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Design and modeling of nanophotonic beam structures as optical NEMS sensors

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ABSTRACT

Silicon photonic crystal (PhC) waveguide based resonator is designed by introducing a micro-cavity within the line defect so as to form the resonant band gap structure for PhC. Free-standing silicon beam comprising this nanophotonic resonator structure is investigated. The output resonant wavelength is sensitive to the shape of air holes and defect length of the micro-cavity. The resonant wavelength shift in the output spectrum is a function of force loading at the center of a suspended beam with PhC waveguide resonator. The sensing capability of this new nanomechanical sensor is derived as that vertical deformation is about 20nm at center and the smallest strain is 0.005% for defect length.

Keywords: Nanophotonics, MEMS, NEMS, Sensor

1. INTRODUCTION

In recent years, nanometer scale photonic crystals (PhCs) are attractive optical structures for controlling and manipulating the flow of light. Various devices such as smaller optical waveguides, microscopic optical cavities and the photonic bandgap structures, open up various possibilities for novel photonic devices. The two-dimensional (2-D) silicon based PhCs typically comprise a group of air holes and the local electromagnetic field is modified by surface state of air holes. W. Suh et al., has proposed a new displacement sensing mechanism based on due to photon tunneling and Fano interference in two slabs of PhC. Transmission contrast of 20-dB is obtained regarding to a distance change between the two PhC slabs for about 1% of operating wavelength [1, 2]. O. Levy et al. have proposed a novel displacement sensor comprising two planar photonic crystal waveguides (PhCWGs) aligned along the same axis of light propagation. The output light intensity is strongly dependent on the alignment accuracy, i.e., the coupling efficiency between input and output PhCWGs. Any deformation of structure, i.e., considering as displacement, will lead to misalignment so as to reduce the output light intensity. They provided simulation results to prove this device concept [3]. Based on a similar concept of two PhCWGs where one in stationary and the other is movable, Z. Xu et al., placed air hole on both sides of PhCWGs and created an optical resonator structure with Q-factor of 40. The resulted intensity reduction in output port is in linear proportion to the longitudinal displacement between PhCWGs [4]. The above results shows that silicon 2-D PhCWG is a very attractive sensing platform for displacement measurement. Moreover, O. L. J. Pursiainen et al., created a flexible three-dimensional (3-D) PhC by using a self-assembly fabrication process. This flexible 3-D PhC contains multi-shelled polymer spheres of high-refractive-index and absorbing materials filled in the interstitial space surrounding said spheres. The dimension of this device is a 1-cm wide strip film. This device was placed on top of a sample holder and was uniformly stretched in micrometer scale while the optical property is measured in situ. They demonstrated a result of 50% reduction of transmission intensity at only 1% strain that is corresponding to about 5nm wavelength shift of the resonant peak in the reflection spectrum [5]. However, good discrimination of resonant wavelength shift regarding to 1% strain may not be easily due to very low quality factor of the resonant wavelength peak. Recently I. EI-Kady et al., proposed a new device concept of detecting submicron crack of substrates based on using a 3-D PhC structure as the physical sensor. It reported that a PhC sensor was attached on a polymer substrate. According to the simulated results derived by using the FDTD (finite difference time domain) approach, this PhC sensor experienced changes in its band gap profile when micro-damage is induced in said substrate [6].

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Interestingly either the intensity reduction of output peak or resonant wavelength shift has been deployed as the sensing scheme for PhC based physical sensors, i.e., displacement and strain sensors. Thus we measure the change in optical signals and correlate such changes with physical parameters, like, displacements and strains. For instance, 1% strain represents about 1nm–5nm deformation in hole diameter for silicon 2-D PhCs devices. Since the typical size of point defects, i.e., air holes, in silicon PhC is about 100–450nm. It implies silicon PhC based physical sensors should exhibit outstanding performance intrinsically. It’s worthwhile to mention that movable suspended silicon waveguides of 1μm have been applied to modify the resonator characteristics of a microtoroidal structure [7]. It’s an example of deploying MEMS (Microelectromechanical Systems) technology for enabling tunable nano/micro photonics.

In this paper, we proposed a free-standing bridge beam structure comprising PhCWG for strain and force sensing, where a beam structure is a common mechanical structure used in MEMS based physical sensors. Thus we apply the resonator characteristics of PhCWG for sensing strain and loaded force. This a new concept of nanomechanical sensor based on using the nature of silicon PhCWG. It may open a new window for a new research field of optical nano-electromechanical systems (NEMS).

2. DESIGN OF PHOTONIC CRYSTAL RESONATORS

The term of PhC means a subclass of materials where a periodic modulation of the refractive index (RI) exists for a given material. PhCs may possess a photonic band gap (PBG) upon the exact periodic modulation. Thus, a given bandwidth of light cannot be transmitted through such material. A PhCWG is considered as a planar PhC with a line defect in the periodic structure, where a line defect is considered as a silicon waveguide typically [8]. The basic property of a PhCWG is that a given bandwidth of light can be guided in the silicon waveguide as the light is confined laterally by the PhC and vertically by total internal reflection (TIR), in which it is similar to conventional waveguide structures. On the other hand, four air holes, i.e., a sort of point defects, have been introduced at the center of said silicon waveguide of PhCWG to form a resonator structure. It is reported that two of high-Q resonances centered at wavelengths 3.621 and 3.843 μm. The quality factors of these two resonant wavelength peaks were measured as 640 and 190, respectively [9]. V. Sandoghdar et al. have applied scanning near-field optical microscopy (SNOM) to visualize the optical intensity topography around these four air holes of this microresonator structure. The peak intensity of resonance shown at 3.84μm has been observed [10]. These evidences point out that silicon PhCWG with four air holes along the embedded silicon waveguide is a good design of optical resonator. In our proposed device configuration, we deploy this 4-holes based microresonator structure as our fundamental design, as shown in Fig. 1. The configuration of PhCWG is a hexagonal array of air holes in a silicon substrate with lattice constant, a, and all holes in the structure with the same radius of r. A linear waveguide is created by removing a column of air holes among the hexagonally arranged holes patterns. We insert one pair of 2 air holes into the linear waveguide as two reflectors, i.e., 4 holes in total. Thus a point defect is defined between the two reflectors to form a micro-cavity. The width of the micro-cavities is defined as the defect length, i.e., L_d, the spacing between the pair of two holes as shown in Fig. 1. The length and width of this PhCWG are 1 = 6.4 μm and w = 4.8 μm. By performing the planewave expansion method, we can obtain the normalized frequency of the photonic band gap for the TE mode exists between 0.28 and 0.32. The corresponding band gap in wavelength is between 1563 and 1786 nm. The 2-D finite-difference time-domain (FDTD) method is performed to simulate the propagation of the electromagnetic waves in the waveguides. The lithography and etching based CMOS fabrication technology have been reported to be good at making PhC structure from a SOI (silicon-on-insulator) wafer [11]. A silicon SOI substrate with device layer of 200nm and SiO2 insulation layer of 1μm is selected as the basic device configuration first. We conduct the simulation throughout the whole study upon this assumption. In contrast to the case of that the layout dimensions used in Refs. [9, 10], i.e., designing for resonant wavelengths in far infrared region, we optimize our PhCWG designs to enable the output resonant wavelength peaks appeared in the wavelength range of 1450nm to 1620nm, i.e., the near infrared region. The common optical spectrum analyzer (OSA) used in optical communication industry can give us down to 0.1nm resolution of measuring resonant wavelength within this region.

As we highlighted in previous paragraphs, the resonant wavelength of PhCWG is strongly affected by surface state of holes. For the SOI wafer with the air holes, there are three regions in consideration for the calculation of the effective refractive index, viz. air above the wafer (n_1), silicon device layer (n_2) and underlying silicon oxide layer (n_3). The respective refractive indices are n_1 = 1.0, n_2 = 3.46 and n_3 = 1.48. K. Kawano and T. Kitoh have described a way of calculating effective refractive index [12]. Solving for the principal electromagnetic fields in the y-direction and applying appropriate boundary conditions at interface of silicon and SiO2, the effective refractive index (n-eff) was calculated to

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be 2.74 for silicon device layer thickness of t = 200 nm. As the defect length, $A_d$, depicted in Fig. 1, we may explore different PhCWG resonator configurations in terms of the micro-cavities with various $A_d$. Fig. 2 shows the simulated output spectrums for these devices. Additionally, the Q-factor of resonant peak of $A_d = 2a-2r$ (Fig. 2a) and $A_d = 4a-2r$ (Fig. 2f) is calculated as 832 and 936, respectively, while the Q-factor of resonant peak of $A_d = 2.4a-2r$ (Fig. 2b) and $A_d = 3.6a-2r$ (Fig. 2e) is calculated as 66 and 98, respectively. Besides, the intensity of resonant peak of devices of $A_d = 2a-2r$ (Fig. 2a) is much larger than the one derived for $A_d = 4a-2r$ (Fig. 2f). By comparing these data, apparently we can conclude that PhCWG device with $A_d = 2a-2r$ is the best design as a PhCWG resonator. On the other hand, we may derive the output resonant wavelength peaks for hole-radii changing from 150 nm to 185 nm regarding to the same lattice constant, a, of 500 nm in Fig. 3. It is observed that the resonant wavelength shifts toward shorter wavelength as the radius increasing.

Fig. 1 Layout drawing of PhCWG using hexagonal array of holes, with lattice constant, a, $A_d$ is the distance between two holes in the center of micro-cavity (defect length), and r is the radius of the cavity. Pulsed light is launched from the left (arrow) and the output is measured at the right (time monitor).

Fig. 2 The output spectrums of PhCWG resonator devices with various defect length of microcavity, where the defect length, $A_d$, is 2.0a-2r for (a), 2.4a-2r for (b), 2.8a-2r for (c), 3.2a-2r for (d), 3.6a-2r for (e), and 4.0a-2r for (f), where the a=450nm and r=140nm are used in the above simulation.
The refractive index of silicon is known to be sensitive to ambient temperature. We need to look into the temperature dependence of PhCWG resonator characteristics. To characterize the resonant wavelength shift corresponding to the temperature drift, we need to study two major effects. First of all, the change in defect length due to volume expansion attributed to increased temperature should be characterized. By using FEM approach, we derived the volume change of radius and defect length first. The resulted shift in resonant wavelength is simulated as +/-0.05nm for 25°C +/- 10°C. Secondly the refractive index of silicon at various temperatures deviated from room temperature, i.e., 25°C, can be calculated by using the approach reported by J. A. McCaulley et al., [13]. The calculated refractive index change of silicon is shown in Fig. 4. The resulted resonant wavelength peaks derived by using the refractive index of silicon discussed in Fig. 4 are shown in Fig. 5. Thus the shift in resonant wavelength is calculated as +/-0.95nm for 25°C +/-10°C, +/-0.43nm for 25°C +/- 5°C and +/-0.12nm for 25°C +/- 1°C. It means we have to include the temperature effect.
on the change of silicon refractive index into our design now. It implies that we need to deploy a temperature stabilizer, eg. thermoelectric-cooler, to maintain the PhCWG resonator at an ambient temperature with temperature drift less than +/- 1°C. Thus the resolution of PhCWG resonator based sensors can be maintain at 0.1nm wavelength shift level without considering the background noise contributed by temperature drift.

Fig. 5. Calculated resonant wavelength peaks versus different silicon refractive index at various ambient temperatures from 15°C up to 35°C.

3. MODELING AND OPTIMIZATION OF NEMS SENSORS

In order to apply the PhCWG to creating a MEMS/NEMS structure which is sensitive to deformation or deflection under an applied force, we proposed a suspended bridge beam with PhCWG along the center as shown in Fig. 6(a) and (b). Regarding to the fabrication process, the PhCWG structure is defined by deep UV photolithography and front side silicon DRIE (deep reactive ion etching) technique first. In the case of making such a suspended silicon PhCWG beam, we can use the front-side KOH based bulk silicon micromaching. This approach will under cut the bulk silicon from the substrate surface and release the PhCWG beam structure. Dimensions of this suspended PhCWG bridge beam are as follows: length of 20 µm, width of 5 µm, and thickness of 200 nm, while the PhCWG resonator with lattice constant, a, of 500 nm, radius, r, of 180 nm and defect length, A_d, of 640 nm is used in the following simulation. To successfully release the beam with width of 5 µm, under-cut of 3 µm at both ends of silicon substrate is typically required. Thus we need to include 3 µm of under-cut at both sides of silicon substrate at end of bridge. It means that the actual deformable length is taken as 26 µm along the longitudinal direction of the suspended beam. Thus we will have a suspended bridge beam comprising PhCWG structure as illustrated in Fig. 6 (b) eventually. As we mentioned that the effective refractive index is highly sensitive to the thickness of device layer and the surface state as well, we need to calculate effective refractive index (n-eff) for suspended silicon beam in which it is considered as “air-Si-air” configuration instead of “air-Si-SiO_2” configuration in conventional silicon waveguide case, i.e., discussed in previous section. The derived effective refractive index is 2.6916. It has been observed that such a decrement in the effective refractive index leads to shift in the resonant wavelength toward shorter wavelength region. For example, in the design of a = 500 nm and r = 180 nm, the resonant wavelength is shifted from 1553.3 nm to 1529.4 nm for the PhCWG beam structure changing from configuration of “air-Si-SiO_2” to configuration of “air-Si-air”, respectively.
In addition to the lattice constant $a$, hole radius $r$, effective refractive index, number of air holes to form the two reflectors, and the defect length $A_d$ are also critical to the resonant wavelength and $Q$ factor of resonant peak. Moreover, we need to consider the influence contributed by the displacement and deformation of the these holes along $x$ and $y$ directions and elongation of the PhCWG in $x$ and $y$ directions, when said suspended PhCWG beam structure is under deformation due to externally applied force. In other words, for the operation of this nanomechanical sensor as either a strain sensor or a force sensor, it is important that changes of such physical parameters have to be taken into account upon applied force. Thus we conduct the FEM (finite element method) simulation by using a commercial software, i.e., CoventorWare [14]. In fact the PhCWG bridge beam as shown in Fig. 6 (b) was built by using this tool and optimized in terms of deformation sensitivity for being a strain sensor or a force sensor.

Assuming there is no change in $r_x$ and $r_y$, i.e., the radius along the $x$ and $y$ directions, it was noted that 0.2 nm increase in the defect length will lead a 0.14 nm increment in the resonant wavelength. However, a 1 nm elongation or displacement of these 4 holes in the $y$-direction individually, i.e., no change in $A_d$ and $r_x$ at this time, will not introduce any observed resonant wavelength shift. In contrast to cases of elongation or displacement happened along $y$-direction, a 1 nm elongation of these 4 holes along the $x$-direction (eg. $r_x' = r_x + 0.5$ nm) leads a resonant wavelength shift of 0.93 nm toward short wavelength region. It was concluded from this study that a change in the defect length coupled with an elongation and/or deformation in the $x$-direction would be the most sensitive parameters to resonant wavelength shift. As a result, to make the PhCWG device sensitive to change of strain or applied force, it would be necessary to design and layout the PhCWG along a direction such that the device would experience the force along the $x$-direction as much as possible. Apparently we need to check the strain distribution along $x$-direction of this suspended beam structure first.

In the FEM simulation, we apply constant pressure loads of 1 to 5 MPa in which it is calculated as 0.7 to 4 $\mu$N regarding to a loading area of 500 nm in diameter, i.e., $7.85 \times 10^{13}$ $\text{m}^2$ at the center of suspended beam in the $z$-direction (into the plane of the beam). The resulted displacement of this beam along $x$-direction with respect to pressure load of 1.0 MPa, eg. calculated as 0.785 $\mu$N, is shown in Fig. 7. As we mentioned in previous paragraph, the actual deformable length is taken as 26 $\mu$m along the longitudinal direction in the FEM model. Thus we can see $x$-directional displacement of 0.5 nm at the edge of both sides of substrate in Fig. 7. It is seen here that the deformation increases with distance increasing from the center of the beam and reduces again as it approaches the fixed ends of the beam. It is observed that the change in defect length reaches maximum at a distance of 3 $\mu$m from the center of the beam, while it is illustrated by the yellow and orange regions in Fig. 7. In other words, the drastic change of vertical position means largest strain area or largest deformation along the longitudinal direction of beam. We arranged the two reflectors of four holes at this 3 $\mu$m point in order to take advantage of that this position will lead our PhCWG exhibits the most sensitive behavior regarding to strain and force. Since the induced strain will be perfectly reflected in the change of $A_d$ and $r_x$ so as to gain in largest resonant wavelength shift. Upon the derived topographic data in FEM simulation regarding to the pressure loads from 1 to 5 MPa.
with 1 MPa difference, we may derive relative changes in \( r_x \) and \( r_y \) for all the holes and \( A_d \), \( r_x \) and \( r_y \) for micro-cavity. Then such derived parameters are fed into a commercial software, i.e., Rsoft, for conducting FDTD simulation. Finally we derived the resonant wavelength shift based on the simulated output spectrum.

Fig. 6(b). Three-dimensional top-side view of the bridge structure as depicted in Fig. 6(a).

Fig. 7. Beam structure of PhCWG showing the displacement of each point on the bridge along x-direction upon application of force, \( F = 0.79 \) µN at the center of the beam into the plane of the paper. The displacement in the x-direction increases as the distance from the center and the beam ends increases. Maximum change in \( A_d \) is seen at a distance of 3 µm from the center (small yellow bar closer to the center of the beam).
Fig. 8. Shift in the resonant peak due to force applied (1.0 MPa - 2.0 MPa in steps of 0.20 MPa).

Fig. 9. Shift in the resonant peak due to force applied (1.0 MPa - 5.0 MPa in steps of 1 MPa).
Besides, we noticed that very sensitive behavior of resonant wavelength shift versus loading force is observed in the small loading force region. As a result, we conducted comprehensive simulation work in this region. The simulation has been conducted in more detailed analysis for cases of loading pressure from 1 to 2 MPa with 0.2 MPa difference between two data points. Fig. 8 shows the simulated various resonant wavelength peaks with respect to different applied pressure from 1 to 2 MPa with 0.2 MPa increment of each step. The shift to shorter wavelengths corresponds directly to the reduction in $A_d$ and an elongation of $r_x$. Besides, the actual shifts in the resonant wavelength after simulations by said FDTD method for loading pressure from 1 to 5 MPa with 1 MPa increment of each step can be figured out from Fig. 9, i.e., the derived resonant wavelength peaks. We may combine the data points shown in Fig. 8 and Fig. 9 and present such data in terms of loading force as shown in Fig. 10. Within the range of 0.7 to 1.7 µN loading force, rather linear behavior observed for the shift of resonant wavelength regarding to the applied force. For force loads between 2 µN and 4 µN, it is seen that the relationship is best described by a second order equation. For the overall data, a polynomial regression line of degree two fits well with the data points.

Fig. 10. Force applied on suspended beam versus resonant wavelength shift of PhCWG.

Fig. 11. Deflection in the z-direction versus resonant wavelength shift of PhCWG.
The resonant wavelength shift is derived as a function of vertical deflection at center of suspended beam, as shown in Fig. 11. It shows that a second order equation can fit this data points, while the minimum detectable vertical deflection is measured as about 20-25 nm in terms of 0.1 nm resonant wavelength shift. A relatively linear relationship is observed for vertical deflections from 75 nm to 160 nm. In consideration of that the most sensitive parameter to resonant wavelength shift is the defect length, i.e., $A_d$, the strain in PhCWG is defined as a ratio of the change in defect length, i.e., $\Delta A_d$, to the original $A_d$. In other words, it is the percentage change in the defect length. Fig. 12 shows the relationship between the shift in resonant wavelength of the PhCWG and the absolute value of strain regarding to $A_d$. Although another polynomial regression line of degree two fits the overall data perfectly, it is also observed that the change in resonant wavelength fits in linear behavior for strain within 0.03%, referring to red dashed line. Again the detectable smallest strain is derived as 0.005%. It is a significant improvement with three orders of magnitude than previous strain sensing data reported by Ref. [5].

4. CONCLUSION

The force and strain sensing capability of a novel silicon bridge beam with PhCWG based resonator has been studied. We insert one pair of 2 air holes into the silicon linear waveguide as two reflectors. The point defect, i.e, a micro-cavity, is defined between the two reflectors. By introducing such a point defect, this suspended beam structure becomes a silicon nanophotonic resonator. It generate clear resonant wavelength peak with Q factor as high as 936. The deformation of the suspended beam could be detected by measuring the resonant wavelength shift. Longitudinal deformation of air holes and change in defect length of micro-cavity contribute resonant wavelength shift effectively. In terms of the percentage change in the defect length due to loading force, such strain can be detected as low as 0.005% regarding to a force load of 0.25 $\mu$N. It concludes that the minimum detectable force and the minimum detectable vertical deflection are 0.25 $\mu$N and 20-25 nm, respectively.

In summary, the derived simulation results show that this device concept could be applied to the force sensing, strain detection and displacement measurement. The main advantage provided by this new sensing concept is ultracompact device footprint. Simply speaking, the applications may be ultra-compact gyroscopes, accelerometers and biosensors, etc. This new nanomechanical sensor will lead to a new research field of optical NEMS.
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