On-chip readout plasmonic mid-IR gas sensor

Qin Chen1.*, Li Liang1, Qilin Zheng1, Yaxin Zhang2 and Long Wen1*

1Institute of Nanophotonics, Jinan University, Guangzhou, 511443, China; 2University of Electronic Science and Technology of China, Chengdu, 610054, China.

*Correspondence: Q Chen, E-mail: chenqin2018@jnu.edu.cn; L Wen, E-mail: longwen@jnu.edu.cn

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Section 1. Electrical resistance for VO₂ film
In our simulation, the electrical resistance of the VO₂ film versus temperature is from the literature as shown in Fig. S1.

Fig. S1 | The electrical resistance R of VO₂ as a function of its temperature.

Section 2. Refractive index of MOF with adsorption of CO₂
MOF is a new type of nanoporous crystalline material consisting of metal ions and organic ligands. It can selectively adsorb certain gas molecules and concentrate them into the nanopores. In Ref.², at least 200 times increase of the adsorption of CO₂ was observed at various concentration due to the physical adsorption of a type of MOF (zeolitic imidazolate framework, ZIF-8) layer with a thickness of 2.7 μm. Considering the void fraction of ZIFs is approximately 0.47³, the refractive index of MOF in a protecting gas (Ar) environment can be calculated following the effective material theory

\[ n_{\text{MOF}} = 0.53 \times n_1 + 0.47 \times n_{\text{Ar}} \]  

where \( n_1 \) is the refractive index of solid ZIF-8 material, and \( n_{\text{Ar}} \) is the refractive index of Ar at a standard atmospheric pressure. The \( n_{\text{MOF}} \) is set to be 1.326 in Ref.² and the same value is used in our simulation.

As we know, the change of refractive index of gas is directly proportional to the change of the number of gas molecule per unit volume⁴,

\[ n_{\text{gas}} = n_0 + kN \]  

where \( n_{\text{gas}} \) is the refractive index of gas, \( n_0 \) is the refractive index of vacuum, \( N \) is the number of gas molecule per unit volume, and \( k \) is a constant. Therefore, the ZIF-8 can concentrate CO₂ molecules by at least 200 times. When this MOF layer is placed in a gas mixture with 10% CO₂ and 90% Ar as the simulation in Fig. 5, its refractive index (real part) can be calculated by combining (1) and (2),

\[ n_{\text{MOF}} = 0.53 \times n_1 + 0.47 \times [1 + (n_{\text{CO₂}} - 1) \times 10\% \times 200] + 0.47 \times [1 + (n_{\text{Ar}} - 1) \times 90\%] \]  

The imaginary part raised by the CO₂ molecules can be easily calculated by \( 0.47 \times k_{\text{CO₂}} \times 10\% \times 200 \), where \( k_{\text{CO₂}} \) is the imaginary part of the refractive index of CO₂ obtained from HITRAN web. Please note it is a coarse evaluation of the refractive index of MOF as the pressure, temperature, volume and so on can all change the refractive index. The formula (3) is to give a hint of the influence of MOF on the CO₂ sensing.

Section 3. Gas sensors optimized for the absorption bands of different gases
As discussed in Fig. 2, the resonant absorption of the gas sensor is based on the SPP, whose resonant wavelength is determined by the grating period. Thus, it is easily tuned to match the fingerprint absorption wavelength of various gases to further improve the sensitivity. As shown in Fig. S2, narrowband (Q>250) resonance with high absorption (>90%) can be obtained for various gases such as CH₄, CO₂, CO, SO₂, SF₆ and NO₂ by tuning the structure dimensions. For an extreme optimization, nearly unity absorption with a Q over 1200 is demonstrated for SF₆. In this case, a small amount variation of the gas concentration induces a large change on absorption.
Fig. S2 | Absorption spectra with absorption peaks at the absorption bands for (a) CH₄ at 3.3 µm, (b) CO₂ at 4.26 µm, (c) CO at 4.65 µm, (d) SO₂ at 8.83 µm, (e) SF₆ at 10.55 µm, (f) NO₂ at 11.85 µm. The structural parameters and the Q factors are shown in the figures.

Section 4. On-chip spectroscopy based on the plasmonic sensor array

In simulation, the spectrum of the broadband source refers to the IR light source in a FTIR spectrometer (MIR8035TM), which is shown in Fig. S3(a). The absorption coefficient of CO₂ is from the HITRAN database as shown in Fig. S3(b). 80 narrowband plasmonic sensors like the one in Fig. 4 are chosen and the spectra are shown in Fig. S3(c), where the pink shadow area indicates the wavelength region in the spectrum reconstruction in Fig. 6.

Fig. S3 | (a) The spectrum of the broadband source used for gas molecular absorption spectrum reconstruction. (b) The absorption line intensity of CO₂ is from the HITRAN database. (c) Spectra of 80 narrowband plasmonic sensors.
Section 5. Size effect of plasmonic structure in mid-IR gas sensor

Fig. S4 | The absorption spectra of the plasmonic structures shown in Fig. 2 with different number of grating periods at the resonance around (a) 3.3 μm and (b) 8.8 μm. (c) The absorption spectra for the structures (with 15 gratings) with reflectors at both ends for different reflector heights. (d) Effect of the grating length along the z direction (Fig. 1) on the absorption spectrum. Spectra of the periodic structures are shown for comparison.

Reference