Nanomechanical Photonic Microsensor for Ultrasensitive Explosive Detection

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ABSTRACT

A novel ultrasensitive integrated nanomechanical optical sensor for the detection of vapour explosive is proposed. The photonic device consists of a silicon nitride disk resonator formed by a horizontal slot-waveguide acting as a circular cantilever. The overall device sensitivity is enhanced by the combined sensitivities of the slot-waveguide and the disk resonator. A detection level of 0.27 ppq for pentaerythritol tetranitrate (PETN) is predicted, representing an enhancement of 4 orders of magnitude as compared to state-of-the-art microcantilever explosive sensors.

1. INTRODUCTION

Some of the current techniques for the detection of explosives are ion mobility spectroscopy (IMS) [1], negative-ion atmospheric pressure chemical ionization mass spectrometry [2] and laser induced fluorescence [3]. Limits of detection of 80 pg and 300 pg for common explosives used in terrorist bombings such as pentaerythritol tetranitrate (PETN) and hexahydro-1,3,5-triazine (RDX), respectively, have been reported. Although extremely sensitivity can be achieved with these detection schemes, they are bulky and expensive and cannot be miniaturized. It is desirable to develop extremely sensitive and inexpensive sensors than can be mass produced so that the cost of detection by law enforcement will be less than the cost of deployment by terrorists.

Micro-opto-electro-mechanical (MOEM) devices based on the principles of integrated optics and micromachining technology on silicon are good candidates for such miniature detectors. In particular, selective-coated microcantilevers can be used as ultrasensitive nanomechanical sensors for explosive vapor detection [4,5]. Differential surface stress due to vapor recognition leads to bending of the cantilever and a laser beam reflected off the cantilever surface is monitored with a position-sensitive photodetector. Thus, detection levels of 100 ppt for DNT have been obtained by using polymer-coated cantilevers.

Integrated optical microresonators have been also shown to be efficient sensing devices [6]. Optical enhancement produced in disk and ring resonators makes the response of these photonic structures very sensitive to small variations of its optical length, which can be originated by, for example, chemical reactions on its surface, pressure changes, mechanical stress or temperature variations.

Barrios, C.A. (2007) Nanomechanical Photonic Microsensor for Ultrasensitive Explosive Detection. In *Prediction and Detection of Improvised Explosive Devices (IED)* (pp. 6-1 – 6-10). Meeting Proceedings RTO-MP-SET-117, Paper 6. Neuilly-sur-Seine, France: RTO. Available from: http://www.rto.nato.int.

A sensor combining the advantages of both of the aforementioned devices (microcantilever and optical microresonator), would benefit from the high sensitivity of both structures leading to an overall enhanced deflection sensitivity. In this paper, I propose a novel configuration consisting of a recently invented photonic structure called slot-waveguide [7] integrated in a disk resonator in order to implement such a sensor. A slot-waveguide consists of two stripes or slabs of a high index material separated by a thin low-index region (slot region). In such a structure, the electric (E)-field discontinuity at the interface between high-index-contrast materials enables to guide and to confine light inside a nanometer-size area of low-index material. This discontinuity is such that the field is much more intense in the low-refractive-index slot region than in the high-index regions. Given that the width of the slot is comparable to the decay length of the field, the electrical field remains high across the slot, resulting in a power density in the slot that is much higher than that in the high index regions. Due to the high field concentration in the slot region, the slot-waveguide is very sensitive to small variations of the slot distance.

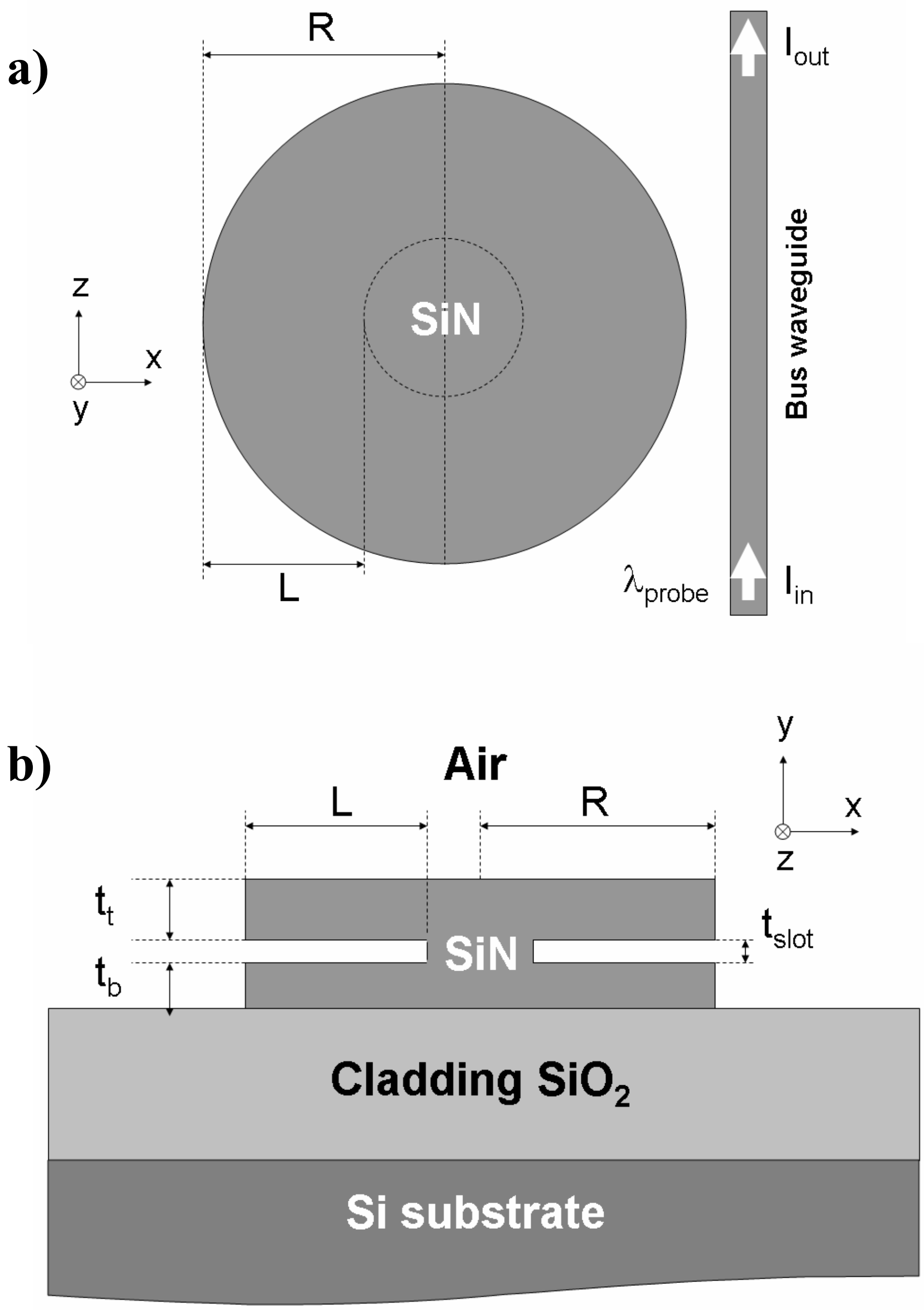

Fig. 1. Schematic top view (a) and cross-section (b) of a horizontal slot-waveguide disk resonator for the detection of nanomechanical forces.

2. DEVICE STRUCTURE

Figs. 1(a) and 1(b) show schematic top view and cross-section of the proposed device, respectively. It consists of a disk resonator of radius R formed by a Si_3N_4 horizontal slot-waveguide on a SiO_2 cladding layer. The horizontal slot-waveguide consists of a top Si_3N_4 disk of thickness t_t and a bottom Si_3N_4 disk of thickness t_b separated by an air gap (slot) of thickness t_{slot}. The top Si_3N_4 disk acts as a circular cantilever supported by an inner Si_3N_4 disk of radius (R-L). The sensing area of the device is the top surface of the Si_3N_4 disk cantilever.

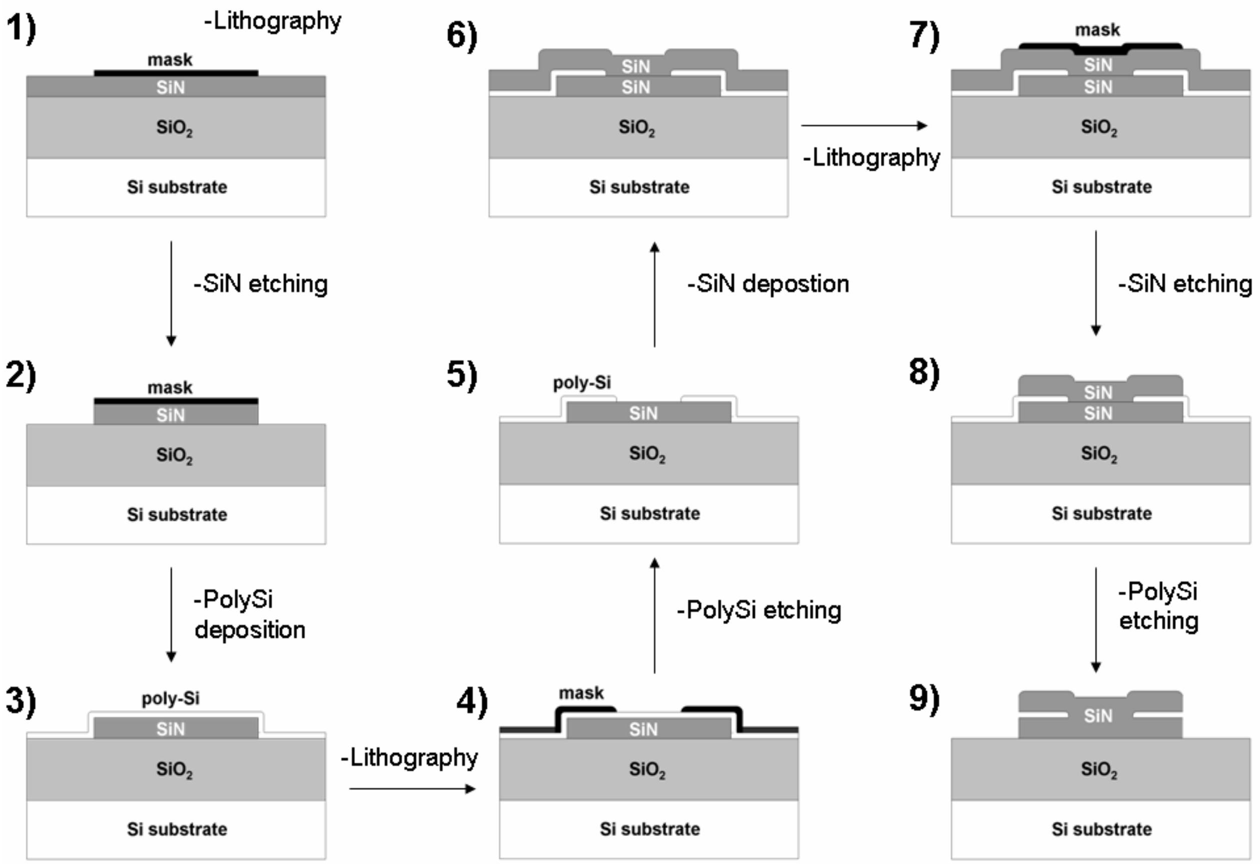

Fig. 2. Schematic process flow for the fabrication of the proposed device.

A practical realization of the proposed device is schematically illustrated and described in the abbreviated diagram of a process flow shown in Fig. 2. Conventional CMOS processing techniques such as chemical vapor deposition (CVD), lithography, reactive ion etching (RIE) and selective wet chemical etching can be employed. The sensing top surface can be functionalized so that a given molecular species will be preferentially bound to that surface upon exposure of the device to a vapour stream. For example, a monolayer coating of 4-mercaptobenzoic acid self-assembled (4-MBA SAM) could be formed on the sensing surface of the device in order to detect PETN and RDX.

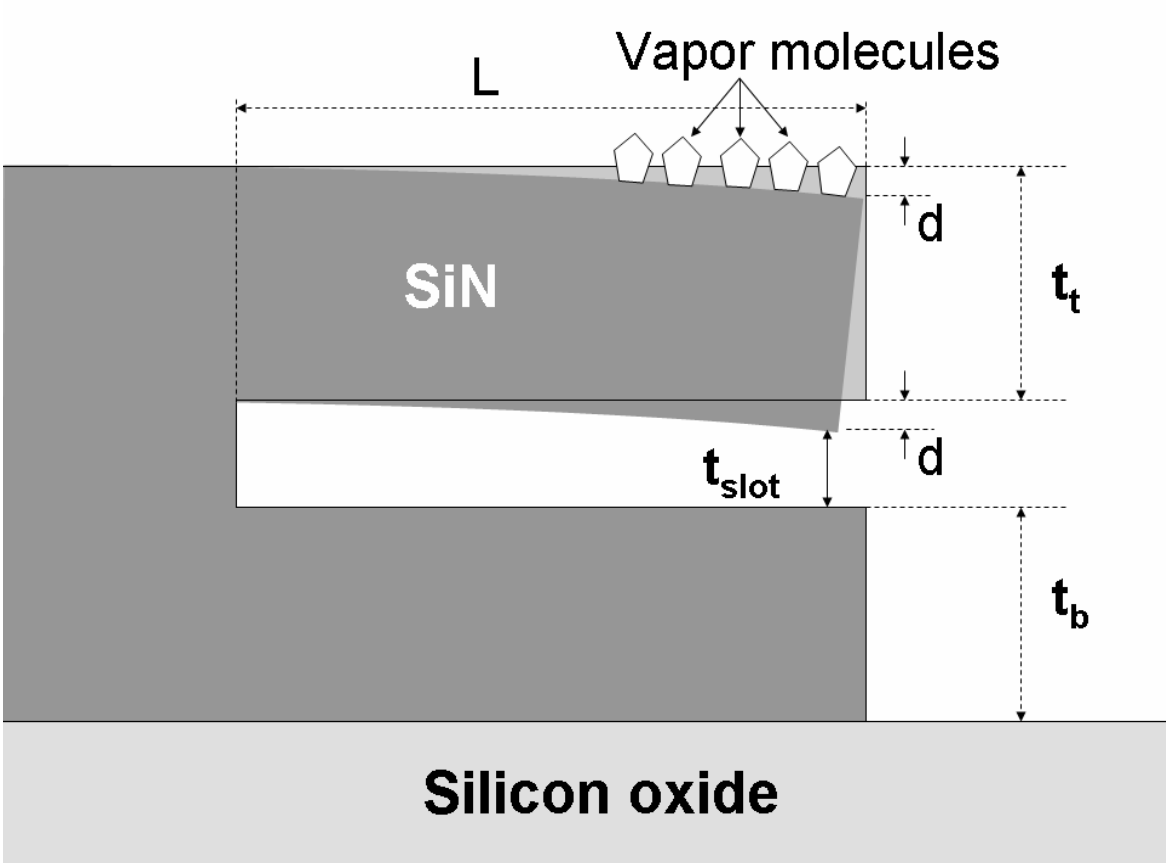

Fig. 3. Sensor device operation. Cantilever deflection (d) due to vapour molecules adsorption varies the distance t_{slot}, which in its turn changes the optical properties of the disk resonator.

3. PRINCIPLE OF OPERATION AND MODEL

The mechanical response of a sensitive layer applied onto the Si_3N_4 cantilever upper surface to the adsorption or recognition of explosive vapour molecules from the environment produces a surface stress that results in a static bending of the cantilever as shown schematically in Fig. 3. This bending corresponds to a deflection given by:

$$d = 3\left(\frac{1-\nu}{Et_t^{\ 2}}\right)L^2(\Delta\sigma_u - \Delta\sigma_l) \qquad (1)$$

where ν is the Poisson coefficient, E is the Young´s modulus, t_t is the cantilever thickness and $\Delta\sigma_u$ and $\Delta\sigma_l$ are the surface stress changes of the upper and lower sides of the cantilever, respectively. The deflection of the disk cantilever in response to an external force modifies the distance between the Si_3N_4 slabs, that is, it changes the slot distance t_{slot}, which in its turn changes the effective refractive index of the optical mode circulating in the disk resonator. This index (phase) variation can be read out as a resonant wavelength shift of the disk resonator, showed as an output intensity (I_{out}) variation at a given probe wavelength λ_{probe}.

SiO refractive index (λ=1.3 μm)	1.46
Si_3N_4 refractive index (λ=1.3 μm)	2.0
Air refractive index (λ=1.3 μm)	1.0
t_b (nm)	200
t_t (nm)	200
t_{slot} (nm) at zero defection (d=0)	100
R (μm)	150
L (μm)	125

Table 1. Materials parameters and dimensions used in the simulations.

The modal characteristics of the slot disk resonator were calculated by using the finite difference beam-propagation method (BPM). The material parameters and dimensions used in the simulations are shown in Table 1. The operation wavelength is 1.3 μm. It is also assumed that the deflection is the same along the whole perimeter of the circular cantilever.

4. RESULTS AND DISCUSSION

Figs. 4(a) and 4(b) show de optical field distribution for the transverse-magnetic (TM) and transverse-electric (TE) polarization modes, respectively, for the lowest order disk resonator modes. In both cases, a percentage of the optical field is observed in the slot region between the two SiN layers. This percentage is particularly significant for the TM mode polarization due to the slot effect (electric field discontinuity).

Fig. 5 shows the calculated effective index change (Δn_{eff}) for the TM and TE polarization modes as a function of the deflection, d, for the simulation parameters given in Table 1. For both TM and TE, Δn_{eff} varies linearly for $d \leq 20$ nm, with a slope (slot-waveguide sensitivity) of $S_{slot} = 1.15\times10^{-3}$ RIU/nm (RIU=refractive index unit). Note that for d>20 nm, Δn_{eff} for TM changes more dramatically than that for TE. This occurs because of the higher optical field confinement in the slot region for the former mode polarization (slot effect).

The deflection sensitivity (S_{def}) of the studied sensor, defined as the variation of the normalized detected output intensity (I_{out}) per unit displacement of the cantilever, is given by the expression:

$$S_{def} = \frac{\partial I_{out}}{\partial d} = S_{disk} S_{slot} = \left(\frac{\partial I_{out}}{\partial(\Delta n_{eff})}\right)\left(\frac{\partial(\Delta n_{eff})}{\partial d}\right) \quad (2)$$

where S_{disk} is the refractive index sensitivity of the disk resonator defined as the variation of the normalized detected output intensity signal per RIU.

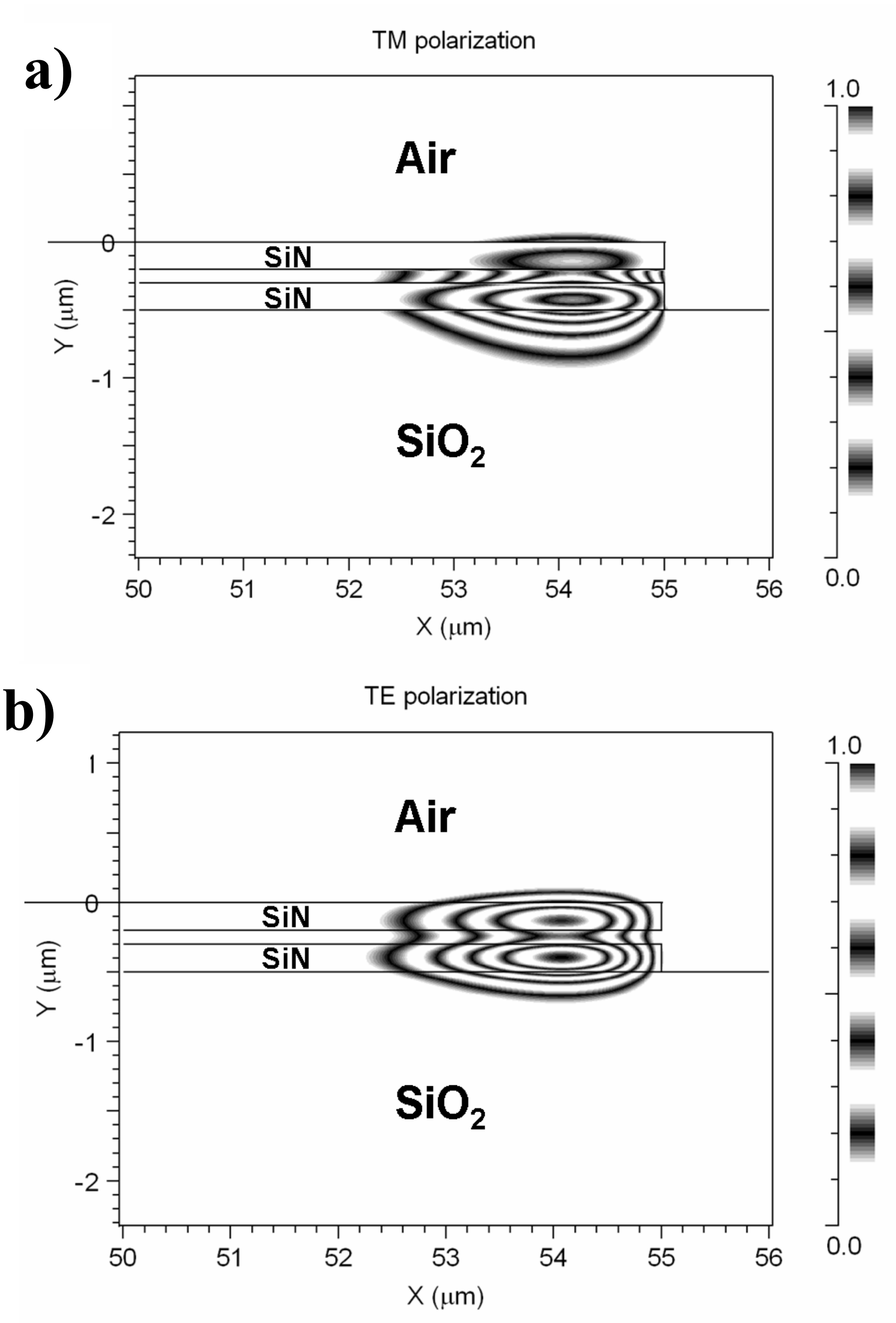

Fig. 4. Optical distribution of the lowest TM (a) and TE (b) modes of the horizontal slot-waveguide disk resonator.

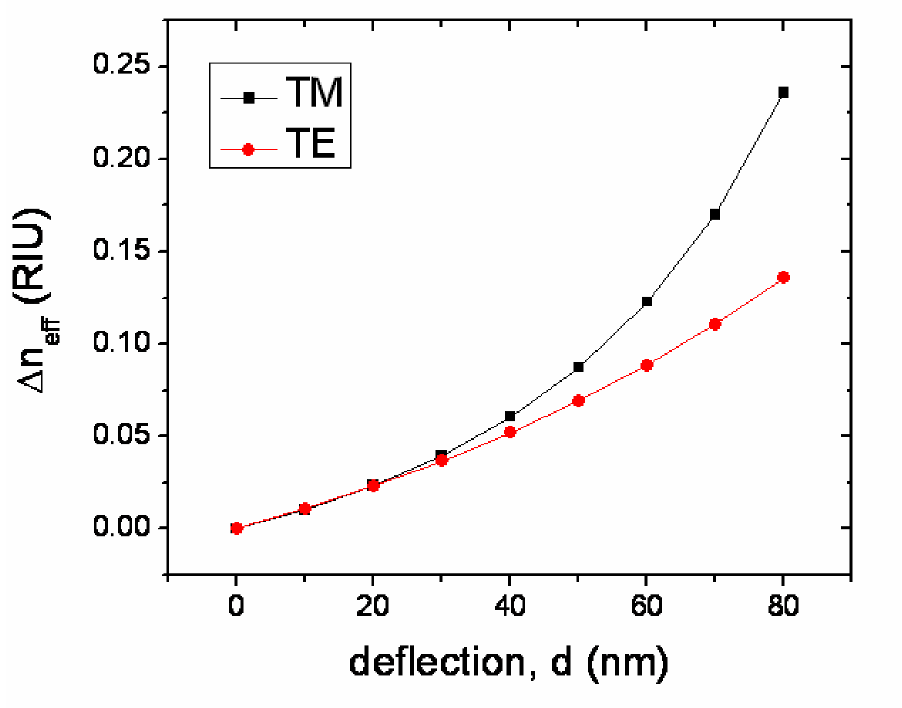

Fig. 5. Variation of the effective refractive index of the disk TM (squares) and TE (circles) optical modes as a function of the deflection d.

$Si_3N_4/SiO_2/Si$ horizontal slot-waveguide disk resonators have been demonstrated to exhibit quality factor (Q) as high as 30,000 for 250 μm-diameter disks [8]. Resonators with such a Q values have been shown to be able to detect effective index variations of $\Delta n_{eff,min}=10^{-6}$ RIU [9]. Assuming that the minimum output intensity (I_{out}) that can be detected is 1% of the normalized maximum output power (a conventional photodetector can easily detect 1 μW over 100 μW of maximum power), the index sensitivity of the considered disk resonator would be $S_{disk}= 10^4$ RIU^{-1}.

Therefore, the deflection sensitivity, S_{def}, of the proposed device is (1): $S_{def}= 10^4$ $(RIU^{-1}) \times 1.15\times10^{-3}$ (RIU nm^{-1}) = 11.5 nm^{-1}. This value is 4 orders of magnitude higher than the typical sensitivity exhibited by state-of-the-art microcantilever sensors [10,11]. The estimated deflection detection limit of the slot-waveguide disk resonator sensor would be $\Delta d_{min}=\Delta n_{eff,min}$ / S_{slot} = 10^{-6} (RIU) / 1.15×10^{-3} (RIU/nm) = 8.7×10^{-4} nm, which is two orders of magnitude smaller than that shown by waveguide microcantilever sensors [11].

As a particular application we can consider the detection of PETN. The detection sensitivity for PETN of a conventional Si microcantilever is 14 ppt, which corresponds to a minimum detectable surface stress of 3.7 mJ/m^2 [4]. The stress sensitivity of the proposed device can be calculated from Eq.1 by using E=96 GPa and ν=0.27 for Si_3N_4; thus, S_{stress}= 11.9 $nm/(mJ/m^2)$. That is, the minimum surface stress that can be detected is $\Delta\sigma_{min}=\Delta d_{min}$ / S_{stress}= 8.7×10^{-4} (nm) / 11.9 $[nm/(mJ/m^2)]$ = 7.3×10^{-5} mJ/m^2. This means that the PETN limit of detection of the proposed sensor would be 0.27 ppq, that is, 4 orders of magnitude smaller than that estimated for a conventional Si microcantilever sensor [4].

5. SUMMARY

A CMOS-compatible novel ultrasensitive integrated nanomechanical photonic microsensor for the detection of vapour explosives is presented. The device consists of a microdisk optical resonator formed by a slot-waveguide containing a mechanical sensing element (cantilever). The overall sensitivity of the device results from the product of the high sensitivity of the effective index of the waveguide to small cantilever deflections and the high sensitivity of a disk resonator to small effective refractive index variations. Calculations indicate a deflection sensitivity of 11.5 nm^{-1} and a limit of detection for PETN of 0.27 ppq, which represents an improvement of 4 orders of magnitude as compared to state-of-the-art nanomechanical explosive sensors based on microcantilevers.

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