Photonic Crystal Resonator in the Millimeter/Terahertz Range as a Thin Film Sensor for Future Biosensor Applications

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Abstract

With recent developments, terahertz (THz) technology has attracted great interest in many different fields of research and application. In particular, biosensors that detect a thin film of captured pathogens are in high demand for rapid diagnosis. Based on the interaction between analytes under test and electromagnetic (EM) field, THz resonators are sensitive to changes in the permittivity of the analyte and have the potential to become sensitive thin-film sensors. However, conventional metamaterial methods have low $Q$ factors, leading to small amplitude variations and ambiguous detection. Here, we present a photonic crystal (PhC)–based resonator with a high $Q$ factor that is sensitive to a monolayer of beads in the µm size range. The PhC resonator made of high resistivity silicon (HRSi) shows a $Q$ factor of 750, which is much higher compared to metamaterial-based methods. Its resonance shift is linearly related to the coverage of the micron-sized beads on its surface. Moreover, simulation results with a thin film model of a single layer of the beads showed agreement with the experimental results. Although the achieved sensitivity needs to be improved by enhancing the field concentration on the analyte, our results suggest that THz PhC resonators with high $Q$ factor are promising for biosensing applications. We anticipate our work to be a starting point for biochips with improved sensing capabilities and more functionality.

Keywords THz · Thin film sensing · Photonic crystal · High $Q$

1 Introduction

In recent decades, terahertz (THz) technology has attracted great interest in many application areas such as spectroscopic sensing, nondestructive testing [1], and high-speed wireless communications [2]. In particular, applications in sensing
have gained popularity because THz radiation has many positive properties, including the short wavelength associated with high spatial resolution [3], spectral fingerprinting of specific molecules, and low photon energy [4]. THz sensors are based on the interaction between THz electromagnetic (EM) fields and the analyte to be detected. A change in the permittivity of the analyte alters the distribution of the EM field, which can be observed as a change in capacitance, transmission, or resonant frequency [5]. This enables a qualitative or quantitative measurement.

In sensing applications, one challenge is to reliably characterize a thin film when only a small amount of the sample is available. This is the case in pathogen detection, where the target pathogens, such as bacteria, are captured by specific antibodies on the surface of the biosensor [6]. The bacteria form a monolayer with a thickness in the micrometer range [7]. Hence, thin film sensors are of great interest for point-of-care (PoC) devices in the healthcare market since they can detect pathogens in close proximity to the patient [8].

In recent years, THz sensors based on metamaterials or metasurfaces have emerged as a promising method [4, 9]. Metamaterial sensors consisting of periodic split ring resonators show EM resonances which strengthen the interaction between the EM field and the analyte. It is most sensitive to the captured analyte at the gap of the ring. Geng et al. presented a THz metamaterial biosensor integrated with microfluidics for detection of liver cancer biomarker [10]. However, the resonance shift for detecting a micrometer thin film is small compared to the 3-dB bandwidth or full width at half maximum (FWHM), leading to small amplitude variations and ambiguous detection. The sensing performance can be improved by enhancing the EM field on the site of the analyte by increasing the quality factor (Q factor). Taleb et al. presented a free-standing metamaterial resonator with an asymmetric structure leading to a Fano resonance with a high Q factor [11]. Weisenstein et al. presented an asymmetric metasurface on a quartz glass substrate, where a specific undercut was etched [12]. However, the Q factor is still limited due to the losses of the metal. Furthermore, a complex measurement setup and costly fabrication are required.

A promising approach for achieving better performance is to utilize an all-dielectric resonator with a high Q factor [13, 14]. Recently, silicon resonators with ultra-high Q factors based on photonic crystals (PhC) have become popular for THz sensing applications. The small structures can be fabricated by micro- and nanotechnology and show potential of high sensitivity, compact size, and integration in a portable PoC device [15]. Hanham et al. demonstrated a PhC slab resonator at 100 GHz with a Q factor of 5800 [16]. As a demonstration, a few nanoliters of water–ethanol mixture in a quartz capillary through the resonator were measured. Okamot et al. showed a PhC resonator at 318 GHz with a Q factor of 10,800 [15]. Resonance shifts of about 300 MHz were observed by placing a 5-µm-thick dielectric polyester tape on top of the resonator. These results give an idea of the potential of PhC resonators for biosensor applications. However, so far, PhC resonators have not been used in scenarios where a micrometer thick analyte film, which corresponds to the thickness of most bacteria, must be detected.
In this article, a silicon THz PhC resonator is proposed for sensing thin films in the micrometer thickness range for future biosensing applications. A fabricated PhC resonator in the millimeter range is characterized using microbeads, which can be interpreted as a thin film of analytes. Firstly, the working principle of the PhC resonator and its sensing capability are described. Then, the preparation of the analyte (SiO₂ beads) and the measurement setup are explained. At last, the measurement results are interpreted in an EM view and compared with simulation results.

2 Concept

The PhC structure consists of a periodic lattice of alternating materials, which leads to a photonic bandgap characteristic. The photonic bandgap enables the confinement of EM waves to achieve a resonator with a high $Q$ factor. The shift of its resonance frequency due to a changed permittivity around it can be used for thin-film sensing. In this section, the working principle of the PhC resonator and thin-film sensing is explained, and the sensing performance is analyzed through EM simulations.

2.1 PhC Resonator

The PhC structure was initially used for optical control and manipulation by the bandgap characteristics [17]. Nowadays, it is the fundamental building block of various THz components [18, 19]. A PhC is a periodic array of two dielectric materials with different permittivities. At each interface of the different materials, one part of an incident EM wave is reflected, and the other part is transmitted. In a certain frequency range, the reflected waves interfere with each other constructively. The transmitted wave decays exponentially and is hence an evanescent wave. After a certain number of periods, the transmitted wave can be neglected. This can be understood as an optical bandgap. The bandwidth of the bandgap can be increased by using two materials with a high contrast of permittivity [17].

Considering the convenience of production, a PhC based on a silicon slab can be fabricated using micro- and nanotechnology. For the fabrication, high resistivity silicon (HRSi) wafers with high resistance (> 10 kΩcm), high permittivity ($\varepsilon_{Si} = 11.68$), and low loss tangent (0.00015) are typically used to realize PhCs with a good performance [20]. A typical PhC slab has a triangular lattice of air holes ($\varepsilon_{air} = 1$), which can be described by the period (the distance between the centers of two adjacent holes) $a$, the radius of the holes $r$, and the thickness of the slab $h$ as shown in Fig. 1a. In our design, the parameters of the PhC are chosen as: $r = 0.28a$ and $h = 0.81a$. A standard HRSi wafer with a thickness $h = 725\mu m$ is used for fabrication. The parameters are correspondingly calculated as $a = 900\mu m$ and $r = 255\mu m$.

Based on the bandgap characteristics, a PhC resonator with two waveguides as input and output paths for power coupling is realized as shown in Fig. 1a as schematic and in Fig. 1b as a photograph of the fabricated device. The two PhC waveguides are realized with a line of defect holes. A wave within the bandgap frequency
transmits only in the waveguide because of the wave restriction in the PhC slab, while the wave outside of the bandgap frequency scatters in the slab which leads to minimal transmission. To couple energy into the PhC waveguides, WR10 rectangular metallic waveguides were used. The simulations showed that the impedance of the WR10 waveguide and the PhC waveguide at 88 GHz are 507 Ohm and 125 Ohm, respectively. To minimize reflections between them and improve energy coupling, impedance matching was realized using a taper structure that provides a continuous transition between them. Its length was chosen as 5 mm to achieve a good transition and ease of fabrication. The PhC resonator is realized by eliminating a single hole in the slab and forming a microcavity. The microcavity can be seen as a terminated waveguide in the x direction. The travelling wave in it meets multiple adjacent holes (marked as 1, 2, and 3 in Fig. 1a) and is reflected at each interface. The phase mismatch of the reflected waves results in radiation losses and reduces the Q factor. The Q factor can be improved by shifting adjacent holes [21]. In the proposed resonator, the first adjacent holes along the microcavity are shifted 90 µm towards the outside and the second and the third hole 90 µm towards the inside.

The performance of the resonator is analyzed with the EM simulation tool CST Microwave Studio. In the simulations, a frequency domain solver is used to get rapid and precise results for the resonator simulation. Frequency samples to sweep were set to automatic type. A tetrahedral mesh type with adaptive mesh refinement was chosen. The boundaries were set to open boundary conditions, which extends the touching geometry virtually to infinity by using a perfectly matched layer (PML) boundary. Two waveguide ports were set up on the WR10 waveguides to simulate S parameters. The WR10 waveguide has a height of 1.27 mm and a width of 2.54 mm, with a recommended single mode frequency range from 75 to 110 GHz. A dominant
TE10 mode was excited in the WR10 waveguides with the electric field oriented parallel to the PhC slab. The simulated electric field distribution at the resonance frequency is shown in Fig. 1c and d. The EM wave propagates through the input taper and waveguide and then is coupled into the microcavity. Within this region, the wave is restricted and forms a strong oscillation at the resonance frequency. Finally, the oscillating wave is coupled to the output waveguide for detection. It should be noted that the absolute value of the electric field is not a realistic value, because the default input power of the waveguide port in the simulation is 0.5 W, which is much higher than the values of the experiments.

The simulated transmission parameter $S_{21}$ is used to evaluate the transmission spectrum of the resonator as shown in Fig. 2. The simulation shows a stopband from 80 to 105 GHz and a resonance frequency at $f_r = 88.23$ GHz. The resonance peak has a FWHM of 113 MHz. Its $Q$ factor can be calculated using the following:

$$Q = \frac{f_r}{\text{FWHM}},$$

(1)

The simulated $Q$ factor is calculated to be 783, which is much higher than achieved in metamaterial sensors [4].

2.2 Sensing Principle

Among the applications thin film sensing, pathogen diagnose is of great interest. To detect the pathogen specially, the surface of the sensor must be functionalized with specific antibodies. After the reaction with them, the goal pathogen, e.g., bacteria, is immobilized on the surface as shown in Fig. 3. After immobilization, the surface can be dried by heating [4] or blowing $N_2$ [10]. Then, a monolayer of the captured bacteria forms a thin film and alters the permittivity. This influences the electric field distribution and results in a shift of the resonance frequency $\Delta f_r$.

If the analyte and its permittivity are assumed to be very small, the perturbed EM field can be approximated by the original field. This approximation is valid since the analyte is in the micrometer range which is much smaller compared to the thickness.
of the PhC resonator with 725 µm. The frequency shift caused by the analyte can be analyzed using perturbation theory [22]:

$$\Delta f = -\frac{1}{2} \Delta \varepsilon ' \frac{\iiint V_s dV |\vec{E}|^2}{\iiint V_0 dV |\vec{E}|^2},$$

(2)

where the $V_0$ is the volume of the resonator and its surroundings and $V_s$ is the volume of the analyte. The analyte changes the complex relative permittivity $\Delta \varepsilon = \Delta \varepsilon ' + j \Delta \varepsilon ''$ in the volume $V_s$. According to Eq. (2), the shift of the resonance frequency depends on the real part of the changed permittivity and the electric field distribution. It can be enhanced by strengthening of the electric field concentration at the site of the analyte.

To evaluate the overall sensing performance independent of the permittivity, a figure of merit (FOM) parameter is defined [10]:

$$FOM = \frac{\Delta f}{FWHM \cdot \Delta \varepsilon}.$$  

(3)

The goal is to have a shift in resonance frequency which is greater than the $FWHM$ of the resonance to enable unambiguous detection of an analyte. From Eqs. (1) (2) and (3), it can be derived:

$$FOM = \frac{1}{2} Q \frac{\iiint V_s dV |\vec{E}|^2}{\iiint V_0 dV |\vec{E}|^2},$$

(4)

Equation (4) shows explicitly that the FOM parameter is proportional to the $Q$ factor. A resonator with a high $Q$ factor has a small $FWHM$ and eases the signal detection. Furthermore, the strong oscillation increases the field strength and hence the interaction with the analyte which leads to stronger shifts of the resonance frequency.

Furthermore, to evaluate the performance of sensors with different configurations and applications, different factors can be considered, such as the thickness and the amount of analyte, resonance frequency, and the transmission intensity [23]. In this article, it is important to evaluate the sensing performance for the thin film, so a $FOM_h$ parameter regarding to unit thickness of the analyte is defined as follows [4]:

$$FOM_h = \frac{FOM}{h_a},$$

(5)
where $h_a$ is the thickness of the analyte.

### 2.3 Simulation of Sensing Performance

To give an insight into the sensing performance of the proposed THz PhC resonator, the dependences of the resonance shift, $FOM$, and $FOM_h$ on the permittivity, the thickness of the analyte and the resonance frequency are investigated by EM simulations. In the simulation, a thin film analyte is modeled as a round spot on the resonator with the radius $r_a = a$ and the thickness $h_a$ as shown in Fig. 4. It is a homogeneous material with the permittivity $\epsilon_a$. Since the thickness of the PhC slab is much larger than the thickness of the film, errors may occur during the simulation. For a reliable simulation, the mesh of analyte must be kept consistent and fine enough. The thin film model is set as an independent mesh with fine mesh step width in the local mesh properties. Only the permittivity of the model is changed from 1 (air) to $\epsilon_a$ to simulate the empty and analyte-loaded resonator. The frequency domain solver in CST is used to achieve high accuracy for the determination of the resonance shift.

Firstly, the dependence on the permittivity of the analyte is investigated by sweeping $\epsilon_a$ from 1 to 4 with a step size of 0.5. The thickness of the analyte was kept constant ($h_a = 1\text{mm}$). As shown in Fig. 5a, the resonance shift shows a linear relationship with the permittivity. Then, the $FOM$ and $FOM_h$ were calculated using Eqs. (3) and (5) and are depicted in Fig. 5b. The $FOM$ and $FOM_h$ (about $0.012 \text{ (µm \cdot PU)}^{-1}$) show only a small variation. The results reveal that the frequency shift is linearly related to the permittivity and the $FOM$ and $FOM_h$ are permittivity independent.

Next, we investigate the dependence on the thickness of the analyte by sweeping $h_a$ from 0.5 to 3 µm with a step size of 0.5 µm. The permittivity was kept constant ($\epsilon_a = 2$). As shown in Fig. 6a, the resonance shift is linearly dependent on the thickness. Figure 6b shows the dependence of the sensing performance, where the $FOM$ shows a linear relationship with the thickness, and the $FOM_h$ (about

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![Fig. 4](image) Modelled thin-film analyte on the surface of the PhC resonator in CST

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0.012 (μm • PU) shows only a slight variation. The results indicate that the resonance shift and the FOM are linearly dependent on the thickness, while the FOMh is independent of the thickness of the analyte.

Finally, the dependence on the resonance frequency was investigated by scaling the resonator with a constant Q factor to higher frequencies. Within the PhC, the period of the holes was varied ($a = 265\mu m, 159\mu m, 114\mu m, 88.3\mu m, and 72.2\mu m$) while the ratio of the parameters was kept constant ($r = 0.28a$ and $h = 0.81a$) to achieve a resonance frequency at 300, 500, 700, 900, and 1100 GHz, respectively, with a constant Q factor ($Q \approx 780$). The permittivity and thickness of the analyte were kept constant ($\varepsilon_a = 2$ and $h_a = 1\mu m$). In Fig. 7a, the resonance shift increases with increasing resonance frequency. Figure 7b shows that the FOM and FOMh are linearly related to the resonance frequency. The results reveal that the sensing performance improves with the increase of the resonance frequency.

Based on the above simulation results, it can be concluded that the resonance shift is linearly related to the permittivity and thickness of the analyte. The FOMh is independent on the permittivity and thickness, but only dependent on the resonator’s
own characteristics. Overall, it can be observed that the sensitivity scales with frequency. In addition, the size of the sensor reduces with increasing frequency, allowing the realization of a very compact and thus cost-efficient devices that are ideally suited for PoC applications.

3 Measurement Setup

3.1 Fabrication of the PhC Resonator

Although resonators with increased resonance frequency have better sensing performance, the fabrication cost increases due to the requirement of nonstandard wafers and technology. Considering the cost, a standard HRSi wafer with a thickness 725 µm was used for fabrication of the resonator at 88.23 GHz in the millimeter range to prove the concept and validate the theoretical analysis. With the standard wafer, a deep reactive ion etching (DRIE) process from Fraunhofer IMS [20] was used to achieve vertical sidewalls with a high aspect ratio. On the topside of the wafer, a 12-µm-thin layer of photoresist was coated and then patterned by photolithography. An UV curable tape was covered on the backside as an etch-stop layer. After that, the wafer was etched by the DRIE process until the holes reached the backside. The fabricated resonator is shown in Fig. 1b.

3.2 Preparation of the Analyte

As described in Sect. 2.2, the resonance shift depends on the permittivity and volume of the analyte. In general, the size of bacteria is in the micrometer range (about 0.5–8 µm) [24]. In practice, the functionalization and immobilization processes are time-consuming and require specialized laboratory, which complicates the work with actual samples. Furthermore, functionalized biosensors are difficult to clean and cannot be reused. In this work, commercial SiO₂ beads were used as

Fig. 7 Simulation of the PhC resonator of varying resonance shift with the analyte: a resonance shift; b FOM and $FOM_h$

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a substitute for biomolecules to simplify the measurement process. The coverage of the beads on the surface of the resonator can be estimated as described below.

Firstly, the beads were prepared as a solution. Commercial SiO₂ beads with diameters of 0.5, 1, and 2 µm were bought from Merck. They are suspended in water with a known solid content \( s = 5\% \), which is the weight ratio of the SiO₂ in the entire suspension. The SiO₂ concentration \( C \) is defined as the amount of the SiO₂ particles in 1 mL suspension and can be calculated as follows:

\[
C = \frac{m_{\text{bead}}}{V_{\text{bead}} \rho_{\text{bead}} + m_{\text{water}}/\rho_{\text{water}}},
\]

where \( m_{\text{bead}} \) and \( m_{\text{water}} \) are the weight of beads and water in 1 g suspension (0.05 g and 0.95 g), respectively. \( \rho_{\text{bead}} \) and \( \rho_{\text{water}} \) are the density of SiO₂ and water, respectively. \( V_{\text{bead}} \) is the volume of a single bead. Based on the calculated concentration, the original suspension can be diluted to the desired concentration.

A small volume of the diluted suspension is transferred onto the surface of the resonator using a pipette. After the suspension dries, only the SiO₂ beads remain on the surface as shown in Fig. 8a. Since the volume and concentration are known, the number of the beads in one drop \( N_{\text{drop}} \) can be calculated as follows:

\[
N_{\text{drop}} = V_{\text{drop}} \cdot C,
\]

where \( V_{\text{drop}} \) is the volume of one drop. The coverage \( R \) of the analyte is defined as the number of beads on 1 µm² area and can be expressed as follows:

\[
R = \frac{N_{\text{drop}}}{S_{\text{drop}}},
\]

where \( S_{\text{drop}} \) is the area of the dried drop. The coverage \( R \) and \( S_{\text{drop}} \) can be adjusted by the volume of one drop \( V_{\text{drop}} \) and the dilution ratio. In our test, the water droplet

![Fig. 8 a Dried drop on the resonator surface; b measurement setup: The PhC resonator is fixed with rectangular waveguides (WR10) and a 3-D printed support](image-url)
shows a coffee ring effect, which leads to an inhomogeneous distribution with a strong concentration of the microbeads in the outer ring. The water dries slowly, which increases the measurement time. This can be compensated by using an ethanol solution. Ethanol supports the spreading of the droplets, reduces the coffee ring effect, and dries faster. After testing different water–ethanol ratios and drop volumes, measurements were performed using a ratio 1:1 and a volume of 0.2 µL. Using this setup, the droplets can spread well and stay only on the surface as shown in Fig. 8a. After observing the dried beads on the resonator, $S_{\text{drop}}$ is defined as the area of the circle with the radius of the period of the PhC $a$.

### 3.3 Experimental Setup

The experiments were performed using a Keysight PNA-X network analyzer (NWA) N5247B with a Keysight millimeter test set N5292A. The Keysight broadband frequency extender N5295 is used for W band (75–110 GHz) measurements. WR10 rectangular metallic waveguides are connected with the extenders. As shown in Fig. 8b, the resonator was held using a 3-D printed support made of Polyamid 12. The tapers of the PhC resonator are used for impedance matching and energy coupling between the WR10 waveguide and the PhC waveguide. The influence of the depth of the tapers in the WR 10 waveguides was investigated by simulations. The simulation results showed that the resonance frequency does not change and the amplitude at the resonance frequency shows minimal difference when the depth is varied. Thus, to maintain the same position of the resonator in each measurement, the tapers were completely inserted into the WR10 waveguides. The transmission parameter $S_{21}$ is measured to observe the frequency spectrum of the resonator. The frequency resolution was set to 100 kHz. Before measurements, the device is calibrated using through waveguide, offset waveguide and short termination. However, the parasitic effects of the devices cannot be eliminated completely. To obtain reliable measurement results, the averaging function and the smoothing function of the NWA were used. Each curve was averaged from 10 scans and smoothed by computing a moving average over 1% of the trace. As shown in Fig. 9, the measured transmission parameter $S_{21}$ presents a stop band from 80 to 105 GHz and a resonance at 88.51 GHz with a $\text{FWHM}$ of 118 MHz. The $Q$ factor is calculated to be 750. The measured results agree well with the simulated result. The small difference between the simulated and measured resonance frequency may be due to variation in the permittivity of the silicon and fabrication tolerances.

### 4 Measurement Results

With this experimental setup, the sensing performance of the resonator was characterized with a diluted solution of SiO$_2$ beads as described in Sect. 3.2. First, the resonator was connected to the NWA and its original resonance frequency was determined. Then, 0.2 µL of the diluted SiO$_2$ suspension was dropped on the resonator using a pipette. A decrease in $S_{21}$ amplitude can be observed, which is due to the losses in water and
ethanol. As the drop dries, the transmission is increasing. The drying of the drop ends when the $S_{21}$ parameter becomes static. Then, the shifted resonance frequency was recorded. After this, the resonator was washed with ethanol to remove the beads. Since the use of the pipette leads to slight variances in drop volume and position, this procedure was repeated 10 times and their average was calculated to minimize random effects. The procedure was repeated for different concentrations as well as for different sizes of the beads. The different bead concentrations provide information about the coverage. Different sizes of the beads give an idea of the effect of the analyte size. To interpret the biological information as EM parameters, a thin-film model with effective permittivity was created in CST.

4.1 Modelling as Thin Film

The coverage of the analyte on the resonator surface was interpreted as an EM analysis that models it as a thin film medium with homogenous permittivity. This allows us to predict the sensing performance by simulation. In the model of the thin film, the thickness is equal to the diameter of the bead, and the area is equal to the area of the dried drop. The permittivity of the film is set as the effective permittivity of the SiO$_2$ beads and their surrounding air. The SiO$_2$ beads are seen as SiO$_2$ spheres with a permittivity $\varepsilon_{\text{bead}} = 4.5$ [25], and the permittivity of air is approximated with $\varepsilon_{\text{air}} = 1$. The effective permittivity $\varepsilon_{\text{eff}}$ can be estimated by effective medium theory [26]:

$$\varepsilon_{\text{eff}} = v_{\text{bead}} \varepsilon_{\text{bead}} + (1 - v_{\text{bead}}) \varepsilon_{\text{air}},$$

(9)

where the $v_{\text{bead}}$ is the volume fraction of the beads. The effective permittivity depends on the calculated coverage ratio $R$ from the preparation.

4.2 Sensitivity to the Beads of Different Concentrations

In the first measurement, 2-µm beads were diluted into different concentrations as shown in Table 1. $A = 6.4 \cdot 10^8$ particles/mL is defined as the unit concentration. A
maximum concentration was calculated, with which a layer of beads is fully covering the surface. Then, the concentrations used were chosen to be less than the maximum concentration. The coverage and effective permittivity of the dried 0.2-µL drop were calculated as explained in Sect. 3.2 and listed in Table 1.

The measurements were repeated 10 times for each concentration. The calculated mean and standard deviation of the resonance shifts for different concentrations are listed in Table 1 and plotted in Fig. 10a. The resonance shift shows a linear relationship with the concentration, which in turn is linearly related to the coverage. The calculated coefficient of determination is 0.9883. This can be explained by Eq. (2): As the number of the beads increases, the volume of the analyte $V_s$ becomes larger and the resonance shift increases. The deviation stems from the tolerances of the manual processing and the measurement environment. The standard deviations are between 0.40 MHz and 0.60 MHz. Figure 10a shows the simulation results for the thin film model with the effective permittivity. The simulated resonance shift is linearly related to the variation of the permittivity with a coefficient of determination of 0.9993. As shown in Fig. 10b, the simulated $FOM_h$ is about 0.012 ($\mu$m $\cdot$ PU)$^{-1}$. The measured $FOM_h$ with the calculated effective permittivity are in good agreement with the simulated results.

### 4.3 Sensitivity to the Beads of Different Sizes

As a next step, the PhC resonator was characterized with beads of different diameter to investigate the effect of different analyte sizes. The beads with 0.5, 1, and 2 µm diameter were diluted into concentrations of 64A, 16A, and 4A, respectively, so that the effective permittivity remained constant, as shown in Table 2.

The mean and standard deviation of the resonance shifts were calculated for 10 measurements as shown in Table 2. The resonance shift increases with the increase of the bead diameter. The standard deviations are between 0.40 and 0.60 MHz. In the simulations, the thickness of the analyte was equal to the diameter. Thin films with an effective permittivity of 2.94 and thicknesses of 0.5, 1, and 2 µm were simulated. The simulated and measured results show good agreement as shown in Table 3. The relationship between the resonance shift and the thickness can be

| Concentration | Coverage (particle/µm²) | Effective permittivity | Mean resonance shift (MHz) | Standard deviation (MHz) |
|---------------|-------------------------|------------------------|---------------------------|--------------------------|
| A             | 0.07                    | 1.48                   | 1.86                      | 0.46                     |
| 1.5A          | 0.10                    | 1.73                   | 2.25                      | 0.54                     |
| 2A            | 0.13                    | 1.97                   | 2.64                      | 0.40                     |
| 2.5A          | 0.17                    | 2.21                   | 3.43                      | 0.49                     |
| 3A            | 0.20                    | 2.45                   | 3.92                      | 0.58                     |
| 3.5A          | 0.23                    | 2.70                   | 4.54                      | 0.52                     |
| 4A            | 0.26                    | 2.94                   | 5.34                      | 0.53                     |
explained by Eq. (2). The resonance shift is linearly related to the concentration of the electric field in the analyte volume $V_s$ for the same variation of the permittivity, where the area of the analyte is constant. Thus, the resonance shift increases with the increasing thickness. The simulated $FOM_h$ is about 0.012 (μm $\cdot$ PU)$^{-1}$, which is consistent with the measured results.

It can be noted that the measured standard deviations are between 0.40 and 0.60 MHz for all concentrations and sizes and do not increase with the increasing resonance shift. This may have two reasons: temperature variations of the environment and tolerances in the liquid transfer. In practice, it is difficult to precisely reach a constant temperature and an identical transfer of the liquid. However, improving the resonance shift and the sensitivity may reduce the impact of these factors. Furthermore, this issue may be addressed by using a reference channel and a micro-fluidic channel in future works. More details on possible solutions are discussed in Sect. 5.

To investigate the sensing performance of the PhC resonator, it was characterized with beads with different concentrations and different diameters. The resonance shift is linearly related to the coverage and the effective permittivity and increases with increasing diameter. The simulation results using the thin film model are consistent with the experimental results. In addition, the $FOM_h$ measured with the beads of different diameters shows agreements with that measured with the beads of different coverage ($FOM_h = 0.012$ (μm $\cdot$ PU)$^{-1}$). However, despite the high $Q$ factor,

![Fig. 10](image.png)

**Fig. 10** Two-micrometer beads of different concentration: a mean value of the measured frequency shift compared to simulation; b $FOM_h$ of the measurement and the simulation

| Diameter (μm) | Concentration | Coverage (particle/μm²) | Effective permittivity | Mean resonance shift (MHz) | Standard deviation (MHz) |
|---------------|---------------|--------------------------|------------------------|---------------------------|--------------------------|
| 0.5           | 64A           | 4.23                     | 2.94                   | 1.98                      | 0.40                     |
| 1             | 16A           | 1.06                     | 2.94                   | 2.65                      | 0.59                     |
| 2             | 4A            | 0.26                     | 2.94                   | 5.34                      | 0.53                     |

![Table 2](image.png)

**Table 2** Beads of different diameters
the achieved $FOM_h$ is still unsatisfactory. Observing Eq. (4), the $FOM$ parameter depends on both $Q$ factor and field concentration at the site of the analyte. Figure 1 (d) shows that the electric field is mainly concentrated inside the silicon, but the beads were placed on the surface of the silicon. The $FOM_h$ parameter can be improved by enhancing the overlap of the electric field and the analyte. A possible solution is explained in Sect. 5. Furthermore, the simulation results in Sect. 2.3 show that the $FOM_h$ increases with increasing resonance frequency. This suggests that our sub-terahertz resonator should be extended to higher frequency to obtain a higher $FOM_h$.

5 Conclusion and Future Works

In this work, we proposed a THz sensor based on a high-$Q$ PhC resonator as a thin-film sensor for the potential applications in bacteria detection. The PhC slab consisting of a HRSi plate with air holes restricts EM wave propagation within the bandgap frequency. The PhC slab resonator is realized by introducing a defect hole in the PhC structure, into which the EM wave enters through evanescent wave coupling. The $Q$ factor is improved by adjusting the position of the adjacent holes. The simulations show the working principle of the PhC resonator as a thin film sensor and the dependence of the sensing capacity on the permittivity, thickness of the analyte, and the resonance frequency. Considering the production cost, a standard HRSi wafer was used to fabricate the PhC resonator at 88.51 GHz in the millimeter range using a DRIE process. The resonator shows a high $Q$ factor of 750. Since the sensing performance depends on the $Q$ factor and the concentration of the electric field on the site of the analyte, the PhC resonator, as a thin film sensor, offers advantages over existing methods such as metasurface.

To verify the sensing performance for small particles in the micrometer range, we utilized commercial SiO$_2$ beads with diameters of 0.5, 1, and 2 µm as analyte. SiO$_2$ microbeads were prepared as a water–ethanol mixture. The coverage of the beads on the surface of the resonator was calculated. Solutions of different concentration and beads of different sizes were characterized. The resonance shift is linearly related to the coverage. Furthermore, a thin-film model with calculated effective permittivity was created in CST. The simulated results show good agreement with the measured results. The thin-film model gives a good explanation for the effect of the coverage and the bead diameter.

| Diameter (µm) | Measured resonance shift (MHz) | Simulated resonance shift (MHz) | Measured $FOM_h$ ((µm • PU)$^{-1}$) | Simulated $FOM_h$ ((µm • PU)$^{-1}$) |
|---------------|-------------------------------|-------------------------------|-------------------------------------|-------------------------------|
| 0.5           | 1.98                          | 1.60                          | 0.0173                              | 0.0129                        |
| 1             | 2.65                          | 3.00                          | 0.0116                              | 0.0121                        |
| 2             | 5.34                          | 5.80                          | 0.0117                              | 0.0117                        |
The experiments show that the $FOM_h$ of the PhC resonator to be 0.012 ($\mu$m $\cdot$ PU)$^{-1}$. However, the sensitivity is inferior compared to the state-of-the-art THz metamaterial biosensor ($FOM_h$ of 0.2 ($\mu$m $\cdot$ PU)$^{-1}$) [11]. The first reason is that the resonance frequency in [11] is at 435 GHz, which is 5 times higher compared to our work. Increasing the resonant frequency leads to shorter wavelengths and higher concentration of the electric field, which enhance the sensitivity. The second reason is that the electric field is mainly concentrated within the silicon as shown in Fig. 1 (d), where the analyte is not positioned. As shown in Eq. (4), the $FOM$ parameter depends on both $Q$ factor and field concentration at the site of the analyte. The field concentration can be greatly enhanced by introducing an open area, such as a slot, at the location of the maximum electric field. This will enhance the interaction with the analyte and improve the $FOM_h$ greatly. Therefore, improving the sensitivity is the focus of our current work.

In the experiments, the results showed high standard deviations, that may lead to erroneous results in potential biosensing applications. The first reason is the environment of the measurement, including the temperature and the device noise. According to the measurements, the deviation of the resonant frequency over temperature is $-66$ ppm/$^\circ$C [27]. A possible solution is a PhC chip with two channels. One is the sensing channel, and the other is the reference channel. These two channels respond to the environment in the same way. Therefore, the influence of the environment can be compensated. The second reason is the manual transfer of the liquid. It introduces tolerances in the drop volume and drop position. This problem can be solved by a microfluidic channel which manipulates the liquid automatically. Furthermore, by improving the sensitivity of the resonator, the resonance shift can be greatly increased. Based on this, the error will be much smaller compared to the resonance shift. This ensures unambiguous measurement results.

However, defining the minimum detectable amount of the analyte remains a difficult task. Whether a difference due to analytes can be detected with an acceptable confidence depends on many factors, such as the sensitivity of a sensor, tolerances, frequency/amplitude resolution of the measurement device, measurement setup, analyte preparation, and data processing techniques. A possible way to define an acceptable confidence is that a frequency shift must be higher than 3 times standard deviation of the entire measurement process, such that this shift has a 99.73% possibility of correlating to a shift caused by analyte. In our experiments, the measured standard deviations are between 0.4 and 0.6 MHz, which come from the whole system tolerances of our measurement procedure. But 10 times measurements are still a small number to evaluate the system standard deviation. In future works, we will further investigate how to characterize and reduce the system tolerances.

Nevertheless, the PhC resonator is promising for thin film sensing applications and shows many advantages. First, the PhC resonator can be easily mass-produced from silicon fabrication to reduce costs. Second, the high $Q$ factor is beneficial to ease the measurement and enable high sensitivity. Third, the resonator can be coupled from waveguides, freeing it from the high free-space losses in THz free space transmission, which reduces the requirement for high-power components and simplifies the measurement setup. Furthermore, multiple channels can be implemented on a small
PhC chip to eliminate environmental factors and detect several pathogens simultaneously. This approach shows high potential for desirable biosensing applications.

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