Effects of dispersion, absorption and interface fluctuation on the reflection spectra of porous silicon microcavity devices*

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One problem associated with microcavity devices is the significant difference between the reflection spectra of fabricated porous silicon microcavity (PSM) devices and those obtained by theoretical calculation of ideal microcavity devices. To address this problem, studies were carried out to determine the effects of the refractive index dispersion, the absorption of the porous silicon layer and the fluctuation of the dielectric interface on the reflection spectra of PSM devices. The results are in good agreement with those obtained experimentally from the fabricated PSM devices, which provides a theoretical basis for the design of PSM sensors.

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Porous silicon has been widely used in optical biosensors because of its good biocompatibility, and it can be easily made into various photonic devices[1-3]. Among these porous silicon devices, porous silicon photonic crystals with microcavity structures have been extensively studied[4-8]. A porous silicon microcavity (PSM) sensor is used to detect organisms by using the change in the reflectance spectrum or angular spectrum induced by a change in refractive index, which is caused by biological reaction in the device[9,10]. However, compared with the theoretical results, the experimental reflectance spectra reported in previous studies have the problems of narrow bandgap, low reflectivity, large defect half-width ratio and high reflectivity at the central wavelength. The main reason is that they have considered porous silicon as a non-absorbing, non-dispersive and smooth dielectric[11-13] and considered the microcavity device as an ideal one. However, because silicon is a semiconductor material, it exhibits dispersion and absorption. The interface of a PSM is obtained by applying different electrochemical corrosion currents and generating random fluctuations at the interface of porous silicon. Therefore, there are some differences between the results from experimental and ideal PSM devices, which will affect the reflection spectra of the devices. As a result, it is highly important to study the effects of dispersion, absorption and interface fluctuations in porous silicon on the optical properties of PSM devices. In this paper, such a research was carried out for a PSM sensor using the transmission matrix method and the Gaussian probability distribution method[14].

The PSM devices are composed of two identical Bragg mirrors and a defective layer of high-porosity silicon in the middle. Bragg mirrors are composed of alternating high- and low-porosity silicon layers. PSM devices were fabricated electrochemically. The silicon wafers are p-type with a resistivity of 0.01—0.05 Ω·cm. The etchant is composed of HF and C_2H_5OH solution with volume ratio of 1:1. The refractive index of the Bragg mirror in the PSM devices varies over 16 cycles. Porous silicon layers with high and low porosity were etched at 110 mA and 60 mA for 3 s and 4.5 s, respectively. The defective layers were etched at 110 mA for 6 s. The reflection spectra of the PSM devices were measured using a Hitachi U-4100 spectrophotometer. The defect state wavelength of the PSM devices is λ_0=1 628 nm.

The dielectric thicknesses of the Bragg mirror and the defect layer in the PSM devices should meet the following relationship:

$$n_1 d_1 = n_2 d_2 = \frac{\lambda_0}{4} \ , \tag{1}$$

$$n_3 d_3 = m\frac{\lambda_0}{2} \ , \tag{2}$$

where n_1 and n_2 are the refractive indices of high and low porosity silicon samples, d_1 and d_2 are the thicknesses of them, respectively, n_3 is the refractive index of the defect layer, d_3 is its thickness, and m is an integer.

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The SEM images of the PSM devices show that d_1, d_2 and d_3 are 290 nm, 240 nm and 580 nm, respectively. The refractive indices of the porous silicon layers with high and low porosity are n_1=1.403 4 and n_2=1.695 8, and the refractive index of the defect layer is n_3=1.403 4, calculated by Eqs.(1) and (2).

Using the above-mentioned parameters, the reflection spectrum of a PSM device is calculated by the transfer matrix method, and the result is also presented in Fig.1.

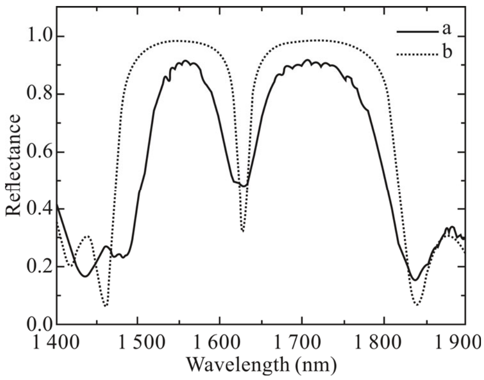

Fig.1 Reflection spectra of the prepared PSM device and the theoretically calculated one

From Fig.1, there is a large gap between the reflection spectra of the PSM device calculated theoretically and the fabricated PSM device. This gap is mainly caused by neglecting the dispersion and absorption of the porous silicon layer, and the PSM reflection spectrum is influenced by the fluctuation of the porous silicon layer interface with different porosities (refractive index).

Porous silicon can be considered as an optical dielectric material with a uniform mixture of air and silicon. The material's effective refractive index n_{eff} is expressed as follows:

$$(1-\rho)\frac{n_{\mathrm{si}}^2-n_{\mathrm{eff}}^2}{n_{\mathrm{si}}^2+2n_{\mathrm{eff}}^2}+\rho\frac{n_{\mathrm{air}}^2-n_{\mathrm{eff}}^2}{n_{\mathrm{air}}^2+2n_{\mathrm{eff}}^2}=0\,, \tag{3}$$

where ρ is the porosity of porous silicon, n_{si} is the refractive index of silicon, n_{eff} is the refractive index of porous silicon, and n_{air} is the refractive index of air.

The Cauchy dispersion formula is used to calculate the refractive indices of porous silicon at different wavelengths. The refractive indices of high and low porosity are n_1=1.403 4 and n_2=1.695 8, and the refractive index of the defect layer is n_3=1.403 4 at the central wavelength of the reflection spectrum of PSM devices. The refractive index dispersion relations of porous silicon layers with high and low porosity are obtained using the Cauchy dispersion formula and Eq.(3). The results are shown in Fig.2.

The incident light is considered as a TE wave and in normal direction. The refractive indices of the porous silicon layers with high and low porosity are selected to be n_1 and n_2 in Fig.2. The thicknesses are d_1=290 nm and d_2=240 nm, the refractive index of the defect layer is n_3=n_1, the thickness is d_3=580 nm and the total number of medium layers is 33. The transfer matrix method is used to simulate the reflection spectra of PSM devices. The results are shown in Fig.3.

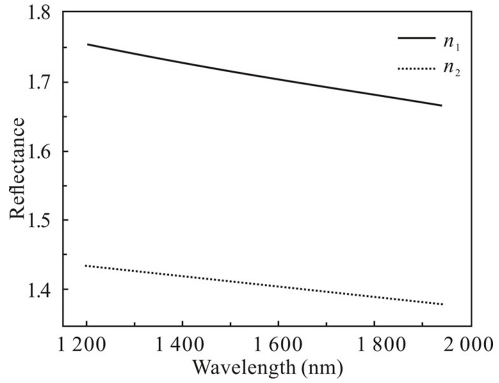

Fig.2 Refractive index curves of porous silicon samples with high and low porosity

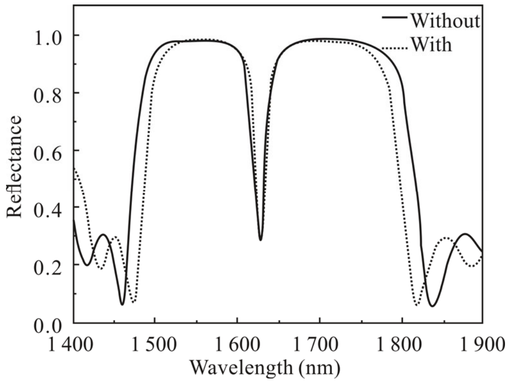

Fig.3 Reflection spectra of PSM devices with and without the refractive index dispersion of porous silicon

A comparison in Fig.3 shows that for PSM devices, the refractive index dispersion of the porous silicon layer will narrow the bandgap of the reflection spectrum, but will not affect the wavelength of defect states or the reflectivity in the bandgap.

For PSM devices, the complex refractive index is introduced to describe the refraction and absorption of light waves simultaneously:

$$\hat{n}=n+\mathrm{i}\kappa\,, \tag{4}$$

where n is the refractive index of porous silicon, and $\hat{e}$ is the extinction coefficient of porous silicon.

When the transfer matrix method is used to address the effect of absorption on the reflection spectrum of PSM devices, in the formula, the refractive index n, which needs to be replaced by a complex refractive index, corresponds to a transparent medium.

The central wavelength of the reflection spectrum of the PSM devices fabricated in this study is λ_0=1 628 nm. The total number of dielectric layers is 33. The complex refractive indices of porous silicon with high and low porosity are $\hat{n}_1$=1.403 4+0.001i and $\hat{n}_2$=1.695 8+0.001 5i. The layer thicknesses are d_1=290 nm and

d_2=240 nm. The complex refractive index of porous silicon in the defect layer is $\hat{n}_3$=1.403 4+0.001i, and the layer thickness is d_3=580 nm (the *k* method described above is used). The transfer matrix method is used to calculate the reflection spectra of the PSM devices, and the results are shown in Fig.4.

In Fig.4, a comparison of the two curves shows that the absorption of porous silicon decreases the reflectivity of PSM devices, particularly in the defect state. At the same time, the defect half-width increases but does not change the defect state wavelength λ_0.

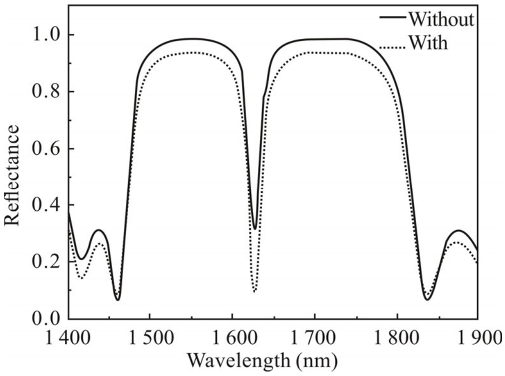

Fig.4 Reflection spectra of PSM devices with and without porous silicon absorption

The PSM devices produced by electrochemical etching are not smooth. Electron microscopy results show that the porous silicon layer of PSM devices is rough at the interface, and there are different undulation heights at different points. Because of the fluctuation of the porous silicon layer, the thicknesses at the incident points of each porous silicon layer are different, which causes the reflection spectrum to be blue-shifted or red-shifted relative to that of the ideal device. The reflection spectrum of PSM devices is composed of the reflection spectra at different incident points.

The interface fluctuation probability of porous silicon satisfies the following Gaussian distribution:

$$f(x)=\frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(x-u)^2}{2\sigma^2}) \quad , \tag{5}$$

where $f(x)$ is the probability of undulation height, x is the magnitude of the undulation, u is the average of the undulations, and ó is the standard deviation of the undulation height distribution.

To study the influence of dielectric interface fluctuation on PSM devices, the refractive indices of the high and low porosity silicon layers are designed to be n_1=1.403 4 and n_2=1.695 8, and the thicknesses are set to be d_1=(290+x) nm and d_2=(240+x) nm. The defect layer refractive index is n_3=1.403 4, and the thickness is d_3=(580+x) nm. The maximum fluctuation is assumed to be 25 nm, and the minimum is assumed to be 25 nm. First, the probability of different undulation heights of each layer is calculated using the Gaussian distribution probability function, and then the reflection spectra of the porous silicon layer under different undulation heights are calculated using the transfer matrix method. Finally, the reflection spectra of PSM devices with different undulation heights are synthesized, and the results are shown in Fig.5.

In Fig.5, the fluctuation of the dielectric interface decreases the bandgap reflectivity and increases the half-width of the PSM, but will not cause the central wavelength to shift.

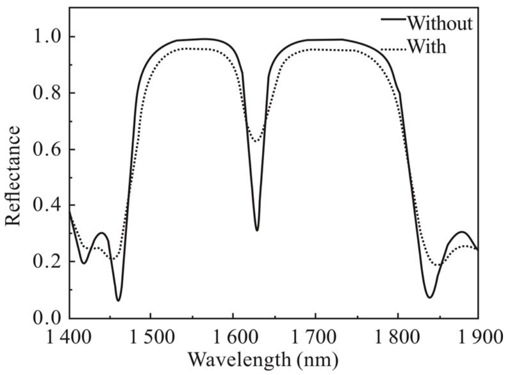

Fig.5 Reflection spectra of PSM devices with and without the dielectric interface fluctuation

Considering the refractive index dispersion and absorption of porous silicon and the fluctuation of the porous silicon interface, the PSM reflection spectra are calculated theoretically and compared with the reflection spectra of the fabricated PSM device and ideal PSM device as shown in Fig.6.

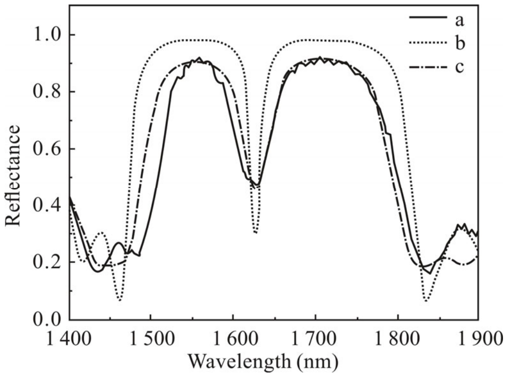

Fig.6 Reflection spectra of (a) a fabricated PSM device, (b) an ideal PSM device, and (c) a PSM device considering porous silicon dispersion, absorption, and interface fluctuation

The extinction coefficients $\hat{e}_1$ and $\hat{e}_2$ of high- and low-porosity silicon layers are obtained by transfer matrix fitting according to the experimentally obtained reflection spectrum. Fig.6 shows that the PSM reflection spectrum c is in good agreement with the experimentally obtained one.

The refractive index of porous silicon increases under the effects of a specific biological reaction in the pores of porous silicon, resulting in a red shift of the defect state wavelength of the reflection spectrum of a PSM device. Therefore, biological response information can be obtained by measuring the red shift of the reflectance spectrum. The quality factor Q of a PSM device is defined as the ratio of the central wavelength to the half-width of the defect state, which reflects the sensitivity of the biosensor. As shown in Fig.6, the ideal PSM device's Q value is 86, and the experimental PSM device's Q value is 48. Taking the refractive index dispersion and absorption of porous silicon and the fluctuation of the porous silicon interface into consideration, the Q value is 54, which is close to the experimentally determined value. Thus, the proposed approach provides a method for designing PSM biosensors.

It can be concluded that the refractive index dispersion of porous silicon narrows the bandgap of the PSM reflection spectrum. Moreover, the absorption of porous silicon decreases the bandgap reflectivity of the PSM reflection spectrum and enlarges the bandwidth of the defect state. The fluctuation of the porous silicon interface in a PSM device decreases the bandgap reflectivity, but the reflectivity at the central wavelength of the defect state increases, and the half-width of the defect state increases. Therefore, the dispersion and absorption characteristics of porous silicon and the effect of the fluctuation of the porous silicon interface on the reflection spectra of PSM devices must be fully considered in the preparation of PSM sensors.

References

[1] Urmann K, Arshavsky-Graham S, Walter J G, Scheper T and Segal E, Analyst **141**, 5432 (2016).

[2] Li S, Huang J and Cai L, Nanotechnology **22**, 425502 (2011).

[3] Rossi A M, Wang L, Reipa V and Murphy T E, Biosensors & Bioelectronics **23**, 741 (2007).

[4] Krismastuti F S H, Pace S and Voelcker N H, Advanced Functional Materials **24**, 3639 (2014).

[5] Ramakrishan S K, Fernandez M M, Cloitre T, Agarwal V, Cuisinier F J G and Gergely C, Sensors & Actuators B Chemical **272**, 211 (2018).

[6] Zhang H, Jia Z, Lv X, Zhou J, Chen L and Liu R, Biosensors & Bioelectronics **44**, 89 (2013).

[7] Bao Wu, Guoguang Rong, Junwei Zhao,Shulin Zhang, Yongxin Zhu and BoyongHe, Nano **07**, 1250049-1 (2012).

[8] Levitsky I A, Euler W B, Tokranova N and Rose A, Applied Physics Letters **90**, 1781 (2007).

[9] Li P, Jia Z, Lü Xiaoyi, Liu Y, Ning X and Mo J, Optics Express **23**, 24626 (2015).

[10] Ouyang H, Striemer C C and Fauchet P M, Applied Physics Letters **88**, 2519 (2006).

[11] Qiao H, Guan B, Gooding J J and Reece P J, Optics Express **18**, 15174 (2010).

[12] Zhang H, Lv J and Jia Z, Sensors **18**, 105 (2018).

[13] Huimin Ouyang, Delouise L A, Miller B L and Fauchet P M, Analytical Chemistry **79**, 1502 (2007).

[14] Ren X C and Guo L X, Journal of Applied Optics **29**, 144 (2008).