

Physics-Based Power-Law Discrimination of CO₂ and Isoprene Using a Single NdFeO₃ Perovskite Sensor

Abhijit Narayan Eshore¹, Subhobrata Banerjee², Priyanka Dutta³, Prasanta Kumar Guha^{3*}

¹ Advanced Technology Development Centre (ATDC), IIT Kharagpur, India

² School of Nano Science and Technology, IIT Kharagpur, India

³ Department of Electronics and Electrical Communication Engineering, IIT Kharagpur, India

Corresponding Author: pkguha@ece.iitkgp.ac.in

Summary:

A physics-based framework is presented for NdFeO₃ gas sensors, where gas-specific power-law scaling arises from coupled defect transport and surface reactions. At 250° C, CO₂ response follows the expected scaling with exponent agreement $\Delta\alpha < 0.05$ (measured $\alpha = 0.297 \pm 0.007$ vs predicted 0.25; $R^2 = 0.987$), identifying the validity regime of the model. Mixed-gas response is analyzed using the shifted power-law formulation without normalizing or masking. The isoprene contribution exhibits enhanced current-response scaling, indicating competitive site-blocking that modulates carrier density at this temperature. These results demonstrate that the scaling exponents can serve as physically interpretable descriptors for dual-analyte discrimination.

Keywords: NdFeO₃, gas sensing, power-law scaling, mixed gas, isoprene, competitive adsorption

Background, Motivation and Objective

Metal oxide gas sensors exhibit excellent robustness and sensitivity, yet simultaneous surface interactions often limit selectivity in mixed gas conditions [1]. In perovskite oxides such as NdFeO₃, sensing behavior is governed by oxygen vacancy defects and surface adsorption that modulate charge transport across grain-boundary barriers [2, 3]. While CO₂ adsorption typically forms carbonates at basic sites, altering carrier density [4], hydrocarbon (e.g., isoprene) interactions are strongly temperature-dependent and favor site competition over complete oxidation at moderate temperatures [5, 6]. This study examines whether these distinct reaction pathways yield characteristic steady-state power-law exponents suitable as single-sensor discrimination descriptors, and identifies the temperature window for model validity.

Description of the New Method or System

The heart of the resistive sensor was nano-material-based sensing layer (NdFeO₃). It was synthesized using sol-gel technique and drop-casted on interdigitated electrodes to fabricate the device. The sensing layer was characterized using XRD (orthorhombic perovskite phase found) and SEM (agglomerated grains with porous morphology observed) (shown in Fig 1). The dynamic response was measured using a custom-made gas test set up. The sensing response is described using a coupled transport-reacting framework, where oxygen vacancy

transport within the bulk is governed by a Nernst-Planck relation and coupled to surface reactions through boundary kinetics [2]. The electrical response is determined by grain-boundary modulation expressed as

$$I = I_0 \exp(-q\Phi_s/K_B T) \dots (i)$$

where I is the measured current, I_0 is the pre-exponential baseline current, q is the elementary charge, k_B is the Boltzmann constant, and T is the absolute temperature, and Φ_s is the surface potential governed by the charge state of adsorbed species [3]. Under steady state conditions, gas-specific scaling exponent (α) relations emerge between response R and concentration (C) as

$$R = AC^\alpha \dots (ii)$$

The carbonate formation in CO₂ sensing depletes electrons producing a positive scaling exponent, validating theoretical value of $\alpha \approx 0.25$ [4]. For isoprene, shifted power law in equation (iii) gives the net empirical response. This positive response change implies adsorption on surface oxygen sites rather than oxidative dehydrogenation at 250° C, and the mechanistic assignment is under ongoing investigation. The mixed-gas response is expressed as:

$$R_{\text{mix}} = R_{\text{base}} + A_{\text{iso}} C_{\text{iso}}^\alpha \dots (iii)$$

Where, R_{base} corresponds to the CO₂ baseline contribution, without normalisation; log-log curvature reflects the superposition of two surface processes. Throughout this work, sensor re-

sponse R is defined as the ratio of steady-state current under gas exposure to current in air (at a constant applied voltage), $R = I_{\text{gas}}/I_{\text{air}}$; a response value greater than unity therefore indicates a decrease in resistance consistent with enhanced carrier density.

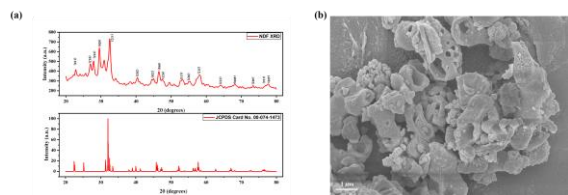


Fig. 1. Structural and morphological characterization of NdFeO_3 . (a) X-ray diffraction (XRD) pattern with indexed diffraction peaks. (b) Field-emission scanning electron microscopy (FESEM) image at the micrometer scale.

Results

At 250°C , CO_2 response follows a power-law with $\alpha_{\text{CO}_2} = 0.297 \pm 0.007$ (predicted theoretically 0.250; $R^2 = 0.987$), confirming the model across 10–160 ppm. The deviation satisfies $\Delta\alpha < 0.05$. For mixed gas conditions (160 ppm CO_2 , and isoprene varying between 0.1 ppm and 5 ppm, as shown in Fig 2b), the response was analyzed using a shifted power-law formulation without baseline subtraction or normalization. The extracted isoprene contribution gives $\alpha_{\text{iso}} = 0.852 \pm 0.021$. The extracted exponent of 0.852 is treated as an experimentally characterised discriminator.

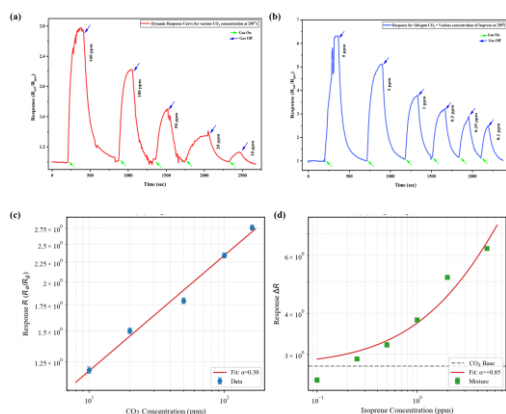


Fig. 2. Gas sensing characteristics of NdFeO_3 at 250°C . (a) Dynamic response of the sensor to varying CO_2 concentrations. (b) Dynamic response under mixed gas exposure (CO_2 + isoprene). (c) Log–log plot of steady-state response versus CO_2 concentration showing power-law scaling with fitted exponent. (d) Mixed-gas response as a function of isoprene concentration, fitted using a shifted power-law model. The presence of a baseline contribution from CO_2 results in curvature in the log–log representation.

Response values increase across 0.1–5 ppm; ΔI is predominantly positive, with a small nega-

tive deviation at 0.1 ppm near the detection limit (ΔI), which may arise from noise or competing surface processes near the detection limit. At 250°C , isoprene adsorbs on vacancy sites, modifying surface oxygen kinetics and enhancing carrier density. The difference between scaling exponents provides a measure of discrimination capability $|\alpha_{\text{iso}} - \alpha_{\text{CO}_2}| = 0.555$. This separation indicates that the contributions of CO_2 and isoprene can be distinguished within a single sensor response. At 200°C , deviations from ideal scaling ($\alpha_{\text{CO}_2} = 0.189 < 0.25$) confirm the model boundary and are excluded from validation in this manuscript.

Conclusion

A physics-based framework for gas sensing in NdFeO_3 has been established using steady-state power-law scaling. At 250°C , the CO_2 response demonstrates strong agreement with theoretical predictions (0.297 ± 0.007 vs. 0.250; $\Delta\alpha < 0.05$; $R^2 = 0.987$), validating the coupled transport-reaction model. Mixed-gas response is accurately described using a shifted power-law formulation, enabling extraction of the isoprene contribution without normalization artifacts. The positive current response and elevated exponent (0.852 ± 0.021) indicate competitive site-blocking at surface oxygen sites. The exponent separation of 0.555 provides a direct, physically interpretable metric for dual-analyte discrimination, offering a streamlined approach for compact mixed-gas monitoring platforms.

References

- [1] S. Kanaparthi, S.G. Singh, Discrimination of gases with a single chemiresistive multi-gas sensor using temperature sweeping and machine learning, *Sensors and Actuators B: Chemical* 348, 130725 (2021); doi: 10.1016/j.snb.2021.130725
- [2] F.A. Kröger, H.J. Vink, Relations between the concentrations of imperfections in crystalline solids, *Solid State Physics* 3, 307–435 (1956); doi: 10.1016/S0081-1947(08)60135-6
- [3] N. Bârsan, U. Weimar, Conduction model of metal oxide gas sensors, *Journal of Electroceramics* 7, 143–167 (2001); doi: 10.1023/A:1014405811371
- [4] Y. Chen et.al., CO_2 sensing properties and mechanism of PrFeO_3 and NdFeO_3 thick film sensor, *Journal of Rare Earths* 37, 80–87 (2019); doi: 10.1016/j.jre.2018.06.007
- [5] J. Casanova-Chafer et.al., Enhanced CO_2 sensing by oxygen plasma-treated perovskite–graphene nanocomposites, *ACS Sensors* 9, 830–839 (2024); doi: 10.1021/acssensors.3c02166
- [6] A.T. Güntner, et.al., Selective sensing of isoprene by Ti-doped ZnO for breath diagnostics, *Journal of Materials Chemistry B* 4, 5466–5474 (2016); doi: 10.1039/C6TB01335J