



# Gas sensing performance of high-Q photonic crystal nanocavities based on a silicon-on-insulator platform

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## Abstract

We have proposed and theoretically analyzed the gas sensing performance of the photonic crystal (PhC) nanocavities based on a silicon-on-insulator platform. To assess the gas sensing performance of the proposed PhC nanocavities, the effect of the etch-depth of the circular air holes in the substrate on the quality factor, mode volume, and resonant wavelength have been analyzed. Numerical analysis carried out using the three-dimensional finite-difference time-domain method and filter diagonalization approach shows that the etch-depth significantly perturbs the electric field profile of the original cavity mode. By tuning this parameter, the antinodes of the electric fields are relocated to the air regions of the etch-depth, which leads to an increase in the quality factor and reduction in the mode volume. In this case, the quality factor is found to increase with increasing etch-depth, but still remains as high as 5170 with a small modal volume of  $0.95 (\lambda/n)^3$ . In addition, using the perturbation method, we have demonstrated that the proposed PhC nanocavities possess the capability of detecting the change in the refractive index of the surrounding gas target with a high sensitivity of 322 nm/refractive index unit (RIU) and a detection limit of  $10^{-3}$  RIU. We believe that our proposed PhC nanocavities, which exhibit excellent sensing performances, ultra-small mode volume, and a compact footprint, may offer the potential to develop on-chip sensing devices for applications in gas detection.

**Keywords** Point-defect PhC nanocavities · Silicon-on-insulator platform · 3D-FDTD · Perturbation theory · Photonic integrated sensors · Gas sensor

## 1 Introduction

Recent developments in the field of nanophotonic devices have increased the demand for reducing their cost and size in order to facilitate their large-scale integration. Silicon-on-insulator (SOI) is one of the most important existing material systems used for the development of integrated nanophotonic devices. This technology is compatible with the well-established complementary metal oxide semiconductor (CMOS) process and has a high

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refractive index (RI) contrast which enables strong mode field confinement (Ramirez et al. 2019). Furthermore, the SOI technology allows for a monolithic integration of optical and electronic devices which permits avoiding the use of hybrid packaging techniques (Ramirez et al. 2019). On the other hand, the focus of recent research studies has been the development of sensors based on PhC structures because of the tremendous demand for sensing platforms especially in the detection of chemicals and gases (Clerbaux et al. 2003; Kassa-Baghdouche and Cassan 2018a, b, 2019). In fact, current developments on photonic technology are focused on the realization of high-performance sensing devices in terms of their sensitivity, detection limit, and response time.

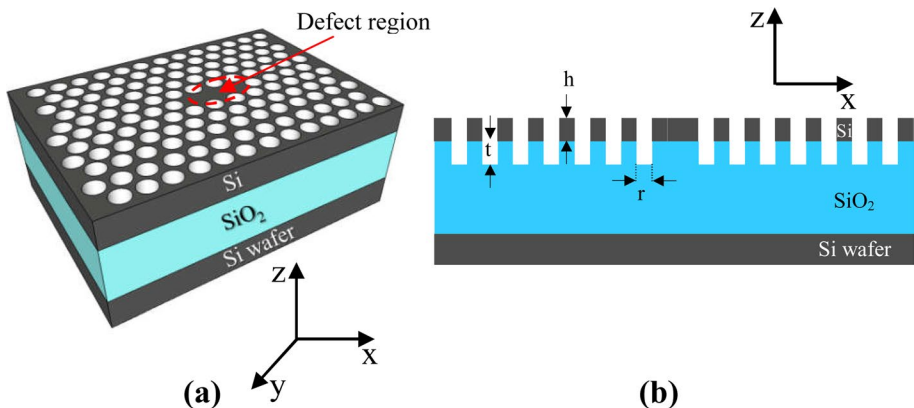
One of the most important properties that should be considered while producing commercial and low-cost photonic gas sensors is their compactness and fabrication feasibility using the existing CMOS and SOI technologies. In practice, to improve the characteristics of the sensing devices based on the SOI platform, several designs have been proposed such as nanobeam photonic crystal (PhC) cavities (Rahman et al. 2012; Zhang et al. 2015; Vaškevičius et al. 2017), slot PhC cavities (Caër et al. 2014; Yang et al. 2016), and PhC waveguides (Goyal and Pal 2015), which are fairly complex to fabricate in order to achieve high sensitivity. As a state-of-the-art sensor technology, PhC nanocavities can be nominated as a potential candidate for various optical sensing applications due to their unique properties such as long photon lifetime (high-Q), small mode volume, and low extinction loss (Yang et al. 2011; Kassa-Baghdouche 2019; Kassa-Baghdouche and Cassan 2020). As a typical structure type, a PhC cavity is formed by introducing point-defects in the orderly arranged lattices (i.e the defect is created by removing one or three holes in the center of triangular lattice PhC) (Kassa-Baghdouche and Cassan 2020). In the case of sensing applications, the strong electromagnetic field confinement in the defect region makes the resonant wavelength of the optical mode of the PhC nanocavity very sensitive to the variations of the RI of its surrounding medium. Such PhC nanocavities, the so-called point-defect PhC nanocavities, have been demonstrated to provide a quality factor that is a few orders of magnitude larger than the conventional PhC nanocavities (Kassa-Baghdouche et al. 2015a, b). Such an extraordinary quality factor capability has a profound impact on the light confinement. By locally controlling the confined fields in the defect region, a high sensitivity of optical response to the variation of RI in the air holes and the cladding could be achieved. As a result, a significant enhancement in the sensitivity of the PhC nanocavity-based gas sensors devices can be achieved. When a miniaturized gas sensor based on the point-defect PhC nanocavities is demonstrated in an SOI platform, a straightforward integration of the photonic sensors in the silicon photonics platform is achieved while providing compliant mechanical stability (Dong et al. 2017).

Therefore, the present paper describes the results of a simulation and theoretical calculations of our optimized point-defect PhC nanocavities based on the SOI platform. First, the proposed in-plane PhC nanocavities have been engineered using simulations for achieving a strong light confinement enhancement and thus to obtain a high-quality factor,  $Q$ , and a small mode volume,  $V$ . Next, the sensing characteristics of the optimized PhC nanocavity structures based on SOI have been studied by the combining the perturbation theory with the three-dimensional finite-difference time-domain (3D-FDTD) method. By fine-tuning the etch-depth of the air holes made into the substrate, we demonstrate strong light confinement and thus prove the successful design of the PhC nanocavities based on SOI exhibiting a high-quality factor and a small mode volume. On measuring the resonant wavelength shift of the point-defect PhC nanocavity sensor immersed in propane ( $C_3H_8$ ) gas, a sensitivity of 322 nm/RIU has been achieved, while the quality factor has been kept to be more than 3400 with a detection limit of  $10^{-3}$  refractive index unit (RIU). The size of the

sensing region of the proposed gas sensor is only  $36\ \mu\text{m} \times 16\ \mu\text{m}$ , making the high Q and high-sensitivity point defect PhC nanocavity sensor based on the SOI platform attractive for realizing on-chip sensor arrays.

## 2 Design methodology and theoretical modeling

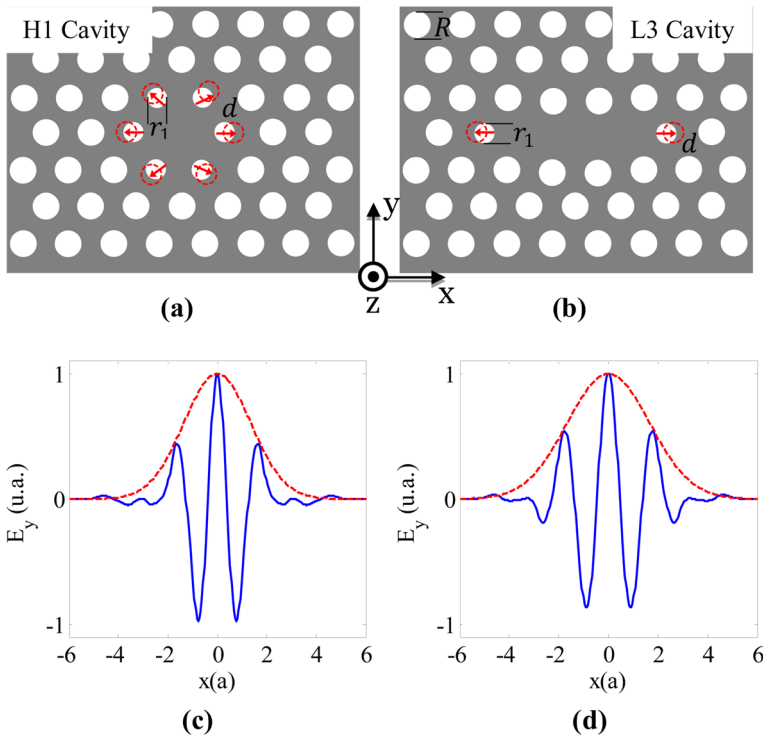
The mid-infrared (mid-IR) wavelength band, i.e., the band having a wavelength range of  $2 - 20\ \mu\text{m}$ , has been gaining importance in recent years for realizing mid-infrared devices (Dong et al. 2017; Hu et al. 2017; Lin et al. 2017). In fact, such a mid-IR band is an ideal wavelength range for realizing absorption-based photonic sensors, since the molecular fingerprints of many chemical species in their gaseous forms dropping in the mid-IR band (Dong et al. 2018; Chang et al. 2020). In this work, in order to select a proper geometry and material to build an effective silicon photonic gas sensor, SOI has been chosen since it has a high RI contrast between the silicon core and the cladding (air and  $\text{SiO}_2$ ). This high RI contrast allows the light to be efficiently confined in the nanocavity. The 3D schematic of the designed PhC-nanocavity-based gas sensor is shown in Fig. 1a. An SOI platform with a 500 nm thick Si device layer and a  $2\ \mu\text{m}$  thick silica buffer layer has been used in our work. The RIs of the silicon core and the silica buffer layer are 3.42 and 1.44, respectively. Taking advantage of the negligible RI variation of silicon in the mid-IR wavelength range, the proposed PhC nanocavity sensor has been designed to operate at a wavelength of  $3.7\ \mu\text{m}$ . In doing so, the period has been chosen to be  $a = 1060\ \text{nm}$ . The PhC sensor is coated with an air top layer. In order to explore the operational principle of the proposed sensor device, it is important to describe the crucial sections and geometrical parameters of the PhC sensor design. A schematic representation of the proposed sensor in the  $x$ - $y$  plane ( $z = 0$ ) is presented in Fig. 1b. The proposed structure consists of two different operating layers, namely, the monomode confining layer and the  $\text{SiO}_2$  layer. The monomode PhC confining layer includes a triangular lattice of circular air holes etched in silicon where a PhC nanocavity is created at the center of the PhC that allows light to be confined with small volume confinement. The  $\text{SiO}_2$  layer provides adequate optical isolation of the PhC



**Fig. 1** **a** Schematic showing the configuration of the point-defect planar PhC nanocavities suspended in a  $\text{SiO}_2$  substrate. Above the silicon membrane, there is a layer of air, while the bottom layer of the membrane consists of silica ( $\text{SiO}_2$ ). **b** Side view of the proposed PhC nanocavities

nanocavity core from the silicon substrate. In the designed PhC cavities based on the SOI platform, the air holes have an etch-depth,  $t$ , underneath the buried oxide layer.

The main concern of the paper was to design a PhC nanocavity that can potentially lead to a high-quality factor and low mode volume. Thus, two types of PhC nanocavities were formed by removing one (H1) or three (L3) air holes from the center of the PhC consisting of the triangular lattice of air holes. Such a defect supports an optical mode having a frequency located within the photonic bandgap. In the proposed PhC nanocavities, light is localized in three dimensions with small values of mode volume  $V$ . In fact, light is localized in the horizontal plane due to a distributed Bragg reflection, while it is localized in the vertical direction due to total internal reflection. The electric field profiles for the two types of PhC nanocavities, shown in Fig. 2b, follow a Gaussian distribution. This means that the optical mode of the PhC nanocavity is gently confined in the defect region, which plays a major role in increasing  $Q$ . Such point-defect nanocavities have a considerable potential for their use in realizing liquid and gas sensors (Kassa-Baghdouche 2019; Kassa-Baghdouche and Cassan 2020; Kassa-Baghdouche 2020). In fact, these types of PhC nanocavities based on the SOI platform support modes in certain wavelengths, and the confined beam encounters interactions with the gas samples inside the defect-region. This will result in a shift in the wavelengths of the transmitted light spectrum depending on the RIs of the samples. Point-defect PhC nanocavities based on the SOI platform can be fabricated using electron-beam (e-beam) lithography or deep ultraviolet (UV) lithography methods (Borel et al. 2004). Both methods allow defining



**Fig. 2** **a, b** Schematic structures of the H1 and L3 point-defect PhC nanocavities. **c, d** Normalized  $E_y$  profiles along the  $x$ -axis for H1 and L3 PhC nanocavity modes

the hole patterns in a resist spun on top of the SOI wafer (Borel et al. 2004). Furthermore, the major advantage of deep UV lithography is its inherent capability for mass fabrication of PhC structures, while the major advantage of e-beam lithography is that it allows fabrication of holes of special shapes and sizes, even down to very small feature sizes (Borel et al. 2004). Using the e-beam resist as a mask, the written patterns were transferred to the Si layer by reactive ion etching

The point-defect PhC nanocavities have an important parameter, namely, the lateral displacement,  $d$ , that can be tuned to change the condition for confinement (see Fig. 2a). For H1 PhC nanocavity,  $d$  is optimized because it creates the space to confine light. On the other hand, in the L3 PhC nanocavities,  $d$  defines the confined field envelope in the cavity without a significant shift of the confined wavelength (Kassa-Baghdouche et al. 2014, 2015a, b, c). Therefore, in this work, in order to design PhC nanocavities with a high Q and small V, by minimizing the propagation losses and thus reducing the unwanted reflection due to mismatch, we have carried out a geometrical optimization of the proposed nanocavities. We follow a step-by-step approach, as shown in Fig. 2a, to reach the final design that achieves strong light confinement and localization in the nanocavity. The geometry of the studied PhC nanocavities is adjusted by reducing the radius of the air holes nearest to the defect region and then by laterally displacing these air holes by an amount  $d$  in the outward direction (Kassa-Baghdouche et al. 2014, 2015a, b, c). In each step, the values of Q, V, and the resonant wavelength,  $\lambda_c$ , of the fundamental transverse-electric (TE) mode of the PhC nanocavities are calculated by employing the 3D-FDTD algorithm using MEEP software (Oskooi et al. 2010). The resonance wavelength and quality factor of the proposed PhC nanocavities are calculated by employing the “*harminv*” software, which employs the filter diagonalization method to extract the decay patterns in time-series data (Mandelstam and Taylor 1997). For the optimum values of the displacement  $d$  nearest to the defect region, the corresponding values of Q, volume, and  $\lambda_c$  are given in Table 1. From the results, it can be seen that there is a significant enhancement in the quality factor of the cavity’s resonant mode, of the order of  $10^3$ , for the H1 and L3 nanocavities based on the SOI platform. Further, the optimized PhC nanocavities have a high Q/V value of the order of  $10^3$ . Consequently, a strong light-matter interaction can be achieved which indicates that the optimized PhC nanocavity design can be used for enhancing the sensitivity of the gas sensors. The optimized PhC nanocavities have a relatively smaller mode volume of  $0.55 (\lambda/n)^3$ , which indicates a stronger light localization. Thus, the designed nanocavities are relatively compact in size ( $36 \mu\text{m}$  (length)  $\times$   $16 \mu\text{m}$  (width) and  $3 \mu\text{m}$  high).

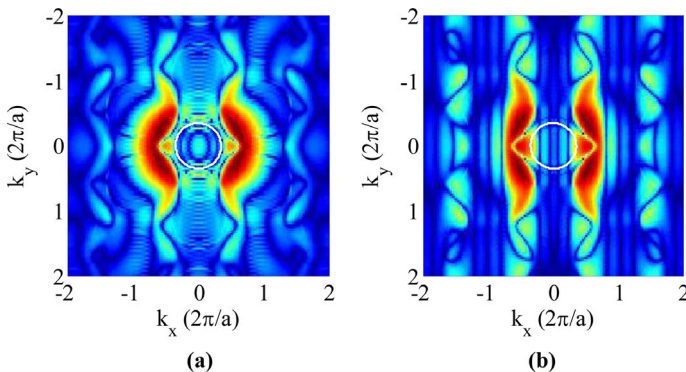
In the designed PhC nanocavities based on the SOI platform, the in-plane confinement of the optical mode is controlled by the distributed Bragg reflection of the surrounding photonic lattice, while the vertical confinement is due to the standard wave guiding by total internal reflection. Specifically, when the magnitude of the in-plane momentum component,  $k_{\perp}$ , is inappropriate to support guiding a vertical radiation loss occurs. In the proposed PhC nanocavities,  $k_{\perp}$  defines a cone in  $(k_x, k_y, \omega)$  space, commonly referred to as the “*light cone*”. Modes that radiate vertically will have small in-plane momentum components that lie within the light cone of the cladding. This simple rule serves as our fundamental guideline in designing the point-defect PhC nanocavities

**Table 1** The optimum values of Q, V, Q/V, and  $\lambda_c$  of the optimized PhC nanocavities

Type of cavity	Q	V $(\lambda/n)^3$	Q/V $(\lambda/n)^{-3}$	$\lambda_c$ ( $\mu\text{m}$ )
H1 PhC cavity	$2 \times 10^3$	0.556	$3.6 \times 10^3$	3.77
L3 PhC cavity	$1.7 \times 10^3$	0.987	$1.7 \times 10^3$	3.78

based on the SOI platform that limit vertical radiation loss. In particular, we seek out structures that support the resonant modes whose in-plane momentum components are primarily situated outside the cladding light cone. The Fourier transform decomposes the  $y$  component of the electric field,  $E_y$ , into a set of wave-vector components of a plane wave and allows analyzing the leaky wave-vector components in the light cone. In other words, this spatial change redistributes the field components in the momentum space ( $k$ -space) after the Fourier transform and the right amount lightens the field components inside the light cone ( $k < 2\pi/\lambda$ ) liable for out-of-plane radiation losses, thus enhancing the photon lifetime inside the cavity (Srinivasan and Painter 2002). The spatial Fourier transform of  $E_y$  of the fundamental mode of the designed PhC nanocavities as a function of real space coordinates of the cavity is plotted in Fig. 3. It is evident from this figure that the spatial Fourier transform of  $E_y$  exhibits an odd symmetry in the  $x$ -direction, which leads to a negligible portion inside the radiation light cone. As indicated by the white circles, there are little wave-vector components inside the light cone. This is due to a reduction in the energy losses or leaky modes that couple to the continuum of the radiation modes in the light cone. In fact, in our nanocavity design, by reducing the radius of the first nearest-neighbor air holes and displacing their position, a high  $Q$  of the order of  $10^3$  is obtained as compared to that obtained for non-optimized PhC nanocavities. This indicates that the enhanced value of  $Q$  during the optimization process results not only from a smoother field profile, but also from a more confined field which is essential for enhancing the light-matter interaction and for designing a high sensitivity gas sensor. As a result, this design process, based on the 3D-FDTD simulations, was important because we started by designing optimized PhC nanocavities with a high  $Q/V$  value.

For sensing applications, it is important to note that the designed PhC-nanocavity-structure device responds to the local variations in RI in the area of the individual sensor. Therefore, the magnitude of the resonant wavelength shift,  $\Delta\lambda$ , will depend on the effective change in the RI of the gas targets. In this work, the gas sensing mechanism has been used for monitoring  $\Delta\lambda$  on account of the analyte-induced RI variations in the near-field of the PhC nanocavity. According to the perturbation theory (Joannopoulos et al. 2008),  $\Delta\lambda$  generated by a small index perturbation,  $\Delta n$ , of the surrounding gas analytes can be approximated as:



**Fig. 3**  $E_y$  field distribution in the Fourier space for the designed, **a** H1 PhC nanocavity and **b** L3 PhC nanocavity based on the SOI platform with the optimal displacement,  $d$ , of the single air holes

$$\frac{\Delta\lambda}{\lambda_o} \approx \frac{\Delta n}{n_o} \frac{\int_{V_{Gas}} \epsilon(\mathbf{r})|\mathbf{E}(\mathbf{r})|^2 d^3(\mathbf{r})}{\int_{V_{Total}} \epsilon(\mathbf{r})|\mathbf{E}(\mathbf{r})|^2 d^3(\mathbf{r})} = \frac{\Delta n}{n_o} \Gamma_{Gas} \tag{1}$$

where  $\Gamma_{Gas}$  is the ratio between the electric field energy in a volume  $V_{Gas}$  of the gas and the total electric field energy in the cavity volume  $V_{total}$ . It describes the filling factor of the electric field energy stored in the surrounding gas analytes and is essential for assessing the sensing characteristics of PhC nanocavities when immersed in a gas analyte.

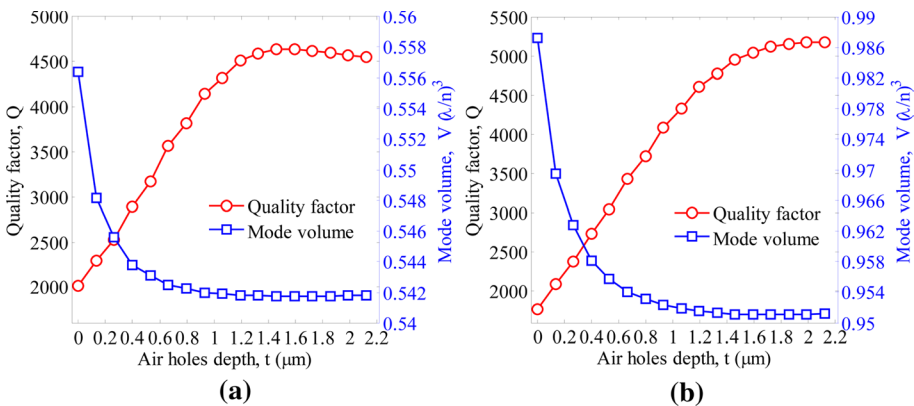
In order to analyze the sensing characteristics of the proposed PhC nanocavities immersed in a gas with a small variation in the RI (the RI of the gas is of the order of  $10^{-3}$ ), the sensitivities should be defined. Therefore, the sensitivity,  $S_\lambda$ , is defined as the ratio of  $\Delta\lambda$  in the cavity to the change in RI,  $\Delta n$ :

$$S_\lambda \approx \frac{\Delta\lambda}{\Delta n} = \frac{\lambda_c}{n_o} \Gamma_{Gas} \tag{2}$$

From Eq. 2, it can be clearly understood that a smaller cavity V and a stronger light confinement in the perturbed region can lead to a larger  $\Delta\lambda$ , thus resulting in a higher sensitivity. To achieve high sensitivity, the optical mode of the PhC nanocavity should be distributed more into the target analytes. Therefore, the optimized PhC nanocavities are preferred for the realization of high-performance gas sensors due to their strong light-matter interaction between the optical fields and the analytes.

### 3 Dependence of the optical properties on the etch-depth

In the proposed PhC nanocavities based SOI platform, the etch-depth of the air holes in the oxide layer is an important parameter. Thus, in this section, we investigate the influence of the etch-depth,  $t$ , on the optical mode properties of the PhC nanocavities. Here, the etch-depth has been varied from 0 to 2.2  $\mu\text{m}$  and the optical properties of the proposed PhC nanocavities have been calculated for different values of this parameter.



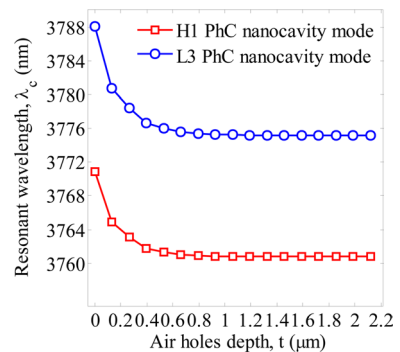
**Fig. 4** Plot showing the variation of the quality factor,  $Q$ , and the mode volume,  $V$ , of the fundamental resonant mode in the **a** H1 PhC nanocavity and **b** L3 PhC nanocavity based on the SOI platform, as a function of the etch-depth,  $t$  (in  $\mu\text{m}$ )

Figure 4 shows the dependence of  $Q$  on the value of  $t$ . The value of  $V$  corresponding to each value of  $Q$  has also been shown in the figure. From the figure, it can be seen that for the two types of PhC nanocavities, as the etch-depth of the air holes increases, the quality factor (red circle) increases exponentially initially with increasing etch-depth, owing to the strengthened optical confinement by the increased PhC mirror periods, until it finally levels off when the etch-depth is greater than  $1.4 \mu\text{m}$ . Since the lower etch-depth, in turn, narrows the photonic band gap and decreases the in-plane as well as vertical confinement of light, as the etch-depth of the air holes increases from  $1.4$  to  $2.2 \mu\text{m}$ , the optical confinement by total internal reflection becomes stronger and the quality factor increases significantly. The optimum mode confinement and, thus, a maximum quality factor of  $4600$  and  $5170$  would be expected for H1 and L3 PhC nanocavities, respectively.

The mode volume of the proposed PhC nanocavities also exhibits a strong variation when the etch-depth of the air holes is changed. From Fig. 4, we notice that  $V$  of the nanocavity modes decreases exponentially with increasing  $t$  until it finally levels off when  $t$  is greater than  $1.4 \mu\text{m}$ . Hence, the mode volume can be decreased by adjusting this parameter, and a small mode volume of the order  $0.542 (\lambda/n)^3$  and  $0.951 (\lambda/n)^3$  could be obtained for H1 and L3 PhC nanocavities, respectively. Therefore, an important property of a PhC nanocavity based on the SOI platform is that it is sensitive to the etch-depth of the air holes. Since the aim of this work is to analyze the gas sensing performance of the high- $Q$  PhC nanocavities based on the SOI platform, in the next section we will study the gas sensing characteristics of the nanocavities for different values of the etch-depth of the air holes.

Further, we investigate the effect of the etch-depth of air holes on the resonant wavelength ( $\lambda_c$ ) of the proposed PhC nanocavities modes. From Fig. 5, it can be seen that the resonant wavelength of the PhC nanocavities based on the SOI platform is indeed independent of the etch-depth. The value of  $\lambda_c$  decreases with increasing  $t$  until it finally levels off when  $t$  is greater than  $0.4 \mu\text{m}$ . As follows from this figure, the shift in the resonant mode is kept constant with  $t$ . Despite the optimum mode confinement, which implies that a maximum  $Q$  is expected for each cavity mode lying close to the band gap wavelength of the structure, these cavity modes exhibit a maximum  $Q$  at the resonant wavelengths of  $3.76\text{--}3.77 \mu\text{m}$  for H1 and L3 PhC cavity, respectively.

**Fig. 5** Plot showing the variation of the resonant wavelength,  $\lambda_c$ , of the fundamental resonant mode in the **a** H1 PhC nanocavity and **b** L3 PhC nanocavity based on the SOI platform, as a function of the etch-depth of air holes,  $t$  (in  $\mu\text{m}$ )



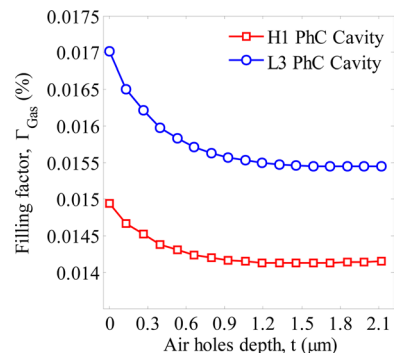


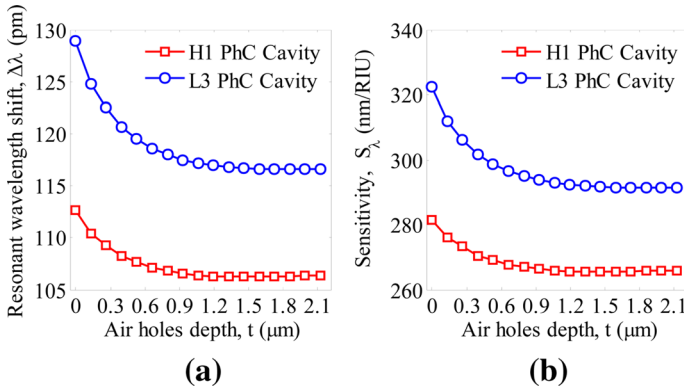
#### 4 Gas sensing performance for the designed structures

Recently, gas concentration measurement has played an important role in many industrial, biomedical and environmental applications (Clerbaux et al. 2003). Thus, in this work, the gas sensing characteristics of the designed PhC nanocavities, which have the capability of confining light according to its wavelengths, has been studied extensively to develop high-sensitivity miniaturized optical gas sensor. Such PhC nanocavities based on the SOI platform can be used for measuring and implementing a high-precision, low-power, and portable detection of low concentration of a gas with fast analysis time and reduced reagent consumption. In order to analyze the sensing characteristics of these nanocavities, it is necessary to scan the cavity's geometrical parameters. Thus, we first investigated the influence of the etch-depth of the air holes on the filling factor,  $\Gamma_{Gas}$ . As can be seen from Fig. 6, the filling factor decreases slowly with the increasing the etch-depth. In addition, it is nearly invariant under different etch-depth of the circular air holes; even when  $t$  is as high as  $1.0 \mu\text{m}$ ,  $\Gamma_{Gas}$  is still as high as 0.015% for the proposed H1 and L3 PhC nanocavities. The variation in the filling factor of the PhC nanocavities with the etch-depth can be explained by the profile of the electric field of the fundamental mode (see Fig. 2b). The electric field,  $E_y$ , is mainly confined in the central region of the nanocavity (defect region) and decays rapidly near its edge, resulting in a very small light confinement in the perturbed region. Therefore, the etch-depth has nearly no influence on the filling factor and can lead to a smaller wavelength shift, resulting in a lower sensitivity.

Next, we measure the resonant wavelength shift  $\Delta\lambda$  of the PhC nanocavity modes when it is immersed in a gas analyte. For the majority of the optical gas sensors, the common gases having RI slightly larger than 1, such as propane, are utilized for investigating optical gas sensing. Since the RIs of the gases generally depend on the concentration, temperature, and pressure, in this work, the changes in the RI of the detected gas is assumed to be of the order of  $10^{-3}$ . By changing the RI of the surrounding gas (the air holes and the top cladding of the PhC nanocavities), the variation of the resonant wavelength shift ( $\Delta\lambda$ ) of the fundamental mode of the proposed PhC nanocavities with the etch-depth are calculated and the results thus obtained are shown in Fig. 7a. As anticipated, the resonant wavelength shift indeed decreases with the increasing etch-depth of the circular air holes. The etching of the circular air holes in the  $\text{SiO}_2$  layer has no influence on the  $\Delta\lambda$  of the fundamental mode of the PhC nanocavities based on the SOI platform. Consequently, the resonant wavelength of the nanocavities does not change significantly when it is immersed in a gas, the RI of which varies from 1.000 to 1.001. While detecting the propane gas, a variation in

**Fig. 6** Plot showing the variation of the filling factor,  $\Gamma_{Gas}$ , as a function of the etch-depth of the air holes,  $t$ , for the two types of point-defect PhC nanocavities





**Fig. 7** Plot showing the variation of the resonant wavelength shift,  $\Delta\lambda$ , and the sensitivity,  $S_\lambda$ , for the **a** H1 PhC nanocavity and **b** L3 PhC nanocavity based on the SOI platform, as a function of the etch-depth of the circular air holes,  $t$  (in  $\mu\text{m}$ )

the refractive index in the surrounding medium induces a larger resonant wavelength shift of the L3 PhC nanocavity mode than that observed in the case of the H1 PhC nanocavity. In fact, a resonance wavelength shift of 282 pm and 322 pm, are induced for H1 and L3 PhC nanocavities respectively.

The sensitivity of the optimized PhC nanocavities based on SOI platform can be calculated using Eq. (2). As can be seen from Fig. 7b, while detecting the propane gas, the measuring sensitivity curves for the PhC nanocavity modes with the etch-depth exhibit the same variation as that observed for the resonant wavelength shift. The corresponding resonant wavelength, mode volume, sensitivity, quality factor, and detection limit for the optimized PhC nanocavities are summarized in Table 2. The sensitivity values of the L3 PhC nanocavity remain slightly higher as compared to those obtained with an H1 single defect introduced at the center of the PhC, and the detection limit for the optimized PhC nanocavities based on SOI platform is the order of  $10^{-3}$ . The higher values of the sensitivity of the proposed PhC nanocavities can be explained to be due to the strong light-matter interaction between the optical fields and the gas analytes. Further, for the two types of PhC nanocavities, the mode volume is lower due to the geometry of the PhC nanocavities, where the confined optical mode is strongly confined in the defect region created in silicon core, which has a high RI material. The quality factor of the PhC nanocavities generally remains high ( $Q$  greater than  $10^3$ ), which also testifies to the absence of a large number of field components in the cone of light. This is because the confinement of the optical mode in the silicon layer is large, and the optical mode of the PhC nanocavity is distributed more into the target analytes. These results indicate that the optimized PhC nanocavities based

**Table 2** Optimum values of  $Q$ ,  $V$ ,  $S_\lambda$ , DL, and  $\lambda_c$  for the designed point-defect PhC nanocavities based on the SOI platform

Type of cavity	$Q$	$V (\lambda/n)^3$	$S_\lambda$ (nm/RIU)	DL (RIU)	$\lambda_c$ ( $\mu\text{m}$ )
H1 PhC cavity	2900	0.543	282	$4.6 \times 10^{-3}$	3.76
L3 PhC cavity	3400	0.954	322	$3.4 \times 10^{-3}$	3.77

on SOI platform can be used for realizing miniaturized integrated gas sensors having high sensitivity.

It should be mentioned here that a few other sensing devices based on slotted and point-defect PhC cavities based on the SOI platform have been reported in the literature. For example, in Caër et al. (2014) proposed a slotted PhC cavity in a non-free standing membrane configuration and demonstrated the device exhibiting a sensitivity of 235 nm/RIU, a high value of  $Q$  of 25,000, and a detection limit of  $1.25 \times 10^{-5}$  RIU. Yang et al. (2016) proposed an  $\alpha$ -H0-slot PhC microcavity and demonstrated the device exhibiting a sensitivity of 200 nm/RIU and  $Q$  of  $10^4$ . In addition, Yang et al. (2011) also proposed an H0-nanocavity PhC cavity operating in the wavelength range of 1.4 to 1.6  $\mu\text{m}$  and demonstrated the device exhibiting a sensitivity of 31.90 nm/V. Zhou et al. (2014) proposed the integration of H2 PhC nanocavity and broadband W1 waveguide, which demonstrated a sensitivity of 131.70 nm/RIU and a detection limit of approximately  $3.797 \times 10^{-6}$  RIU. Chakravarty et al. (2014) proposed L13 PhC microcavities with nanoholes and demonstrated the device exhibiting a sensitivity of 112 nm/RIU and a detection limit below  $1 \times 10^{-7}$  RIU. However, both these devices work at the telecommunication wavelength. As compared to the above-mentioned sensing devices, our designed point-defect PhC nanocavities have a small mode volume and a very small sensing area, such that very small amounts of gas analytes will shift the resonant wavelength of the nanocavities, thus exhibiting a very high sensitivity. This is of huge importance when we want to detect very small analytes, such as propane gas targets with quality factors greater than  $10^3$ .

We believe that the results of this work will be valuable for understanding the influence of the design parameters on the optical properties of the PhC nanocavities based on the SOI platform, and for designing highly sensitive, robust, and PhC gas sensors capable of a large range of measurement. Furthermore, our designed PhC nanocavities can be readily integrated into optical chips that are compatible with the well-established CMOS technology and have high compatibility with external waveguides. Considering the above mentioned advantages, these optimized PhC nanocavities based SOI platform can be used in a variety of sensor applications. The experimental realization of the optimized PhC nanocavities structure is generally technically achievable with classical nanofabrication techniques, such as electron-beam lithography followed by reactive ion etching (Borel et al. 2004). However, since the circular air holes can be etched only up to a certain depth in the  $\text{SiO}_2$  layer, the major fabrication challenge for the realization of the designed PhC-nanocavity-based gas sensor device is that its realistic implementations are prone to nonidealities, including distortions to the shape or position of the holes which can be introduced in the fabrication process. Nevertheless, in order to fabricate structures with dimensions very close to the designed values, further optimization of the fabrication process is required.

## 5 Conclusions

In conclusion, we have proposed and theoretically analyzed point-defect PhC nanocavities based on the SOI platform that is used for refractive index sensing in a gaseous environment. By increasing the etch-depth of the circular air holes in the buried oxide layer, the quality factor of the proposed PhC nanocavities has been found to increase and still remains as high as  $10^3$  with a highly concentrated field in the defect region with an ultra-small mode volume. In addition, for sensing purposes, a RI based gas sensing mechanism has been used, which is based on the measurement of the resonant wavelength shift corresponding

to the RI of the propane gas analytes. The results obtained from this work show that the proposed PhC nanocavities simultaneously possess a high-quality factor of  $10^3$  and a sensitivity of 322 nm/RIU at a resonant wavelength near 3.7  $\mu\text{m}$ . All these factors suggest the potential use of the proposed PhC nanocavities based on the SOI platform for gas sensing applications. Furthermore, owing to the simplistic, high-quality factor, high sensitivity, and lower detection limit of the designed PhC nanocavities, we believe that the results reported in this paper are important steps on the path to developing on-chip devices for applications in gas detection.

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