Data-Driven Prediction and Discrimination of Mixed-Gas Environments Using rGO/In_2O_3 Nanocomposite-Based Chemiresistive Sensors Assisted by Machine Learning

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Selectivity toward specific analytes and reliable detection at sub-ppm concentrations remain persistent challenges for chemiresistive gas sensors, particularly under complex, mixed-gas environments. Hybrid sensing materials that combine reduced graphene oxide (rGO) with semiconducting metal oxides have emerged as promising candidates due to their enhanced charge transport, high surface reactivity, and superior sensitivity at ultralow gas concentrations. In this work, rGO/In_2O_3 nanocomposite thin films were fabricated by incorporating rGO synthesized via a modified Hummers method into nanocrystalline In_2O_3, followed by spin coating and post-deposition thermal annealing to achieve stable and reproducible sensing layers.

Comprehensive structural and morphological characterization confirmed the formation of phase-pure cubic bixbyite In_2O_3 with uniform dispersion of rGO sheets throughout the oxide matrix. The intimate interfacial coupling between rGO and In_2O_3 provides abundant defect sites, enhanced adsorption centers, and efficient conductive pathways, which collectively facilitate improved gas-solid interactions and charge transfer. As a result, the optimized rGO/ In_2O_3 sensor demonstrated excellent sensitivity and long-term stability toward H_2S, achieving a detection limit as low as 100 ppb under controlled conditions.

Despite these improvements, accurate identification and quantitative estimation of target gases in mixed and interfering environments remain a major bottleneck for single-sensor platforms. To overcome this limitation, a machine-intelligent framework was implemented for simultaneous gas classification and concentration prediction using dynamic response features extracted from the sensor's transient behavior. The trained model successfully discriminates between different analyte clusters with an accuracy of 99.7% and reliably predicts previously unseen concentrations of H_2S, NH_3, and CO in mixed-gas scenarios.

The synergistic integration of rGO/In_2O_3 nanocomposite sensing with machine-learning-assisted inference enables robust, low-concentration gas detection using a single sensor, offering a viable pathway toward intelligent chemiresistive systems for real-world environmental monitoring, industrial safety, and health-related applications.

KEYWORDS: rGO, Mixed-gas environment, Gas Sensors, Chemiresistive sensor, Machine learning, PCA, Cluster analysis, H_2S detection