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Ultra-Responsive Methane Sensing by 2D ZnO Nanoparticle Based MemS Gas Sensor-an Artificial Intelligence Based Study

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INTRODUCTION

Methane (CH₄) gas is aggressively unstable and flammable when admixed with air, posing a risk of explosions, causing asphyxiation due to displacing oxygen in confined or poorly ventilated spaces.[1] Therefore, creating a dependable and affordable methane gas sensor is a critical question, in the environment and in coal mines to protect human lives. Metal oxides prove themselves as efficient methane gas sensing element, due to semiconducting nature. ZnO is a low cost and higher conducting metal oxide, preferably employed in CH₄, H₂ sensing as it is wide band gap (3.2 to 3.4 eV), electron dominated compound semiconductor, easily synthesized even at room temperature [1], high compatibility with silicon. Presently ZnO with its several morphology [1] are becoming prevalent in the ultra-responsive nano-dimensional gas sensors. Microheater-based micromachined silicon structures provides lots of advantages over traditional gas sensors, such as size-compactness, low power consumption, with cost-effective fabrication. They also provide high quality, excellent thermal efficiency, increased sensitivity, fast thermal response time, and long-term reliability. Although existing reports documented ZnO nanostructure based CH₄ sensing with MEMS based Si platform at lower operating temperature but the forecasting in CH₄ sensing is not reported comprehensively.[2] Artificial Intelligence (AI) based forecasting is a promising area of research now-a-days. In this present work, 2D ZnO nanoparticle based CH₄ sensor with Pd-Ag contact and DILVER P1 based MEMS platform is documented. The sensing mechanism, V-I characteristics, dynamic response, long term stability study were investigated at lower temperature range (150- 200°C). The novelty of the present work is the successful implementation of Gradient Boosting Regression algorithm, to predict the CH₄ sensing where the performance of the model is measured by MSE(Mean Squared error) and R-squared value.

MATERIALS AND METHODS

Zinc Sulphate (ZnSO₄·7H₂O), Sodium Hydroxide (NaOH), Palladium Chloride (PdCl₂) were procured from Merck, India. All reagents were used without any further purification. P-type polished Si was purchased from Ultra nanotech Private Limited, Bengaluru, India. Google Collaboratory was used for development of our model as the platform is a free python platform and works fine in cloud architecture. The training data set comprises of operating temperature and CH₄ concentration as input whereas response magnitude (RM), response time(RT) are treated as output.

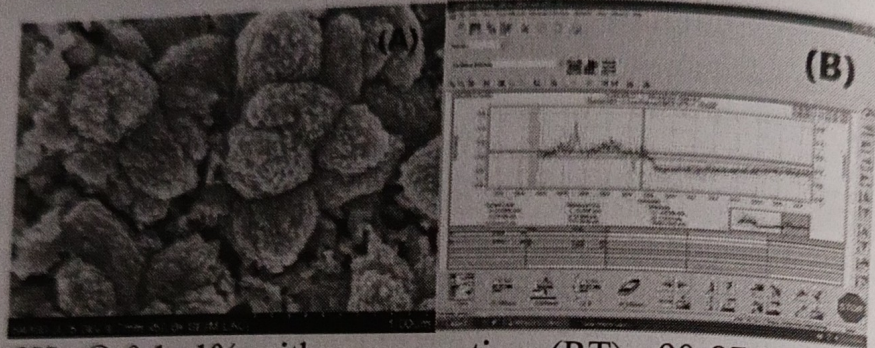
- A. p-Si substrate Preparation
- B. Synthesis of Nanocrystalline ZnO
- C. Characterization- XRD, FESEM, FTIR, UV-Vis spectroscopy.
- D. Fabrication of MEMS based nanocrystalline ZnO based CH₄ gas sensor
- E. Gas Sensing Measurement
- F. ML model- Gradient Boosting Regression implementation

RESULTS AND DISCUSSION

The XRD pattern confirms the formation of wurtzite structured ZnO nanoparticle with grain size of 41.06 nm. FTIR study is also in good agreement with XRD result due to availability of hydroxyl group(O-H stretch, H-bonded) and Zn-O bond at 479 cm⁻¹. The Scanning ElectronMicroscopy revealed 2D flake like structure of the as prepared ZnO layer. FESEM study explores 2D flake like morphology of ZnO thin film consisting of hexagonal needle like structures with ~40-70 nm size and pores with average diameter of ~80nm. The film thickness is

measured and it is found to be 250 nm. The UV-Vis spectra unshielded green defect (significant absorption at 561 nm) enriched ZnO nanostructure. The band gap energy was found to be 3.326 eV.

Figure 1. (A) FESEM micrograph of as synthesized ZnO film, (B) ZnO film thickness profile



The sensor starts sensing CH_4 @ 0.1 -1% with response time (RT) ~90-87s at 125°C . The optimized temperature of the gas sensor is evolved as 200°C as the RM becomes 88.48% for 1% CH_4 and RT was be 40s. The Pd-Ag (70%) contact exhibited excellent ohmic behavior. The sensor exhibited fairly stable response both for N_2 and for 1% CH_4 in N_2 . The Gradient Boosting Regression model has depicted the prediction sensing in terms of MSE (0.7148) and R-squared value (0.9994). (from Table 1)

Table 1. Prediction performance of CH_4 sensing by Gradient Boosting Regression model

Temperature(x1)	Methane conc(x2)	Predicted magnitude(output)	Actual magnitude	Error
238.24	0.64	82.537	83.89	1.353
246.12	0.33	82.537	81.8819	-0.6551
166.35	0.33	74.2779	75.7608	1.4829
188.15	0.82	88.3453	86.9133	-1.432
130.23	0.07	44.4055	43.4314	-0.9741
224.86	0.22	85.2338	83.3102	-1.9236
189.33	0.43	85.5308	83.7936	-1.7372
211.41	0.5	86.5308	85.7576	-0.7732
228.9	0.44	82.537	84.011	1.474
226.18	0.05	79.3098	81.265	1.9552

CONCLUSION

Conclusively, the present investigation explored excellent and stable CH_4 sensing at low temperature by ZnO nanoparticle. The ML modelling has predicted the gas sensing with high level of regression.

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