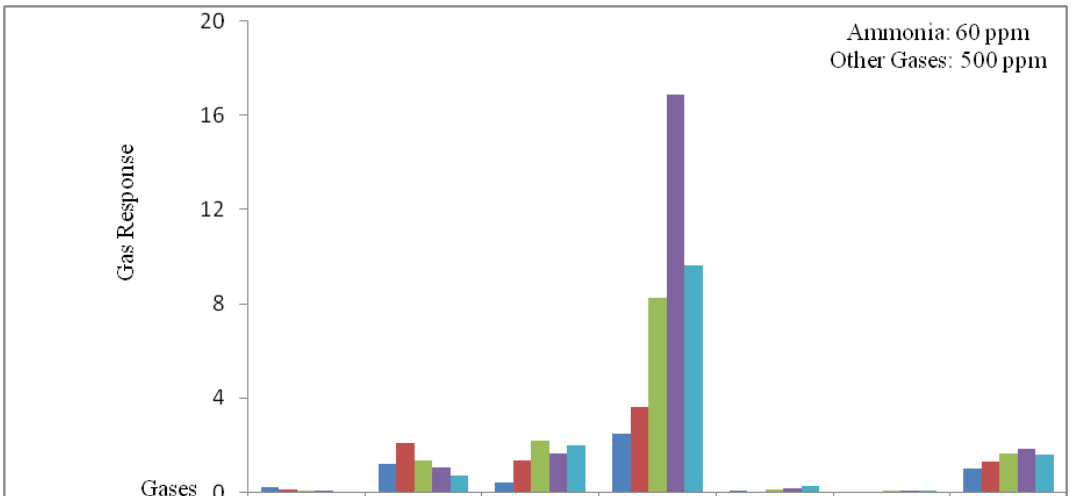
Figure 1. Response of CdO- MgO nanocomposites towards ammonia (60 ppm) as function of operating temperature.

Figure 1. illustrate response of CdO- MgO nanocomposites towards ammonia (60 ppm) as function of operating temperature. Gas response for all the samples of CdO-MgO nanocomposites increased with operating temperature, ranging from room temperature to 350°C towards ammonia gas (60 ppm). This rise in gas response with increasing operating temperature can be attributed to the semiconducting properties of the CdO-MgO nanocomposite thick films. From 250^{0}C to 350^{0}C, gas response increases, with a sharp rise beyond 250 ^{0}C. As shown in the figure, gas response of CdO-MgO nanocomposites (60:40) was higher as compared to other composition of CdO-MgO nanocomposites. This difference could be due to the intergranular potential barriers and grains of grains of varying nature. This modification leads to the formation of heterogeneous inter-grain boundaries in the CdO-MgO nanocomposite, which increases the barrier heights in these regions and may contribute to the reduced conductivity [24-27]. Specifically CdO-MgO (60:40) exhibited highest gas response (16.89) than other composition of CdO-MgO nanocomposites towards NH_3 gas (60 ppm) at 350 ^{0}C.

3.2 Selectivity for NH_3 against various gases

The Figure 2 depicts the gas response of the CdO-MgO nanocomposite thick films towards Ammonia gas (60 ppm) and other gases (500 ppm) at 350 ^{0}C. The sensor showed high selectivity to NH_3 against LPG, CO_2, C_2H_5OH, Cl_2 and H_2S gases. There is smaller gas response for CO_2, C_2H_5OH and H_2S gases whereas no gas response for LPG, $H_2$and Cl_2 gases at 500 ppm at operating temperature 350 ^{0}C. CdO-MgO (60:40) showed higher gas response i.e. 16.89 than other concentration of CdO-MgO nanocomposites to NH_3 (60 ppm) at operating temperature 350 ^{0}C.

The superior response of CdO-MgO (60:40), compared to other concentrations of CdO-MgO nanocomposite thick films, is likely due to the optimal distribution of CdO grains on the surface, as opposed to MgO. If the CdO content is below the optimal level, the number of misfit CdO grains may be insufficient to uniformly cover the surface, resulting in weaker gas interactions and a smaller response. Conversely, if the CdO content exceeds the optimal amount, it could mask the MgO base material, hindering NH3 gas from reaching the CdO-MgO surface. As a result, the gas response would not change significantly, leading to a smaller response [28].



	LPG	CO2	Ethanol	NH3	H2	CL2	H2S
CdO-MgO (90:10)	0.21	1.22	0.44	2.47	0.08	0.01	1.03
CdO-MgO (80:20)	0.14	2.07	1.34	3.61	0.04	0.02	1.31
CdO-MgO (70:30)	0.08	1.33	2.19	8.27	0.11	0.05	1.66
CdO-MgO (60:40)	0.07	1.05	1.67	16.89	0.16	0.07	1.84
CdO-MgO (50:50)	0.03	0.73	1.98	9.61	0.27	0.06	1.58

Figure 2: Gas response for CdO-MgO nanocomposites thick film towards NH3 (60 ppm) gas and other gases (500 ppm) at 350 ^{0}C.

3.3 Effect of NH_3 gas concentration:

Figure 3 illustrates the variation in gas response of the CdO-MgO (60:40) nanocomposite thick films to different concentrations of NH_3 at 350 ^{0}C. The CdO-MgO (60:40) nanocomposite thick film was exposed to a range of NH_3 concentrations from 20 ppm to 120 ppm. As the gas concentration increased up to 120 ppm, the response of the CdO-MgO (60:40) films showed a continuous rise. The rate of increase in gas response was significant up to 60 ppm, after which it increase slowly. Therefore, the active region of the sensor is considered to be from 60 ppm to 80 ppm at 350 ^{0}C. At lower gas concentrations, a unimolecular layer of gas molecules forms on the sensor surface, which interacts more effectively, resulting in a higher gas response. However, at higher concentrations, multiple layers of gas molecules accumulate on the surface, leading to a saturation of the response beyond 80 ppm.

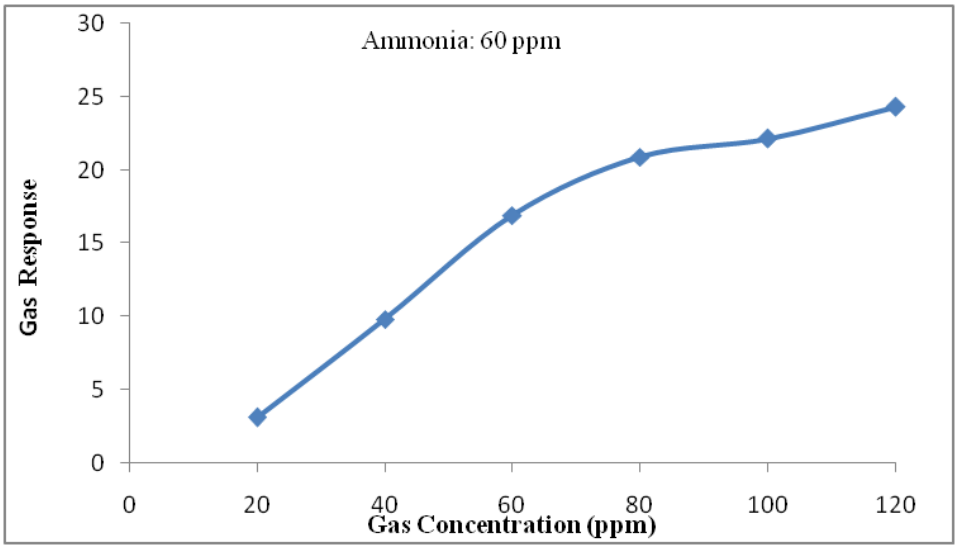


Figure 3: The Gas response of CdO-MgO (60:40) nanocomposite thick films at 60 ppm of NH_3, as a function of the different concentration

3.4 Response - Recovery Characteristics

Response time (RST) is defined as the time it takes for a sensor to reach 90% of the maximum increase in conductance after exposure to a test gas, while recovery time (RCT) refers to the time required for the sensor to recover 90% of its maximum conductance in air [29].

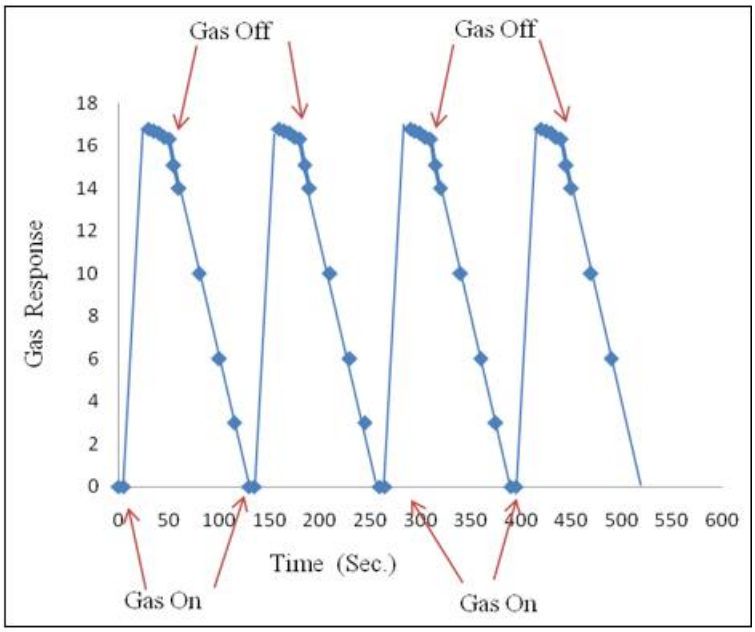


Figure 4: Repeatability graph of Gas response verses time in second for ammonia gas (60ppm) at 350 ^{0}C particularly for the CdO-MgO (60:40) nanocomposite thick film.

Figure 4. illustrates the response and recovery characteristics of the CdO-MgO (60:40) nanocomposite thick film toward ammonia gas (60ppm) at 350 ^{0}C. CdO-MgO (60:40) nanocomposite thick film exhibited a rapid response (~25 s) towards of ammonia at 60 ppm, while the recovery was notably swift (~75 s) at 350 ^{0}C operating temperature. The quick gas response to ammonia and the fast recovery to its initial chemical state can be attributed to the minimal amount of surface reaction products and their high volatility.

3.5 Mechanism of Gas Sensing for CdO-MgO Nanocomposite Thick Film:

1) Chemical Reaction and Conductivity Enhancement:

- Upon exposure to NH_3 gas, the CdO-MgO nanocomposite interacts with NH_3 molecules, leading to a surface reaction that alters the electrical properties of the material. The primary reaction can be represented as:

$$2NH_3+3O^-\rightarrow N_2+3H_2O+3e^-$$

- This reaction releases free electrons into the conduction band leading to a decrease in resistance for the n-type CdO-MgO composite, thus enhancing sensor response to NH_3 [30-32].

2) Heterojunction Transformation

- The CdO-MgO nanocomposite forms an n/n heterojunction due to the combination of n-type CdO and n-type MgO.
- Upon NH_3 exposure, electron transfer occurs at the CdO-MgO interface, altering the charge distribution and modulating the sensor's electrical response. This transformation contributes to the selective and enhanced response characteristics toward NH_3 gas.

3) Recovery Process:

- The adsorbed NH_3 molecules gradually desorb from the sensor surface at room temperature, but complete recovery can be slow under ambient conditions.
- To expedite the recovery process, mild heating (~150-200^{0}C) in air facilitates the oxidation of residual NH_3 species and restores the sensor to its original n-CdO/n-MgO state, enabling repeated sensing cycles.

This mechanism aligns with findings on metal oxide-based NH_3 sensors, where electron transfer, surface reaction, and heterojunction modulation play a crucial role in selectivity and sensing performance. The CdO-MgO nanocomposite, with its high surface area and tunable electronic properties, demonstrates excellent sensitivity, selectivity, and stability for NH_3 gas detection [33-37].

3.6 Stability of the CdO-MgO Nanocomposites:

The long-term stability of gas sensors is a critical parameter for their practical applications in environmental monitoring and industrial safety. To assess the stability of the synthesized CdO-MgO (60:40) nanocomposites as depicted in **Figure 5**, NH_3 gas sensing tests were repeated for the CdO-MgO (60:40) at interval of 10 days upto 90 days of storage under ambient conditions. The results revealed that the performance of the CdO-MgO (60:40) nanocomposite remained consistent over time, demonstrating minimal degradation in their gas sensing response, selectivity, and response-recovery characteristics toward NH_3 gas.

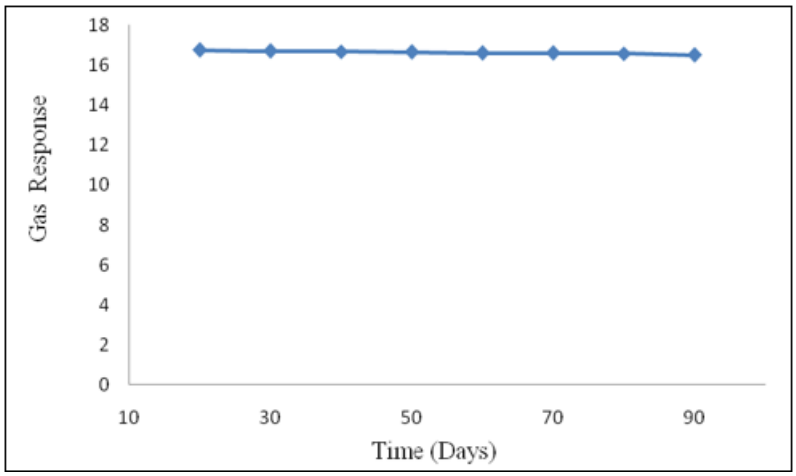


Figure 5: Stability of CdO-MgO (60:40) nanocomposites over time.

The sustained performance of the material indicates that the CdO-MgO nanocomposites possess excellent structural and chemical stability. Several factors contribute to this stability [38-39]. The CdO/MgO nanocomposite demonstrated exceptional stability due to its robust metal-oxide bonding, where strong ionic and covalent interactions within the lattice structures prevented phase decomposition or significant morphological changes over time. Minimal surface degradation was observed, as the material remained free from substantial oxidation, contamination, or decomposition, ensuring that NH_3 gas sensing processes were unaffected. Additionally, the stable n-CdO/n-MgO heterojunctions preserved their structural and electronic integrity, maintaining consistent charge transfer mechanisms crucial for reliable sensing performance. Furthermore, the nanocomposite exhibited resilience to environmental conditions, effectively resisting atmospheric moisture and minor temperature variations that could otherwise induce surface hydroxylation or chemical degradation, thereby reinforcing its durability and long-term functionality.

4. Discussion

The gas sensing analysis provided compelling evidence of the high sensitivity, selectivity, and rapid response-recovery behavior of the CdO-MgO nanocomposites, particularly toward NH_3 gas at an optimal operating temperature of 350^0C. Among the various compositions tested, the CdO-MgO (60:40) nanocomposite exhibited superior gas response, reaching a maximum of 16.89 at 60 ppm NH_3. This enhancement can be attributed to the optimal distribution of CdO grains, leading to increased surface oxygen vacancies and improved charge carrier mobility, facilitating more effective gas adsorption-desorption processes. Selectivity studies confirmed that the CdO-MgO (60:40) nanocomposite preferentially detected NH_3 over other gases such as CO_2, C_2H_5OH, H_2S, and Cl_2, with negligible response toward LPG and H_2, emphasizing its potential application as a selective NH_3 sensor.

The response and recovery time analyses highlighted the rapid sensing behavior of the CdO-MgO (60:40) nanocomposite, with response and recovery times of approximately 25 s and 75 sec., respectively. This fast response-recovery characteristic is indicative of efficient charge transfer mechanisms facilitated by heterojunction formation between CdO and MgO. The gas sensing mechanism was further explained through surface reaction kinetics, where NH_3 interaction with oxygen species led to electron donation and subsequent conductivity modulation, enhancing the sensor's response. Additionally, the presence of an n-CdO/n-MgO heterojunction played a significant role in modulating charge distribution and improving sensing stability [40].

Long-term stability assessments indicated that the CdO-MgO nanocomposite retained its structural and functional properties even after 90 days of ambient storage. The robustness of metal-oxide bonding within the composite, minimal surface degradation, and resilience to environmental variations ensured sustained sensing performance over time. The material exhibited high resistance to moisture-induced surface hydroxylation and minor temperature fluctuations, further reinforcing its suitability for real-world applications [41].

In conclusion, the strategic incorporation of MgO into CdO significantly improved the material's gas sensing properties, particularly for NH_3 detection. The superior response magnitude, excellent selectivity, fast response-recovery times, and long-term stability position CdO-MgO nanocomposites as promising candidates for advanced gas sensor technologies. Future work could explore doping strategies and compositional tuning to further enhance performance parameters, paving the way for their integration into commercial gas sensing devices for environmental and industrial safety monitoring.

5. Conclusion

The CdO-MgO (60:40) nanocomposite demonstrated exceptional NH_3 sensing performance, exhibiting high sensitivity, selectivity, and rapid response-recovery characteristics. Its stability and robustness over extended periods make it a promising candidate for advanced gas sensor applications in environmental and industrial safety monitoring.

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