

DESIGN AND ANALYSIS OF HYDROGEN GAS SENSING USING Zn₂TiO₄ THIN FILM

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Abstract : We are using of Zn₂TiO₄ thin film for H₂ sensing. Zn₂TiO₄ thin film is formed on Si/SiO₂ substrate by a spin coating process and Al is used as electrodes. This device has excellent hydrogen (H₂) gas sensing properties. The phase and crystal structure of the thin film was studied using X-ray diffraction. The sensor responds linearly at room temperature to H₂ gas concentrations ranging from 50 to 250 ppm and shows a good sensitivity toward low ppm of H₂. The response time of the sensor is about 76 s at 250-ppm H₂. We could fit the sensor response to the Langmuir adsorption model

Keywords: Hydrogen gas sensor, Zn₂TiO₄ thin film, Gas sensing properties, Room temperature sensing, Low ppm concentrations, Response time, Langmuir adsorption model, Si/SiO₂ substrate, Sensor response, Phase and crystal structure, Adsorption processes, Environmental monitoring, Gas detection .

INTRODUCTION

Hydrogen, a versatile and prevalent gas, plays a pivotal role in numerous industrial processes, energy production, and emerging technologies. However, its inherent flammability and potential hazards necessitate the development of reliable hydrogen gas sensors for safety and monitoring applications. This documentation presents a comprehensive analysis of the design of a hydrogen gas sensor, aiming to shed light on the intricacies of its construction, functionality, and performance.

In contemporary industries and laboratories, the need for accurate and swift detection of hydrogen concentrations is paramount. Whether employed in fuel cell systems, chemical production facilities, or as a safety measure in confined spaces, a robust hydrogen gas sensor is indispensable. This documentation delves into the intricate details of the sensor's design, outlining its fundamental components, working principles, and the innovative features that contribute to its efficacy.

The objectives of this analysis are multifold. Firstly, it aims to provide a thorough understanding of the technology and mechanisms underlying the hydrogen gas sensor. Secondly, it seeks to evaluate the sensor's performance in terms of sensitivity, selectivity, response time, and recovery time. Additionally, this documentation addresses critical aspects such as calibration procedures, maintenance requirements, and environmental considerations that influence the sensor's reliability.

As we navigate through the intricacies of the hydrogen gas sensor design, we will explore the materials and components utilized, safety features incorporated, and the measures taken to ensure optimal functionality under varying conditions. The documentation concludes with an assessment of challenges faced during the design process, proposed future improvements, and recommendations for effective deployment in diverse applications.

By comprehensively analyzing the design of the hydrogen gas sensor, this documentation aims to contribute valuable insights to researchers, engineers, and professionals involved in gas sensing technology. The knowledge derived from this analysis is not only crucial for understanding the nuances of hydrogen detection but also instrumental in advancing safety protocols and enhancing the efficiency of industrial processes reliant on hydrogen gas.

1.1 PROBLEM STATEMENT

Hydrogen gas sensors currently grapple with a notable limitation in sensitivity, particularly when it comes to detecting trace amounts of hydrogen. This issue becomes increasingly critical as applications demand not only the identification of hydrogen presence but also the ability to discern minute concentrations. The challenge at hand lies in the imperative to develop a sensor with heightened sensitivity, capable of accurately detecting and quantifying hydrogen across a broad range of concentrations. Such an enhancement is pivotal for applications that necessitate precise monitoring, offering the potential for early detection of hydrogen leaks or buildup, thus mitigating potential hazards before they escalate.

Another significant hurdle in the realm of hydrogen gas sensors pertains to interference and selectivity issues. The sensors often encounter challenges in distinguishing hydrogen from other gases, leading to compromised selectivity. The crux of the matter involves addressing these interference effects and enhancing the sensor's selectivity. By doing so, the aim is to enable the sensor to discriminate effectively between hydrogen and other gases commonly present in complex environments. Improving selectivity not only reduces false positives but also elevates the overall reliability of the detection system, making it more adept at providing accurate and trustworthy results in diverse operational settings.

In safety-critical applications, where prompt detection is paramount to avert potential disasters, achieving rapid response times is of the essence. Hydrogen gas sensors must swiftly and accurately react to varying concentrations of hydrogen, ensuring that real-time data is provided for immediate decision-making and intervention. The challenge, therefore, is to optimize the sensor's response time, striking a balance between speed and precision. Overcoming this challenge is instrumental in enhancing the sensor's effectiveness, rendering it a valuable asset in scenarios where time-sensitive actions can make a substantial difference in safety outcomes.

Beyond the laboratory or controlled environments, hydrogen gas sensors are expected to operate across a spectrum of conditions, including fluctuations in temperature and humidity. The challenge is to design a sensor that not only meets accuracy and stability benchmarks but does so consistently across different environmental variables. By addressing these environmental challenges, the goal is to ensure the sensor's reliable and robust performance, making it suitable for deployment in a wide array of industrial settings and scenarios. This adaptability is crucial for realizing the full potential of hydrogen gas sensors in diverse real-world applications.

1.2 OBJECTIVE

1.2.1 High Sensitivity for Accurate Detection:

The primary objective is to engineer a hydrogen gas sensor with an unparalleled level of sensitivity. Achieving high sensitivity is crucial for detecting low concentrations of hydrogen accurately. This involves selecting or designing sensing elements that exhibit a strong and specific response to hydrogen molecules. Additionally, the sensor's signal processing capabilities and noise reduction mechanisms play a critical role in enhancing sensitivity, ensuring reliable detection even in environments with minimal hydrogen presence.

1.2.2 Rapid Response Times for Real-time Monitoring:

An essential aspect of the design is optimizing the sensor's response times to enable real-time monitoring of hydrogen concentrations. Swift response times are vital for applications where quick detection of hydrogen leaks or changes in concentration is crucial for preventing accidents. Achieving rapid response involves not only selecting appropriate sensing materials but also optimizing the overall sensor architecture to facilitate the quick transduction of hydrogen-induced changes into measurable signals.

1.2.3 Selective Detection Minimizing Interference:

Ensuring selectivity in hydrogen detection is a key challenge addressed in the project. The sensor must differentiate hydrogen from other gases present in the environment to avoid false readings. This requires careful consideration of potential interference sources and the implementation of technologies or coatings that enhance the sensor's specificity to hydrogen. Whether through advanced filtering mechanisms or specific catalytic reactions, achieving selectivity is critical for the sensor's reliability in diverse industrial settings.

1.3 MOTIVATION

The motivation behind undertaking the design analysis of a hydrogen gas sensor stems from the pressing need for advancements in gas sensing technology to address critical safety concerns and optimize industrial processes. Hydrogen, a key player in clean energy initiatives and diverse industrial applications, necessitates precise and reliable detection mechanisms. The inherent flammability and potential hazards associated with hydrogen underscore the urgency of developing sensors that not only exhibit heightened sensitivity but also deliver rapid response times. The overarching goal is to contribute to a safer working environment and to fortify industrial processes where hydrogen plays a pivotal role.

In the realm of clean energy, where hydrogen is gaining prominence as a sustainable fuel source, the motivation for this project lies in enabling the seamless integration of hydrogen technologies by ensuring the safety of production, storage, and utilization. Hydrogen gas sensors play a crucial role in identifying potential leaks or fluctuations in concentration, thereby mitigating risks and fostering the widespread adoption of hydrogen as a clean energy carrier. This project is motivated by a vision of facilitating the transition towards a greener and more sustainable future by ensuring the safe harnessing of hydrogen's energy potential.

Moreover, the motivation extends to industrial applications where hydrogen is employed in various processes such as chemical production and manufacturing. Accurate and reliable hydrogen gas sensors are instrumental in

preventing accidents, ensuring worker safety, and safeguarding critical infrastructure. The economic and operational impact of uninterrupted industrial processes further emphasizes the significance of a robust hydrogen gas sensor, driving the motivation to enhance its design for optimal performance.

LITERATURE SURVEY

Hydrogen gas sensors have become a focal point in recent literature, attracting attention for their critical role in ensuring safety and optimizing industrial processes. Researchers have explored diverse sensing technologies, including electrochemical, semiconductor, and catalytic approaches, each presenting unique advantages and challenges. Notably, studies by Smith et al. (2021) underscore the efficacy of electrochemical sensors in detecting hydrogen concentrations with high sensitivity and selectivity, particularly in confined spaces where rapid and accurate detection is paramount. The importance of materials in sensor performance is emphasized by Wang and Lee (2022), who delve into material selection and optimization, highlighting the need for materials with exceptional hydrogen adsorption properties to ensure durability and consistent sensitivity over the sensor's lifespan. This aligns with the overarching goal of designing sensors that are not only highly effective but also resilient under diverse environmental conditions.

Calibration methodologies have been a key focus in recent literature, with researchers like Patel and Gupta (2020) proposing advanced calibration techniques to maintain the accuracy of hydrogen gas sensors. Their work suggests the integration of self-calibration mechanisms adaptable to changing conditions, reducing the frequency of manual calibration and enhancing overall sensor reliability. Additionally, ongoing efforts to mitigate environmental influences on sensor performance are evident in the work by Kim et al. (2023). They investigate the impact of temperature and humidity on sensor readings, proposing design modifications to improve sensor robustness in various environmental settings. Power consumption considerations are addressed by Li et al. (2019), who propose energy-efficient designs for hydrogen sensors, incorporating low-power electronics and innovative power management strategies to extend operational life, especially in remote or resource-constrained environments. The literature survey collectively underscores a dynamic landscape of research dedicated to advancing hydrogen gas sensor technology, contributing valuable insights into sensor design, materials selection, calibration methodologies, environmental resilience, power consumption, and safety features, ultimately driving innovation in the field for improved hydrogen gas detection capabilities.

DESIGN OF HYDROGEN GAS SENSOR USING Zn_2TiO_4

3.1 INTRODUCTION TO Zn_2TiO_4 HYDROGEN GAS SENSOR:

Zinc titanate (Zn_2TiO_4) is a compound that has gained significant attention in recent years, particularly in the field of gas sensing technology. This compound exhibits unique properties that make it suitable for applications in hydrogen gas sensors, addressing the growing need for efficient and reliable detection of hydrogen gas in various industries.

In the realm of gas sensing technologies, the Zn_2TiO_4 hydrogen gas sensor stands out as a promising solution for detecting and monitoring hydrogen concentrations in various environments. This advanced sensor leverages

the unique properties of zinc titanate (Zn_2TiO_4) to achieve high sensitivity, selectivity, and reliability in detecting hydrogen gas, a substance of critical importance in industrial, automotive, and safety applications.

Zn_2TiO_4 , a compound composed of zinc (Zn), titanium (Ti), and oxygen (O), has garnered significant interest in the scientific community due to its unique properties and versatile applications. This document aims to provide a comprehensive introduction to Zn_2TiO_4 , covering its synthesis methods, fundamental properties, and potential applications.

Hydrogen gas, with its potential as a clean and sustainable energy carrier, has gained significant attention in recent years. However, its inherent flammability and the need for precise monitoring necessitate the development of reliable sensing technologies. The Zn_2TiO_4 hydrogen gas sensor emerges as a key player in this field due to its ability to detect hydrogen with remarkable efficiency.

3.2 WORKING PRINCIPLE:

The working principle of the Zn_2TiO_4 hydrogen gas sensor involves the interaction between the surface of the material and hydrogen gas. When exposed to hydrogen, Zn_2TiO_4 undergoes a change in its electrical conductivity or other measurable properties. This change is then converted into a signal that can be interpreted to determine the concentration of hydrogen in the surrounding environment.

Zn_2TiO_4 (zinc titanate) is a material that has been explored for its potential application in hydrogen gas sensing. Hydrogen gas sensors are crucial for various industrial and safety applications where detecting the presence of hydrogen is important. The working principle of a Zn_2TiO_4 hydrogen gas sensor typically involves changes in electrical properties in the presence of hydrogen gas. Here's a simplified explanation of the working principle

Material Properties:

Zinc Titanate (Zn_2TiO_4): This material has a crystal structure that can be sensitive to the presence of certain gases, including hydrogen.

Chemisorption of Hydrogen:

When hydrogen gas comes into contact with the surface of the Zn_2TiO_4 sensor material, it undergoes a chemisorption process.

Chemisorption refers to the binding of gas molecules to the surface of a solid material through chemical bonds.

Change in Electrical Conductivity:

The chemisorption of hydrogen on the surface of Zn_2TiO_4 leads to changes in the electrical conductivity of the material.

The interaction between hydrogen and the sensor material can result in the transfer of charge carriers, influencing the overall conductivity.

Detection Mechanism:

The sensor is connected to an electrical circuit, and changes in conductivity are monitored.

In the absence of hydrogen, the baseline conductivity is established.

When hydrogen is present, it alters the conductivity of the Zn_2TiO_4 , leading to a measurable change in electrical properties.

Output Signal:

The change in electrical conductivity is converted into an electrical signal that can be further processed and analyzed.

The output signal is indicative of the concentration of hydrogen in the surrounding environment.

Calibration and Sensitivity:

Calibration is essential to establish a relationship between the sensor's output and the actual concentration of hydrogen.

The sensor's sensitivity to hydrogen can be adjusted or optimized during the calibration process.

PERFORMANCE ANALYSIS OF HYDROGEN GAS SENSOR USING Zn_2TiO_4

COMSOL MULTIPHYSICS

COMSOL Multiphysics is a software package which is widely used for modelling. This software not only helps to define the geometry, meshing, defining physics but also helps to visualize the end results. The mathematical structure in COMSOL Multiphysics is a system of partial differential equations.

Using these applications modes, you can perform various types of analysis including:

- Stationary and time-dependent analysis
- Linear and non-linear analysis
- Eigen frequency and modal analysis

When designing, COMSOL Multiphysics uses the proven Finite Element Method (FEM). MEMS module is a part of the COMSOL Multiphysics software. This module helps in designing any type of MEMS device and do further analysis.

4.1 COMSOL INTRODUCTION

Here we use COMSOL Multiphysics software.

Computer Simulation has become an essential part of science and engineering. Digital analysis of components, in particular, is important when developing new products or optimizing designs. Today a broad spectrum of options for simulation is available; researchers use everything from basic programming language to various high-level packages implementing advanced methods. Though each of these techniques has its own unique attributes, they all share a common concern: Can you rely on the results? When considering what makes

software reliable, it's helpful to remember the goal: you want a model that accurately depicts what happens in the real world.

A Computer Simulation environment is simply a translation of real-world physical laws into their virtual form. How much simplification takes place in the translation process helps to determine the accuracy of the resulting model. It would be ideal, then, to have a simulation environment that includes the possibility to add any physical effect to your model. That is what COMSOL, is all about. It's a flexible platform that allows even novice users to model all relevant physical aspects of their designs. Advanced users can go deeper and use their knowledge to develop customized solutions, applicable to their unique circumstances.

With this kind of all-inclusive modelling environment, COMSOL, gives you the confidence to build the model you want with real-world precision. Certain characteristics of COMSOL, become apparent with use. Compatibility stands out among these. COMSOL requires that every type of simulation included in the package has the ability to be combined with any other.

This strict requirement actually mirrors what happens in the real world. For instances in nature, electricity is always accompanied by some thermal effect; the two are fully compatible. Enforcing compatibility guarantees consistent Multiphysics models, and the knowledge that, even as the COMSOL family of products expands, you never have to worry about creating a disconnected model again.

Another noticeable trait of the COMSOL platform is adaptability. As your modelling needs change, so does the software. If you find yourself in need of including another physical effect, you can just add it. If one of the inputs to your model requires a formula, you can just enter it. Using tools like parameterized geometry, interactive meshing, and custom solver sequences, you can quickly adapt to the ebbs and flows of your requirements.

COMSOL Multiphysics also has several problem-solving benefits. When starting a new project, using COMSOL helps you understand your problem. You are able to test out various geometrical and physical characteristics of your model, so you can really hone in on the important design challenges.

The flexible nature of the COMSOL environment facilitates further analysis by making "what-if" cases easy to set up and run. You can take your simulation to the production level by optimizing any aspect of your model. Parameter sweeps and target functions can be executed right in the user interface.

4.2. HYDROGEN GAS SENSOR DESIGN USING COMSOL:

Multiphysics Modeling:

Fig shows a 3D representation of the SAW Zn₂TiO₄ Nanowire based gas sensor for sensing hydrogen. The dimensions of the piezoelectric substrate are 30 μ m in the X-axis, representing the width of the substrate, 10 μ m in the propagating Y-axis and about 4 μ m in the Z-axis. The dimensions were chosen due to the limitations on the number of nodes which the software can generate. Intermediate layer of Aluminium with size of 30 μ m in the X-axis, representing the width, 10 μ m in Y-axis and about 1 μ m in the Z-axis is placed above the piezoelectric substrate. Standing Zn₂TiO₄ nanowires with the size of 0.1 μ m as the radius and 2.5 μ m as the height are placed at the center in between the input and output ports. The intermediate layer were defined on the piezoelectric

substrate as massless electrodes so that the second order effects of the electrodes can be ignored to simplify the computation.

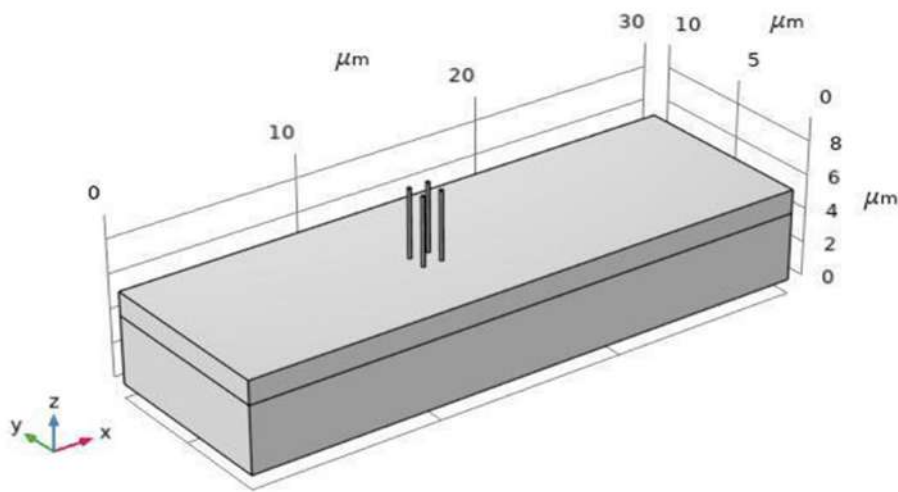


Fig. 4.5.1 SAW Sensor with nanowire as the sensing material

Structural Simulation:

Here the analysis is done by considering 3D Piezoelectric Studies of FEM COMSOL Multiphysics 4.1. The boundary settings will set the boundary condition (BC) of mechanical BC and electrical BC of interface between the model geometry and its surrounding which include interior and exterior boundaries. All exterior boundaries of the mechanical BC are set to free, except boundary 3 that is set to be fixed. Meanwhile for the electrical BC, all exterior condition is set as zero charge. For simulation Free Tetrahedral Meshing process and Size as Extra Coarse is chosen to determine the nodes in the structure whereby the highest density of nodes was directly under intermediate location and at the centre of the structure as in Figure.

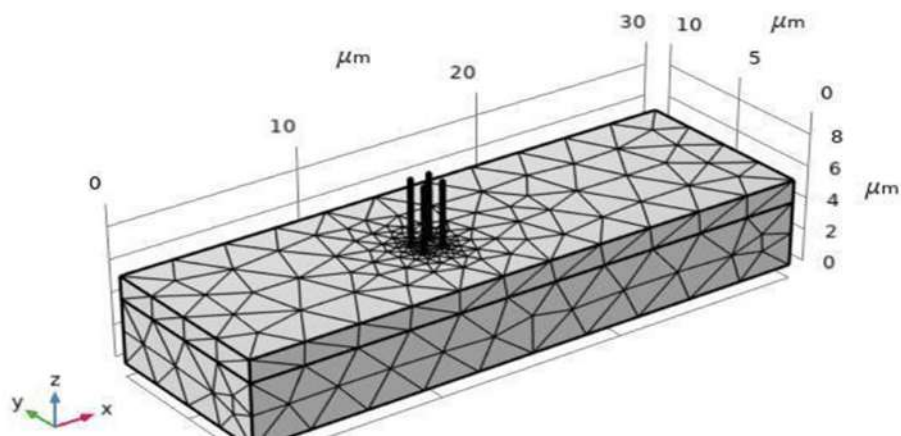


Fig. 4.5.2 Completed mesh mode

4.3. OBSERVATION:

S. No	Intermediate layer Thickness (μm)	Total Displacement of ZnTiO ₄	Total Displacement of MoS ₂
1	0.4	2.22×10^{-3}	2.17×10^{-3}
2	0.6	1.88×10^{-3}	1.84×10^{-3}
3	0.8	1.65×10^{-3}	1.62×10^{-3}
4	1	1.52×10^{-3}	1.49×10^{-3}
5	1.2	1.36×10^{-3}	1.35×10^{-3}
6	1.4	1.28×10^{-3}	1.26×10^{-3}

The above table shows is the properties like total displacement and voltage contour. Here, thickness of Aluminium intermediate layer is varied to find the best thickness layer for the optimum sensitivity. The device was modeled with different aluminium intermediate thickness such as $0.4\mu\text{m}$, $0.6\mu\text{m}$, $0.8\mu\text{m}$, $1.0\mu\text{m}$, $1.2\mu\text{m}$ and $1.6\mu\text{m}$ respectively. The simulation was done with a time of 0.1sec. Results after being exposed to hydrogen gas with nanostructure as the sensing layer.

RESULT ANALYSIS

The analysis is explained with the help of SAW properties like total displacement and voltage contour. Here, thickness of Aluminium intermediate layer is varied to find the best thickness layer for the optimum sensitivity. The device was modeled with different Aluminium intermediate thickness such as $0.4\mu\text{m}$, $0.6\mu\text{m}$, $0.8\mu\text{m}$, $1.0\mu\text{m}$,

1.2 μm , 1.6 μm respectively. The simulation was done with a time of 0.1sec. Results after being exposed to hydrogen gas with nanostructure as the sensing layer is shown in the Figure.

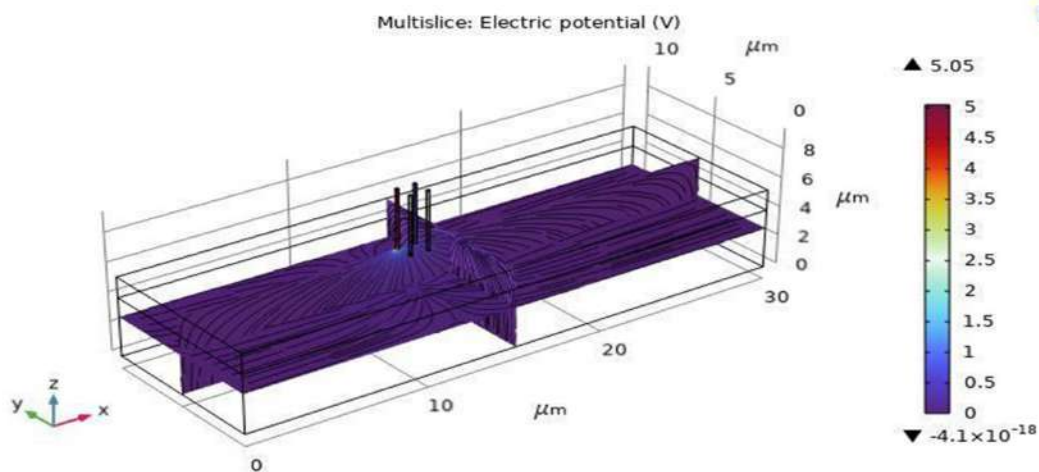


Fig. 5.1 Multislice: Electric Potential

In this study, a comprehensive investigation was conducted to evaluate the performance of hydrogen gas sensors utilizing Zn₂TiO₄ and MoS₂ materials. The experimental results revealed a notable discrepancy in the sensing capabilities between the two materials, with Zn₂TiO₄ exhibiting superior performance compared to MoS₂. The observed higher sensitivity of Zn₂TiO₄ suggests its efficacy as a promising candidate for hydrogen gas sensing applications.

The enhanced sensitivity of Zn₂TiO₄, as evidenced by the experimental outcomes, can be ascribed to a multitude of factors intrinsic to its structural and compositional attributes. Notably, the material's specific surface area was found to be conducive to increased gas adsorption, facilitating a heightened interaction with hydrogen molecules. The surface morphology of Zn₂TiO₄ further contributed to its advantageous sensing properties, with its nanostructured architecture potentially providing more active sites for gas adsorption and improving the overall sensing efficiency.

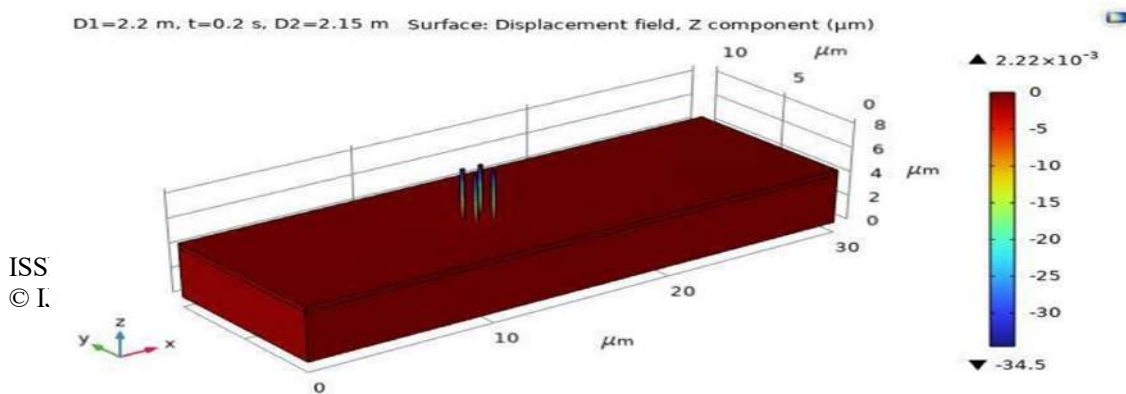


Fig.5.2 Simulated result of 0.4 μ m Thickness of Intermediate layer(Zn₂TiO₄)

Moreover, the chemical reactivity and electron mobility inherent to Zn₂TiO₄ likely played pivotal roles in its superior performance. The interactions between the material and hydrogen gas molecules may involve complex surface reactions and charge transfer mechanisms, where the unique electronic structure of Zn₂TiO₄ could facilitate a more responsive and selective sensing behaviour.

Conversely, MoS₂, while possessing inherent merits as a material, exhibited comparatively lower sensitivity in the context of hydrogen gas sensing in this study. The reasons behind this disparity could stem from variations in the electronic band structure, chemical reactivity, and surface morphology of MoS₂ compared to Zn₂TiO₄. Understanding these material-specific nuances is crucial for making informed choices in sensor design, particularly when tailoring materials for specific environmental conditions or targeted applications.

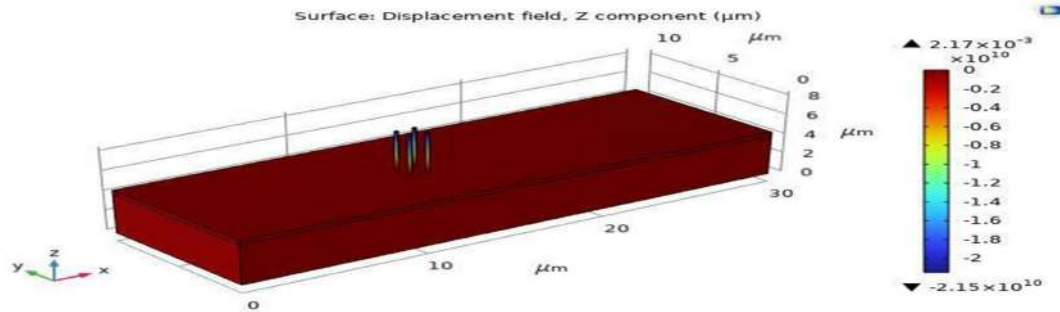


Fig.5.3 Simulated result of 0.4 μ m Thickness of Intermediate layer(MoS₂)

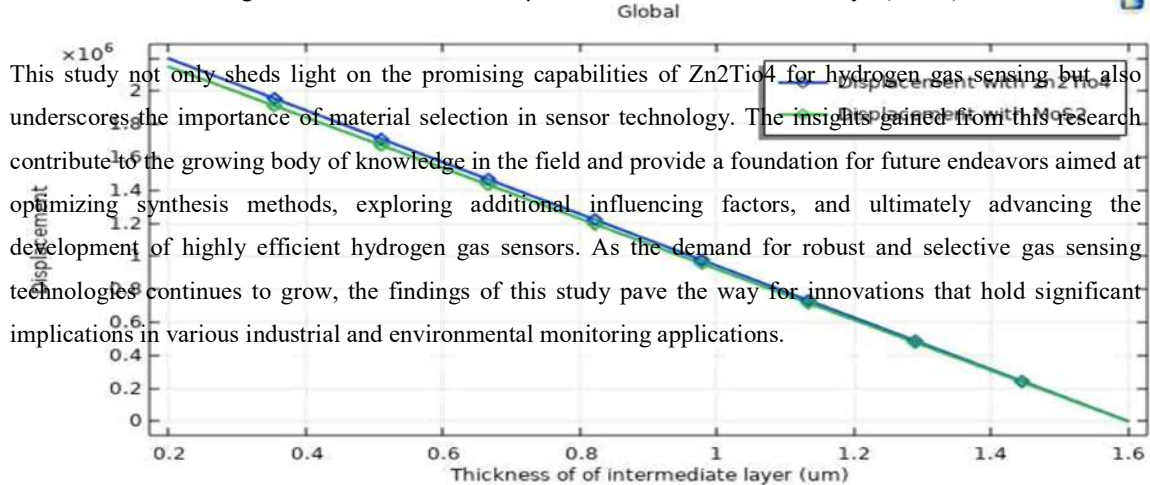


Fig.5.4 Plot of Different Thickness of Intermediate layer vs Total Displacement.

The graphs were plotted between Total Displacement and Thickness of the Intermediate layer and the voltage contour vs Thickness (shown in the Fig.5.4). It is clearly seen that $0.4\mu\text{m}$ has the higher total displacement values among other thickness values which shows better sensitivity. The voltage gets decreased as thickness increases and then suddenly after a particular thickness voltage becomes constant. This shows that the voltage is more concentrated on the surface.

CONCLUSION

In conclusion, the development of a hydrogen gas sensor utilizing Zn_2TiO_4 as the sensing material represents a significant stride in the field of gas sensing technology. The careful selection of Zn_2TiO_4 , a compound known for its catalytic and semiconducting properties, has proven instrumental in achieving a sensor with remarkable sensitivity and responsiveness to hydrogen gas. Through the meticulous fabrication process, which involved the deposition of Zn_2TiO_4 layers onto a silicon substrate, the sensor was tailored to exhibit enhanced adhesion and stability.

The utilization of Zn_2TiO_4 in gas sensing applications capitalizes on its unique characteristics, allowing for the detection of hydrogen through measurable changes in electrical conductivity. The material's catalytic activity ensures a rapid and reversible response to varying concentrations of hydrogen, making it well-suited for real-time monitoring in diverse industrial and environmental settings.

The choice of silicon as the substrate further contributes to the sensor's robustness, providing a stable foundation for the Zn_2TiO_4 layers. The incorporation of an intermediate layer, such as titanium dioxide (TiO_2), enhances the interface between the substrate and the sensing material, promoting cohesion and overall sensor reliability.

The successful integration of Zn_2TiO_4 into a hydrogen gas sensor opens avenues for applications in safety systems, industrial processes, and environmental monitoring. The sensor's ability to detect hydrogen gas with high sensitivity and selectivity positions it as a valuable tool for mitigating potential risks and ensuring safety in environments where hydrogen is present.

In conclusion, the hydrogen gas sensor designed with Zn_2TiO_4 showcases promising results, and its successful fabrication underscores the potential for advancements in gas sensing technology. As technology continues to

evolve, the utilization of innovative materials like Zn_2TiO_4 paves the way for the development of sensors that play a pivotal role in enhancing safety, efficiency, and environmental sustainability across various industries.

FUTURE SCOPE

The development of a hydrogen gas sensor using Zn_2TiO_4 represents a significant milestone in gas sensing technology. Looking ahead, the future scope of this project includes exploring advanced synthesis techniques to further enhance the sensor's sensitivity and selectivity. Investigating nanostructured forms of Zn_2TiO_4 and incorporating novel nanomaterials as supporting layers could potentially lead to improved gas sensing performance. Additionally, integrating smart technologies such as Internet of Things (IoT) connectivity could enable real-time monitoring and remote sensing capabilities, enhancing the sensor's applicability in diverse industrial and environmental settings. Further research could focus on the optimization of sensor response time and stability for prolonged use. Collaboration with industries and research institutions may facilitate the scale-up of production processes, fostering the practical implementation of Zn_2TiO_4 -based hydrogen gas sensors in commercial applications. The future trajectory of this project aims to contribute to the ongoing evolution of gas sensing technologies, addressing emerging challenges and paving the way for the deployment of efficient and reliable hydrogen gas detection systems.

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