## An ammonia gas sensor with two chambers based on U-bending microring resonator<sup>\*</sup>

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A compact ammonia gas sensor with two gas chambers is proposed in this paper, whose core sensing device is a U-bending microring resonator. The waveguides of ring part and feedback part in this resonator are made of silicon on insulator (SOI) ridge waveguide covered with ZnO nanocrystals which are sensitive to ammonia gas. The sensor can measure two groups of gas samples simultaneously. By computer simulation, we obtain the clear sensitivity curves of two gas chambers in ammonia sensor when the gas concentration increases from 0 to 4‰. The gas concentrations in two chambers can be obtained from one output spectrum, which significantly reduces the material and time consumption.

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Currently, there are four types of sensors using different principles for detecting  $NH_3$  gas<sup>[1,2]</sup>. Semiconductor metal oxide (SMO) sensor<sup>[3,4]</sup> is the most widely used and successful in commercial detection so far. However, most semiconducting sensors have to be heated up to comparatively high temperature (300–700 °C) for the electrical response to gas concentration<sup>[5]</sup>. Therefore, the whole sensing system should be complicated including special heater, thermal isolation and so on. Surface acoustic wave (SAW) sensors are based on detecting the frequency change of SAW resulting from the adsorption of ammonia into an elastic membrane which is coated on piezoelectric crystal<sup>[6]</sup>. Since optical absorption spectrometric sensors are deficient in compactness and sensitivity, optical chemical sensors both on fiber and waveguide draw much attention in recent years.

Particularly, owing to the development of silicon on insulator (SOI) fabrication, microring resonators are extensively used in add-drop filters, optical switches, wavelength division multiplexing (WDM) multiplexers and lasers, showing attractive and potential features for sensing ability<sup>[7-10]</sup>. The U-bending microring resonator<sup>[11-14]</sup> was reported as a modulator to alter the output light signal, like using electro-optic method or thermo-optic method to shift the resonant waveguide, to change the bandwidth and to widen the free spectral range (FSR).

However, the chemical optical gas sensor usually needs relatively long reaction time. In this paper, we design a two-chamber ammonia gas sensor based on U-bending microring resonator chip. The chip is in micrometer scale, and it can measure two gas samples synchronously. The concentrations of the two samples are both included in the output spectrum, which doubles the sensing efficiency and greatly decreases the material and time consumption.

Fig.1(a) depicts the cross section of ridge waveguide designed for gas sensing. The SOI ridge waveguide is coated by ZnO porous layer which is composed of ZnO nanocrystals. Ammonia gas molecule can react with the ZnO molecule on the surface of nanocrystals. The tinier the ZnO particles are, more sufficient the reaction can be. When the temperature is kept at 150 °C, the chemical reaction on the surface of crystals is

$$2NH_3 + 3O^{-} \leftrightarrow N_2 + 3H_2O + 3e^{-}.$$
 (1)

If this waveguide is surrounded by ammonia gas, due to its affinity property, ammonia molecule can be attracted by ZnO, fills into the gap in ZnO nanocrystals, adheres to the surface of ZnO crystals, and renders the change of refractive index of the covering layer. It is not uncommon to use Lorentz-Lorenz equation in the computation of refractive index of composite medium, which can be expressed as

$$\frac{n^2 - 1}{n^2 + 2} = \frac{4\pi}{3} N\alpha , \qquad (2)$$

where *n* is the refractive index of the material, *N* is the molar mass, and  $\alpha$  refers to polarizability. For ZnO porous layer after gas adsorption, the refractive index  $n_1$  can be estimated by

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$$\frac{n_{1}^{2}-1}{n_{1}^{2}+2} = \frac{3N_{a}}{4\pi N_{\rm NH_{i}}} \left(\frac{n_{\rm NH_{i}}^{2}-1}{n_{\rm NH_{i}}^{2}+2}\right) + \frac{3N_{b}}{4\pi N_{\rm ZnO}} \left(\frac{n_{\rm ZnO}^{2}-1}{n_{\rm ZnO}^{2}+2}\right), \quad (3)$$

where  $N_a$  and  $N_b$  refer to the molar masses of NH<sub>3</sub> and ZnO in porous layer,  $N_{\rm NH_3}$  and  $N_{\rm ZnO}$  are the molecular weights of NH<sub>3</sub> and ZnO,  $n_{\rm NH_3}$  and  $n_{\rm ZnO}$  are the refractive indices of NH<sub>3</sub> and ZnO, respectively. Hypothesize the gap between ZnO nanocrystals occupies 40% space of covering layer, namely the porosity is 40%, and the refractive index  $n_{\rm ZnO}$  is 1.93. According to Eq.(3), when no cladding interaction with ammonia occurs, the refractive index of ZnO covering layer is 1.483.



## Fig.1 (a) The cross section of the ridge waveguide for ammonia sensing; (b) The structure of U-bending microring resonator

Fig.1(b) shows the U-bending ring structure in this gas sensing device<sup>[12]</sup>. Define the radius of ring as  $R=25 \mu m$ , effective index of waveguide as  $n_{\rm eff}$ =3.34, the coupling coefficient of two couple sections as k=0.047 (critical coupling) and the length of feedback waveguide as  $L=2\pi R$ . We use the transmission matrix and the theory of couple modes to construct a mathematic model, and simulate the output spectrum shown in Fig.2(a). The FSR of this structure is 9.7 nm, and the ring resonator works as a narrow-wave filter, making the resonant notches obviously distinguished with each other. On the other hand, as this U-bending structure has a piece of feedback waveguide, we can modulate the output spectrum by varying the refractive index of feedback waveguide. Fig.2(b) shows the output power of light signal at  $\lambda$ =1549.7 nm changing with the increase of index.

As can be seen from Fig.2(b), the output power rockets from bottom to top in half period ( $\Delta n=0.005$ ), and thus the ring resonator is very sensitive to the variation of index of feedback waveguide.



Fig.2 (a) Output spectrum of U-bending microring resonator; (b) Relationship between output intensity and effective index of feedback waveguide at  $\lambda$ =1549.7 nm

Combining the gas sensitive waveguide and U-bending waveguide structure described above, we can design a gas sensor based on the principle as depicted in Fig.3.

The schematic diagram in Fig.4 describes the setup of the designed sensor. The semicircular part of the structure refers to the gas sensing waveguide coated with ZnO nanocrystals, and the straight part is made of ordinary SOI ridge waveguide which is not able to absorb ammonia gas. A glass window is set on the side face of gas chamber. A coupling fiber from a tunable laser is aligned to the input grating coupler, and the light from the output grating is collected by a detector. Then the data can be processed by computer and then turned into output spectrum.



Fig.3 Flow chart of the gas sensing procedure

According to Ref.[15], ZnO crystals can be prepared

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based on the wet chemical procedure at room temperature. Using this method, ZnO nanocrystals with diameter ranging from 2.5 nm to 4.5 nm can be obtained. The sample gas is mixed by different proportions of ammonia and pure nitrogen. The parameters of U-bending structure are the same as introduced above. In ridge waveguide, H=250 nm, h=100 nm, and the refractive indices of Si and SiO<sub>2</sub> are 3.44 and 1.46, respectively. In order to simplify the calculation method, we assume that the porosity of ZnO is 40%, and the center wavelength of laser signal is 1550 nm.



Fig.4 Structure of the two-chamber ammonia sensor

If we input ammonia-nitrogen mixed gases with different concentrations into gas chamber, supposing the reaction time is enough, we obtain the relationship between effective index variation  $\Delta n$  and gas concentration, which is shown in Fig.5.



Fig.5 Effective index change vs. ammonia concentration

On one hand, if we only fill the sample gas into gas chamber A, we can obtain the sensitivity curve with different gas concentrations shown in Fig.6(a), where the vertical axis refers to the normalized output power of light at 1549.7 nm. Fig.6(a) indicates 8 groups of data we obtained, and the curve is a simulation trend. In this structure, changing the refractive index of feedback waveguide can not move the resonant wavelength, but it can change the depth of resonant notch. On the other hand, if we only fill sample gas into chamber B, the sensitivity curve is recorded in Fig.6(b). At this time, only the index of ring waveguide is changed, and thus the resonant wavelength red-shifts from 1554.7 nm to 1552.3 nm in output spectrum when the concentration changes from 0 to 4‰. The sensitivity of index on ring can be expressed as

$$\Delta\lambda_{\rm res} = \frac{\Delta_{\rm con} n_{\rm eff} \lambda_{\rm res}}{n_{\rm g}}, \qquad (4)$$

where  $\Delta \lambda_{\text{res}}$  is the wavelength shift, the  $\Delta_{\text{con}} n_{\text{eff}}$  is the change of effective index caused by the change of gas concentration, and  $n_{\text{g}}$  is the group index. Thus, the sensitivity trend of chamber B is linear theoretically.



Fig.6 (a) The output intensity with only chamber A filled with sample gas and (b) the shift of resonant wavelength with only chamber B filled with sample gas in different ammonia concentrations

If we pump the gas into both the two gas chambers in the meantime, the output transmission spectra in different situations are shown in Fig.7. According to Fig.7, it is obvious that resonant wavelength is determined by the concentration in chamber B. If we compare the three spectra with the same resonant wavelength, it is easy to find that only when the gas concentrations are the same in two gas chambers, the complete extinction in resonant wavelength can be realized in the situation of critical coupling. On the contrary, if there is a huge difference between the concentrations in two chambers, the filtering is not significant any more, as shown in Fig.7(c) and (g).

Fig.8 describes the sensitivity of concentration difference between two gas chambers, where  $\Delta C = C_A - C_B$  and the vertical axis refers to output transmission at resonant wavelength. The NH<sub>3</sub> concentration in chamber B can be obtained from the shift of resonant wavelength. Meanwhile, the concentration difference between chambers A and B can be obtained by measuring the output intensity at resonant wavelength. According to the sensitivity in Fig.6(b) and Fig.8, if we know which concentration is greater in value, the gas concentrations in two chambers can be obtained simultaneously.



Fig.7 Output spectra when two chambers with different concentrations



Fig.8 Relationship between output intensity and concentration difference between two gas chambers

In this paper, we design the two-gas-chamber  $NH_3$  sensor with a U-bending microring resonator. The proposed structure keeps the compact size and doubles the sensing efficiency, which shows great potential in future optical gas sensor.

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