

Nondispersive Infrared Ray CH₄ Gas Sensor Using Focused Infrared Beam Structures

JongSeon Park and SeungHwan Yi*¹

Research Center of ALT Semicon, ALT Semicon Corporation,
1112-7 NamchonRi, Oksan Myeon, CheongwonGun, Chungbuk 363-911, Korea

¹Department of Mechanical Engineering, Chungju National University,
123 GeomDanRi, IryuMyeon, Chungjushi, Chungbuk 380-702, Korea

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We propose a concave optical cavity structure for use in a high-performance nondispersive infrared ray (NDIR) methane gas sensor module. By using a concave mirror structure, the maximum output voltage and voltage difference between 0 and 9,500 ppm increased by more than 160% compared with using a vertical mirror structure. The output voltage dependence of the thermopile location was tested in the case of a concave mirror structure. The output voltage increased from 2.75 to 3.63 V with the thermopile detector placed at distances of 2 and 3 mm from the reference position. It was found that the output voltage of the sensor decreased by more than 45% from 2.16 to 1.18 V after three years of operation in the case of the vertical mirror structure.

1. Introduction

As a clean energy source, liquid natural gas (LNG) is widely used in homes and factories. The main components of LNG are methane (CH₄), ethane (C₂H₆), and other gases. The lower explosive limit (LEL) of methane is 5% in air ambient,⁽¹⁾ so when there is a leakage of methane in the air, an explosion could be prevented using safety methods such as a methane detector with high accuracy and reliability, and adequate ventilation. Moreover, methane is very hazardous to humans because it may induce dizziness, headaches, and nausea, and can cause suffocation if inhaled at high concentrations.⁽²⁾ Methane can be released from waste disposal sites (particularly from the anaerobic decay of food and from agricultural areas) and residential gas distribution systems. In addition, methane causes more greenhouse effects than carbon dioxide. Therefore, a small and low-cost methane sensor module is needed to warn of the release of methane in industrial and residential environments.

*Corresponding author: e-mail: isaac_yi@cjnu.ac.kr

Currently, there are two types of sensor used to detect methane gas. One is based on the catalytic combustion method,^(3,4) and the other is semiconductor-based.⁽⁵⁾ In addition, an optical sensing method using nondispersive infrared rays (NDIRs) or a near-infrared (IR) compact gas sensor⁽¹⁾ has been introduced into the market with the help of cost reduction and miniaturization of the main components (optical cavity, light source, and infrared detector). The catalytic gas sensor has some advantages such as small size, short response time, and a relatively simple circuit to manipulate the signal conditioning. However, it exhibits poor selectivity to other gases in ambient air, and shows some reliability problems over time. The NDIR gas sensor has some unique properties compared with other methane sensors: high reliability and accuracy, and selectivity as a result of using the optical properties of the subject gas. However, the NDIR methane gas sensor used in the market shows a long-optical-path structure to increase the sensitivity, since the band intensity of methane is roughly ten times smaller than that of carbon dioxide.⁽⁶⁾ Thus, if the sensor structure is exactly the same except for the IR detector for methane gas sensing, the output voltage of the NDIR methane gas sensor will be much smaller than that of an NDIR CO₂ gas sensor with the same configuration at the same gas concentration. To improve the sensitivity of methane gas sensors, optical lenses can be used to achieve high output voltages, or a pyroelectric sensor can be used with high sensitivity to IR radiation.

In this study, we simulated unique optical cavity structures to obtain a novel NDIR methane gas sensor and to improve the sensitivity to methane gas without optical lenses or pyroelectric devices. After prototyping optical cavities on the basis of simulation results, an NDIR methane gas sensor module was built and tested to compare NDIR sensor modules with different cavity structures.

2. Sensor Design

2.1 Theoretical review

Thermal radiation is emitted by a black body (or an IR radiator) as a result of a temperature difference between the black body and the ambient. The thermal radiation per unit area follows Stefan-Boltzmann's law and is described as

$$R_T = \sigma \cdot (T_{\text{body}}^4 - T_{\text{amb.}}^4), \quad (1)$$

where $\sigma = 5.67 \times 10^{-8} \text{ W}/(\text{m}^2 \cdot \text{K}^4)$ is the Stefan-Boltzmann constant, T_{body} is the temperature of the black body emitting thermal radiation, and $T_{\text{amb.}}$ is the surrounding ambient temperature.⁽⁷⁾

The absorption of radiation energy by gas molecules is described using the Lambert-Beer law:⁽⁸⁾

$$I_d = I_o \cdot \exp(-\alpha \cdot x \cdot L), \quad (2)$$

where I_o is the light intensity at the source (W/m^2), I_d is the light intensity on the detector side (W/m^2) at room temperature, α is the absorption coefficient per molecule of target

gas, x is the concentration of molecules of gas, and L is the optical traveling length (m) from the source to the detector. By placing the silicon thermopile on the detector side, a thermal electromotive force is induced at the output terminals, and the output voltage⁽⁹⁾ is described as

$$V = \int_{T_{\text{amb.}}}^{T_{\text{body}}} n \cdot \Delta\alpha \cdot dT = n \cdot \Delta\alpha \cdot (T_{\text{body}} - T_{\text{amb.}}), \quad (3)$$

where $\Delta\alpha$ is the difference in Seebeck coefficients of thermopile materials and n is the number of couples in the thermopile detector.

If there is no loss of light traveling through the optical cavity except the absorption of light, then eqs. (1) and (2) would be the same. After rearranging these equations and combining them into eq. (3), we obtain

$$\begin{aligned} V &= n \cdot \Delta\alpha \cdot \frac{I_0}{\sigma \cdot (T_{\text{body}}^2 + T_{\text{amb.}}^2) \cdot (T_{\text{body}} + T_{\text{amb.}})} \cdot \exp(-\alpha \cdot x \cdot L) \\ &= \eta \cdot \exp(-\alpha \cdot x \cdot L), \end{aligned} \quad (4)$$

where η is a proportionality constant that is affected by light intensity I_0 coming from the IR source, the blackbody temperature T_{body} emitting IR rays, and the ambient temperature $T_{\text{amb.}}$. Furthermore, when we consider the focused bundle of the radiating beam,⁽¹⁰⁾ eq. (4) can be described as

$$V = \xi \left(\frac{r_i}{r_s} \right)^2 \exp(-\alpha \cdot x \cdot L), \quad (5)$$

where ξ is a new proportionality constant that includes the reflection coefficient of the coating material of the optical cavity, r_i is the radius of a parallel bundle beam of the IR ray, and r_s is the radius of the focused beam in the cavity structure.

From eq. (5), we can infer that the output voltage of the thermopile detector is increased by the square of the beam radius ratio between r_i and r_s . Thus, the focused beam increases the output of the thermopile detector if the optical cavity is designed to concentrate the radiated beam into a spot instead of a parallel beam.

2.2 Design of optical cavities

Currently, there are four different optical cavity structures used in NDIR gas sensor modules. The first structure uses a square or cylindrical tube with one IR source and detector.⁽¹¹⁾ The second has two IR sources with one detector^(12,13) for thermal aging compensation of the IR source. The third uses a cylindrical tube for its optical cavity and a Fabry-Perot filter⁽¹⁴⁾ to select the target gas wavelength. The fourth structure consists of one IR source and detector; however, it uses a structure with three elliptical mirrors to increase the optical path within a small cavity volume.⁽¹⁵⁾

To obtain a design concept for our cavity structure, we surveyed a commercial cavity

structure that was filed as an international patent.⁽¹⁵⁾ When we divided the cavity into subsidiary parts, it appeared to use three circles of different radii. After rearranging the three circles and inlet part of the light beam, we constructed an optical cavity structure using the TracePro® commercial optical simulation tool. The simulation results of the optical path in the previously described structure are shown in Fig. 1. As shown in the figure, the light bundle coming from the upper right corner was reflected five times in the cavity and then reached the detector side located at the lower left corner.

After reviewing the current optical cavity structures, we tried to develop a unique optical cavity for the NDIR sensor module. As a result, we designed cavities that have two circular mirrors with optimal optical paths and light intensities, as shown in Figs. 2(a) and 2(c). The design parameters of each structure are listed in Table 1. Figure 2(a) shows the previously described optical cavity structure⁽¹⁶⁾ that has vertical mirror surfaces. The vertical mirror surface is perpendicular to the top surface of the optical cavity structure as shown at the left side of Fig. 2(b). The dotted-line circle in Fig. 2(c) represents the filter area of the thermopile detector. In this case, a parallel light bundle (coming from the lower right corner) is reflected twice at the mirror surfaces, and finally converges at the detector side, as shown in Fig. 2(a). However, the focused beam pattern looks like a cat's eye as shown in the left side of Fig. 2(c). Thus, a focused beam was not effective in collecting all the incident rays onto the active area ($0.7 \times 0.7 \text{ mm}^2$) of the thermopile, which was used to detect IR rays in the NDIR sensor module. To enhance the light intensity, we revised the proposed optical cavity structure by curving the mirror surface with the defined radius of curvature listed in Table 1. The left and right sides of the mirror surfaces have 17 and 30 mm radii of curvature; thus, the mirror surfaces of each side have a uniformly curved surface on the inner surfaces of the mirrors as can be seen at the right side of Fig. 2(b). In the case of the concave mirror surfaces, the optical path was almost the same as that of the vertical mirror structure shown on the left side of Fig. 2(a). However, since the mirror surfaces have a concave structure, the light is

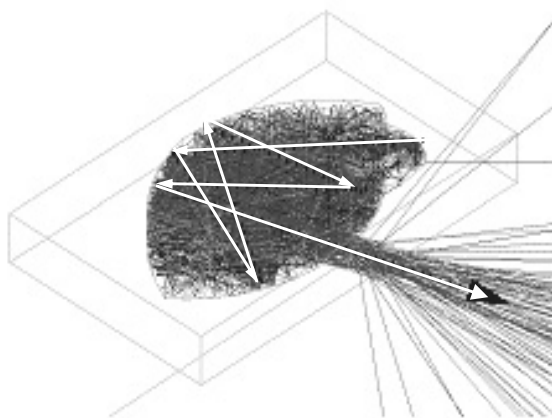
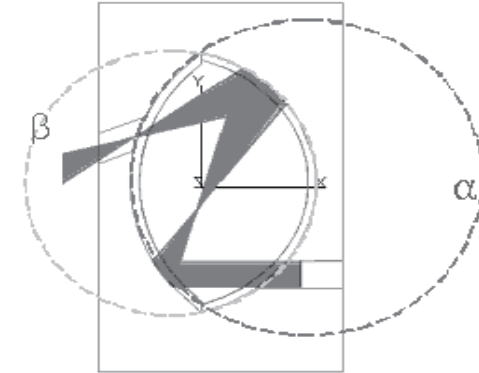
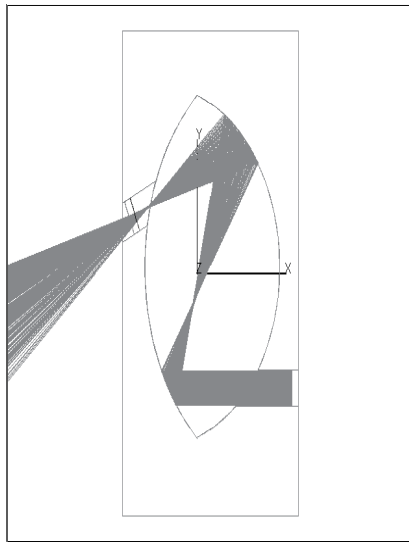


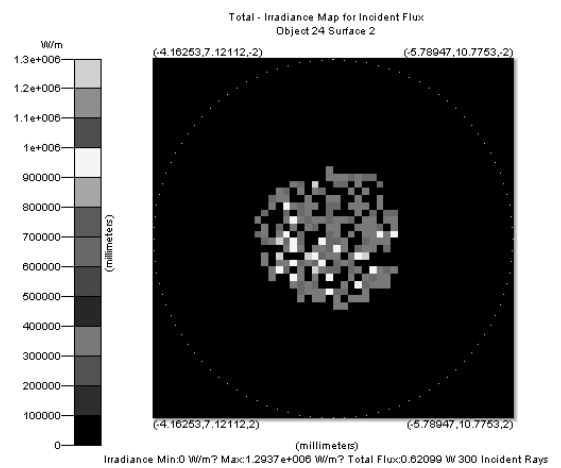
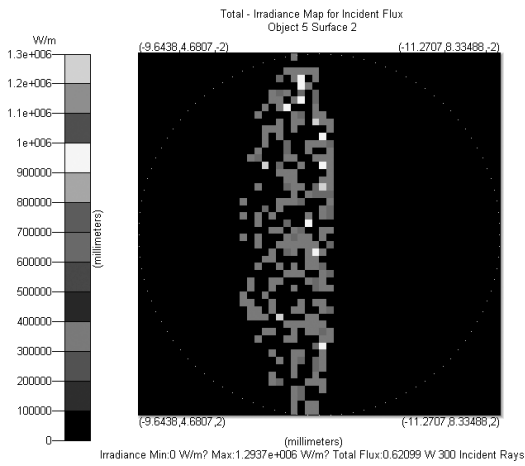
Fig. 1. Simulation result of commercialized cavity structure.



(a)



(b)



(c)

Fig. 2. Simulation results of optical path and light intensity for novel NDIR gas sensors: (a) with vertical mirror surfaces and (b) with concave mirror surfaces.

Table 1
Design parameters of optical cavity structures.

Category	Radius (mm)		Radius of curvature (mm)	
	A	B	α	β
Vertical mirror	24.9	20	—	—
Concave mirror	24.9	20	30	17

focused more effectively onto the thermopile detector, and the focused beam showed a circular pattern as seen on the right side of Fig. 2(c). Therefore, we inferred that the IR ray can be focused onto a spot to increase the output voltage of the thermopile detector as suggested in eq. (5). In both structures, the cavity volume is about 4.5 cm³ and the optical path length is about 65 mm.

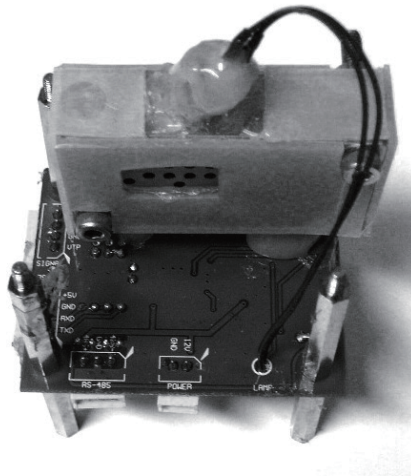
3. Sample Preparation and Experimental Setup

3.1 Sample preparation

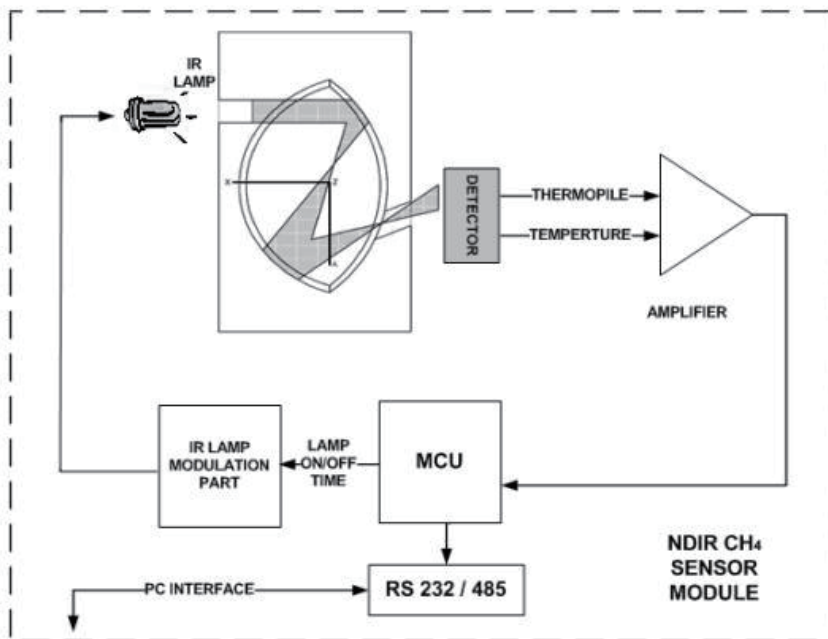
On the basis of simulation results, we built a sensor module using the proposed cavity structure design. The design has four parts as shown in Fig. 3: 1) a gas sensing cell with an IR source, a thermopile detector, and a proposed cavity; 2) IR pulse modulation and signal amplification circuits; 3) an ADUC 848 (Analog Device Inc.) microcontrol unit (MCU) for signal conditioning and storage of the measured data; and 4) a data communication port between the main computer and sensor modules (RS485 and RS232 interfaces). We used an infrared light source that emitted infrared light in the 1 to 5 μm range. In addition, we used a thermopile infrared detector (ZTP-315 GS provided by General Electric Sensing, Korea) modified for our gas sensing application by replacing the general optical filter (that passed infrared light above 5 μm) with a CH₄ filter having a center wavelength of approximately 3.3 μm and a 20 nm full width at half maximum (FWHM). To modulate a pulse signal of IR light, an IR lamp was turned on for 350 ms and turned off for 5 s. We specified the on-time to be 350 ms so that the thermopile detector had a response time lag of approximately 200 ms. Furthermore, the thermopile detector has the highest output voltage at that modulation period. In the amplification circuit, an AD 8628 (Analog Device, Inc.) was used as an operational amplifier with a low offset voltage (less than 5 μV), which was necessary because the output voltage of the thermopile detector was around 300 μV . For signal conditioning and to obtain a high output voltage at 0 ppm CH₄ concentration, we used second-order amplification circuits with an LM 385 (National Semiconductor, Inc.) reference voltage driver. After acquiring the amplified signal, the signal was fed to the MCU for further signal conditioning and data storage in an Electrically Erasable Programmable Read-Only Memory (E²PROM) implemented in the MCU.

3.2 Experimental setup

Figure 3 shows our proposed NDIR gas sensor module and its functional block diagram. The cavity has two main parts: a parabolic reflector to create a parallel light



(a)



(b)

Fig. 3. NDIR CH₄ gas sensor module consisting of optical cavity with concave mirror surfaces: (a) photo of prototype sensor module, (b) its functional block diagram.

bundle from the light coming from the IR lamp (which is located below the optical cavity), and a pair of circular mirror surfaces with concave optical mirrors (whose design is based on the simulation results) to focus the light bundle into a circular shape, thereby enhancing the light intensity.

After assembling each part onto a printed circuit board (PCB) as shown in Fig. 3, the sensor modules were tested in a gas chamber. To accurately monitor the gas concentration in the chamber, we connected a photoacoustic multigas analyzer (INNOVA 3012, INNOVA Inc.) to the gas chamber in order to detect the gas concentration accurately in the chamber as a function of time. The overall function of the measurement system is described in a block diagram shown in Fig. 4. The gas chamber was placed inside a constant-temperature/humidity chamber because the thermopile detector is very sensitive to fluctuations in ambient temperature. The output voltage signals were stored in a computer through the data acquisition board, and the temperature of the chamber was set to within $\pm 0.3^\circ\text{C}$ of the target temperature. Methane gas was injected in 1,000 ppm steps with a preset time period, and the concentration was continuously monitored using a multigas analyzer. The monitored CH_4 concentration and output voltage value from the sensor module were automatically stored in the main computer via the data acquisition board, and were compared with each other. After finishing the test at a particular temperature, the gas chamber was purged with synthetic air for several minutes to achieve a nearly 0 ppm methane gas concentration.

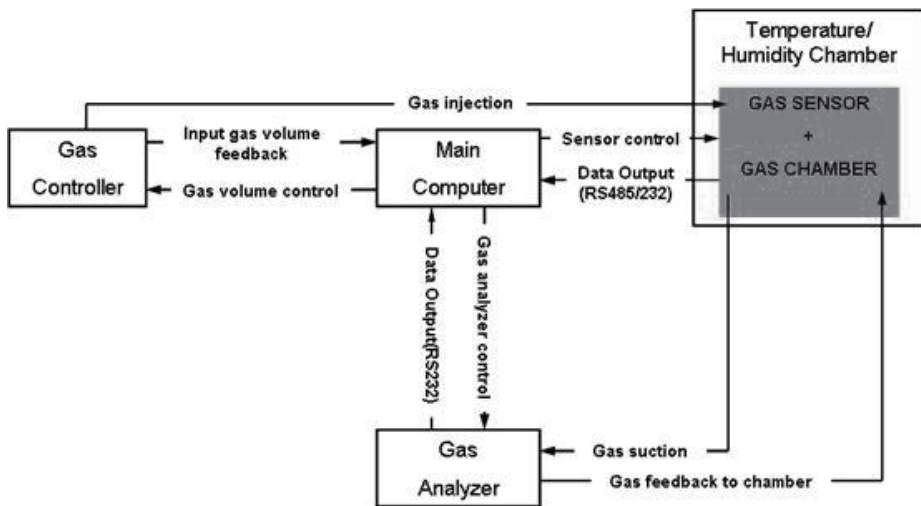


Fig. 4. Block diagram of gas measurement system.

4. Experimental Results and Discussion

Figure 5 shows a comparison of output voltages of the prototype NDIR methane gas sensors with two different reflecting mirrors: one has vertical mirrors, and the other has concave mirror surfaces. The output voltage of the concave mirror sensor was 3.63 V and that of the vertical mirror sensor was about 2.16 V at 0 ppm methane gas concentration. Thus, the concave mirror sensor voltage was 168% higher than the vertical mirror sensor voltage.

In the case of a concave mirror, when the positions of the IR detector were 2 and 3 mm away from the reference position (i.e., the left side of the optical cavity structure through which the IR ray is passing, as shown in Fig. 2(a)), the amplified output voltages of the IR detector were significantly affected by the location of the thermopile detector. The voltage difference between the two was more than 30% at 0 ppm methane gas concentration, as shown in Fig. 6.

The output voltages of fresh and aged samples were tested and the results are shown in Fig. 7. The output voltage of the fresh sensor decreased from 2.154 to 2.056 V for a methane gas concentration of 0 to 9,500 ppm. However, the output voltages of sensor modules operated for three years were attenuated by more than 50% from their initial values within the same gas concentration range. However, it gave a similar tendency with the measured methane gas concentration.

Our experimental results are summarized in Table 2. The maximum voltages of each sensor module showed their relevance to the optical cavity structures. Comparison of the concave structures showed that the maximum output voltages and voltage difference were strongly dependent on the position of the thermopile detector. By manipulating the

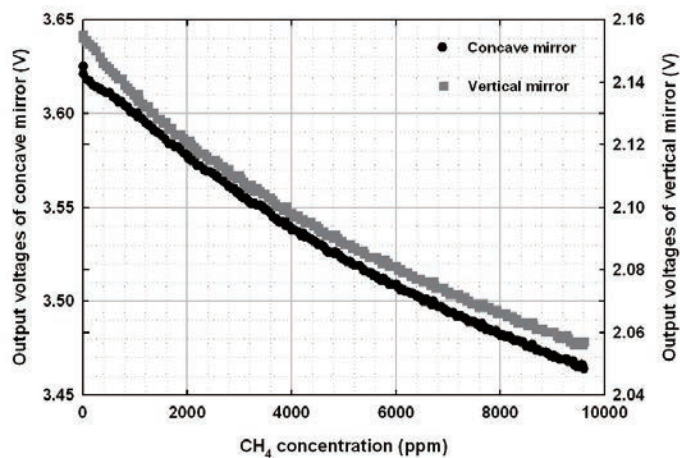


Fig. 5. Output voltages of NDIR methane gas sensors with different optical cavity structures.

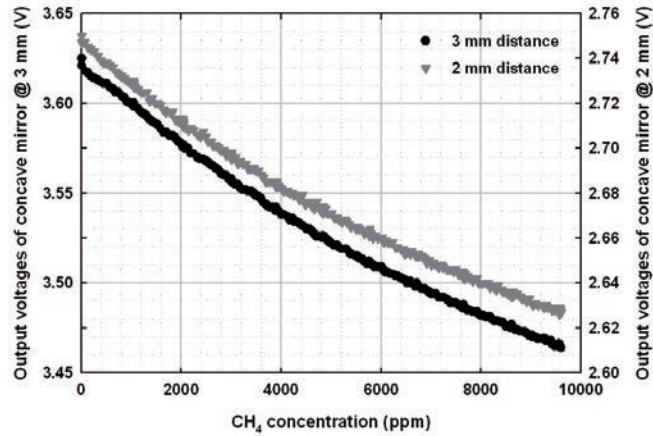


Fig. 6. Output voltages as a function of methane gas concentration according to the optical distance from the reference position.

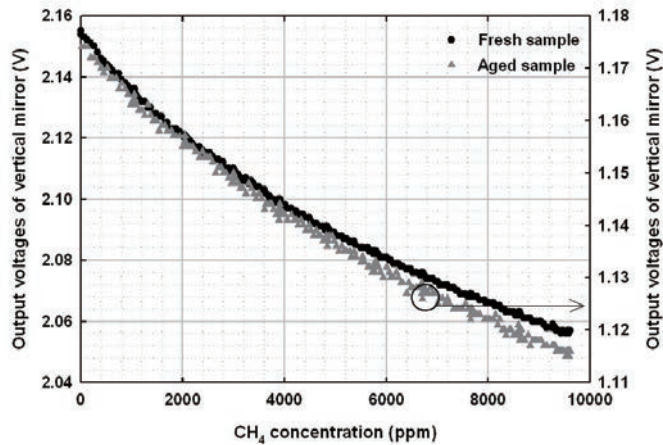


Fig. 7. Comparison of output voltages due to the aging of Au-coated surfaces.

detector position in the same optical cavity, the output voltage and voltage difference, which were used to define the sensitivity of the sensor module, increased by 130%. This means that the thermopile detector should be carefully positioned to produce a high-sensitivity sensor module.

Table 2
Summary of experimental results.

Category of sensor module	Maximum voltage at 0 ppm (V)	Voltage difference between 0 and 9,500 ppm (mV)
Concave mirror with 3 mm distance from reference	3.63	159
Concave mirror with 2 mm distance from reference	2.75	123
Vertical mirror with fresh Au coating	2.16	98
Vertical mirror after 3 years of operation	1.18	58

Comparison of the cavity structures showed that the concave mirror has a higher output performance than the vertical mirror, because the maximum output voltage and voltage difference of the concave mirror were both greater than those of the vertical mirror. Therefore, we used the concave mirror structure to determine more accurately the concentration of methane gas from the experimental results.

The characteristics of the output voltages changed over the three years of operation of the sensor module. This may have been caused by two factors: one is the worn-out filament of the IR lamp, the other is a property change of the Au-coated surfaces. To examine the possibility of changing surface properties, a new IR lamp was installed in both a fresh and an aged sensor module. We then measured the output voltage of the sensor module. The results show that the maximum output voltages and voltage difference are quite similar to the trends listed in Table 2. Thus, the decrease in output voltage of the aged sensor is affected by the properties of the Au film coated onto the metal cavity structures. Therefore, anti-aging protection methods should be implemented to ensure stable output voltage characteristics of the sensor module.

5. Conclusions

A concave optical cavity structure was proposed after surveying currently available commercial structures. The operation of the device was simulated to aid in designing a high-performance NDIR methane gas sensor module. A circular mirror cavity with a vertical mirror structure focuses an irradiated IR beam onto a thermopile detector. In contrast, a concave mirror structure concentrates an incoming IR beam onto a small spot without requiring an optical lens to magnify the IR intensity per unit area. By using a concave mirror structure, the maximum output voltage and voltage difference between 0 and 9,500 ppm increased significantly to determine the concentration of methane gas in air. Thus, the proposed optical cavity structure can be useful for implementation in commercial products.

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