



Design and Simulation of a Novel Tunable Terahertz Biosensor Based on Metamaterials for Simultaneous Monitoring of Blood and Urine Components

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Received: 6 November 2020 / Accepted: 4 February 2021 / Published online: 9 March 2021
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Abstract

In this essay, a tunable metamaterial-based biosensor is proposed for simultaneous monitoring of blood components including cells, plasma, water, thrombus, and urine components as well as glucose, albumin, and urea. The proposed biosensor is based on optical sensors, and it provides real-time, label-free, and direct detection, small size, and cost-effectiveness that can be an alternative tool to other conventional methods. The influence of operating frequency, sample thickness, temperature, and radiation angle on the performance of the sensor is investigated by the finite element method (FEM). Numerical results show that the maximum sensitivity and figure of merit (FoM) in the high frequency are 500 (nm/RIU) and 2000, and for low frequency are 136 ($\mu\text{m}/\text{RIU}$) and 155, respectively. The footprint of the structure is $0.34 \mu\text{m}^2$, which is remarkably smaller than the other reported biosensing structures. The proposed biosensor has the potential to provide high sensitivity, high FoM, and a wide operating range for biomedical applications.

Keywords Nano-biosensor · Biomaterial · Biosensor · Metamaterial · Blood

Introduction

Today, prostate cancer is one of the most common diseases in men, especially adults. This disease may not appear in the early stages; in more advanced stages, it can cause problems in urinating, blood in the urine, or pain in the pelvic and waist regions during urination. Another symptom that occurs later is the low level of red blood cells [1–11]. For these reasons, the use of extremely accurate and rapid biosensors can be very useful in examining the components of blood and urine. Biosensors are highly effective tools for clinical and diagnostic, industrial, environmental monitoring, food industry, and so on [12–23]. The biosensor must be very accurate, highly sensitive, and show linear behavior relative to different concentrations. They should be small and not damage biological tissue for use in clinical trials. Also, a biosensor must perform real-time analysis that can be used to quickly measure analytes from human samples. The analyte should be

stable and specific under normal storage conditions, and the biosensor must be portable, cost-effective, small, and usable by semi-skilled operators. They have several types including electrochemical, amperometric, potentiometric, thermometric, optical, and luminescent [24–33]. Amongst these, optical sensors are good candidates because of their high sensitivity, portability, sample-free label, and low-cost and high-speed for sample preparation [34–37]. The main problems of optical biosensors are related to the interaction of biological molecules with the sensor surface, as well as their integration for making small devices. The environmental monitoring sensors with high sensitivity are other important sensors. Based on their structure, optical sensors include different types such as photonic crystals [38, 39], metamaterials (MMs) [40, 41], optical fibers [42], plasmon-induced transparency [43], and so on [44–64]. The unique properties of MMs are the negative refractive index and confining electromagnetic waves [65, 66]. MMs were introduced theoretically in 1968 by the Russian physicist Victor Veselago. Unlike natural materials, MMs can have a negative refractive index; therefore, they are not found in nature. To achieve such a structure, we use a combination of resonators (with negative μ) and an array of thin metal wires (with negative ϵ), which ultimately leads to a negative refractive index ($n = \sqrt{\epsilon\mu}$). MMs have many

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advanced applications such as cloaking [67], miniature antenna [68–74], superlens [75], absorber [76], and so on [13, 56, 77–87]. In several works, MMs are used as a biosensor for the detection of biological tissues. Typically, the main components of MMs are resonators, which have a certain resonance frequency according to their shape and size [88]. The MM biosensors in terms of their operating frequency regime are divided into several groups of microwave [89], terahertz [90], and plasmonic [91]. As the frequency rises, the sensor's dimensions become smaller [15, 92–94]. Thus, they will be able to detect samples with a very small thickness (at nanoscale) [95]. Also, MM biosensors can be used to detect DNA [96], cancer cells [97], and microfluidic applications [40] among other uses. The main factor for detecting the above-mentioned cases is the variation of the dielectric constant of under test cells. For example, a cancerous cell has more water content than a normal cell, which results in a higher dielectric constant and electrical conductivity [98]. Also, blood components such as blood plasma, cells, clots, and water have a certain refractive index. About 55% of blood is made up of plasma, and the rest includes red and white cells and also platelets [99]. The dielectric constant also changes with glucose concentration in blood (or urine) [100]. Therefore, it is the main parameter for detecting glucose concentration. In this regard, several research groups have examined the changes in dielectric constant at different concentrations of glucose-based spectroscopy [101]. For instance, in Robinson and Dhanlaksmi [102], a photonic crystal biosensor is provided to detect the concentration of glucose, albumin, and urea in urine at 1550-nm wavelength. Tao et al. [103] measured experimentally the concentration changes of glucose and urea in the water using MM-based biosensors. MMs used in this work have a substrate of paper. This feature partly defines the practical aspects of this detection method. From a practical perspective, some of these structures suffer from a serious problem, i.e., their big footprint and labeled material detection, which leads to high-cost products [104–113].

In the present works, a MM biosensor structure is designed based on split-ring resonators (SRRs), in which the operating frequency regime can be easily tuned by changing the size of the system or incident angle. The main mechanism of the proposed structure is based on the shift in the resonance frequency. Besides, to show their diagnosis ability, the variations in the transmission and reflection amplitude of waves have been investigated. One of the main advantages of our proposed sensor is the tunability of operation frequency. Hence, the proposed sensor is evaluated for low-frequency operations (1–2 THz) and high-frequency operations (around 193 THz), which perfectly reflect the trait of the tunable sensor. As will be discussed later, environmental parameters such as temperature and thickness of the samples can affect the response and performance of the sensor. Therefore,

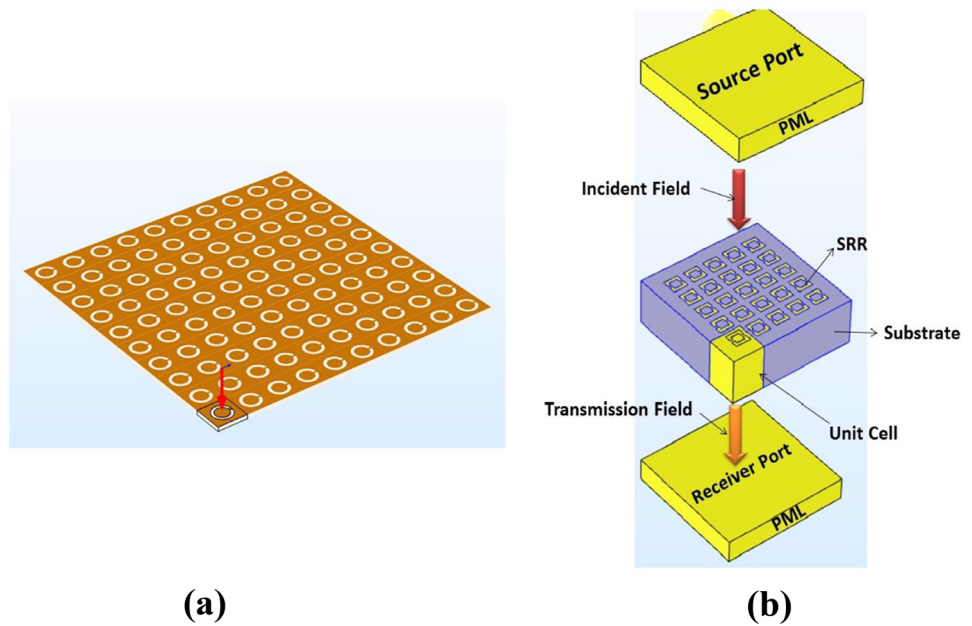
mentioned parameters can be well controlled under laboratory conditions. For computer simulations, a proper physical model is needed for biological tissues. One of the widely used models for this purpose is the Debye model. Finite-element-method (FEM) is applied to calculate the partial differential equations (PDEs) in 3D space. Numerical results show that the maximum sensitivity and figure of merit (FoM) in the high frequency are 500 (nm/RIU) and 2000, and for low frequency are 136 ($\mu\text{m}/\text{RIU}$) and 155, respectively. This study provides a path for the development of novel nano-scale practical biomedical applications.

The Physical Structure and Operation of the Proposed Sensor

In this section, the geometrical parameters of the proposed structure are presented. As we know, the base and foundation of the MM structures are the resonators, which have different geometric shapes. The most common resonator in this regard is the split ring-resonator (SRR). A metal (e.g., copper and gold) resonator is placed on an insulator substrate. Our suggested biosensor structure is based on frequency-selective-surface (FSS) filters. Figure 1a presents an overview of an FSS that includes arrays of SRRs that are located on a sub-layer. The waves fall in the direction of the red arrow. The resonators resonate at a specific frequency, depending on their size and shape, and pass or filter a particular frequency. The main sensor structure is shown in Fig. 1b. Here, the resonator structure is in the form of the square that is located on a Teflon (PTFE) substrate with a dielectric constant of 2.1. Also, we used a perfectly matched layer (PML) to confine the areas of mathematic computational in the simulation process for open-boundary problems.

For the sake of simplicity, the periodic boundary conditions in the FEM analysis, which refer to repeated cells, are considered. The basis of detection in this method is the variation in the refractive index of analytes that are placed on the sensor. Our analytes here are blood and urine. Changes in the level of glucose (urea or albumin) result in the refractive index change of the blood (urine). The proposed sensor has resonators with a specific resonance frequency under normal conditions (without any sample), which is a function of the environmental refractive index. Now, if an analyte is placed on the sensor, the resonance frequency of the sensor will shift. The main objective of this paper is to diagnose blood components such as whole blood, blood cells, blood plasma, thrombus, and water. Also, the concentrations of glucose in the blood and urine, albumin, and urea in urine are calculated. In the next section, we will examine the optical properties of these tissues.

Fig. 1 (a) The overall schematic of a FSS. (b) An overview of the array structure of the biosensor



Fundamental Modeling Data

This section examines the parameters and models that are needed to simulate the biological tissues such as blood and urine components. The biological models are expressed in two frequency ranges from 0.2 to 2 THz (low frequency) and around 193 THz (high frequency). There are two reasons for using high- and low-frequency modes: First, the biosensor can be easily tuned by an only change in the sensor’s unit cell size. Second, the sensor operation at low and high frequencies resolves many challenges. Also, for the mentioned frequency ranges, the experimental refractive index and the dielectric constant of the samples are available. Debye parameters of blood components (BCs) in the 0.2–2 THz regime were extracted from [114].

Modeling of Bio-tissues in the 0.2–2 THz

In this work, the Debye model is used to reveal blood components such as whole blood, blood cells, blood plasma, thrombus, and water, as follows:

$$\epsilon(\omega) = \epsilon_\infty + \sum_{n=1}^i \frac{\Delta\epsilon}{1 + j\omega\tau_n} = \epsilon_\infty + \frac{\epsilon_s - \epsilon_2}{1 + j\omega\tau_1} + \frac{\epsilon_2 - \epsilon_\infty}{1 + j\omega\tau_2} \tag{1}$$

where ϵ_∞ is the real part of the permittivity at a high-frequency limit, ϵ_s and ϵ_2 are static limit permittivity and intermediate dielectric value, τ_1 and τ_2 are relaxation times of the first and second relaxation process, and ω is the angular frequency. The values of these parameters are shown in Table 1 for blood components in the range of 0.2–2 THz [114].

The Debye parameters of single-pole are extracted from [115] according to the glucose concentration in the blood plasma for amounts from 0 to 16,000 (mg/dl).

Modeling of Bio-tissues at High Frequency (1550 nm)

In the following, the concentration of glucose in blood and concentrations of glucose, albumin, and urea in urine are studied. For this purpose, the variation of the refractive index is considered. The refractive indices and electrical conductivities for various concentrations at high frequencies (about 193 THz) are taken from. Considering these values, it is observed that by changing the concentration, the refractive index changes from 1.335 to 1.348. The electrical conductivity values are taken into account for losses, which are modeled as follows [44]:

$$N = n + ik \equiv \sqrt{\epsilon_r} \tag{2}$$

Table 1 Debye parameters belong to blood components in the 0.2–2 THz regime [114]

$\tau_2(ps)$	$\tau_1(ps)$	ϵ_2	ϵ_s	ϵ_∞	Blood components
0.1	14.4	3.8	130	2.1	Whole Blood
0.1	16.1	3.7	130	2.2	Thrombus
1.8	410.8	23.8	2.5	3.4	Blood Cells
0.1	8.0	3.6	78.8	1.7	Blood Plasma
0.1	8.4	4.5	78.8	3.3	Water

$$n = \sqrt{\frac{|\epsilon_r| + \epsilon'_r}{2}}, k = \sqrt{\frac{|\epsilon_r| - \epsilon'_r}{2}} \tag{3}$$

$$\epsilon_r = \epsilon'_r - i\epsilon''_r = \epsilon'_r + i\frac{\sigma}{\omega\epsilon_0} \tag{4}$$

where n and k are real and imaginary parts of the refractive index, respectively; σ refers to the electrical conductivity of the material; and ϵ_0 is the vacuum dielectric constant.

According to the above data, the resonant frequency of the proposed sensor is set in the low frequency (0.2–2 THz) and high frequency (around 193 THz). The results are discussed in the next section.

Results

Low Frequency

In this section, we set the frequency resonance of the system to operate at the frequency range of 0.2–2 THz. Figure 2a shows the accurate dimensions of the sensor unit cell. Figure 2b presents the frequency response of the system.

The blue and red graphs are related to the transmittance and reflectance of the stricter, respectively. The system, in this case, has a resonant frequency, about 1.94 THz.

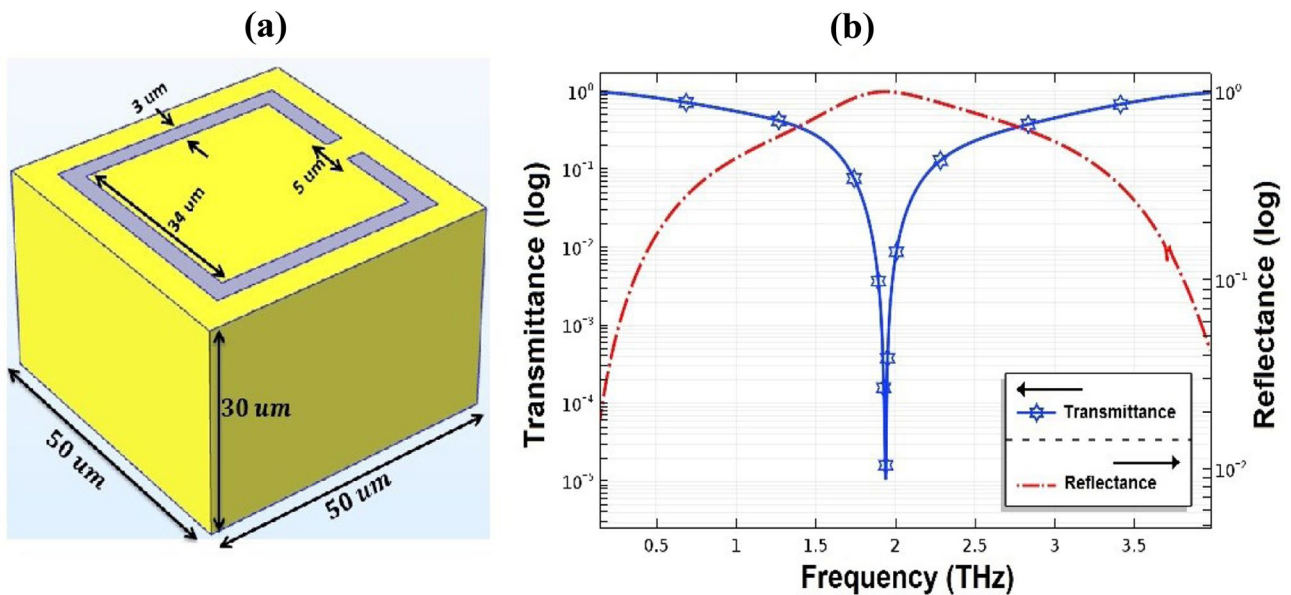


Fig. 2 (a) Structure and dimensions of the proposed sensor unit cell for operation at the low-frequency regime. (b) Frequency response of the proposed sensor at the low-frequency regime

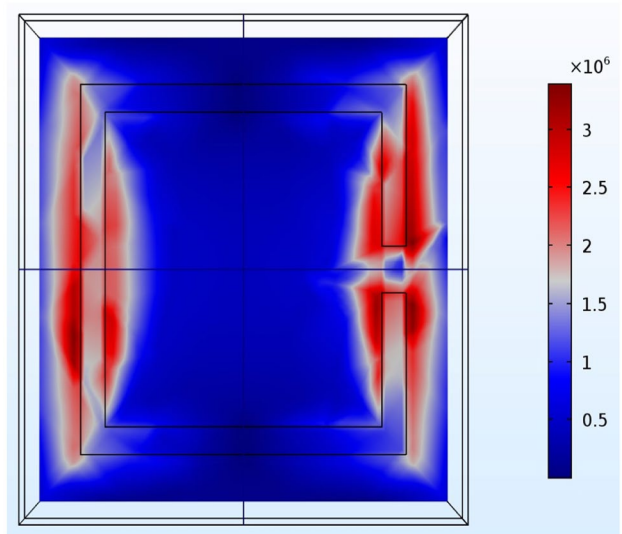


Fig. 3 Electric field distribution at the frequency of $f = 1.94$ THz

Figure 3 shows the distribution of the electric field at the resonant frequency (1.943 THz) of the system.

By placing samples on the sensor, consider into account their dielectric constants, a blue shift occurred at the resonant frequency. Figure 4 presents the frequency response variations for different blood components. The lower and higher resonant frequencies correspond to the blood plasma (1.55 THz) and water (1.37 THz), respectively.

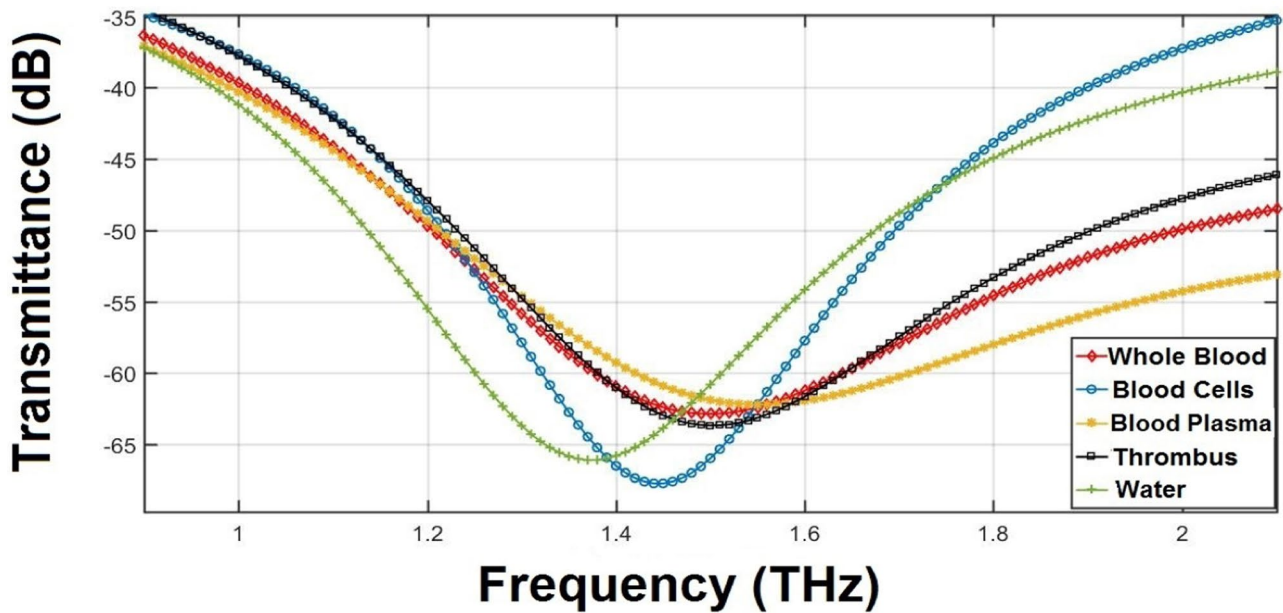


Fig. 4 Variation in the resonance frequency of the system for different blood samples

Figure 5 shows the frequency response of the sensor for different glucose densities in the blood plasma.

The dielectric constant is changed via different glucose concentration, and, therefore, various frequency response is met. Considering no sample state, the minimum and maximum frequency shifts correspond respectively to 1000 and 16,000 mg/dl with the resonance frequency of these concentrations being 1.82 and 1.12 THz.

High Frequency (About 193 THz)

As the operating frequency of the system increases, the dimensions of resonators diminish. Figure 6 presents the unit cell dimensions of the proposed sensor for working near the 193 THz frequencies. The sub-layer used here is Teflon, which has a refractive index of 1.34.

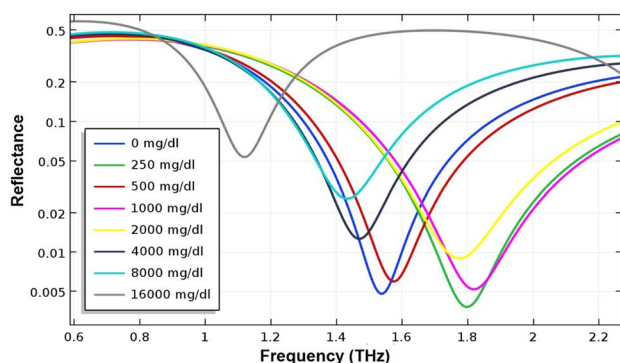


Fig. 5 Frequency response of the sensor as a function of the concentration of glucose in the blood plasma

The transmittance and reflectance diagrams of the sensor for frequencies around 193 THz are shown in Fig. 7. The accurate value of the resonant frequency of the system is 193.4 THz (1550 nm). Figure 8 also illustrates the distribution of the electric field at a frequency of 193.4 THz.

Figure 9 shows the change of the resonance frequency as a function of the blood glucose, urine glucose, albumin, and urea concentrations. As can be seen, with increasing the concentration of these parameters in blood and urine, the resonance frequency of the system shifts to lower frequencies. Although the difference in the refractive indices is very low ($\Delta n = 0.001$), as can be seen, the graphs of each of the concentrations are separated by a good resolution. The minimum resolution between the concentrations is 0.01 THz. The lowest and highest shifts in the frequency response of the system are related to the refractive index of 1.35 (normal concentrations) and 1.348 (10 mg/dl), respectively. The resonant frequency values for these concentrations are 191.6 and 190.81 THz, respectively.

Effective Parameters on the System Response

Thickness of Samples

The thickness of the placed samples on the sensor can somewhat affect the response of the system. Figure 10 depicts the frequency response of the system for different thicknesses of the whole blood. As can be seen, by increasing the sample thickness, the system

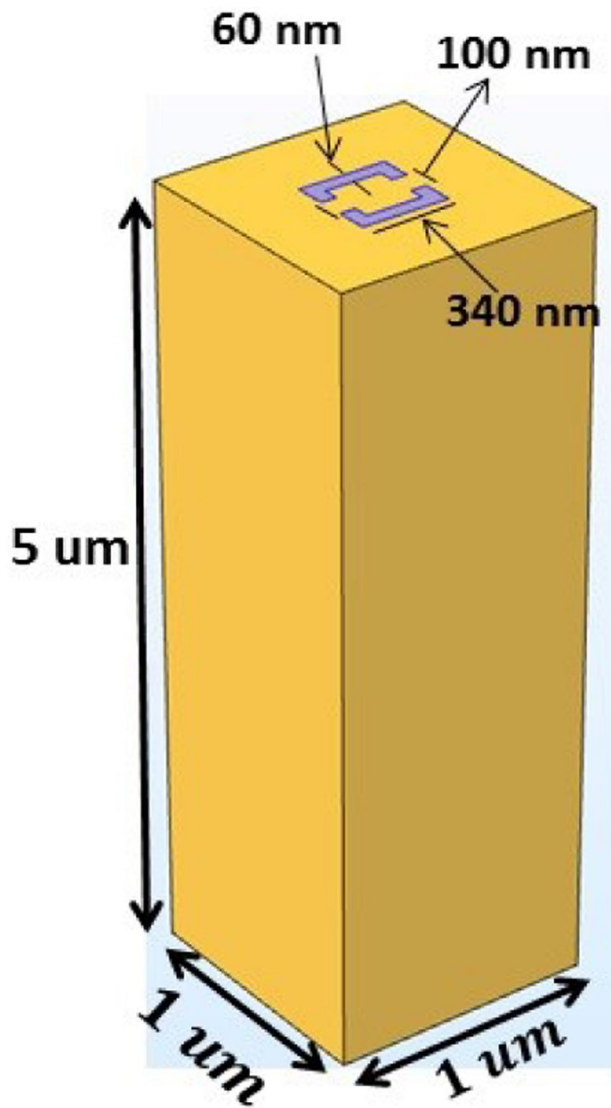


Fig. 6 The sensor unit cell dimensions for operation at a high-frequency regime

resonant frequency moves toward lower frequencies. At high thicknesses, the changes in the resonant frequency become negligible such that only the transmission amplitude is reduced.

Temperature

The ambient temperature can affect the response of the system [116, 117]. The fluid part of the blood, which is called plasma, mainly consists of water. Therefore, the temperature can affect this part of the blood and change its dielectric constant. As temperature rises, the real part of the dielectric constant reduces, and the electrical conductivity increases. Figure 11 presents the thermal effects on the dielectric

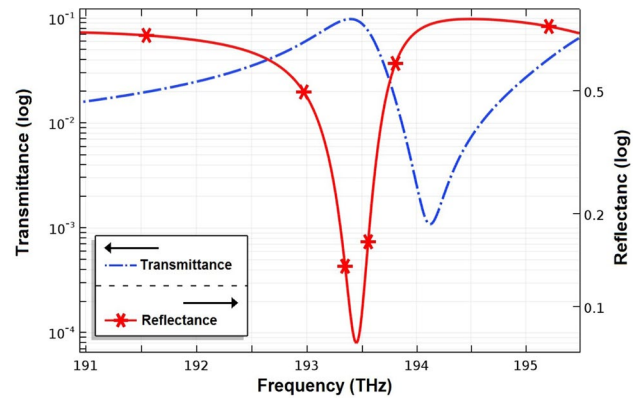


Fig. 7 Transmission and reflection diagram of the proposed sensor at high frequencies

constant and the electrical conductivity of the water. As can be seen, with increasing temperature from 293 to 333 K, the dielectric constant of water decreases from 4.6 to 3.9 and its electrical conductivity rises from 88 to 170 (S/m).

Figure 12 shows temperature changes in the frequency response of the system. According to the simulation results, by increasing temperature, the resonance frequency of the sensor shifts toward higher frequencies (less variation). Also, the transmittance amplitude is reduced, suggesting that the system will have more casualties.

Sensitivity and FoM

In this section, we will review the operation of the system. For this purpose, we use the sensitivity and FoM parameters. These parameters are defined as Sensivity = $\frac{\Delta\lambda}{\Delta n}$ ($\frac{\text{nm}}{\text{RIU}}$) and FoM = $\frac{1}{T} \frac{\Delta T}{\Delta n}$, where $\Delta\lambda$, ΔT , and Δn represent wavelength, transmittance, and refractive index variations, respectively.

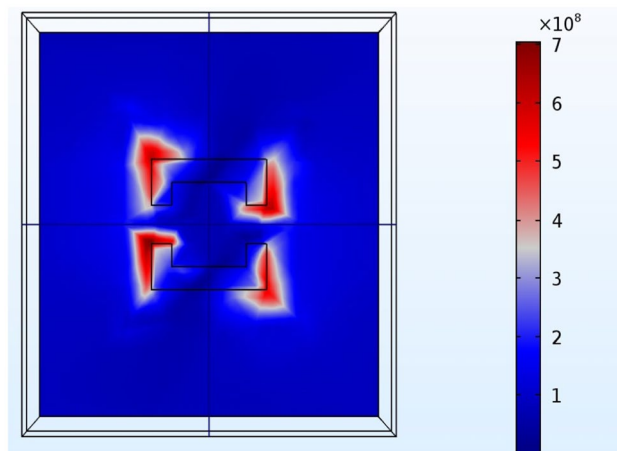


Fig. 8 Electric field distribution at $f_r = 193.4$ THz

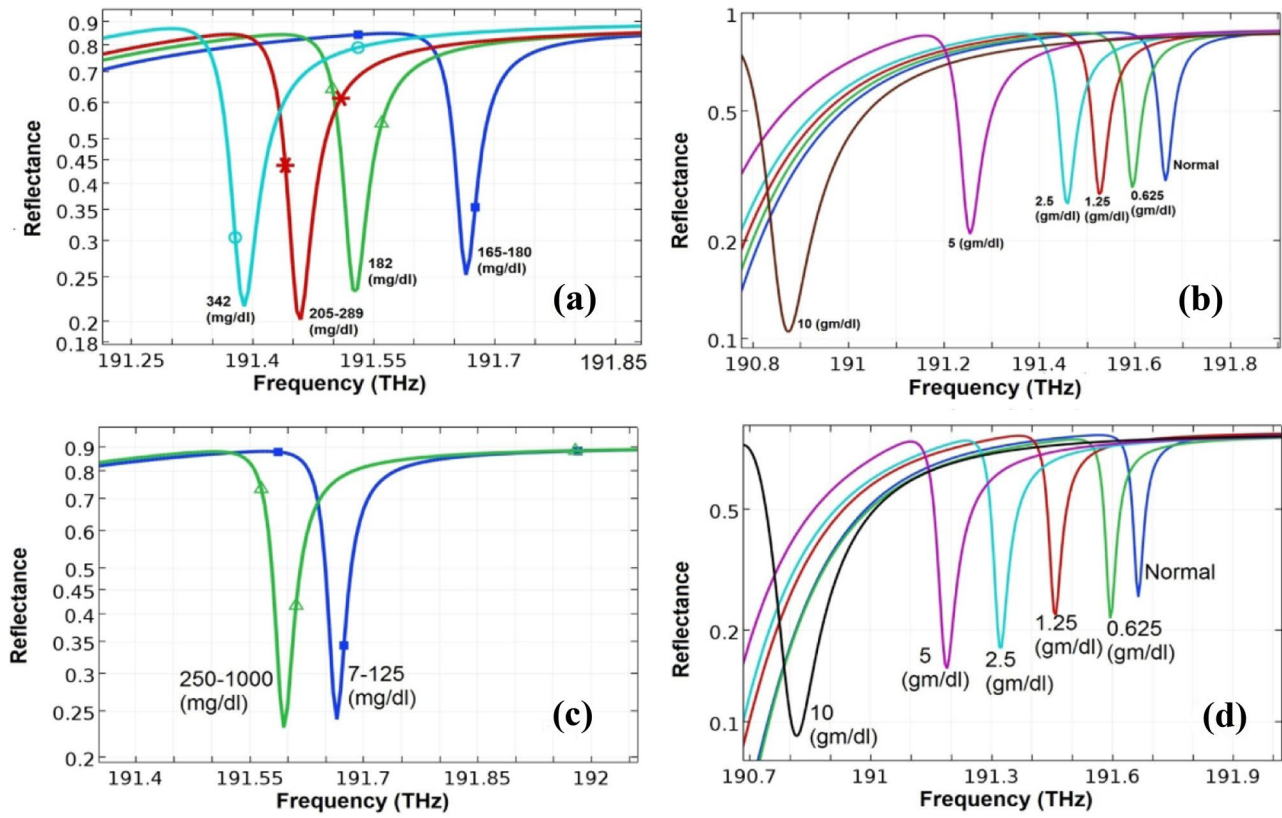


Fig. 9 Resonance frequency of the proposed system as a function of (a) blood glucose concentration, (b) urine glucose concentration, (c) urine albumin concentration, and (d) urine urea concentration

The refractive-index-unit (RIU) is used in optical biosensing, for evanescent wave sensors (optical waveguides, ring resonators, interferometers, and surface plasmon resonance). It is the minimum detectable change in the refractive index of the surface where the evanescent wave is traveling. Also, T is the transmission amplitude at the resonant frequency of the system.

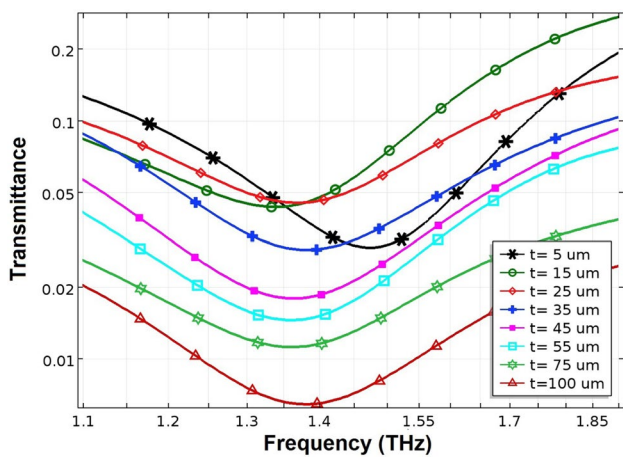


Fig. 10 Effects of sample thickness on the frequency response

Figure 13a shows the sensitivity and FoM for high-frequency mode and Fig. 13b for low-frequency mode. In high-frequency mode, the maximum sensitivity and FoM are 500 (nm/RIU) and 2000, respectively. These values in the low-frequency mode are 136 ($\mu\text{m}/\text{RIU}$) and 155, respectively.

As we know biosensor in different shapes and mechanism are considered by research groups [26, 118–139]. For example, Wang, Minghua, et al. proposed bimetallic

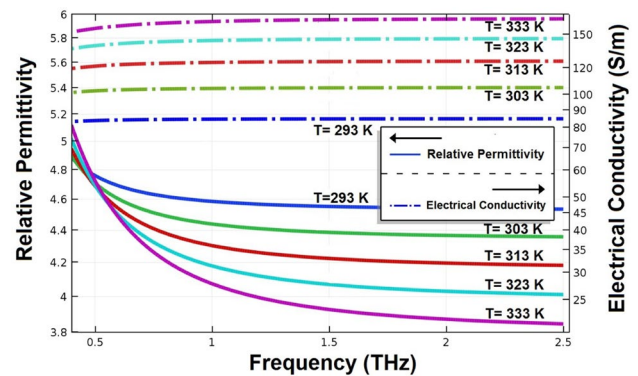


Fig. 11 Relative permittivity and electrical conductivity as a function of frequency at different temperatures

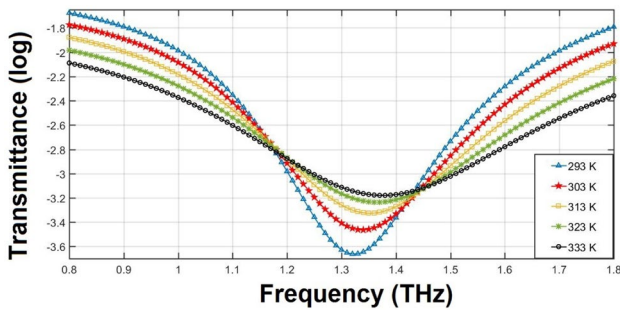


Fig. 12 Temperature changes versus water frequency response

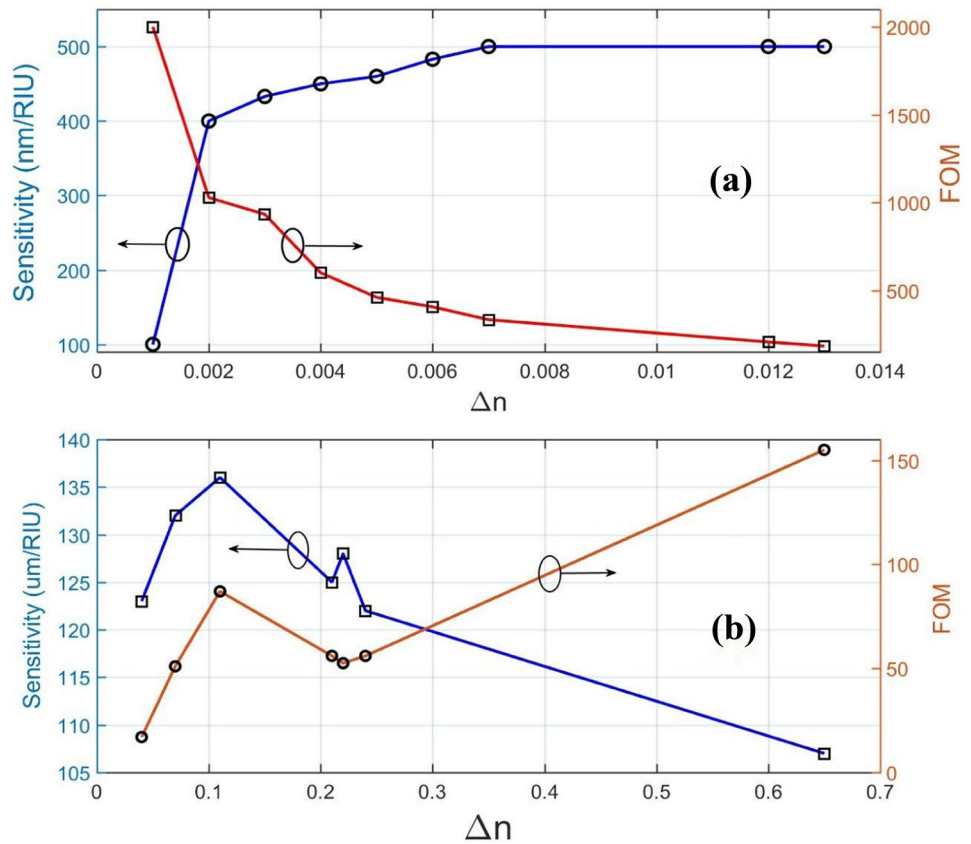
Table 2 Comparison between the suggested design and those reported in the literature

Ref	Structure	Sensitivity (nm/RIU)	FoM	Size (μm^2)
[140]	Metasurface	840	84	1.1
[141]	Dielectric nanostructures	263	88	
[142]	Photonic crystal	6.5		12
[143]	Photonic crystal ring resonators	2500	1400	13
This work	MMs	500	2000	0.34

NiFe oxide structures derived from hollow NiFe Prussian blue nanobox for label-free electrochemical biosensing adenosine triphosphate [120]. Jia, Qiaojuan, et al. proposed Polyoxometalate-derived MoS₂ nanosheets embedded around iron-hydroxide nanorods as the platform for sensitively determining miRNA-21 [131]. Lu and co-worker proposed numerical investigation of narrowband infrared absorber and sensor based on dielectric-metal metasurface [140]. Almpanis used dielectric nanopatterned surfaces for

subwavelength light localization and sensing applications [141]. Chopra research group proposed photonic crystal waveguide-based biosensor for detection of diseases [142]. Tavousi research group proposed high sensitivity label-free refractometer-based biosensor applicable to glycosylated hemoglobin detection in human blood using all-circular photonic crystal ring resonators [143]. Finally, Table 2 compares several types of biosensors with different structures.

Fig. 13 Sensitivity and FoM of the proposed system for (a) low-frequency mode and (b) high-frequency mode



Conclusion

A biosensor was designed to detect blood components and also to measure the concentration of glucose, albumin, and urea in urine and blood. One of the most important features of this sensor is the easy adjustment, which was demonstrated in the present article, as well. To illustrate this important feature, we set the sensor to operate at low frequencies (around 1 THz) and high frequencies (about 193 THz) and then measured different samples. According to the simulation results, the maximum sensitivity at high-frequency is 500 (nm/RIU) and at low frequency is 136 (um/RIU). Also, FoM in the high frequency is 2000 and in the low frequency is 155. The major features of this biosensor include real-time measurement, high speed, very small dimensions, cost-effectiveness, and free-label of the sample.

Author Contribution Hamed Emami Nejad: Software, Data curation, Investigation. Ali Mir: Conceptualization, Methodology, Writing—review and editing. Ali Farmani: Validation, Data curation, Writing—original draft.

Data Availability All data included in this paper are available upon request by contact with the contact corresponding author.

Declarations

Ethical Approval This is a numerical study on plasmonic biosensors.

Consent to Participate This is a theoretical study on the design of plasmonic biosensors.

Consent for Publication All authors of this paper agree to publish our theoretical research.

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