

On-chip CO₂ Sensor Integrated with MEMS Emitter and Pyroelectric Detector

Hong Cai^a, Md Hazwani Khairy^a, Rachel Chen Fang Ang^a, Linfang Xu^a, Doris Keh Ting Ng^a, Nanxi Li^a, Zhonghua Gu^a, Anmin Kong^a, Weiguo Chen^a, Wen Wei Seit^a, Eva Wai Leong Ching^a, Norhanani Jaafar^a, Huanhuan Wang^a, Landobasa Y M Tobing^a, Leh Woon Lim^a, Qingxin Zhang^a, and Lennon Yao Ting Lee^{*a}

^aInstitute of Microelectronics, A*STAR (Agency for Science, Technology and Research),
2 Fusionopolis Way, #08-02 Innovis Tower, Singapore 138634

ABSTRACT

A demonstration of an on-chip CO₂ gas sensor is reported. It is constructed by the integration of a MEMS-based thermal emitter, a scandium-doped aluminum nitride (ScAlN) based pyroelectric detector, and a sensing channel built on Si substrate. The integrated sensor has a small footprint of 13mm × 3mm (L×W), achieved by the replacement of bulky bench-top mid-IR source and detectors with MEMS-based thermal emitter and ScAlN-based pyroelectric detector, with their footprints occupying 3.15 mm × 3 mm and 3.45 mm × 3 mm, respectively. In addition, the performance of the integrated sensor in detecting CO₂ of various concentrations in N₂ ambient is also studied. The results indicate that the pyroelectric detector responds linearly to the CO₂ concentration. The integration of MEMS emitter, thermal pathway substrate, and pyroelectric detector, realized through CMOS compatible process, shows the potential for mass-deployment of gas sensors in environmental sensing networks.

Keywords: Gas sensor, Pyroelectric detector, MEMS emitter, Carbon dioxide,

1. INTRODUCTION

Detection and monitoring of carbon dioxide (CO₂) concentration levels have been attracting considerable attention due to their impacts on diverse areas, including climate change¹, biology, chemical industry², agriculture, food³ and healthcare⁴⁻⁵. For example, with the rising concern about climate change and serious air pollution due to rapid industrialization and urbanization, huge efforts have been made to develop technologies for the evaluation of environmental air quality by monitoring CO₂ concentration levels. Meanwhile, with the technological evolution in the agricultural and food industry, CO₂ concentration control becomes more important including process control and safety assessment. Moreover, research studies have identified that CO₂ concentrations are related to many health issues and could help doctors to diagnose respiratory system problems as well as cardiopulmonary diseases.

Various CO₂ detection techniques and gas sensing applications have been demonstrated⁷⁻¹⁰. However, some of those are costly, lack portability, and demand high operating power, even though they are with high accuracy and precision. For widespread CO₂ gas sensing applications, cost-effective sensing devices with a small footprint and the ability of real-time detection are preferred. On the other hand, advances in modern micro-/nano-fabrication technologies and miniaturizations have enabled sensing technologies to turn to systems on a chip (SOC) scheme. In particular, microelectromechanical system (MEMS) devices have been proven as a promising candidate for the development of SOC technology, due to the maturity of processes and its compatibility with standard complementary metal-oxide-semiconductor (CMOS) technology.

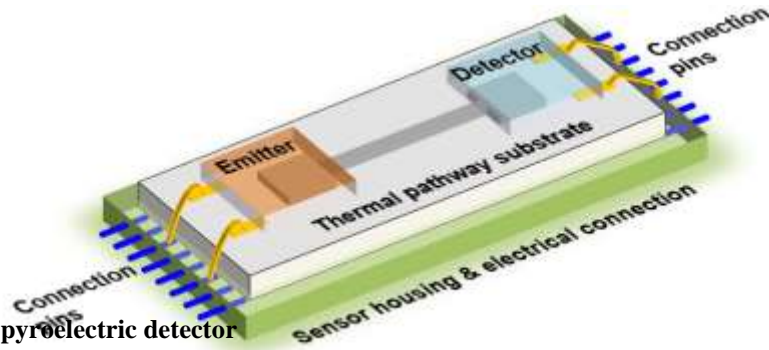
This work demonstrates an on-chip integrated CO₂ sensor, which consists of a MEMS emitter and a pyroelectric detector. Both the emitter and detector are bonded on a thermal pathway substrate. The MEMS thermal emitter acts as a radiation source, while the pyroelectric detector converts the changes in temperature due to CO₂ gas concentration into a current signal. All key components use CMOS compatible fabrication method. The performance of the sensor is tested and discussed. Results indicate that the sensor responds linearly to variations in the CO₂ concentration.

* lennon-lee@ime.a-star.edu.sg, phone 65 67705413, a-star.edu.sg/ime

2. SENSOR DESIGN AND INTEGRATION

2.1 Pyroelectric effect and thermal conductivity

Gas concentration can be measured based on the thermal conductivity of different gases. In principle, when there is a change in the concentration of the gas components under measurement, the thermal conductivity of the gas mixture changes. The rate of change of the temperature can be detected by a pyroelectric detector¹¹, which generates a pyroelectric current proportional to the rate of the temperature change. Therefore, we propose an on-chip CO₂ gas sensor configuration, which consists of a MEMS emitter and a pyroelectric detector, integrated with a thermal pathway substrate, as shown in Fig. 1. Upon detection of the modulated radiation from the emitter, the pyroelectric detector responds to various temperature differences and exhibits different current peak level according to the CO₂ concentration in the sensor.



2.2 MEMS emitter and pyroelectric detector

Within the CO₂ sensor, we use a MEMS thermal emitter¹² as a resistive heater. A meander design is employed to improve the thermal uniformity and temperature distribution in the active region. The MEMS emitters are fabricated on an 8-inch wafer using a CMOS-compatible fabrication facility. The device includes a metal layer acting as a resistor to generate heat when applying an electrical voltage. A top metal layer acts as the interdigitated electrode to ensure homogeneous heat distribution. To achieve thermal isolation from surrounding components, we designed a suspended membrane that is surrounded by air acting as a thermal insulator. The suspended membrane is formed using the deep reactive ion etching (DRIE) process to remove the silicon substrate from the wafer back.

The detector is another critical component in this integrated on-chip CO₂ gas sensor solution. Many studies have demonstrated uncooled thermal detectors, among which pyroelectric thermal detectors have inherent uncooled advantages over other thermal detectors technologies. In particular, aluminum nitride (AlN) based pyroelectric detectors have been reported capable of infrared detection at room temperature operation conditions. In this work, we select a MEMS pyroelectric detector⁷ to be integrated into the gas sensor device. The pyroelectric detector contains multiple layers that provide different functionalities. The top SiO₂-SiN-SiO₂ stack acts as an absorber, which sits on the top electrode layer constructed by TiN layer. The bottom electrode is formed by Mo. A ScAlN pyroelectric film is sandwiched between the top- and bottom- electrodes. In this device, we use Al metal contacts to link respective electrodes. To improve thermal isolation and detection efficiency, the entire film stack membrane is released from the backside Si substrate. Meanwhile, to obtain higher material pyroelectric coefficient, we doped AlN with 12% Scandium (Sc) which has demonstrated a detectivity of up to $\sim 6.08 \times 10^7$ cm²/V $\sqrt{\text{Hz}}$. The whole fabrication process is CMOS compatible. The active region of this detector is 3.45 mm × 3 mm.

2.3 Sensor integration

Flip-chip integration has been widely used in the assembly of MEMS devices¹³, especially with process optimization, low temperature, low bonding force, and short bonding time could enable high yield. In this work, as the MEMS emitter and pyroelectric detector both feature active regions at the top surface, we selected a polyimide material as the bonding



adhesive layer for protection. Before the sensor integration, the polyimide is pre-patterned on the thermal pathway substrate chip, forming a cavity structure to protect the active surfaces of MEMS devices. Plasma treatment on the substrate surface is conducted to improve the adhesion between bonded surfaces. Subsequently, the separate MEMS chips are aligned and bonded to the patterned substrate, forming the integrated sensor chip, as shown in Fig. 2(a). After that, the bonded sensor device is subjected to curing at the temperature of 200°C for 2 hours inside an oven to ensure the bonding quality. For the convenience of external electrical connections and sensor characterizations, the integrated sensor chip is placed inside a bathtub with wire bonding to different leads at two ends of the hybrid package housing, as shown in Fig. 2 (b).

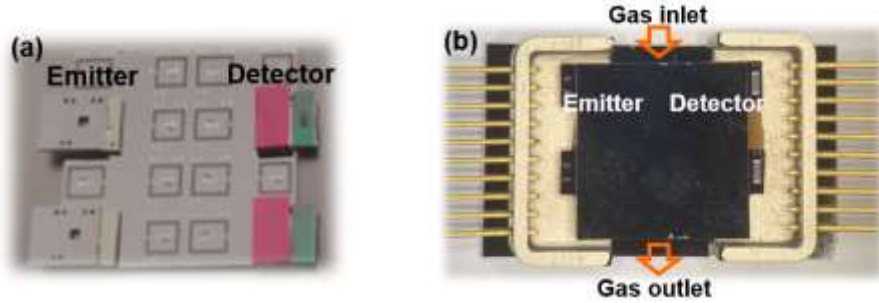


Figure 2 The images of the integrated CO₂ gas sensor. (a) The on-chip integrated CO₂ gas sensor, and (b) the hybrid packaged sensor chip wire-bonded in a bathtub housing.

3. EXPERIMENTAL RESULTS AND DISCUSSIONS

A schematic diagram of the overall gas sensor testing setup is shown in Fig. 3. The 99.8% CO₂ gas source is diluted with 99.99% purity nitrogen (N₂) gas. Varying CO₂ concentrations are obtained by a gas mixing system with computer-controlled mass flow meters for tuning the CO₂ and N₂ gas flow rates. The gas sensor is placed in an environmental control chamber throughout the measurement duration to control and monitor the humidity and temperature. Additionally, N₂ gas is also used for purging and cleaning the measurement chamber. A waveform generator is used to drive the MEMS emitter using a square wave with a modulation frequency of 17 Hz and a peak-to-peak voltage of 1.8 V. The pyroelectric response is proportional to the rate of temperature change, and the signal detected is relatively weak. Therefore, a low-noise current preamplifier with a gain of 10⁹ is used to amplify the signal, which is then captured by a lock-in amplifier (Zurich Instruments HF2LI).

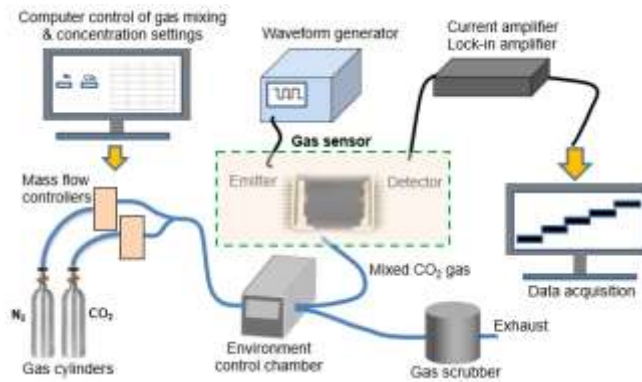


Figure 3 Schematic representation of the CO₂ gas sensor characterization set-up and integrated gas sensor.

Figure 4 plots the measured sensor response to different CO₂ gas concentrations for different ranges. In Fig. 4(a), the CO₂ concentration is varied over a range from 50% to 0% in intervals of 10%. For each concentration level, the duration cycle is 7 minutes, and it switches to the next concentration level through automatic control by the gas mixing system. Each data point in the plot is an average value of the sensor voltage readings over the 7-minute duration. The error bars (i.e., standard deviation) for most experiments are around ~ 5 μV. As shown in both plots in Fig. 4 (a) & 4(b), the sensor response is linear from 0% to 100% CO₂ concentration. We observe a slight difference in the slope for the decreasing (Fig.4(a)) and the increasing (Fig.4(b)) CO₂ concentrations, whose raw data collected are presented in Fig. 4(c) and 4(d),

respectively. The exact cause for such differences requires further investigation, but it could be attributed to experimental nonidealities such as thermal insulation during measurements. The dependence of the slope on the increase/decrease of concentration will be our future studies.

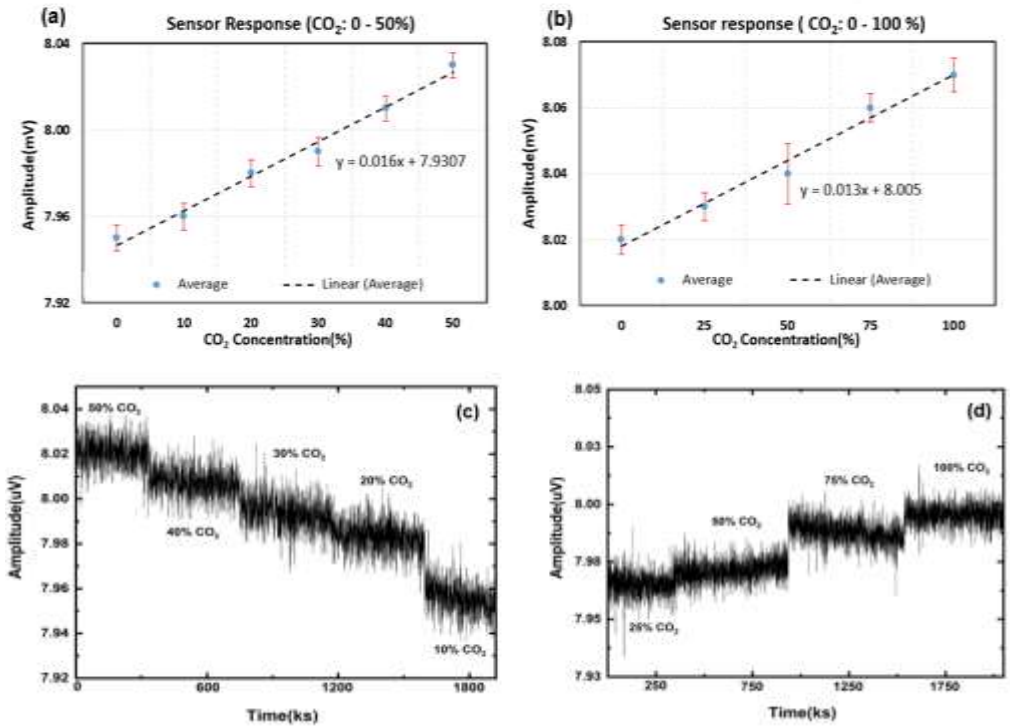


Figure 4 (a) The sensor response to the CO₂ concentration changes over 0%-50% at a step of 10%. (b) The sensor response to the CO₂ concentration changes over 0%-100% at a step of 25%. (c) and (d) are the raw plots of the experimental sensor voltage response (in the time domain) without any signal processing to CO₂ concentrations over 50%-0% and 0%-100%, respectively.

4. CONCLUSION

In summary, an on-chip integrated CO₂ gas sensor with a MEMS-based thermal emitter and a pyroelectric detector is demonstrated. Each component is fabricated using CMOS-compatible processes and the integrated sensor has a small footprint of 13mm × 3mm (L×W). Sensor characterization results show that the sensor response increases linearly with CO₂ concentration over a range from 0 to 100%. The integrated gas sensor is highly promising for other low-cost and miniature gas sensor solutions, and for mass deployment of gas sensors in environmental sensing networks.

ACKNOWLEDGMENTS

This work is supported by Agency for Science, Technology and Research (IAF-PP A1789a0024 and IAF-PP A19B3a0008).

REFERENCES

- [1] Clark, M. A., Domingo, N. G. G., Colgan, K., Thakrar, S. K., Tilman, D., Lynch, J., Azevedo, I. L., Hill, J. D., "Global food system emissions could preclude achieving the 1.5° and 2°C climate change targets," *Science*, 370, 705–708 (2020).
- [2] Otto, A., Grube, T., Schiebahn, S., Stolten, D., "Closing the loop: Captured CO₂ as a feedstock in the chemical industry," *Energy Environ. Sci.*, 8, 3283–3297 (2015).

- [3] Puligundla, P., Jung, J., Ko, S., "Carbon dioxide sensors for intelligent food packaging applications," *Food Control*, 25, 328–333 (2012).
- [4] Zhao et al. 2014, Zhao D, Miller D, Xian X, Tsow F, Forzani ES. , "A novel real-time carbon dioxide analyzer for health and environmental applications," *Sens Actuators B Chem.* 195,171–176 (2014).
- [5] El-Betany, A. M. M., Behiry, E. M., Gumbleton, M., Harding, K. G., "Humidified warmed CO₂ treatment therapy strategies can save lives with mitigation and suppression of SARS-CoV-2 infection: an evidence review," *Front. Med.*, 7, 594295 (2020).
- [6] Gardner, E. L. W., Luca, A. De, Vincent, T., Jones, R. G., Gardner, J. W. and Udrea, F., "Thermal Conductivity Sensor with Isolating Membrane Holes," *IEEE SENSORS*, 1-4 (2019).
- [7] Hagleitner, C., Hierlemann, A., Lange, D. et al. Smart single-chip gas sensor microsystem. *Nature* 414, 293–296 (2001).
- [8] Lochbaum, A., Fedoryshyn, Y., Dorodnyy, A., Koch, U., Hafner, C., Leuthold, J. "On-Chip narrowband thermal emitter for mid-IR optical gas sensing", *ACS Photonics*, 4 (6), 1371-1380 (2017)
- [9] Li, N., Chao, Q., Gu, Z., Song, S., Zhou, Y., Zheng, S., Xu, L., Chua, Y. D., Zhang, Q., Cai, H., Zhang, D., Wang, Q. J. and Lee, L., "Photonic crystal MEMS emitter for chemical gas sensing," *MOEMS and Miniaturized Systems XX 11697*, 145–151, SPIE (2021).
- [10] Zheng, S., Cai, H., Xu, L., Li, N., Gu, Z., Zhang, Y., Chen, W., Zhou, Y., Zhang, Q. and Lee, L. Y. T., "Silicon substrate-integrated hollow waveguide for miniaturized optical gas sensing," *Photon. Res.*, 10(1), 261–268 (2022).
- [11] Ng, D. K. T., Zhang, T., Siow, L. Y., Xu, L., Ho, C. P., Cai, H., Lee, L. Y. T., Zhang, Q., and Singh, N., "A functional CMOS compatible MEMS pyroelectric detector using 12%-doped scandium aluminum nitride," *Appl. Phys. Lett.* 117, 183506 (2020)
- [12] Li, N., Yuan, H., Xu, L., Zeng, Y., Qiang, B., Wang, Q., Zheng, S., Cai, H., Lee, L., Singh, N., and Zhao, D., "Tailorable infrared emission of microelectromechanical system-based thermal emitters with NiO films for gas sensing," *Opt. Express* 29 (12), 19084-19093 (2021).
- [13] Seit, W. W., Chong, S. C., Cai, H., Wai, E. and Ang, R., "Comprehensive Study on Polymer Based Chip-to/chip Bonding for Gas Sensor Application," 2021 IEEE 23rd Electronics Packaging Technology Conference (EPTC), 18-22 (2021).