

“A simulation based study on the selectivity of MoSe₂ for CO and CO₂ gases”

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Abstract:

In this paper, we have examined the vital field of gas sensors, which is crucial for environmental monitoring, industrial safety, and healthcare. One of the most important properties of gas sensors is their selectivity, or their capacity to precisely identify and discriminate particular gases in intricate combinations. Selectivity is influenced by a number of important parameters, some of which were brought to light by our inquiry. These include the choice of sensing material, sensing techniques, operating temperature, humidity levels, cross-sensitivity, sensor geometry, gas preconcentration methods, and the usage of sensor arrays. Additionally, we covered a number of physical and chemical processes, including adsorption and desorption, conductivity changes, capacitance variations, optical absorption, mass loading, chemical reactions, heat production or consumption, ionisation, gas diffusion, and changes in mechanical properties that support gas sensor operations. This study used the gas diffusion method and a variety of sensing materials to evaluate the performance of the MoSe₂. We observed distinct surface concentration levels in response to CO and CO₂ gases on the active surfaces of MoSe₂ thorough simulations. On the other hand, MoSe₂ responded better to CO₂ than to CO. Our results highlight the significance of customising sensor choices based on individual gas detection requirements. As a result, this study clarifies the crucial variables affecting gas sensor selectivity and offers insightful information about the gas-sensing capacities of MoSe₂. Additionally, it highlights the potential uses.

Keywords: Absorption, Diffusivity, Selectivity, Sensitivity, Surface Concentration.

Introduction:

Environmental monitoring, industrial safety, and healthcare are just a few of the fields and applications where gas sensors are crucial. The capacity of gas sensors to accurately detect and distinguish between specific gas analytes in a complicated mixture of gases depends on their selectivity, which is sometimes regarded as their most important characteristic. This paper explores the essential ideas and methods of gas diffusion on the metal oxide semiconductor or transitional metal gas sensor. The key factors that influence the sensitivity of the metal based gas sensor are as follow

- i. Sensing material: One of the key elements impacting selectivity is the selection of the sensing material. Different substances have different affinity for particular gases. Sensing components can be modified or functionalized to increase their selectivity for specific target gases [1].
- ii. Sensing Methods: Gas sensors can use resistive, capacitive, optical, or piezoelectric sensing methods, among others. The selectivity of the sensor depends on how it interacts with gases through its detecting mechanism [2].
- iii. Temperature: A gas sensor's selectivity can be considerably impacted by the temperature at which it operates. At various temperatures, some sensors respond to gases in different ways. Selectivity for particular gases can be increased by modifying the operating temperature [3].
- iv. Humidity: The environment's humidity levels can have an impact on the selectivity of gas sensors, especially for sensors sensitive to water vapour. High humidity can cause interference or drift in sensor responses [4].
- v. Cross-Sensitivity: In gas sensors, cross-sensitivity is a frequent problem. When a sensor reacts to a variety of gases, including ones that are not of interest, it happens [5].
- vi. Sensor Geometry and Design: The selectivity of a sensor can be affected by its physical design, including its size, shape, and arrangement. Gas diffusion rates can be influenced by sensor shape, which in turn can affect reaction times and selectivity [6].
- vii. Gas Preconcentration: Gas preconcentration techniques can be used to increase the concentration of the target gas before it reaches the sensor, which can improve selectivity. This reduces the influence of interference gases and increases the sensor's sensitivity to the target gas [7].
- viii. Sensor Arrays and Multi-Sensor Systems: By integrating several sensors with various selectivity into an array or system, selectivity can be increased overall. The reactions can then be analysed using pattern recognition algorithms to pinpoint particular gases [8].

Some other factors like gas filtration, environment conditions, signal processing and sensor calibration are also influence the selectivity of the gas sensor.

In gas sensors, there are various physical and chemical phenomenon take place that provide the basis for gas sensor operation. These phenomenon quantify the sensor characteristic, which are utilised to identify and measure the presence of particular gases. The physical and chemical phenomenon happen in gas sensor are:

- i. Adsorption and Desorption: The surface of the sensing material is adsorbed with gas molecules from the surroundings. The electrical, optical, or mechanical properties of the material are altered as a result of this adsorption. Gas molecules are released from the surface during desorption, which can either be reversible or irreversible [9].
- ii. Change in Conductivity: Changes in electrical conductivity are used by many gas sensors, particularly those made of metal oxide. Target gas adhering to the surface of the sensor changes the material's electron conductivity, causing a change in resistance or conductivity. This alteration is then correlated with gas concentration.
- iii. Change in Capacitance: Some gas sensors, especially capacitive ones, use variations in capacitance brought on by gas adsorption. The dielectric constant or thickness of the insulating layer of the sensor changes when gas is present, which causes a noticeable change in capacitance.
- iv. Optical Absorption: Gas sensors that rely on optical absorption work by using the fact that some gases absorb particular light wavelengths. The intensity of light that is transmitted or reflected decreases when the target gas is present because it absorbs light at specific wavelengths. To identify and calculate the gas concentration, this change is employed [10].
- v. Mass Loading: The principle of mass loading governs the operation of piezoelectric gas sensors. Gas molecules contribute mass to the sensor by adhering to its surface, changing the sensor's resonance frequency. These fluctuations in frequency are inversely correlated with gas concentration.
- vi. Chemical Reactions: Some gas sensors work by triggering chemical processes between the target gas and the sensing substance. Changes in colour, pH, or other chemical qualities may arise from these interactions; these changes are noted as related to gas concentration.
- vii. Heat Generation or Consumption: When they come into contact with gases, some gas sensors either create or absorb heat. For instance, catalytic combustion sensors measure the heat produced during gas oxidation to identify combustible gases [11]. On the other hand, when gases adsorb onto a sensor's surface, some sensors absorb heat [12].
- viii. Ionisation: Gas molecules must be ionised at the electrode surface of ionization-based gas sensors, such as electrochemical sensors. As a result, a reaction that is proportionate to gas concentration in current or voltage is produced [13].
- ix. Gas Diffusion: The presence of the target gas can affect how quickly gas molecules diffuse through a sensing material. For gas sensing, it is possible to identify and use this variation in diffusion rate [14].
- x. Changes in Mechanical Properties: Some gas sensors (such quartz crystal microbalance sensors) assess changes in mechanical properties, such as the deformation or resonance frequency of a mechanical element. These modifications, which are brought on by gas adsorption, are related to gas concentration.

Selectivity in gas sensing technologies is crucial, and this cannot be emphasised enough. Getting selectivity is essential for accurate and usable data collection in a world where gas mixtures can vary greatly and contain a variety of potentially dangerous or volatile substances. It improves safety and makes environmental monitoring, industrial operations, and medical diagnostics easier when certain gases can be accurately identified and quantified. The transition metal like Molybdenum-diselenide (MoSe_2) are selected for this investigation using the gas diffusion method based on this previously mentioned phenomenon and sensing method.

2. Method

The 2D model of the proposed model is designed in the COMSOL Multiphysics simulator as shown in Fig. 1 for simulation to study the diffusion of gas in the active region of the sensor. The gas is in from the inlet side and out from the outlet side. The Active region is the region where the sensor is put. The length of the active region is 0.1 mm.

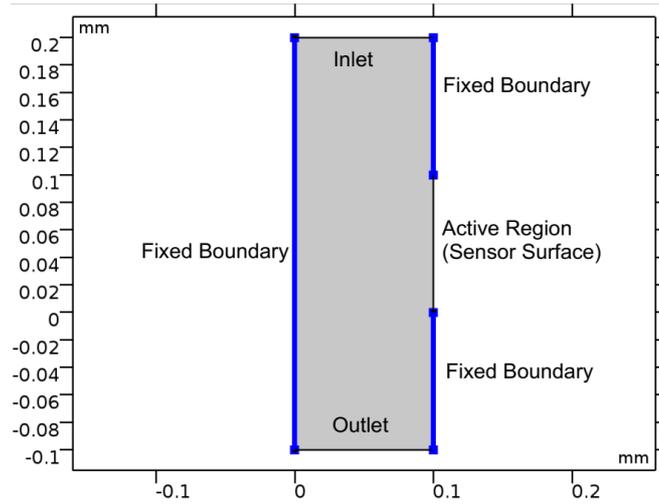


Fig. 1: 2D proposed model for simulation in COMSOL.

After designing the 2D model, the various parameter used in the simulation is defined in the parameter section and the they are tabulated in table 1.

Table 1: Various parameters define in the COMSOL simulation.

Name	Value	Description
C_0	100 mol/m ³	Initial concentration
k_{ads}	1E-6 m ³ /(s·mol)	Forward rate constant
Γ_s	100 mol/m ²	Active site concentration
D_s	0.0012 m ² /s	Surface diffusivity of MoSe ₂
D	2.08E-5 m ² /s	Gas diffusivity of CO
V_{max}	0.001 m/s	Maximum velocity
l	1E-4 m	Length of the active region

For various sensing materials and target gases, they have different values of surface diffusivity and gas diffusivity, respectively. In this study, the combination of transitional metal MoSe₂ with CO₂ and CO gases is done. Later, a comparative study based on diffusivity is done to see which combination is performed better. The surface diffusivity and gas diffusivity taken in this study is tabulated in the table 2 [15-16].

Table 2: Surface Gas Diffusivity and Gas Diffusivity used in Simulation.

Name	Value	Unit	Description
MoSe ₂	1.2E-3	m ² /s	Surface diffusivity
CO	2.08E-5	m ² /s	Gas diffusivity
CO ₂	1.6E-5	m ² /s	Gas diffusivity

The meshing of the design model is done with free tetrahedral shape and the size of the meshing is taken as finer for this simulation. After meshing the study model is show in Fig.2.

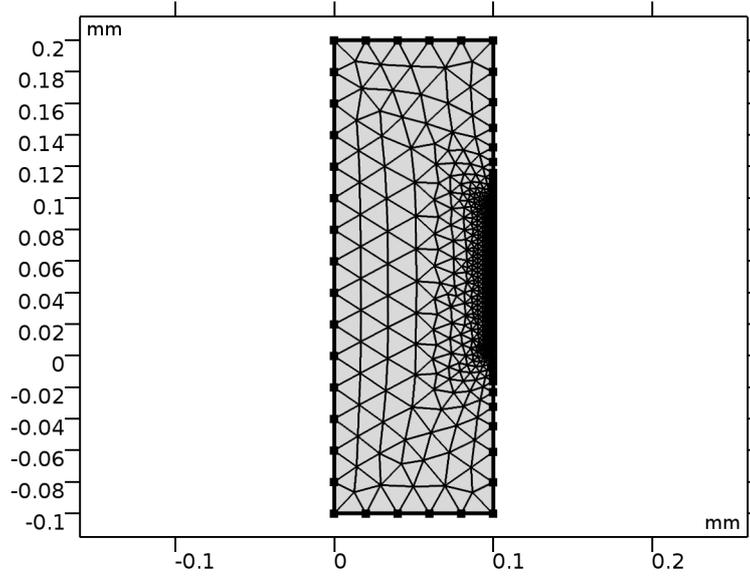


Fig. 2: Meshing of the Design Model.

The mass balance of the CO and CO₂ molecules in the bulk and on the surface are related, and the mass balance of the surface is determined as a boundary condition. This requirement determines the surface reaction rate, which results in a convection diffusion equation equal to the flux of concentration of CO and CO₂ at the boundary.

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i$$

$$\mathbf{N}_i = -D_i \nabla c_i + \mathbf{u} c_i$$

Where, c_i is the concentration of the species (SI unit: mol/m³), D_i denotes the diffusion coefficient (SI unit: m²/s), R_i is a reaction rate expression for the species (SI unit: mol/(m³·s)), \mathbf{u} is the mass averaged velocity vector (SI unit: m/s), \mathbf{N}_i is the inward molar flux from the gas analyte into the sensing and has the unit moles/(m²·s)

3. Result and Discussion

The simulations are run for the combinations of MoSe₂ with CO and MoSe₂ with CO₂. The simulated output of the simulation showing the surface variation of surface concentration in the active region are show in Fig. 3 and Fig. 4.

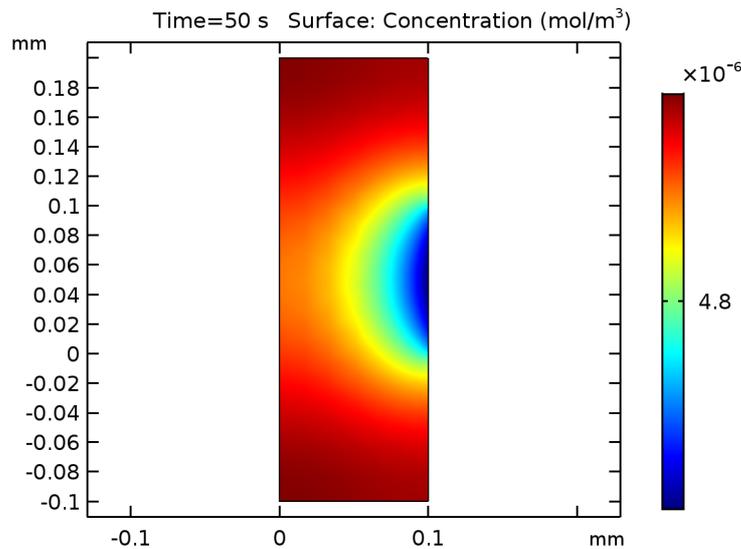


Fig. 3: Simulated output of the surface concentration for MoSe₂ with CO.

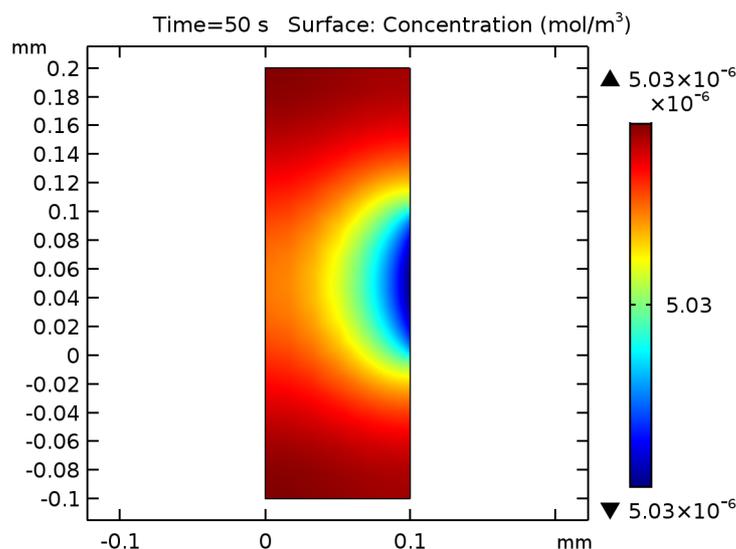


Fig. 4: Simulated output of the surface concentration for MoSe₂ with CO₂.

Table 2: The various surface concentration of the analytes on the active surface

Sl. No.	Combinations	Surface Concentration
1	MoSe ₂ with CO	4.80 E-6 mol/m ³
2	MoSe ₂ with CO ₂	5.03E-6 mol/m ³

From Fig. 3 and Fig. 4, the surface concentration of gas shows different concentration levels. This means that MoSe₂ is able to sense CO and CO₂ gas through the diffusion phenomenon. The various surface concentrations of the analytes on the active surface are tabulated in Table 2. It is also observed from Table 2 that MoSe₂ with CO₂ has higher sensitivity than the MoSe₂ with CO. The MoSe₂ sensing material can be for selection of CO₂ and CO since the deviation of surface concentration on the is 0.23 mol/m³. MoSe₂ is also able to sense CO with less sensitivity as the response is less.

4. Conclusion

In conclusion, the simulated results presented in Fig. 3 and Fig. 5 reveal distinct surface concentration levels, indicating the capability of MoSe₂ to effectively sense CO and CO₂ gases through the diffusion phenomenon. The comprehensive data on surface concentrations is summarised in Table 2, offering valuable insights into the sensor's performance. Selectivity in a gas sensor is often evaluated based on the deviation of the sensor's response to the target gas, and this observation underscores MoSe₂ effectiveness in distinguishing between the two gases. Additionally, it is worth mentioning that MoSe₂ demonstrates a higher surface concentration for CO₂, indicating a stronger sensing response to this gas. MoSe₂ excels in distinguishing between CO and CO₂, making it an ideal choice for applications requiring high selectivity with enhanced sensitivity to CO₂. These findings provide valuable insights into the potential applications of MoSe₂ based gas sensors in various environmental and industrial settings, allowing for tailored sensor selection based on specific gas detection requirements.

Finally, the selectivity of CO and CO₂ can be approved by using an array of sensor with proper Artificial Intelligence classification tools.

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