Ultra-high sensitive 1D porous silicon photonic crystal sensor based on the coupling of Tamm/Fano resonances in the mid-infrared region

Ashour M. Ahmed & Ahmed Mehaney

Porous silicon one-dimensional photonic crystals (PSi-1DPCs) are capable of sensing solutions and liquids based on the smallest variation of the refractive indices. In the present work, we present a novel metal/PSi-1DPC as a liquid sensor based on Tamm/Fano resonances. The operating wavelength range is from 6.35 to 9.85 μm in the mid-infrared (MIR) spectral region. Different metals (Al, Ag, Au, and Pt) are attached to the top surface of the PSi-1DPCs structure to show Tamm/Fano resonances more clearly. To the best of our knowledge, it is the first time that Tamm/Fano resonances exhibit simultaneously in PSi-1DPCs within the same structure. The reflection spectra were calculated for the metal/PSi-1DPC structure by using the transfer matrix method (TMM) and the Bruggeman’s effective medium approximation (BEMA). The simulations show that the Tamm/Fano resonances are red-shifted towards the higher wavelengths with increasing the refractive index of the pores. The Ag/PSi-1DPC sensor showed the highest performance. Its sensitivity can be reached to the value 5018 nm/RIU with a high-quality factor of about 2149.27. We predict the proposed sensors can be easily fabricated and we expect them to show higher performance than other reported sensors of this type. Therefore, it will be of interest in the field of optical sensing in different fields.

Photonic crystals (PCs) are new smart composite structures could control the propagation of electromagnetic waves with different frequencies. The novel phenomenon appeared on PCs is the photonic band gap. Within the band gap, all frequencies of the incident electromagnetic waves are effectively attenuated. Breaking the periodicity of PCs and generating resonant modes inside the photonic band gaps increase the novelty of such periodic structures more than the perfect ones. Based on these remarkable physical and engineering applications, PCs inspired researchers to replicate this idea on different types of waves e.g., elastic, acoustic, surface, electric and magnetic waves. Recently, the process of solutions and liquids sensing by using PCs has attracted great attention due to its major role in many biological, biochemical and engineering applications.

On the other hand, the porous silicon (PSi) can be used as a biosensor due to it has a considerable surface area and versatile surface chemistry. The PSi is a form of the silicon wafer that has introduced nanopores in its microstructure. It can be easily formed by electrochemical etching of silicon wafers in hydrofluoric acid (HF) electrolyte under an applied electric current. The electrochemical process allows for precise control over the properties of PSi such as porosity and thickness of the porous layer by adjusting the etching current density, time interval, and HF concentration. The one-dimensional photonic crystal (1DPC) based on multilayered PSi can be easily fabricated by periodic alteration of the current density during the electrochemical process. The PSi-1DPC offers many advantages such as its high specific surface area, its ease of fabrication and compatibility with standard microelectronics processing. R. Carosselli et al. experimentally developed a highly sensitive PC sensor based on PSi for low refractive index variations. The PSi sensor showed a sensitivity of about 1000 nm/RIU. Also, V. Pham et al. developed a...
1DPC microcavity sensor based on PSi multilayers. The 1DPC sensor showed a sensitivity of about 200 nm/RIU, and it can be used for the determination of organic content in different liquid solutions.

In addition to that, the well-known phenomenon Tamm resonance has been achieved in PCs and it has been used in the optical sensing techniques of PCs structures. Mainly, Tamm resonance is formed at the metal and the Bragg mirror interface. B. Auguié et al. studied theoretically and experimentally Tamm resonance in a PC composed of SiO2 and TiO2 multilayers. The sensitivity of this structure was low of about 55 mm/RIU.

Moreover, Fano resonance was observed in many 1DPC structures, and it can be used as an indicator for many applications such as bio-sensing, switching, photodetector, filter, waveguide, and modulator. V. Klimov et al. proposed theoretically Fano resonances in a 1DPC structure composed of MgF2 and TiO2 layers, the structure was used as a biosensor. In this work, we present a new theoretical study concerning Tamm/Fano resonance in a PSi-1DPC structure. The PSi-1DPC is a ternary structure composed of three different PSi layers repeated in \( N = 25 \) unit cells with a metal layer on the top of the ternary structure; Si/[PSi1/PSi2/PSi3]N=25/metal. Also, we will study the optical properties and sensitivity of the proposed metal/PSi-1DPC sensor. The paper is organized as follows; In the first, we present the design of a metal/PSi-1DPC sensor. Secondly, the theoretical basis equations of PSi and its relation with the refractive index of the void (the material filling the pores) are presented. Finally, the output simulated results and the sensitivity analysis of the metal/PSi-1DPC sensor are introduced and discussed.

**Results**

**Design of PSI-1DPC sensor.** The proposed configuration of the biosensor is a ternary Si/[PSi1/PSi2/PSi3]N=25/metal as shown in Fig. 1. Recently, the periodic ternary 1D-1DPC structures have attracted the researchers attention due to their high sensing performance compared with the binary systems. For refractive index detection, the target solution is injected inside the flow cell in contact with the top surface of the PSi-1DPC in order to fill the pores as shown in the schematic diagram of Fig. 1. For an optimization purpose, the number of periods is chosen to be \( N = 25 \). Rea has fabricated experimentally and determined the porosity ratio in the PSi layer in the range from 56% to 81%. Therefore, the calculated porosity here in this paper was determined and confirmed experimentally for the proposed PSi layers. The values of the different parameters of the materials used in the calculations are given in Table 1. These values are given after optimization to get the best sensor performance. See Table S1 in the supplementary data.

![A schematic diagram of the metal/PSi-1DPC sensor structure.](image)

\[
\begin{align*}
R &= 100 \left( \frac{M_{11} + M_{12} q_i}{M_{11} + M_{12} q_i} * q_0 + (M_{21} + M_{22} q_i) \right)^2 \\
&= \frac{M_{11} + M_{12} q_i}{M_{11} + M_{12} q_i} * q_0 - (M_{21} + M_{22} q_i) \\
&= (M_{11} + M_{12} q_i) * q_0 - (M_{21} + M_{22} q_i)
\end{align*}
\]

where \( M_{11}, M_{12}, M_{21}, \) and \( M_{22} \) are the elements of the total transfer matrix of the proposed structure. The \( q \) values of air and substrate are given by the equations \( q_0 = n_0 \cos \theta_0 \) and \( q_s = n_s \cos \theta_s \), respectively.

The angles of incidence of each layer are related to the angle of incidence \( \theta_i \) in the air by Snell’s law as follows,

\[
n_0 \sin \theta_0 = n_i \sin \theta_i, \quad i = 1, 2, 3, m, s,
\]

where the order numbers 1, 2, 3, 4 and 5 represent the PSi1, PSi2, PSi3, metal, and substrate, respectively.

The detailed analysis of the TMM and the characteristics matrix details can be found extensively in literatures.
Porosity/refractive index relations of PSi. The effective refractive index of the PSi layer can be obtained by the Bruggeman’s effective-medium approximation (BEMA) as follows:

\[
P \frac{n_v^2 - n_{\text{eff}}^2}{n_v^2 + 2n_{\text{eff}}^2} + (1 - p) \frac{n_{\text{Si}}^2 - n_{\text{eff}}^2}{n_{\text{Si}}^2 + 2n_{\text{eff}}^2} = 0,
\]

where \(n_{\text{Si}}, n_v, \) and \(n_{\text{eff}}\) are the refractive indices of silicon, the material inside the pore and the whole PSi layer, respectively. \(P\) is the porosity ratio.

Equation 3 can be rewritten in a new form to shows \(n_{\text{eff}}\) as a function of \(P\) and \(n_v\) as follows:

\[
n_{\text{eff}} = 0.5 \sqrt{3P(n_v^2 - n_{\text{Si}}^2) + (2n_{\text{Si}}^2 - n_v^2) + \sqrt{(3P(n_v^2 - n_{\text{Si}}^2) + (n_{\text{Si}}^2 - n_v^2))^2 + 8n_{\text{Si}}^2n_v^2}}.
\]

For porosities 65%, 77%, and 85%, the corresponding refractive indices at a wavelength 8 \(\mu\)m are 1.6826, 1.381 and 1.2199, respectively.

According to Bruggeman’s model, Fig. 2(A) shows the dependence of the effective refractive index of the PSi on the porosity variation. With increasing the porosity value, the effective refractive index of the PSi will be decreased for all wavelength values in the range from 6.35 to 9.85 \(\mu\)m. Therefore, the effective refractive index of the PSi can be controlled from the range 3.4203 to 1 based on the porosity variation. Also, According to Fig. 2(B), \(n_{\text{eff}}\) increases linearly with increasing the refractive index of voids for the three porosities. Also, it is well-known that the effective refractive index does not vary in the mentioned operating wavelength range.

Discussion
Perfect PSi-1DPC. The reflectance of the incident electromagnetic wave for the perfect PSi-1DPC; Si/[PSi1/PSi2/PSi3]N=25 is plotted versus the incident wavelength. A ray of light is normally incident on the PSi-PCs structure (with an angle of incidence = zero degrees). As shown in Fig. S2 in the supplementary data, the reflectance was calculated at different void refractive indices \((n_v = 1\) to \(1.5\)) as shown in this Figure, wide photonic band gaps appeared for each \(n_v\) value. These gaps resulted from the constructive interference of electromagnetic waves at the interface between each two layers, since the width of the band gap increases with increasing the mismatch between the constituent materials. With increasing the refractive index of the void, the photonic band gap
decreases due to decrement the contrast of the refractive indices between the PSi and Si substance. Also, the spectrum is red-shifted towards the higher frequency range with increasing $n_v$ value.

Metal/PSi-1DPC sensor. In Fig. 3(A), the reflectance of the metal/PSi-1DPC structures as a function of the wavelength at $n_v = 1.1$, respectively. Fig. 3(B) A comparison between the reflectance of the PSi-1DPC and Ag/PSi-1DPC at $n_v = 1.1$.

![Graph](image)

Figure 3. (A) The reflectance of the Ag/PSi-1DPC, Au/PSi-1DPC, Al/PSi-1DPC and Pt/PSi-1DPC structures as a function of the wavelength at $n_v = 1.1$, respectively. (B) A comparison between the reflectance of the PSi-1DPC and Ag/PSi-1DPC at $n_v = 1.1$.

Table 2. Drude model parameters for metals that used in the calculations.

| Metal | Plasma $\omega_p x10^{11}$ (rad/Sec) | Damping $\gamma x10^{11}$ (rad/Sec) |
|-------|-------------------------------------|-------------------------------------|
| Al    | 224107.9                            | 1242.952                            |
| Au    | 137101.3                            | 404.909                             |
| Ag    | 136913                              | 273.4494                            |
| Pt    | 78155.29                            | 1050.859                            |

Table 2. Drude model parameters for metals that used in the calculations.

![Table](image)

The refractive index of metals can be described by a complex dielectric function. According to the Drude model, the dielectric function of a metal can be given by the following relation,

$$\epsilon_m = 1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)} = \epsilon_1 + i\epsilon_2,$$

where $\omega_p$ is the plasma frequency and $\gamma$ is the damping frequency term (inverse of the relaxation time). $\epsilon_1$ and $\epsilon_2$ are the real and imaginary part of the dielectric function, respectively. Thus, the refractive index of a metal is given by the following relation $n_m = \sqrt{\epsilon_m}$.

Table 2 summarizes the $\omega_p$ and $\gamma$ values for Ag, Au, Al, and Pt, respectively.
It is important to mention that attaching metal to the PSi-1DPC structure will induct the appearance of resonant wavelengths as shown in Fig. 3(A). Those resonant wavelengths or Tamm resonance is due to the interference of electromagnetic waves at the interface between the PSi layers and the metals. 

Also, Fig. 3(B) shows a comparison between the reflectance of a PSi-1DPC and Ag/PSi-1DPC at a void refractive index $n_v = 1.1$. It can be seen that the width of the photonic band gap of the Ag/PSi-1DPC is wider compared with the PSi-1DPC due to the existence of the Ag layer on the top of the PSi-1DPC. Also, Fig. 3(B) shows a narrow peak (resonant mode) inside the photonic band gap of the Ag/PSi-1DPC at $\lambda_r = 6.7965 \mu m$, which is called Tamm/Fano resonance. Furthermore, the number of ripples in the reflectance spectrum outside the photonic band gap of the PSi-1DPC and Ag/PSi-1DPC is equal.

Moreover, the reflectance of the four metals on the PSi-1DPC at different $n_v$ values is shown in Fig. S3 in the supplementary data. As shown in Fig. S3(A) in the supplementary data, with increasing $n_v$, the intensity of the resonant wavelengths was decreased and red-shifted towards the higher wavelengths. Also, the photonic band gaps became flat and had a narrower FWHM due to the damping properties of Ag. Moreover, Fig. S3(B) represents the reflectance spectrum of the Au/PSi-1DPC. The Au/PSi-1DPC spectrum is similar to the Ag/PSi-1DPC spectrum, this is due to the great convergence in the optical properties between Ag and Au as indicated in Table 2.

A motivating phenomenon appeared when the Al layer attached to the PSi-1DPC sensor structure as shown in Figs 3(A) and S3(C,D) in the supplementary data. Not only resonant peaks appeared due to Tamm resonance, but also Fano resonance appeared for each $n_v$ value. As is well-known, Fano resonance is asymmetric line shape and results from the interference between slow-varying background (Here is the PSi-1DPC mode) and narrow-band resonance (Tamm resonance). Fano resonance appeared in Al/PSi-1DPC because the damping constant of Al is greater than of Ag or Au. So that the photonic narrow-band (resonance mode) appears clearly in the case of Al than Ag, which in turn produces Fano resonance. Confirming the inspections made above, Fano resonance is sharply observed when Pt is attached to the PSi-1DPC structure as shown in Figs 3(A) and S3(D). The Pt is characterized by high damping constant compared with Al, Au or Ag, which then enhance the appearing of Fano resonance for each $n_v$ much clearer. Therefore, Fano resonance in the case of using Pt is clearer than other metals. However, the Pt/PSi-1DPC has a high bandwidth (FWHM) which decrease the values of quality factor and figure of merit, hence, the sensor performance will decrease.

**Sensor analysis.** The efficiency and performance of any sensor type are determined by the values of many parameters such as the sensitivity ($S$), the figure of merits (FOM) and the quality factor ($Q$). These parameters can be obtained using the following expressions:

$$ S = \frac{\Delta \lambda}{\Delta n}, \quad (6) $$

$$ \text{The figure of merit} \quad \text{FOM} = \frac{S}{\text{FWHM}}, \quad (7) $$

$$ \text{The quality factor} \quad Q = \frac{\lambda_r}{\text{FWHM}}. \quad (8) $$

where, the resonance refractive index and wavelength of the air were used as references to calculate $\Delta \lambda$ and $\Delta n$ for the different media, i.e., $\Delta \lambda = \lambda_r(\text{void}) - \lambda_r(\text{air})$ and $\Delta n = n_v - n(\text{air})$. The FWHM is the full width at half maximum of the resonant peak.

Figure 4 shows the position of the resonant peak wavelength as a function of $n_v$. The positions of the resonant peak are increased linearly with the void refractive index increment for the four metals. The linear fitting of the simulation data for Ag/PSi-1DPC, Au/PSi-1DPC, Al/PSi-1DPC and Pt/PSi-1DPC can be given according to the following equations,
As shown in Table 3, these parameters were calculated beside the resonance mode which has a narrow resonant dip will provide a high detection accuracy of the same measurement. From our A sensitivity of about 4.76631, 4.77217, 4.78146 and 4.78404, the suggested biosensor can be obtained. The slope of each fitting line indicates the sensitivity of the Metal/PSi-1DPC. The proposed metal/PSi-1DPC structure based on Tamm/Fano resonance allows greater and precise control for the measurements of the refractive index than previously reported sensor structures. These sensors include SPR-based optical fiber sensor described by Cennamo et al. and 1DPC and Ag/PSi-1DPC, respectively.

The real and imaginary parts of the refractive index for Ag, Au, Al, and Pt are presented in the supplementary data in Fig. S1. The refractive index is plotted in the wavelength range from 6.35 to 9.85 μm. From this table, the average value of FWHM increases from 0.001274 to 0.019988 and from 0.003508 to 0.028379 with increasing the damping constant of metals. Hence, the value of FWHM at same the refractive index of void as seen in Table 3.

Table 3. The values of S, Rr, FOM, FWHM and Q at n_v = 1.1 for the Ag/PSi-1DPC, Au/PSi-1DPC, Al/PSi-1DPC and Pt/PSi-1DPC sensors, respectively.

| Metal | λ_r (μm) | R_r (%) | FWHM (μm) | S (μm/RIU) | FOM (RIU⁻¹) | Q |
|-------|----------|---------|------------|------------|--------------|---|
| Ag    | 7.2993   | 88.43   | 0.003396   | 5.018      | 1477.54      | 2149.27 |
| Au    | 7.2997   | 91.52   | 0.00496    | 5.0924     | 1026.665     | 1471.65 |
| Al    | 7.29365  | 98.74   | 0.014513   | 5.0315     | 346.68       | 502.55  |
| Pt    | 7.3348   | 76.74   | 0.041341   | 5.013      | 121.25       | 177.42  |

where the RIU is the refractive index unit. The R² is the square of the correlation coefficient between the linear fitting and the simulation data. The calculated R² is equal to 0.999 for all fitting lines. Hence, high linearity of the suggested biosensor can be obtained. The slope of each fitting line indicates the sensitivity of the Metal/PSi-1DPC. A sensitivity of about 4.76631, 4.77217, 4.78146 and 4.78404 μm/RIU for Pt/PSi-1DPC, Al/PSi-1DPC, Au/PSi-1DPC and Ag/PSi-1DPC, respectively.

Using Eqs (9–12), the S, FWHM, FOM and Q are calculated at the peak of Tamm/Fano resonance for the metal/PSi-1DPC structure. As shown in Table 3, these parameters were calculated beside the resonance mode (R_r) for the four metals Ag, Au, Al and Pt at n_v = 1.1, respectively. Also, we can see the effects of the void refractive index on the sensor performance parameters in Table S2 in the supplementary data. From this table, the average sensitivity for all metals is about 4.9 μm/RIU (4900 nm/RIU). Not only we obtained high values for the sensitivity, but also for FOM and Q as well. The FOM and Q determine the efficiency and performance of sensors. At n_v = 1.1 in the Ag/PSi-1DPC sensor, the Q and FOM have the highest values of about 2149 and 1477.54 RIU⁻¹, respectively. The reason of these high values is due to the small broadening in the resonance curve of each Metal/PSi-1DPC structure. Moreover, the trend of all observed calculations is that for higher n_v values the PSi-1DPC sensor has the lowest sensitivity for the four metals.

Table 3. The values of S, R_r, FOM, FWHM and Q at n_v = 1.1 for the Ag/PSi-1DPC, Au/PSi-1DPC, Al/PSi-1DPC and Pt/PSi-1DPC sensors, respectively.
part describes the broadening of the resonance peak\(^6\). In our structure, the total thickness of the structure is Si/PSi\(_1/PSi_2/PSi_3\)\(_N \sim 25\) is very high (62.5 µm). Also, there is a high change in the effective refractive index for the layers PSi\(_i\), PSi\(_i\), and PSi\(_i\) from 1.6825, 1.381 and 1.220 to 2.0905, 1.8605 and 1.722 with increasing the refractive index of the void from 1 to 1.5, respectively. Hence, the effect of the imaginary part of the metals refractive index on the position of the resonance peak is very small.

Conclusions

In conclusion, we successfully studied and developed theoretically a high sensitive sensor based on the PSi-1DPC structure. For the first time, the sensing process is based on the displacement of Tamm/Fano resonances by the variation of liquids refractive indices in a metal/PSi-1DPC structure. For Al and Pt, Fano resonance can occur and couple with Tamm resonance due to the high damping constant of the two elements. Finally, we performed a sensitivity analysis for the proposed PSi-1DPC sensor for the four metals. High sensitivity, quality factor, and figure of merit values were obtained for the four metals Ag, Au, Al, and Pt, respectively. The values of S, Q and FOM for Ag/PSi-1DPC structure are 4784.04 nm/RIU, 2149.27 and 1477.54 RIU\(^{-1}\), respectively. Therefore, Fano resonance in the case of using Pt is clearer than other metals. However, the Pt/PSi-1DPC has a high bandwidth (FWHM) which has a negative effect on the values of quality factor and figure of merit which in turn, will decrease the sensor performance. Finally, it would be interesting to realize the proposed devices and to test them for optical sensing.

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Author Contributions
A.M. Ahmed devised the main ideas and performed numerical simulations. A. Mehaney analyzed the data and discussed the results. All authors contributed to the final manuscript.

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