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## Study on design method of multi-layer film in optical filter for analysis of CO<sub>2</sub> absorption line

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### Abstract

Analysis of gas (especially CO<sub>2</sub>) components in air is very important for many industrial applications such as environmental protection and disaster monitoring. It is essential to distinguish the absorption lines of the measured gas from the mixed spectral lines of the various gases in the spectral measurement for gas analysis. The conventional narrowband filter is not sufficient to separate the sharp spectrum of the CO<sub>2</sub>. In this paper, we present a design method for narrowband optical filter by combining a narrowband filter and a wideband filter.

### Keywords:

#### 1. Introduction

The analysis of CO<sub>2</sub> has a great significance in various fields including environmental protection, disaster monitoring and chemical industry.

Laser spectroscopy is an attractive method for gas analysis in environmental and industrial measurements. A coherent light source with narrow spectral width is appropriate for detecting one absorption line of the material and avoiding signal interference due to other kinds of materials.

A laser photodiode with a wide range of difference frequencies was used for gas detection [1]. Absorption spectra were measured in the range of 2380-2275 cm<sup>-1</sup> (4.2-4.40 μm) of the CO<sub>2</sub> absorption spectrum. S.Robert *et al.* reported on finding the absorption spectra of a new CO<sub>2</sub> isotope on the surface by SOIR spectroscopy [2]. The SOIR spectrometer can measure atmospheric transmittance in the IR (2.2-4.3 μm) range with high resolution (0.15 cm<sup>-1</sup>).

A.Grosch *et al.* used infrared spectrometer with fiber optic sensor to measure the concentration of CO<sub>2</sub> and water vapor in a harsh environment [3]. CO<sub>2</sub> and water vapor have the common absorption spectral bands at about 3700 cm<sup>-1</sup> due to active molecular vibrations. The detecting system consists of a wide-band tungsten halide lamp and two near-infrared detectors coupled with two different optical filters.

Johann Maywoger provided a gas sensor which consists of a TR-source, a sample gas box, a narrow-band filter, and an infrared sensor for CO<sub>2</sub> analysis [4]. They determined concentration of absorbent material by measuring the intensity of light transmitted through the medium and using Lambert-Beer law.

Turner A. F and Baumeister studied Fabry-Perot narrowband filter which had a spacer between two reflecting layers. The drawback of this filter is that it is difficult to fabricate the multilayer film because reference wavelength will change due to the small deviation of film thickness during deposition.

The analysis by periodical symmetric systems is convenient for the band filter. Thelen studied the structural analysis of periodic symmetric systems (0.5 L H 0.5 L) [6].

Absorption spectra of a mixture of gas molecules contain HC (3.4 μm), SO<sub>2</sub> (4 μm), CO (4.7 μm), CO<sub>2</sub> (4.3 μm), H<sub>2</sub>O (1.9 μm) and NO (5.3 μm) and so on.

In this paper, we discuss the design method of CO<sub>2</sub> filter (4.3 μm) with all-dielectric materials, which has broadband suppression and narrowband transmission.

#### 2. Narrowband-pass filter for CO<sub>2</sub>

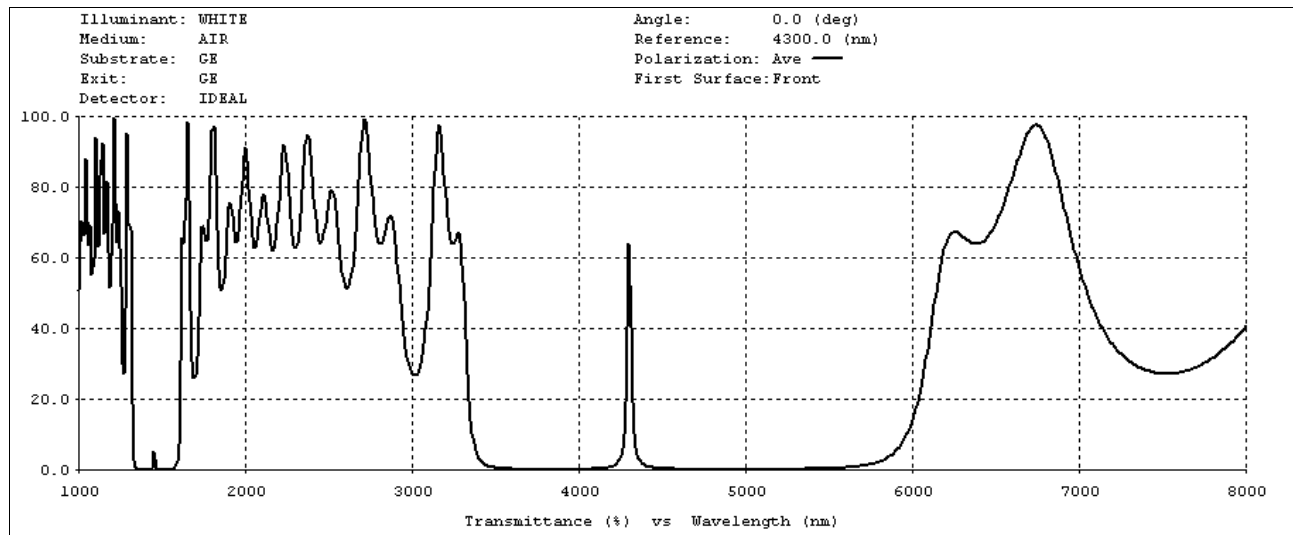
Fabry-Perot interferometer is a typical narrow-band filter to detect the sharp spectrum and its structure is as follows.

$$G/LHLHLHL2HLHLHLHL/A$$

(1)

where  $\text{Ge}(n_{\text{Ge}}=4)$  is high-refractive index layer and  $\text{SiO}(n_{\text{SiO}}=2)$  is low-refractive index. Fig 1 shows

transmittance of single-cavity filter with reference wavelength  $4.3\mu\text{m}$ .



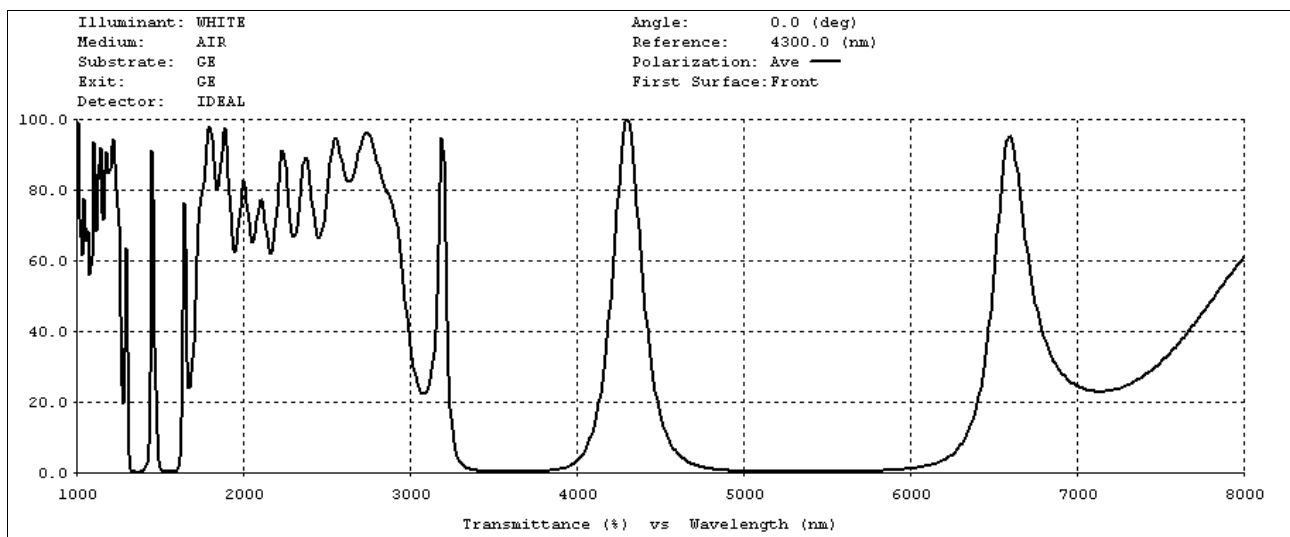
**Fig 1:** Transmittance of Fabry-Perot filter with reference wavelength  $4.3\mu\text{m}$ .

From Fig 1, Fabry-Perot filter has a good spectral selectivity but low transmittance and poor manufacturability at  $\lambda_0=4.3\mu\text{m}$ . We can improve this spectral character by

coupling Fabry-Perot filter in series. the structure of which is as follows.

$$\text{G/LHL(2H)LHLHL(2H)LHL/A} \quad (2)$$

Spectral transmittance of this double half-wave filter is shown in Fig 2.

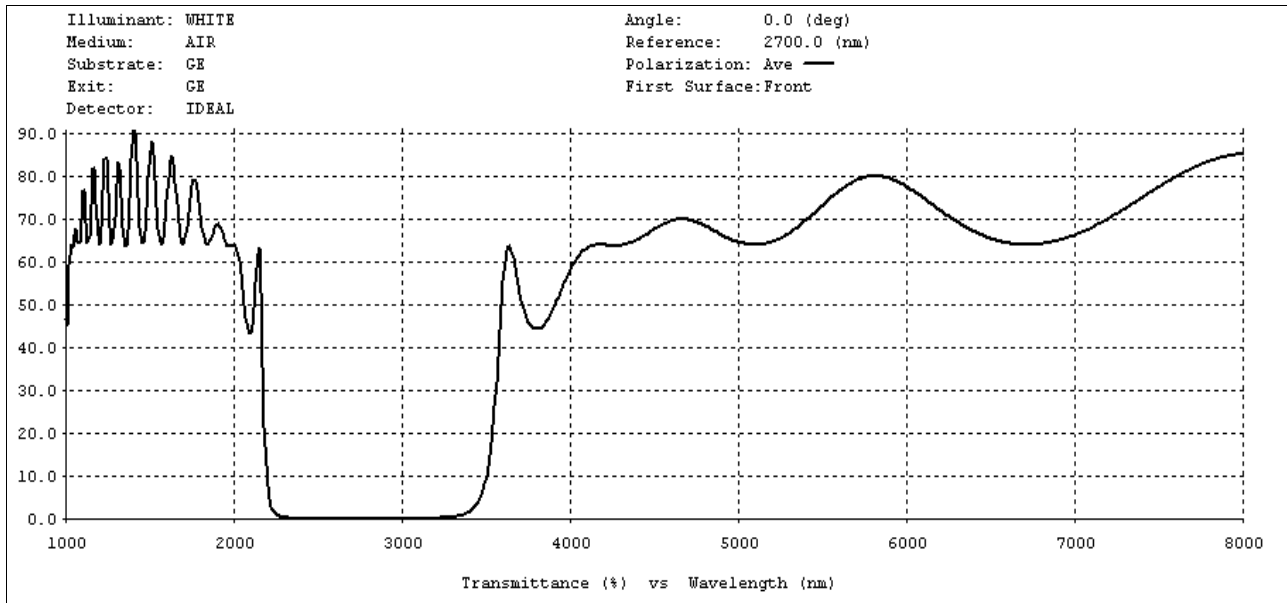


**Fig 2:** Spectral transmittance of middle infrared double Fabry-Perot filter with reference wavelength  $4.3\mu\text{m}$ .

From Fig 2, we can find that the spectral half width of the filter became wider and transmittance at reference wavelength increased as  $T_{\lambda_0}=100\%$ , however it could not remove sideband of  $\text{CO}_2$  ( $4.3\mu\text{m}$ ). Spectral transmittance is calculated by using optical filter design program TFCalc3.5. Because there are other spectral bands for  $\text{H}_2\text{O}$  ( $1.9\mu\text{m}$ ),  $\text{HC}$  ( $3.4\mu\text{m}$ ),  $\text{SO}_2$  ( $4\mu\text{m}$ ),  $\text{CO}$  ( $4.7\mu\text{m}$ ) and  $\text{NO}$  ( $5.3\mu\text{m}$ ) besides  $\text{CO}_2$  ( $4.3\mu\text{m}$ ), it needs to combine an additional broadband filter with narrow-band one.

For this reason, we suggested broad band filter to remove sideband of  $4.3\mu\text{m}$  in Fig 3. Blocking band and transmittance band of the designed broadband filter is  $1.8\text{--}3.3\mu\text{m}$  and  $4.1\text{--}4.5\mu\text{m}$ . When we use Ge as substrate of the filter, blocking band of the filter is  $2\text{--}3.5\mu\text{m}$  because of absorption property of Ge.

From transmittance character of this filter, structure of broadband filter is  $\text{G}/(0.5\text{LH}0.5\text{L})^6/\text{A}$ . where, p is the period of symmetrical system.



**Fig 3:** Transmittance of middle infrared broadband-pass filter G/(0.5LH0.5L)6/A.  $\lambda_0=2.7\mu\text{m}$

From above figure we can find that infrared bandpass filter has the low transmittance of at  $4.3\mu\text{m}$ . This is because of no matching between multi-layer system, substrate and surrounding air. To increase the transmittance at  $4.3\mu\text{m}$ , multi-layer system must be matched with surrounding medium.

According to Thelen' research, the symmetrical period system can be replaced with equivalent single film. Suppose that three-layer symmetric system is ABA, interference matrix of this system is

$$M_{11} = M_{22} = \cos 2\delta_A \cos \delta_B - \frac{1}{2} \left( \frac{\eta_B}{\eta_A} + \frac{\eta_A}{\eta_B} \right) \sin 2\delta_A \sin \delta_B \quad (3)$$

Where

$$M_{12} = \frac{j}{\eta_A} \left[ \sin 2\delta_A \cos \delta_B + \frac{1}{2} \left( \frac{\eta_B}{\eta_A} + \frac{\eta_A}{\eta_B} \right) \cos 2\delta_A \sin \delta_B + \frac{1}{2} \left( \frac{\eta_A}{\eta_B} - \frac{\eta_B}{\eta_A} \right) \sin \delta_B \right] \quad (4)$$

$$M_{21} = \frac{j}{\eta_A} \left[ \sin 2\delta_A \cos \delta_B + \frac{1}{2} \left( \frac{\eta_B}{\eta_A} + \frac{\eta_A}{\eta_B} \right) \cos 2\delta_A \sin \delta_B - \frac{1}{2} \left( \frac{\eta_A}{\eta_B} - \frac{\eta_B}{\eta_A} \right) \sin \delta_B \right] \quad (5)$$

$$M_{ABA} = \begin{bmatrix} \cos \delta_A & j \sin \delta_A / \eta_A \\ j \eta_A \sin \delta_A & \cos \delta_A \end{bmatrix} \begin{bmatrix} \cos \delta_B & j \sin \delta_B / \eta_B \\ j \eta_B \sin \delta_B & \cos \delta_B \end{bmatrix} \begin{bmatrix} \cos \delta_A & j \sin \delta_A / \eta_A \\ j \eta_A \sin \delta_A & \cos \delta_A \end{bmatrix} \quad (6)$$

The symmetrical period system consisted of three-layer symmetric system (ABA) is equivalent to following single film.

$$M_{ABA} = \begin{bmatrix} \cos \delta_e & j \sin \delta_e / \eta_e \\ j \eta_e \sin \delta_e & \cos \delta_e \end{bmatrix} \quad (7)$$

where,  $\delta_e$ - equivalent phase thickness of equivalent single layer,  $\eta_e$ -equivalent optical admittance (Herpin index). Therefore.

$$M_{11} = M_{22} = \cos \delta_e \quad (8)$$

$$M_{12} = j \sin \delta_e / \eta_e \quad (9)$$

$$M_{21} = j \eta_e \sin \delta_e \quad (10)$$

$$\eta_e = \sqrt{\frac{M_{21}}{M_{12}}} = + \eta_A \left\{ \frac{\left[ \sin 2\delta_A \cos \delta_B + \frac{1}{2} \left( \frac{\eta_B}{\eta_A} + \frac{\eta_A}{\eta_B} \right) \cos 2\delta_A \sin \delta_B + \frac{1}{2} \left( \frac{\eta_A}{\eta_B} - \frac{\eta_B}{\eta_A} \right) \sin \delta_B \right]}{\left[ \sin 2\delta_A \cos \delta_B + \frac{1}{2} \left( \frac{\eta_B}{\eta_A} + \frac{\eta_A}{\eta_B} \right) \cos 2\delta_A \sin \delta_B - \frac{1}{2} \left( \frac{\eta_A}{\eta_B} - \frac{\eta_B}{\eta_A} \right) \sin \delta_B \right]} \right\}^{1/2} \quad (11)$$

From expression

$$\delta_e = \arccos \left[ \cos 2\delta_A \cos \delta_B - \frac{1}{2} \left( \frac{\eta_B}{\eta_A} + \frac{\eta_A}{\eta_B} \right) \sin 2\delta_A \sin \delta_B \right] \quad (12)$$

If anti-reflection coating is introduced between above equivalent single layer and incident medium, it can be matched main stack with air.

To ensure maximum transmittance at  $4.3\mu\text{m}$ , we must realize anti-reflection processing at the wavelength. Relative wave number at  $\lambda=4.3\mu\text{m}$ :  $g=\lambda_0/\lambda=0.581$

Phase thickness for the symmetrical periodic system of G/(0.5LH0.5L)<sup>6</sup>/A is as follows.

$$\delta_A = \delta_L = \frac{2\pi}{\lambda} n_L d_L = \frac{2\pi}{\lambda} \cdot \frac{\lambda_0}{8} = \frac{\pi}{4} g = 0.145\pi$$

$$\delta_B = \delta_H = \frac{2\pi}{\lambda} n_L d_L = \frac{2\pi}{\lambda} \cdot \frac{\lambda_0}{8} = \frac{\pi}{4} g = 0.29\pi$$

$$\delta_B = 2\delta_A$$

Equivalent admittance of periodic symmetric system is  $n_{e,0.581}=3.71$  from expression (11). To match main stack with surrounding air, anti-reflection coating is introduced into boundary between equivalent structure and air.

Then, refraction index of matching film is as following.

$$n_j = \sqrt{n_e \cdot n_0} = \sqrt{3.71 \cdot 1} = 1.92$$

where, we select refraction index of the matching film as  $n_{sio} = 2$  which is low-refraction index of the main film.

The geometrical thickness of matching film is

$$d_e = \frac{\lambda_e}{4n_e} = 0.537(\mu\text{m})$$

Because material of the matching film is the same as low refractive index film, the thickness of film that contact with air is  $d_L = 0.537 + 0.156 = 0.693(\mu\text{m})$  and thickness coefficient is  $c = 0.639/312 \approx 2.22$

Therefore, structure of the new broadband filter is denoted as

$$G/(0.5LHLHLHLHLHLHLH2.2L)/A. \quad (13)$$

Structure and spectral transmittance of this multi-layer system is shown in fig 5.

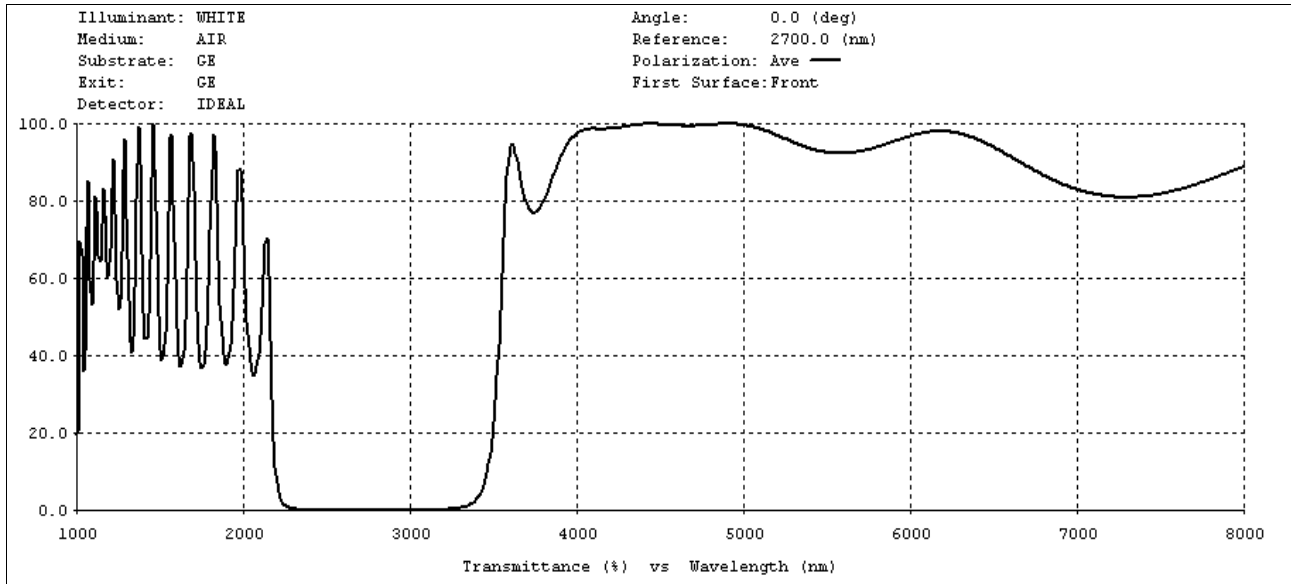


Fig 4: Spectral transmittance of  $G/(0.5LHLHLHLHLHLHLH2.2L)/A$   $\lambda_0 = 2.7\mu\text{m}$

Comparing spectral transmittance of Fig (5) with Fig (4), average transmittance of the filter consisted of symmetrical period system is 65% at  $4.3\mu\text{m}$  but it increased as 100% for equivalent structure.

Finally, combining narrow band filter consisted of double symmetric Fabry-Perot with broad band filter consisted of

periodic symmetric film, we made a filter for  $\text{CO}_2$  absorption analysis.

Multi-layer system of this filter is as follow.

$$A/LHL(2H)LHLHL(2H)LHL/G/(0.5LHLHLHLHLHLHLH2.2L)/A$$

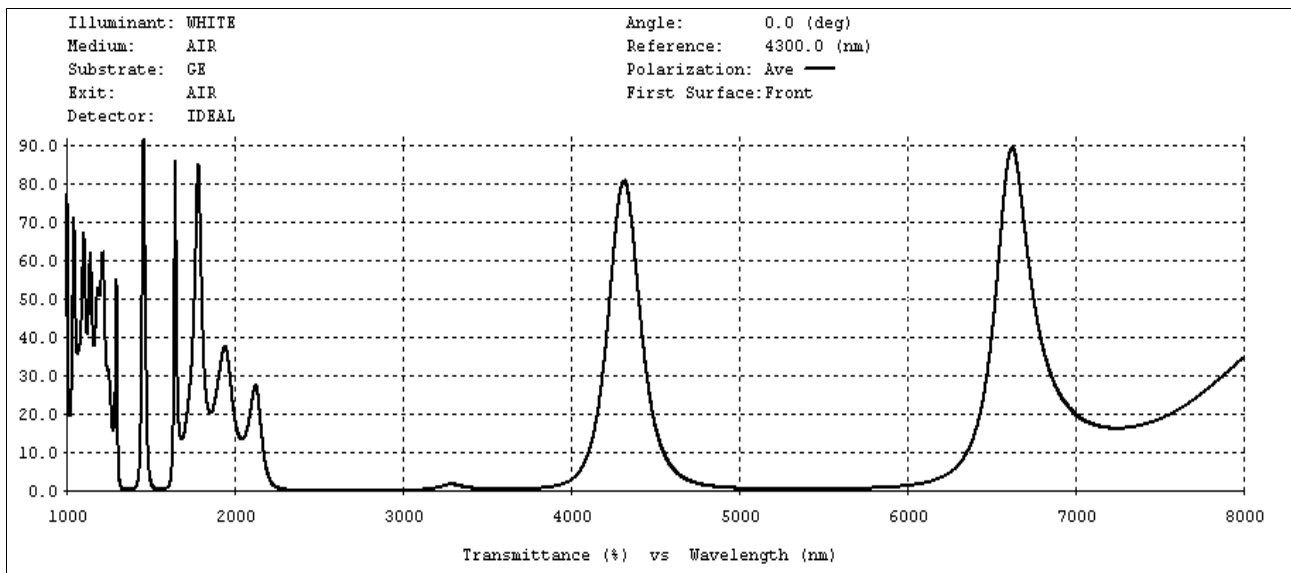


Fig 5: Spectral transmittance of  $A/LHL(2H)LHLHL(2H)LHL/G/(0.5LHLHLHLHLHLHLH2.2L)/A$

From fig 6, the new filter has high transmittance at  $\text{CO}_2$  absorption spectrum ( $4.3\mu\text{m}$ ) and broad sideband suppression

#### 4. Discussion

We discussed the design method of narrowband optical filter for CO<sub>2</sub> gas analysis which are essential for many industrial fields such as environmental protection and disaster prevention. Atmosphere contains NO, CO, water vapor and SO<sub>2</sub> gases in addition to CO<sub>2</sub> and their absorption spectra in the middle infrared range are the same as CO<sub>2</sub>. Therefore, narrowband filter must not only suppress the spectra of other gas components but transmit the absorption spectrum of CO<sub>2</sub>. Proposed narrowband filter design method can satisfy these spectroscopic properties.

#### 5. Conclusion

In this paper, we described the design method of narrowband filter to detect CO<sub>2</sub> gas in a gas mixture. Middle infrared narrowband filter is composed of all-dielectric narrowband single-cavity and broadband filter with reference wavelength 4.3 $\mu$ m. In order to provide a wide-band suppression and high transmittance, we introduced the multi-layer system of double cavity filter and broadband filter that had deposited on front and back of substrate. This structure can avoid spectral change in reference wavelength due to film thickness errors during deposition. To increase the transmittance of the CO<sub>2</sub> absorption spectrum, the equivalent theory of the periodic symmetric film system was applied to achieve the refractive index matching with environment medium.

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#### 7. Conflict of interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

#### 8. Disclosure statement

No potential conflict of interest was reported by the authors.

#### 9. Data Availability

The data that support the findings of this study are available within the article.

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