

Detection and analysis of human hemoglobin HB and HBO₂ with new Nano-sensor based on chiral metamaterials

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Abstract

This article is devoted to the simulation COMSOL Multiphysics of ultra-sensitive nano-sensor based on chiral Metamaterials, which allows us to follow hemolysis with good accuracy. Where we will study the reflected wave in human hemoglobin oxygenated and deoxygenated to determine its concentration. In this paper we also present the numerical results and the equations of variations obtained by Matlab.

Keywords: Chiral Metamaterials; Nano-Sensor; Human Hemoglobin.

1. Introduction

The development of nanotechnology in the last 20 years has allowed the emergence of new materials (Chiral Metamaterials) [1-6], for the electronic field, optics, and other fields. In addition, the artificial composite structures is open a new perspective in the effects of reflection and transmission of an electromagnetic wave. Today, there are several theoretical studies modeling, simulation and experimental work on the Chiral Metamaterials (Figure 1,2). One of the important applications in clinical and bio-photonics is that monitoring hemolysis when hemoglobin leaking out of red blood cells, and therefore, the local concentration of hemoglobin changed quickly [7-11]. The representation of the hemoglobin of refractive index as a complex value [7]:

$$n = n_0 + i * k \quad (1)$$

Where k is the absorption coefficient, n_0 is the refractive index of which is varied in proportion to the hemoglobin concentration, by the relation [7]:

$$n_0 = n_{H_2O} + \alpha C \quad (2)$$

n_{H_2O} : distilled water of refractive index and α is the specific refraction increment.

In our work we will simulate in the COMSOL Multiphysics and study an ultra-sensitive nano-sensor based on Chiral Metamaterials, designed to measure the concentration of deoxygenated and oxygenated hemoglobin human. The simulation results were used as data in a Matlab program we developed to determine the sensitivity maxima (peaks, illustrating the effect of resonance) of the S_{11} parameter (the input port voltage reflection coefficient) characteristic parameter of the nano-sensor, relating to changes refractive indices of the oxygenated and deoxygenated hemoglobin. This will allow us to retrieve the equations of the variation in refractive index depending on the resonant frequency.

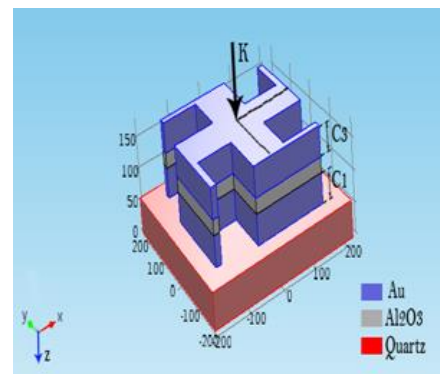


Fig. 1: 3D Representation of the Chiral Metamaterials Structure.

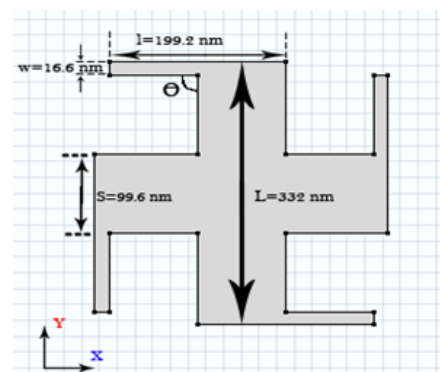


Fig. 2: Chiral Metamaterials Structure.

2. Ultra-sensitive nano-sensor

Our work we will study the reflection of electromagnetic wave to a Chiral Metamaterials detector of oxygenated hemoglobin and deoxygenated human, calculating the S_{11} parameter (the input port voltage reflection coefficient) for left-handed circularly polarized LCP). The cell shown Chiral Metamaterials presented below is

considered in a perfect conductor, dimensions: $420 \times 420 \times 1500 \text{ nm}^3$ and excited by a source of polychromatic rayonnement, according to a circularly polarized wave left LCP. The field $E_0 = 100 \text{ V/m}$, $P_0 = 10 \text{ mW}$, and a range of frequency $\omega \in [720, 780 \text{ THz}]$. While the polarization state, the initial wave (power) is assumed to left circularly propagated along the axis Z. The simulation ultra-sensitive nano-sensor (figure 3,4) of human oxygenated and deoxygenated hemoglobin are done using the variation of refractive index according to their concentrations in blood, made from the linear relationship of variation index based on the concentration [7]:

$$n = n_{H_2O} + \alpha C \quad (3)$$

Where: $\alpha_{HbO_2} = 0.170 (\text{ml/g})$ and $\alpha_{Hb} = 0.146 (\text{ml/g})$
 $n_{H_2O} = 1.343 (37^\circ\text{C})$. For specifics wavelength $\lambda = 401.5 \text{ nm}$. The values of the refractive indices of deoxygenated hemoglobin (Hb) and hydrogen (HbO₂) for a wavelength $\lambda = 401.5 \text{ nm}$, are quoted in the following table [7]:

Table 1: Change in Hb Refractive Indices and HbO₂en Function of Concentration

Concentration (g/l)	Refractive indices of Hb	Refractive indices of HbO ₂
0	1.345	1.345
20	1.349	1.349
50	1.353	1.354
80	1.357	1.359
110	1.362	1.364
140	1.365	1.369

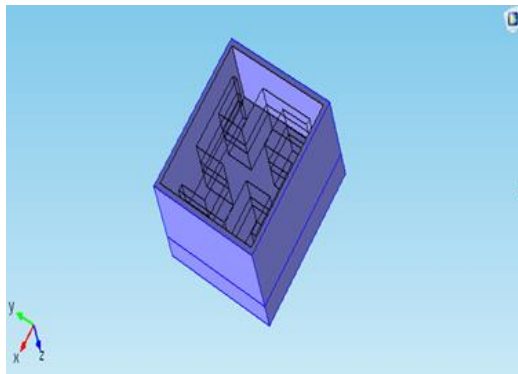


Fig. 3: Representation of the Structure MMC Nano-Sensor without the Hemoglobin.

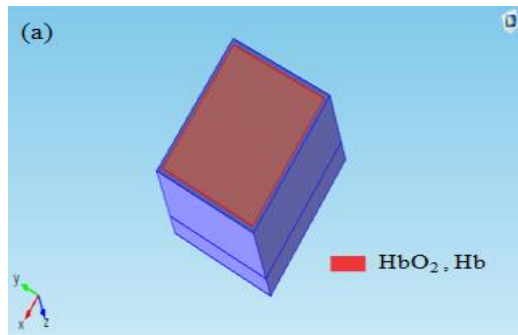
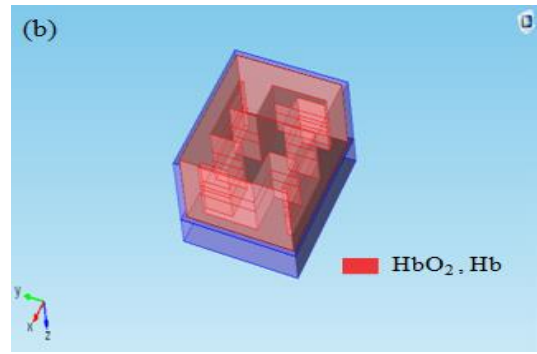


Fig. 4: (A)-Representation of the Analyzed Layer (B) - Representation Of The Cell MMC And Analyzed Layer Transparent

3. Results and discussion

The results obtained by simulation under the environment COM-SOL the change in resonance frequency according to the variation of the concentration of Hb and HbO₂ are represented in the following figures:

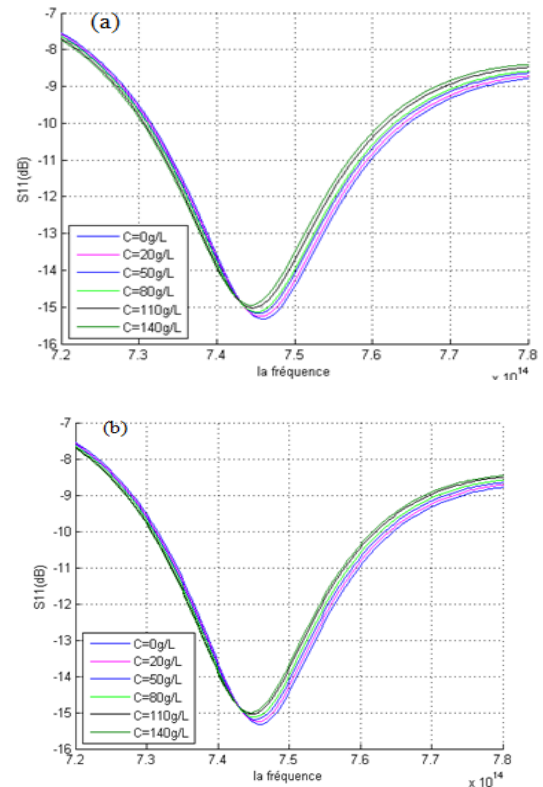


Fig. 5: (A) - The Variation of the Resonance Peaks Depending on the Refractive Indices of HbO₂, (B) - Variation of the Resonance Peaks Based on Hb Refractive Indices.

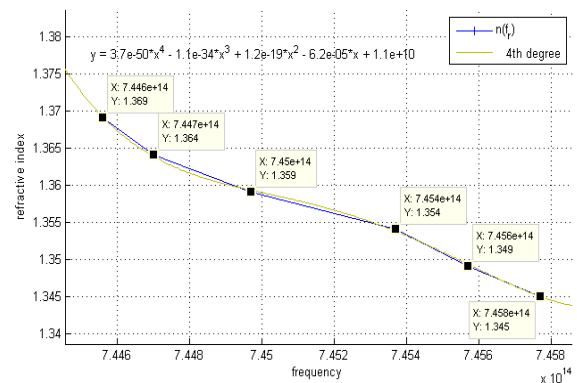


Fig. 6: The Variation of Refractive Indices Depending on HbO₂ Resonance Peaks.

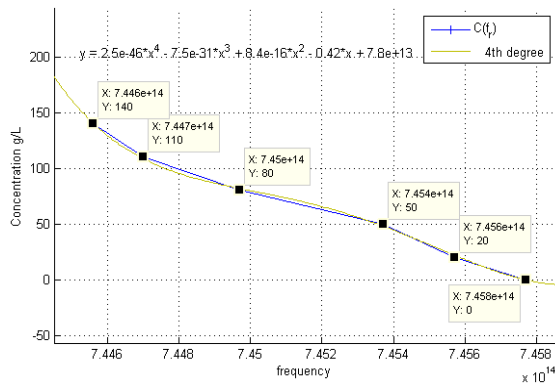


Fig. 7: The Variation of the Concentration Depending on HbO₂ Resonance Peaks.

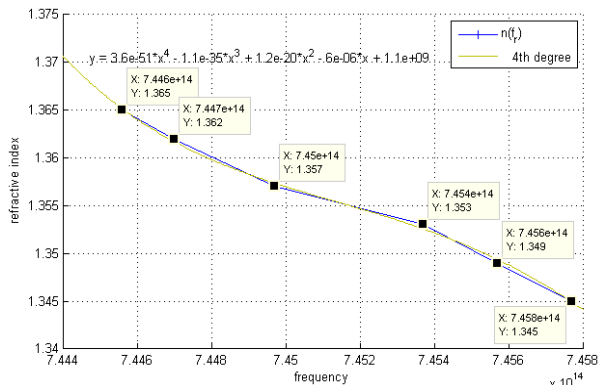


Fig. 8: The Variation of Refractive Indices Depending on Hb Resonance Peaks.

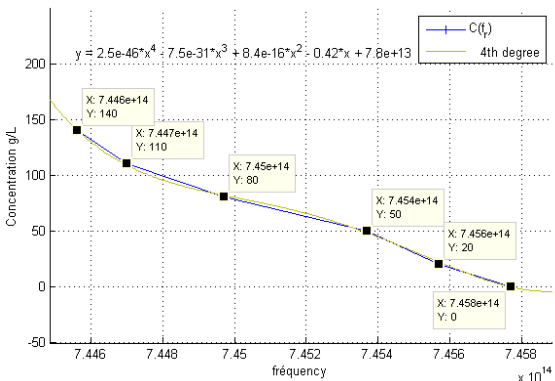


Fig. 9: The Variation of the Concentration Depending on Hb Resonance Peaks.

The curve form illustrating the variation of the refractive indices and concentration according to the parameter S_{11} , for a LCP waves, a curve (regressive) linearly. When the refractive indices or the concentration increase, we note moving resonance peak relative referential peak (lack of hemoglobin) which is seen a decrease in resonance frequencies when the concentration of hemoglobin (with or without oxygen) increases to study this variation, we use Matlab 'basic fit', we have provides the equations of variation of the refractive index and concentration according to the n resonance frequency $n(f_r)$, $C(f_r)$ below:

- For the deoxygenated hemoglobin Hb:

$$n(f_r) = 3.6 * 10^{-51}(f_r^4) - 1.1 * 10^{-35}(f_r^3) + 1.2 * 10^{-20}(f_r^2) - 6 * 10^{-6}(f_r) + 1.1 * 10^9 \quad (4)$$

$$C(f_r) = 2.5 * 10^{-46}(f_r^4) - 7.5 * 10^{-30}(f_r^3) + 8.4 * 10^{-16}(f_r^2) - 0.42 * (f_r) + 7.8 * 10^{13} \quad (5)$$

- for the oxygenated hemoglobin HbO₂:

$$n(f_r) = 3.7 * 10^{-50}(f_r^4) - 1.1 * 10^{-34}(f_r^3) + 1.2 * 10^{-19}(f_r^2) - 6.2 * 10^{-5}(f_r) + 1.1 * 10^{10} \quad (6)$$

$$C(f_r) = 2.5 * 10^{-46}(f_r^4) - 7.5 * 10^{-31}(f_r^3) + 8.4 * 10^{-16}(f_r^2) - 0.42 * (f_r) + 7.8 * 10^{13} \quad (7)$$

These equations have obtained allows us to generalize the study to any concentration and possible clues refraction. And monitoring the variation with good accuracy.

4. Conclusion

The results obtained by simulation and development programs Matlab; led to an interesting characterization of an ultra-sensitive nano-sensor to study the variation in the refractive index of the concentration of oxygenated and deoxygenated hemoglobin human. However, the development of our theoretical calculations based on the 4th order equations allowed us to make our theoretical study generalizes. The studied structure is highly sensitive, and detects the change in the index of refraction 10^{-3} order. This allowed us to interpret correctly identified and the variation of the concentration of hemoglobin in the blood with good accuracy.

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