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Detection of Toxic Gases Using Flexible Metamaterial Absorber at Terahertz Frequencies

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ABSTRACT

The development in technology leads to the release of several gases into the environment. These gases, especially toxic ones, have many negative effects on human life and cause many diseases that will adversely affect human health. In this respect, effective and accurate identification of these gases is important in terms of preventing possible damage. In this study, a sensor design that can detect toxic gases using a metamaterial structure operating in the terahertz frequency range is presented. Metamaterials not found in nature are defined as artificial or synthetic structures and can be used in many applications, including sensors, thanks to their negative index of refraction. Here, a metamaterial-based sensor application for the detection of carbon monoxide, a toxic gas, is investigated. The sensor performance is analyzed by adding 50% and 100% toxic gas to the suggested metamaterial design, and 0.010 and 0.013 THz shifts are obtained in the resonance frequency, respectively. These shifts indicate that this structure is a viable candidate in sensor applications for carbon monoxide.

Terahertz Frekanslarında Esnek Metamalzeme Emici Kullanarak Zehirli Gazların Tespiti

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ÖZ

Teknolojinin gelişimi, çevreye çeşitli gazların salınmasını beraberinde getirmektedir. Bu gazlar, özellikle zehirli olanları, insan yaşamı üzerinde birçok olumsuz etkiye sahip olup, insan sağlığını olumsuz yönde etkileyecek birçok hastalığa neden olmaktadır. Bu açıdan, bu gazların etkin ve doğru tespiti olası zararların önüne geçilmesi açısından önemlidir. Bu çalışmada, terahertz frekans aralığında çalışan bir metamalzeme yapısı kullanılarak zehirli gazları algılayabilen bir sensör tasarımı sunulmaktadır. Doğada bulunmayan metamalzemeler yapay veya sentetik yapılar olarak tanımlanır ve negatif kırılma indisleri sayesinde sensörler dahil birçok uygulamada kullanılabilir. Burada toksik bir gaz olan karbon monoksitin tespiti için metamalzeme tabanlı bir sensör uygulaması araştırılmaktadır. Önerilen yapıya %50 ve %100 zehirli gaz eklenerek sensör performansı analiz edilmiş ve sırasıyla rezonans frekansında 0,010 and 0,013 THz kayma elde edilmiştir. Bu kayma önerilen yapının karbon monoksit için sensör uygulamalarında kullanılabilir bir aday olduğunu göstermektedir.

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1. Introduction

The refractive index (RI) can be obtained by using the parameters permittivity (ε) and permeability (μ), which are used to examine the electromagnetic (EM) properties of a medium. The RI can be defined as a parameter formed by the bending of a light beam as it passes from one medium to another. Numerous research has been carried out since the emergence of the RI concept (Dale et al., 1858; Gladstone et al., 1863), but few of them are related to the negative index materials (NIMs), and these are listed in detail by Moroz (Moroz, 2009). It is theorized by Veselago that the medium could have a negative RI relative to the ε and μ EM parameters in a particular frequency range (Veselago, 1968). Studies about NIMs have increased rapidly due to the fact that the permittivity and permeability of materials are experimentally shown to be negative at the same time, and these materials are referred to as metamaterial (MTM) (Pendry et al., 1998; Pendry, 2000; Smith et al., 2000; Shelby et al., 2001). MTMs not found in nature, which are expressed as man-made structures that can be artificial or synthetic, have many research areas such as MTM absorber (MMA) (Landy et al., 2008; Wang et al., 2017; Xie et al., 2018; Al-Badri, 2021), sensors (Yang et al., 2013; Zhao et al., 2015; Akgol et al., 2017; Altintas et al., 2017), harvesting (Ramahi et al., 2012; Karaaslan et al., 2017; Bakır, 2018), MTM based antennas (Afridi et al., 2013; Tetik et al., 2018), and terahertz (THz) (Ling et al., 2018; Tetik, 2020; Han et al., 2021) applications. MTMs can suppress EM wave propagation in a certain frequency band which exhibits exceptional EM characteristics such as cloaking, backward propagation, and negative refraction. These exceptional characteristics can be controlled by their geometric structure.

Sensor applications, which have an important effect on the world of science, have gained considerable progress with increasing of research in the THz area. Gas sensors, which are preferred to have high performance and low fabrication costs, constitute an important part of these applications. These sensors are generally used in the detection of toxic gases, industrial pollution, and the monitoring of air quality. Hazardous gases have become an important problem that threatens daily life, and therefore their detection is considerably important. There are numerous studies in the literature for the detection of toxic gases in different research areas (Park et al., 2014; E. Tetik, 2014; Xu et al., 2020). Moreover, THz materials, which have potential research areas such as screening, imaging, and biomedical applications, are used in gas sensor studies. In addition, MTM sensors operating in the THz frequency range are important candidates for the detection of toxic gases. In this study, the detection of toxic gases by MTM based sensors, which are not yet in the literature, has been performed in the THz frequency range. In the first stage, the suggested MTM structure is designed and optimized according to its geometric structure. In this way, it is determined that it has a negative RI, which is the main feature of MTM structures. The reflection, transmission, and absorption characteristics of the optimized MTM design are analyzed. Then, CO molecule that is used for detection is generated as the Drude material (Bade, 1957) for the plasma applications and is integrated into the gaps of the proposed MTM structure. Plasma material-based applications created using the Drude dispersion model are preferred especially in antenna and EM material applications (Jafargholi et al., 2015; Golazari et al., 2016). Different volumes of toxic gases are used for detection performance. Finally, it is observed that the suggested MTM model can be used in sensor applications for the CO toxic gas.

The design and simulations of the flexible MTM structure are performed using a full-wave EM solver CST Microwave Studio (Computer Simulation Technology GmbH, Darmstadt, Germany) based on the finite integration technique. CST Microwave Studio is a 3D EM analysis software package used to design, analyze, and optimize EM components and systems and includes various calculation methods such as the Frequency Domain, Time Domain, Multilayer, Eigenmode, and Hybrid Solver. In addition, it has a large material library and macros for creating materials. The proposed structure is created using the frequency selective surface, MTM-unit cell workflow and is performed via using the frequency domain solver. To create the material to be used in the sensor study, the Drude Material Macro is preferred, which allows creating materials for use in plasma applications. The materials created with plasma applications in the CST program enable to obtain many properties of these materials such as EM characteristics.

2. Theory and Simulation Procedures

The proposed MTM structure exhibits flexible properties thanks to its constituent materials. These are the GaAs patch, gold resonator, gold ground plane, and polyimide substrate. The unit cell of its geometric structure is demonstrated in Fig. 1. The gold ground plane and resonator constitute the flexible MTM structure by sandwiching the polyimide substrate with the GaAs patch. Fig. 1b demonstrates the top view and dimensions of the unit cell. EM features of the flexible MTM design can be controlled by geometric parameters. In this context, by performing geometric optimization procedures, negative RI is obtained according to permittivity and permeability parameters. The optimum MTM structure is obtained by changing the values of the d, p, b, c, and g parameters. The length of one side of this structure having a square structure is $d = 42000$ nm. The length of one side of the resonator is $p = 32500$ nm. The resonator has dimensions $c = 4000$ nm, $b = 3000$ nm, and $g = 2100$ nm, respectively. The proposed flexible MTM structure is referred to as resonant electric metamaterials and is designed in different sizes and with different materials (Padilla et al., 2007; Landy et al., 2008).

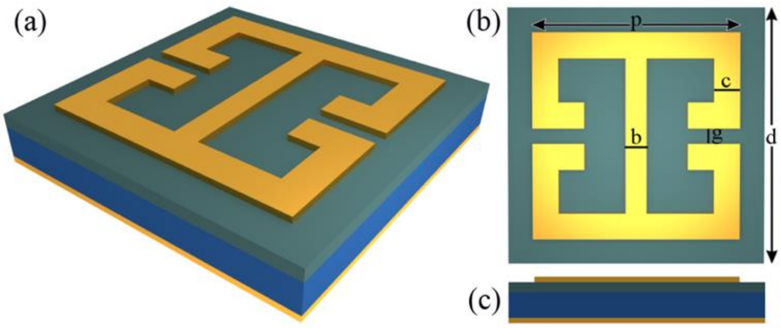

Figure 1. Perspective view (a), top view (b), and left view (c) of the unit cell of the suggested MTM design.

The equilibrium flexible MTM is created with the optimization procedure. As a result of the calculations of the MTM structure, the data in Figure 2 are obtained. MTMs are accomplished by designing microstructures smaller than the wavelength of incident radiation which has negative RI. The RI describing the propagation of an EM wave from one medium to another can be written as:

$$n = \frac{c}{v_{phase}}$$

where c is the speed of light in a vacuum and v_{phase} is defined as the phase velocity of light in the medium. On the other hand, the refraction of light in a structure can be expressed by Snell's law and it can be written as:

$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$

Using Maxwell's equations, the relationship of RI with ε and μ can be given by the following equation:

$$n = \sqrt{\mu_r \varepsilon_r}$$

When the RI equations are evaluated in terms of MTM designs, preferring the negative square root should not cause any problems. In this regard, it can be stated with the Lorentz equation which the ε depends on the frequency of the light. The force ($\boldsymbol{F}$) on electrons can be written in terms of electric ($\boldsymbol{E}$) and magnetic ($\boldsymbol{B}$) fields as follows:

$$\boldsymbol{F} = -e(\boldsymbol{E} + v \times \boldsymbol{B})$$

Assuming that the electrons in an atom/molecule are bound to their equilibrium position through an elastic restoring force, the equation of motion for an electron of mass m is:

$$m\ddot{\boldsymbol{r}} + m\gamma\dot{\boldsymbol{r}} + m\omega_0^2\boldsymbol{r} = -e\boldsymbol{E_0}\mathrm{e}^{-i\omega t}$$

where $\boldsymbol{r}$, ω, and ω_0 are expressed as the displacement vector, the angular frequency of the light, and the resonance angular frequency, respectively. If a solution according to the $\boldsymbol{r} = \boldsymbol{r}_0\mathrm{e}^{-i\omega t}$ equation is applied at this stage, the electron displacement can be expressed as:

$$\boldsymbol{r}_0 = \frac{-e\boldsymbol{E_0}/m}{\omega_0^2 - \omega(\omega + i\gamma)}$$

The total dipole moment per unit volume can be written as the vectorial sum of all dipoles per unit volume. In this case, assuming that there is an average molecular density (N) per unit volume and one dipole per molecule, the total dipole moment can be defined as:

$$\boldsymbol{P} = N\boldsymbol{p} = \frac{Ne^2\,\boldsymbol{E}/m}{\omega_0^2 - \omega(\omega + i\gamma)} = \varepsilon_0\chi_e\boldsymbol{E}$$

In this equation, the dielectric constant is written as χ_e. By rearranging these equations, the $\varepsilon(\omega)$ is expressed as:

$$\varepsilon(\omega) = 1 + \frac{Ne^2/m\,\varepsilon_0}{\omega_0^2 - \omega(\omega + i\gamma)} = 1 + \chi_e(\omega)$$

The same results can be obtained for μ in a similar way. This equation represents the Lorentz formula of dielectric permittivity for the real and imaginary parts. At this stage, using Maxwell's equations for a time-harmonic plane wave, the following equations are obtained:

$$\boldsymbol{k} \times \boldsymbol{E} = \omega\mu_0\mu\boldsymbol{H} \text{ and } \boldsymbol{k} \times \boldsymbol{H} = -\omega\varepsilon_0\varepsilon\boldsymbol{E}$$

where, considering that the parameters ε and μ are less than zero, the vectors $\boldsymbol{E}$, $\boldsymbol{H}$, and $\boldsymbol{k}$ represent a left-handed media. In this case, the Poynting vector $\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$ can be seen as right-handed, but the wave vector and the Poynting vector are anti parallel. On the other hand, the RI can be defined in terms of the Poynting vector as $\boldsymbol{k} = \hat{S}n\omega/c$. The fact that the $\hat{S}$ and $\boldsymbol{k}$ parameters are in the opposite direction means that the RI can take a negative value ($n = -\sqrt{\mu_r\varepsilon_r}$).

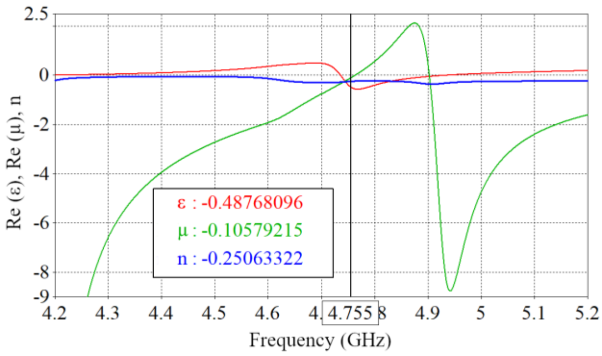

Figure 2. The permittivity (ε), permeability (μ), and refraction index (n) results of the flexible MTM design.

Simulation studies are carried out considering these fundamental principles. The proposed MTM structure has 4.755 THz resonance frequency. The permittivity, permeability, and refraction index of this structure are -0.487, -0.105, and -0.250 at the resonance frequency, respectively. The negative RI shows that the proposed structure exhibits MTM characteristics. Accordingly, this design can be used in numerous applications in areas such as harvesting, sensor, and antenna at THz frequency. In this study, the toxic gas sensor application has been realized with the proposed structure.

3. Calculation Method and Results

After the design and optimization procedure of the flexible MTM design, the simulation calculations have been realized to investigate the absorption (A), reflection (R), and transmission (T) characteristics of the design. These calculations are carried out at 4.2-5.2 THz frequency range and first perfect absorption properties are analyzed. In the calculations, two important features have been primarily focused: the first is impedance matching with the gold resonator and incident medium to provide maximum penetration and the second is gold plate covering the backside to restrain the penetrated wave in the proposed MTM. The absorption features of MTMs can be expressed in terms of frequency depending on the reflection $\mathrm{R}(\omega) = |S_{11}|^2$ and the transmission $\mathrm{T}(\omega) = |S_{21}|^2$, this relationship can be defined with the formula $\mathrm{A}(\omega) = 1 - \mathrm{R}(\omega) - \mathrm{T}(\omega)$. From the calculated results, frequency dependent S parameters are obtained. According to the absorption formula, maximizing frequency value of A (ω) is equivalent to minimizing simultaneously both (T) (ω) and (R) (ω) at the same frequency value. In addition, maximum absorption can only be satisfied by matching the impedance of the MTM to that of the free space with low loss features. In this case, the impedance ($Z(\omega) = \sqrt{\mu(\omega)/\varepsilon(\omega)}$) of the MTM unit cell should be matched to the free space $Z = Z_0$ for the minimum reflection. In this way, by ensuring the maximization of the imaginary part of the RI, the absorption of incident waves is increased. As a result, it is ensured that the MTM design exhibits a high absorption in a particular frequency range.

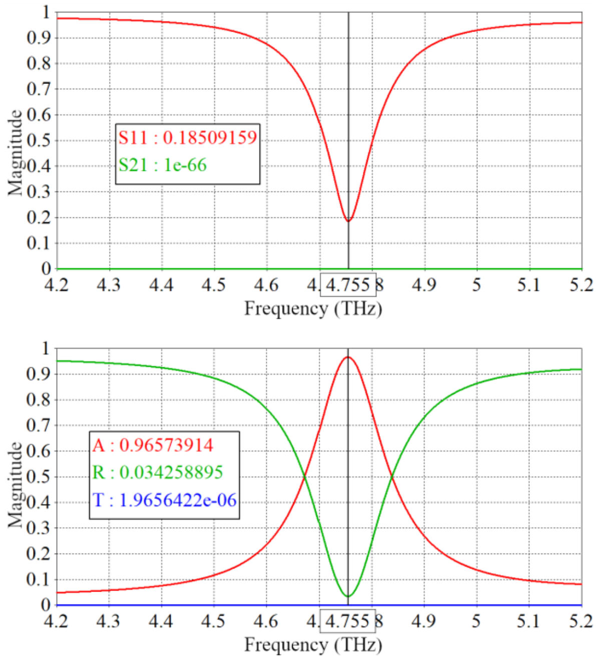

Figure 3. (a) The S_{11} and S_{21} parameters, (b) absorption (A), refraction (R), and transmission (T) results of the flexible MTM design.

At this stage, the suggested design is analyzed to investigate absorption operation mechanism. In the first step, S parameters are calculated and the S_{11} and S_{21} are obtained (Fig. 3a). Then, absorption, refraction, and transmission are calculated using parameters S_{11} and S_{21}. The results obtained are given in Fig. 3b. It is seen that the S_{21} parameter is zero as expected due to the copper plate on the back of the proposed structure. The S_{11} parameter is obtained as 0.18 value at the 4.755 THz resonance frequency. According to the S parameters, the maximum absorption value is around 96.5% at 4.755 THz, and it is seen that the flexible MTM design exhibits excellent absorption. Therefore, the proposed system can be used in sensor applications, and it will be a very good candidate for many sensor projects.

4. Sensor Applications

In this stage, the inorganic molecule CO has been preferred as the toxic gas and formed according to the plasma state. The proposed structure is described by the cold plasma model, also defined as the Drude dispersion model. This dispersion model describes the characteristics of media with two types of charge carriers. The first type (usually electrons) is considered to be freely moving, while the other type (usually slow ions in plasma) is considered stationary. Damping is expressed by elastic collisions of the moving particles with stationary particles using the collision frequency ν_c. The relative permittivity in terms of specific plasma frequency ω_p can be written as:

$$\varepsilon(\omega) = \varepsilon_\omega - \frac{\omega_p^2}{\omega(\omega - i\nu_c)}$$

It is also possible to model dependency of the instantaneous plasma frequency ω_p using the local electric field. The plasma frequency of the CO molecule formed according to this modeling is obtained as 2.805e+10 rad/s and its collision frequency as 3.458e+07 1/s. The proposed MTM design can be prepared by using methods such as conventional photolithography on a high-resistivity substrate (Park et al., 2014).

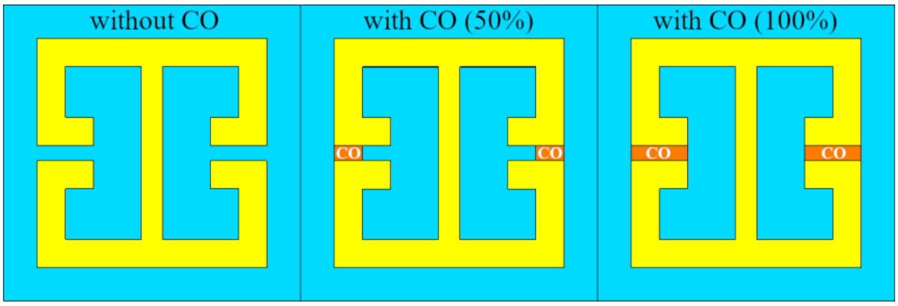

Figure 4. Integration of the CO molecule into the proposed structure (a) without CO, (b) with CO (50%), and (c) with CO (100%).

The placement of the created CO molecule on the gap part of the suggested MTM model is demonstrated in Fig. 4. The structure in Fig. 4a is the proposed basic structure and no toxic gas is added to the gap region. The toxic gas determined as CO is applied in two different amounts as 50% (Fig. 4b) and 100% (Fig. 4c). The volume of the gap area is considered when integrating the CO gas.

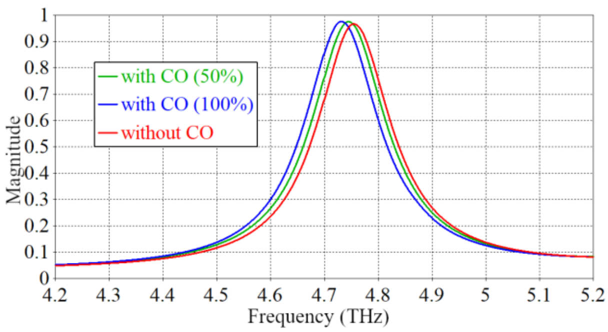

Figure 5. The absorption results of the suggested MTM model according to the amount of toxic gas.

To investigate the sensor performance of the flexible MTM model, the S parameters are calculated for 50% and 100% CO molecule content. The absorption results are obtained using the S parameters. Comparison of these results is given in Fig. 5. With the addition of different amounts of CO gas, a shift in frequency is observed. In the calculation made without adding toxic gas, the magnitude value is obtained as 96.5% at a frequency of 4.755 THz. Then, the CO molecule is placed in both gap regions at the same rate (50%). As a result of the calculation, the magnitude value is obtained as 97.4% at a frequency of 4.745 THz. Similarly, the CO molecule is placed in both cavities at the same rate (100%). In this case, the magnitude value is obtained as 97.4% at a frequency of 4.732 THz. It is seen that the resonance frequency of the proposed MTM structure shifts in direct proportion to the addition rate with the addition of the poisonous gas. In addition, the resonance frequency slightly increases with the addition of toxic gas.

Table 1. The results obtained by adding toxic gas to the proposed MTM structure.

Toxic Gas (CO)	Magnitude	Frequency (THz)	Shift (GHz)
Without	96.5%	4.755	-
50 %	97.4%	4.745	10 GHz
100 %	97.4%	4.732	13 GHz

The results obtained by adding toxic gas to the proposed structure are summarized in Table 1. With the addition of 50% and 100% gas, the amount of shift is obtained as 0.010 and 0.013 THz, respectively. The shift is taken into account in GHz units and the shift amount formed by the addition of 50% and 100% poisonous CO molecule is obtained as 10 GHz and 13 GHz, respectively. The results of the proposed sensor are compared with a similar study, and it is seen that similar results are obtained (Park et al., 2014). In that study, two different micro-organisms are studied using MTM structure, and two different shifts are obtained around 9 GHz and 23 GHz. According to the results, the designed MTM sensor provides perfect absorption at the resonance frequency and can be used in sensor applications for toxic gases such as the CO molecule. This structure can also be used in other frequency ranges and can be a good candidate for the applications where toxic gas sensors are used.

5. Conclusion

In this study, firstly, the absorption characteristics of the proposed MTM structure are investigated and discussed numerically. Then, the sensor characteristics of this MTM structure which exhibits perfect absorption features are analyzed using the toxic CO molecule. Simulation processes are carried out by adding 50% and 100% CO molecules to the two gap regions. Then, shifts in the absorption parameter are investigated. The toxic gas sensor properties of the proposed MTM structure are analyzed from the obtained results. A shift of 10 GHz occurred when 50% CO molecule is added to the gap region of the suggested MTM model. Similarly, with the addition of 100% CO molecule, a shift of 13 GHz is observed. The results obtained are in agreement with the literature. According to these results, the designed MTM sensor can be used in many sensor applications for toxic gases like the CO molecule.

Statement of Conflict of Interest

Authors have declared no conflict of interest.

Author’s Contributions

The contribution of the authors is equal.

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