Design of High-performance Terahertz Sensor Based on Metamaterials

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Abstract—In this paper, a high-performance terahertz sensor is proposed. The sensor obtains a perfect narrow-band transmission spectrum at 3.842 THz with a Q value of 137 at the resonance frequency. The sensitivity reaches 160 GHz/RIU at the thickness of the substance to be measured of 10 μm, with good sensing performance. The results show that it has a promising application in terahertz high-sensitivity biosensing detection.

1. Introduction
At present, terahertz time-domain spectroscopy (THz-TDS) technology[1] obtains scientific research achievement in the identification of drugs, additives, etc. It is widely used as the main means of substance classification and identification[2,3]. Focusing on the issues of noisy spectral data and weak signals caused by the system or environment, many scholars established models for qualitative and quantitative analysis by machine learning and deep learning. However, the detection of trace biological samples and the identification between similar fingerprint spectrum are still challenging.

With the development of micro/nanofabrication technologies[4], the emergence of metamaterials (MMs)[5,6] has compensated to some extent for the hardness of THz-TDS techniques. MMs is an artificially designed electromagnetic composite material. It is composed of periodic subwavelength unit structures with special physical properties that cannot be achieved by natural materials, such as negative refractive index[7,8] and inverse Doppler effect[9,10]. The terahertz metamaterial biosensor[11] is an unlabeled affinity sensor. It is not only able to enhance the local electromagnetic field strength, but also extremely sensitive to the change of dielectric constant in the surrounding environment. This provides a new idea for the detection of micro or trace biological samples. The application prospects of terahertz metamaterial biosensors have been demonstrated in biomedicine, pesticide detection and other fields. However, its performance needs to be further improved to detect minor changes in analytes.

In this paper, we designed a transmissive terahertz sensor with a resonant structure consisting of two typical metal open rings and a short metal wire. Due to the strong interaction between the unit structures,
the transmission characteristic curve has a perfect transmission valley between 3.4 and 4.2 THz. We
used the FIT method to simulate and analyze the formation mechanism of resonance. Moreover, the
influence of refractive index and thickness of the measured object on the sensor performance is
investigated. The sensor designed in this paper achieves high sensitivity in the terahertz band, reaching
160 GHz/RIU, and has a high Q value. This design will be of great advantage in the field of high-
sensitivity detection of micro or trace biological samples.

2. Structural design and mechanism analysis

2.1. Structure design and simulation

The structure of the terahertz sensor designed in this paper is shown in Fig. 1(a), which is composed of
gold/fused quartz material. Fig. 1(b) is a schematic diagram of the structure of this sensor unit, the top
surface is a resonator consisting of two mirror image open rings and a short metal wire, and the structural
parameters are shown in TABLE 1. Among them, the conductivity of gold $\sigma = 4.561 \times 10^7$ S/m and
the relative permittivity of fused quartz $\varepsilon_r = 3.75 + i0.004$.

![Fig. 1 (a) 3D schematic diagram of the sensor structure; (b) Top view of the cell structure](image)

TABLE 1 Geometric parameters of the unitary structure

| Parameter | Value/µm |
|-----------|----------|
| a         | 25       |
| b         | 50       |
| r         | 8        |
| d         | 12.5     |
| w1        | 3        |
| w2        | 2        |
| g         | 2        |
| h         | 20       |
| t         | 0.2      |

We use CST to simulate and analyze the designed structure. The terahertz wave is incident vertically
on the upper surface of the metamaterial structure with the polarization direction along the x-axis. In
addition, periodic boundary conditions are set in the x and y directions, whereas open boundary
conditions are set in the z direction. The transmission spectrum of this structure without covering the
analyte is shown in Fig. 2, from which it can be seen that the designed sensor has a sharp resonance
peak at $f = 3.842$ THz with a minimum transmittance of 0.047. The quality factor Q is one of the
performance indicators of the sensor. Its magnitude is positively correlated with the resolution and
sensitivity. $Q = f / \text{FWHM}$, where $f$ is the resonance frequency and FWHM is the half-peak width.
Therefore, the sensor offers a Q value of 137. The higher Q value indicates that the sensor has a high
frequency selectivity characteristic.
2.2. Resonance mechanism analysis

In order to analyze the resonance mechanism of the sensor, the near-field electromagnetic field and surface current at $f = 3.842$ THz are analyzed in this paper. Through Fig. 3, we can observe that the electric field is mainly concentrated at the opening of the metal ring and the two arms. In this way, the opening can be equated to capacitance $C_1$ and the circle near the metal wire side can be equated to inductance $L_1$. In addition, the electric field intensity at the two arms is significantly larger than that at the opening. Above phenomenon indicates that the transmission valley is mainly formed due to the LC resonance and the interaction between the unit structures.

The surface current distribution is shown in Fig. 4(a). Ring currents with opposite directions are formed on both sides near the metal wire, so we also analyze the magnetic field distribution at $f$, as shown in Fig. 4(b). It can be seen that the surface currents between the left and right open rings of the unit structure circulate along opposite directions to form magnetic dipoles. They are connected at the beginning and end to form a closed ring, forming a toroidal dipole momentum oscillation. As a result, a resonant response of the toroidal dipole is generated in the opposite direction along the y-axis. In this paper, the ring dipole response is weak.

![Fig. 3 Electric field distribution at $f$. (a) top view; (b) front view](image)

![Fig. 4 (a) Surface current distribution at $f$; (b) Surface magnetic field distribution at $f$](image)
3. Characteristics of metamaterial sensors

The thickness and dielectric constant of the analyte to be measured on the sensor surface affect the frequency shift and intensity of the transmission characteristic curve. If the dielectric constant of the analyte is $\varepsilon$, its refractive index can be expressed as $n = \sqrt{\varepsilon \mu}$, where the magnetic permeability $\mu = 1$.

In order to research the influence of the thickness of the analyte to be measured on the sensor performance, let $n = 1.38^{[12]}$. The transmission characteristic curve of $h_1$ varying from 5 $\mu$m to 25 $\mu$m is shown in Fig. 5(a), the resonance frequency appears red-shifted phenomenon. The relationship between the frequency shift and the thickness of the analyte to be measured is shown in Fig. 5(b). It can be clearly seen that as the thickness of the substance to be measured increases, the frequency shift increases and the increase rate gradually tends to saturate. This is because the incident wave will excite the current on the sensor surface to oscillation. The larger the distance, the faster the oscillation attenuation. Therefore, the thickness of the analyte to be measured is preferably 10 $\mu$m.

Fig. 5 Effect of thickness of the analyte to be measured. (a) Transmission characteristics curves at different thicknesses; (b) Variation of frequency shift with analyte thickness

When the sensor surface is covered with 10 $\mu$m analyte of different refractive indices, the corresponding transmission characteristic curves are simulated and plotted, as shown in Fig. 6(a). When the refractive index of the analyte changes from 1.3 to 1.38, the resonance peak shows a distinct red-shift phenomenon, which is due to a significant change in the dielectric constant around the sensor, and the metamaterial sensor reflects this change in the resonance curve. The frequency shift curve of the resonance frequency with the change of refractive index is shown in Fig. 6(b). Sensitivity and FOM values are also indicators of sensor performance. $S = \Delta f / \Delta n$, $\text{FOM} = S / \text{FWHM}$, where $\Delta n$ indicates the amount of refractive index change of the analyte, $\Delta f$ indicates the magnitude of the frequency shift of the center frequency, and the unit of sensitivity is GHz/RIU (Refractive Index Unit). From Fig. 6(b), the refractive index sensitivity of the sensor is 160 GHz/RIU and the FOM value is 5.7. Many substances are distributed in this range of refractive index, so the sensor can be used for the detection of cancerous tissues, pesticide residues, etc.
Fig. 6 Transmission characteristic curve (a) and frequency shift & linear fit (b) of the analyte to be measured with refractive index

4. Conclusion
In this paper, a high-performance terahertz metamaterial sensor is proposed and its physical mechanism and sensing performance are analyzed. The results show that the sensor achieves modulation of terahertz waves with a minimum transmittance of 0.047. The quality factor at the resonance frequency is 137. In addition, it has good detection capability at 10 μm thickness, and the sensitivity is 160 GHz/RIU. The sensor has high quality factor and sensitivity, having potential applications in the detection of trace or micro biological samples.

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