# Metamaterial-based design of biological sensors operating at THz frequencies

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#### Abstract

In this contribution, we present an omega-shaped electromagnetic resonator, which is of potential interest for THz biosensors. A new analytical model for such an inclusion-type is developed, considering the effects of the fringing capacitance. After the development of a proper parametric (analytical and numerical) analysis, we optimize the design in terms of selectivity and sensitivity for the operation of the biosensor at THz frequencies. The obtained biosensor exhibits an higher selectivity and sensitivity compared to similar devices already presented in the literature.

#### **1. Introduction**

The use of bio-electromagnetic sensors is of great interest in many application fields, such as medicine, microbiology, physics, environmental and personal safety. A biosensor has to be sensitive, selective, and immune to external disturbances (pressure, temperature changes, electromagnetic interference). In most integrated optical biosensors proposed in recent years, the presence of the analyte is detected by measuring its refractive index in different ways [1], depending on the specific architecture of the biosensor. Among these architectures, the Mach-Zehnder-based one is widely used [2]-[3], due to its high sensitivity. Interferometer configurations are usually the most sensitive ones, but they also need quite long structures of the order of tens of mm. Photonic sensors, based on micro-resonators, are much more compact (reduction in length of three orders of magnitude) [4] and show a sensitivity which is comparable to that of the Mach-Zehnder-type sensors [5]-[6].

The aim of this study, is to propose nano-sensors operating in the THz frequency range and characterized by high sensitivity and selectivity through the employment of metamaterial resonators. The structures analyzed consist of a planar array of printed metallic particles (squared and circular split-rings, omega inclusions, etc.) placed on a glass substrate through proper adhesion layers.

#### 2. Quasi-static equivalent circuit model

The structure is assumed to be excited by a TM wave, with the electric field parallel to the inclusion gap. In connection with this excitation and with reference to what already exists in the literature [7]-[9], we have developed the equivalent quasi-static circuit model of the single inclusion reported in Figure 1.





In this analytical model, we added to the regular terms already proposed in the literature (see Figure 1b) a capacity term, related to the fringing field in the lateral side of the inclusion, which takes into account for the particle thickness. Such term, connected in parallel to the other capacitances, reads:

$$C_{f}(l,w,h,g,\varepsilon_{r}) = \varepsilon_{0}\varepsilon_{r}\frac{4h}{\pi}\cosh^{-1}\left[\frac{l-g}{g}\right]$$

being l the inclusion length, h the thickness, g the gap length, and w the strip width. In order to consider the effect of the substrate, starting from the assumptions given in [10], we obtained the following analytical expression:

$$\varepsilon_r^{eff}(\varepsilon_r, h, w, s) = 1 + \frac{2}{\pi}(\varepsilon_r - 1)sinh^{-1}\left[\frac{3}{2}\pi\sqrt{\frac{h}{(w+s)}}\right]$$

By replacing the relative permittivity with this effective permittivity expression in the fringing capacitance formula, we derive the final form used to complete the model of Figure 1b. We have considered different inclusion shapes, such as the squared and the circular split-ring resonators and the omega shape. In both cases, we found a good agreement (more than 95%) between the analytical models and the numerical results obtained through CST Studio Suite. In the simulations we have fully taken into account losses and materials dispersion. The results are not shown here for sake of brevity.

#### 3. Choice of the structure: selectivity, sensitivity, and linearity

The resonance frequencies of the different inclusions have been evaluated in terms of their electrical size and obtained bandwidth, as a function of the geometrical parameters (g, l, w, h), distance  $\Lambda$  between resonators), and thickness of adhesion layers. We have selected the shapes and their physical dimensions to maximize the two fundamental characteristics of a biosensor: sensitivity and selectivity.

In order to obtain high selectivity it is necessary to get a narrowband operation, which is strongly linked to the resonant behavior of the inclusions. By using the proposed circuit models, it is possible to derive analytically the Q-factor of the different metamaterial-based biosoensors. We obtained values ranging from 90 and 105. The sensitivity of a sensor, instead, is given in terms of the frequency shift  $\Delta f$  for the unit change of the permittivity  $\varepsilon$  or the refractive index *n* of the analyte placed on top of the sensor. For small variations of permittivity, the input-output relation can be assumed to be linear. CST simulations confirm this hypothesis, as shown in Figure 2 for a couple of representative inclusions, where the wavelength shift  $\Delta \lambda$  is reported against the variation of the refractive index  $(1 \le n \le 3)$ .



Figure 2: Change in wavelength per unit of refractive index for omega and squared split-ring based biosensors.

After a careful evaluation of the resonator types (squared and circular split-ring resonators, omega resonators), we selected the omega particle, which exhibits superior performances in terms of selectivity and sensitivity, and ended up with an optimized setup characterized by the following parameters: omega radius r = 50 nm, g = 15 nm, w = 15 nm, h = 15 nm, spatial period  $\Lambda = 400 \text{ nm}$ . The inclusions have been assumed to be made of gold and in the design we have considered also the presence of an adhesion layer of titanium dioxide (TiO<sub>2</sub>) (thickness 5 nm) and of a glass substrate (SiO<sub>2</sub>) (thickness 50 nm) to support the entire structure.

For a more complete evaluation of the sensor performance, we have considered and evaluated the sensitivity FOM (Figure Of Merit) defined in [3]. The comparison between our proposed design and the configurations proposed in [2] and [11] is reported in Table 2. From such a comparison, we see that the designed omega shape exhibits superior performances with respect to the previously proposed ones.

Single SRR <sub>n</sub>	Single $SRR_w$	Coupled Symmetric-SRR <sub>n</sub>	Coupled Symmetric-SRR <sub>w</sub>	Coupled Asymmetric-SRR	CPS	Omega particle (this paper)
[2]	[2]	[2]	[2]	[2]	[11]	( F. F)
2.08	0.39	1.51	0.19	2.86	0.72	8.48

Table 2: FOM values of biosensors already existing in literature and of the one based on the omega particle.

### 4. Conclusions

In this contribution, we have presented an omega-shaped electromagnetic resonator, which is of potential interest for THz biosensors. We have developed a new analytical model (working at THz frequencies) for such an inclusion, considering the effects of the fringing capacitance, which is of paramount relevance for sensor applications, due to the presence of the analyte on top of the metallic resonators; we have studied analytically and numerically the relationship between the resonance frequency of the proposed particle and the geometrical parameters (shape, size, length, thickness, and distance between the resonators); we have optimized the design in terms of selectivity (Q-factor) and sensitivity (FOM) for the operation of the biosensor at THz frequencies; we have obtained sensor selectivity and sensitivity higher than those of similar devices already presented in the literature.

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