Optik 125 (2014) 2752–2755

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Simulation of ZnO-coated SOI microring resonant shift response to ethanol and ammonia

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ARTICLE INFO

Article history:
Received 8 June 2013
Accepted 7 November 2013

Keywords:
Microring resonator
Gas sensor
Chemisorption
Physisorption

ABSTRACT

A compact silicon-on-insulator microring resonator coated with porous ZnO layer for gas sensing is proposed in this paper. Based on the sensing system designed, we simulated the output spectra of two different sample gases, ethanol vapor and ammonia gas. The variable gas concentration we choose in this work range from 0 to 3‰. The molecule sizes of them are in different orders of magnitude, leading the sensitivity curves to show thoroughly different trends. The significant difference of two curves suggests that these two types of reducing gas obey different absorption principles depending on the size disparity between gas molecules and ZnO nanocrystals coated on ridge waveguide.

1. Introduction

Gas concentration measurement is extensively applied in modern industry, medical detection, and environment monitoring, with great potentials in anti-terrorist as well, such as air quality detection, medical breath analysis, airport security, industry process monitoring, and leak detection of explosive gases. Nowadays, the trend of gas sensor upgrade is to pursue safety, microminiaturization, low power consumption, cheapness, and remote monitoring [1–4]. With the development of modern technology, the demands for gas sensing in many fields are being constantly promoted, making the development of gas sensor has become an urgent mission recently.

Silicon-on-insulator (SOI) is widely used recently as a suitable material to fabricate integrated optical devices because of its compactness and compatibility to complementary metal-oxide-semiconductor (CMOS) [2,3,5–8]. These photonic SOI structures are reported with submicron scale features and can be realized on chips. Due to these advantages, some micron scale gas sensor based on various principles like electro-chemical, biological, and optical detection are proposed in recent papers [5–8]. In these sensors, the electro-chemical method of measuring gas by changing the resistance of metal-oxide-semiconductors (MOS) attracts most attentions [5,6,9–12]. However, MOS sensors usually need a relatively higher temperature to interact with sample gas and the chemical process is irreversible. Thus, the high cost of power and material consumption can be an issue. Besides, the sparking risks associated with the electrical contacts make these sensors potentially unsafe in explosive environment [7].

On the other hand, these weak points can be avoided by using optical detection. In order to keep the miniaturization and integration, some papers suggested to dope a gas sensing chemical or biological film on SOI rectangle waveguide [1–3,7,8]. It is not uncommon in optical sensing because they strongly decrease the interaction length compared with a direct spectroscopic gas analysis. Also, a proper choice of both the sensitive optical component and the chemical coating can lead to a significant enhancement in the sensor sensitivity. Owing to these merits, the research on SOI optical structures is becoming a hot topic in this field.

Some metal oxides like ZnO, WO_3, and NiO are reported able to absorb reducing gases such as hydrogen, ammonia, and ethanol vapor, which are also flammable and explosive in industrial application [13,14].

In this paper, we designed a microring resonator for gas sensing with its ring covered by porous ZnO layer. The porous nature of covering layer provides the space for gas absorption and ZnO is sensitive to several kinds of reducing gas such as ethanol, acetone, TMA, and ammonia. By this structure, the gas concentration around microring can be obtained by measuring the shift of resonant wavelength in output spectrum. NH_3 and ethanol vapor, representing two different situations of gas absorption are analyzed. Their concentrations ranging from 0 to 3‰ are simulated and the different optical outputs are shown in this paper, suggesting that these two categories of sample gas obey different absorption principles.

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0030-4026/$ – see front matter © 2013 Elsevier GmbH. All rights reserved.
http://dx.doi.org/10.1016/j.ijleo.2013.11.037

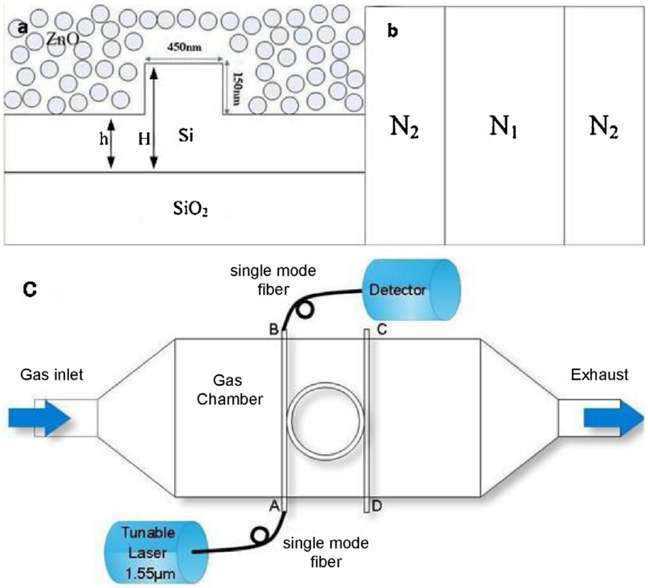

Fig. 1. (a) The structure of waveguide with ZnO crystal covering layer, (b) the equivalent waveguide of ridge waveguide, and (c) schematic of gas sensor setup.

2. The sensor structure

The cross sectional structure of the ring waveguide is shown in Fig. 1(a), including a piece of SOI ridge waveguide and the porous ZnO covering layer coated on it. The porous layer has good performance in gas sensing [15]. Since digging nanoholes in ZnO layer may be very difficult to realize, we can use ZnO nanocrystals as covering layer, and the gap between nanocrystals can be considered as nanoholes. ZnO is easy to attract volatiles, also low cost, low toxicity, and convenient for doping. Besides, ZnO is transparent in the near infrared around 1550 nm, enabling applications based on evanescent field interactions in SOI [7]. Based on the wet chemical procedure, the ZnO crystals doped in this structure is possible to be prepared. 2.5 mol $(CH_3)_4NOH{\cdot}5H_2O$(TMAH), dissolved in 5 ml dry ethanol, is added drop-wise to 15 ml solution of 0.1 M pure zinc acetate in dimethylsulfoxide under 10–15 min vigorous stirring at room temperature [16]. Using this method, ZnO nanocrystals ranging from 2.5 to 4.5 nm in diameter can be obtained. These sizes of nanocrystals are used in our simulation to approach the reality.

Compared with rectangle waveguides, ridge waveguide is better suited in this gas sensing structure. First of all, ridge waveguide allows wide band light signals, which ensures the shift length being detected. Secondly, the theoretical calculation of multimode interference in ridge waveguide is simple, leading to a proper waveguide design to obtain single-mode condition at the output [17].

The schematic of gas sensor with ring resonator is described in Fig. 1(c). As it can be seen in the picture, the microring resonator is sited in the middle of gas chamber. Its ring part is made of the waveguide depicted in Fig. 1(a). In order to keep a constant air pressure in the chamber, sample gas is filled into gas chamber from gas inlet in left and exhausted to right. The light signal from tunable laser comes into Port A and exits from Port B, which can be captured by the detector in the end. Part of incident light field drops into the ring when they pass the coupling section between ring and waveguide. This part of light field dissipates in the evanescent field and is unable to be detected in output spectrum. Based on this principle, some notch wavelengths are visible in the output spectrum. When the sample gas is filled into the chamber, the ring part of microring resonator begins to absorb the sample gas around, rendering the changes in refractive index of ring waveguide. As a result, the resonant wavelength in output spectrum will shift, indicating the changes of gas concentration in the chamber. Following the gas sensing procedure demonstrated above, we can build a mathematical model of this gas sensor to simulate the process and output outcome.

First of all, as it is shown in Fig. 1(a), a 450 nm high and 150 nm wide SOI ridge waveguide is coated by ZnO nanocrystals. Since metal-oxide like ZnO is naturally gas attractive, the sample gas surrounding the waveguide can be easily absorbed into the space within its nanocrystals. To obtain the refractive index of covering layer when gaps are filled with sample gas, the computational method obeys the Lorentz–Lorenz equation.

$$\frac{n^2-1}{n^2+2}=\frac{4\pi}{3}N\alpha \tag{1}$$

Here, n is the refractive index of the material, N is the molar mass, and α means polarizability. Based on this equation, if we define n_a as the refractive index of metal oxide and n_b as the refractive index of sample gas, the equation expressing the changed refractive index of covering layer n_{cover} can be:

$$\frac{n_{cover}^2-1}{n_{cover}^2+2}=\frac{3N_a}{4\pi N_m}\left(\frac{n_a^2-1}{n_a^2+2}\right)+\frac{3N_b}{4\pi N_s}\left(\frac{n_b^2-1}{n_b^2+2}\right) \tag{2}$$

In this formula, N_a and N_b refer to the molecular weight of metal oxide part and the gas part, respectively, while N_m and N_s is the molar mass of metal oxide and sample gas. Assuming the space rate of gaps in ZnO covering layer is 50% and a refractive index of ZnO is 1.93, we obtain the value of n_{cover} 1.3917 when gas is not filled into chamber.

In order to calculate the effective index of waveguide, we should equivalent the ridge waveguide into a three layer planar waveguide as shown in Fig. 1(b). Since only one mode can be output by coupled single mode fiber, the refractive index of conductive layer N_1 and covering layer N_2 in the equivalent planar waveguide for each mode can be separately expressed as:

$$N_1=\left\{n_2^2-\left[\frac{(m+1)\pi}{k\times H_{eff}}\right]^2\right\}^{\frac{1}{2}} \tag{3}$$

$$N_2=\left\{n_2^2-\left[\frac{(m+1)\pi}{k\times h_{eff}}\right]^2\right\}^{\frac{1}{2}} \tag{4}$$

where n_2 is the refractive index of the ridge conductive layer, H_{eff} and h_{eff} is the effective length of H and h in Fig. 1(a), k refers to the wave vector of basic mode, and m is the order of conductive modes in vertical direction. In this case, H_{eff} and h_{eff} can be determined by the equation of $H_{eff}=H+\delta$ and $h_{eff}=h+\delta$, where δ is

$$\delta=\frac{\gamma_1}{\sqrt{k\left(n_2^2-n_1^2\right)}}+\frac{\gamma_2}{\sqrt{k\left(n_2^2-n_3^2\right)}} \tag{5}$$

In Eq. (5) n_1 and n_3 is the refractive index of covering layer and substrate layer in Fig. 1(a). For TE modes, $\gamma_{1,2}=1$; For TM modes, $\gamma_1=(n_1/n_2)^2$, $\gamma_2=(n_3/n_2)^2$. In the structure shown in Fig. 1(a), we choose SOI as the material of ridge waveguide, so the parameters are $n_1=n_{cover}$, $n_2=n_{Si}=3.44$, and $n_3=n_{SiO2}=1.46$. The effective index of waveguide can be calculated by Eq. (3), (4), and (5). When the gas chamber has no gas in it, the effective index is 3.1571. As a result, since we attribute the change of covering layer refractive index to the partially filling of gaps by sample gas, with the increase of gas concentration, the equivalent refractive index of waveguide rises as well.

The mathematical model of light field transmitting in microring resonator can be obtained based on transmission matrix and coupling mode theory [18,19]. For the sake of simplifying calculation, we assume the distance between ring and straight waveguide in two couple sections are same and $k^2+t^2=1$. Here k is couple