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# Numerical analysis of the mechanisms involved in integrated THz imaging with a NIR femtosecond laser illumination

Tatiana E. Itina <sup>\*a</sup> and Xxx Sedao

<sup>a</sup> Laboratoire Hubert Curien, UJM, UMR 5516 CNRS, Saint-Etienne, 18 rue du Prof. Benoit Lauras, Bat F, 42000 France

## ABSTRACT

Femtosecond laser allows the production of THz radiation that is very promising for the imaging of various tissues and, namely, for in vivo cancer detection. Despite numerous very convincing experimental demonstrations, the mechanisms involved in image formation are still under discussion. In this paper, based on modeling, we analyze the major physical processes involved in THz laser interactions with tissues, namely with skin. Particular attention is given to the mechanisms involved in integrated THz imaging with NIR femtosecond laser illumination. An effective medium approach is found to be helpful. The difference in water fraction, pores, and additional nanoparticles and nanorods are shown to play a role in the considered non-invasive optical imaging of skin cancer.

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**Keywords:** femtosecond laser, imaging, THz radiation, cancer

## 1. INTRODUCTION

Cancer is a set of the diseases that are becoming widely spread practically everywhere in the world. In particular, skin cancer is one of the most commonly detected with the age of its appearance constantly decreasing, while the number of new cases dramatically rising. The early detection of this disease is crucial for the success of the following treatment. For this, several non-invasive in vivo methods were proposed. Recently, THz radiation was also used both for detection and for treatment of several carcinomas [1]. Among various sources of this radiation, femtosecond laser interactions with either electron plasmas or with metasurfaces and also with water are promising.

Typical THz imaging systems are based on either transmission or reflection-based geometry. In particular, in the reflection-based imaging, the transmitter (emitter) and receiver (detector) are on the same side of the sample (Figure 1a). The interaction of the electromagnetic waves with the sample provides a THz signal at the receiver. The main advantages of this technology as compared to more traditional imaging techniques is that it should be a non-ionizing, and since, non-invasive technique. The major challenge is in the fact that skin is composed of several layers and is not homogenous (Figure 1b). As a result, the contrast of the obtained images often requires improvements. One of the possibilities to improve the contract is to use additional near-infrared (NIR) femtosecond irradiation and nano-objects, such as nanorods or nanoparticles [2]. When specifically chosen nanoparticles are introduced and are preferably concentrated in the tumor, its optical properties are modified with an increase in the refractive index as common nano-composite materials (Figure 1c). Because of the plasmonic properties, the inclusions are more efficiently heated and give rise the local field enhancement around them. Such materials can be represented by using effective-medium approaches [3-5], or by a detailed multi-physical modeling including Maxwell equations, material ionization and heating, pressure calculations, etc. [6].

Despite many promising results, the underling mechanisms involved are still under discussion. It is well-known that THz radiation is absorbed, and therefore attenuated by water. Because of the a rather important water fraction in biological tissues, and namely in skin, it is commonly attenuated within 1 mm depth. Skin cancer commonly appearing on the surface look particularly suitable for the detection by using THz radiation.

To better understand the mechanisms involved, both electromagnetic and thermo-mechanical modeling are to be performed. Herein, several useful examples are given. In particular, using a modified effective-medium approach in combination with multi-layer equation systems seems promising.

## 2. MODELING AND RESULTS

### Modeling approaches

Figure 1 summarizes the schematics of the detection system (a), of the multi-layer representation of skin (b) and of the tumor layer containing gold nanorods (c). Several effective layer models were proposed in literature, both for spherical nanoparticles and for elongated ones.

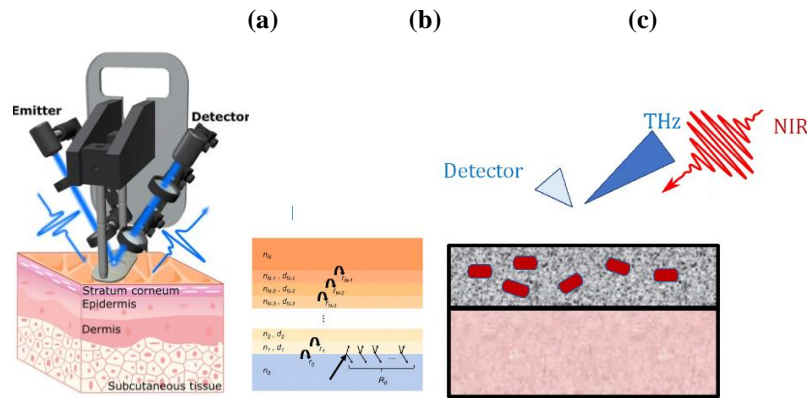


Figure 1. Schematics of the THz detection of surface tumors [7], multi-layer model [8] of skin and effective-medium approximation for NIR-femtosecond laser assisted THz detection with a layer containing gold nanorods.

It should be note that to increase biocompatibility and stability, nanoparticles and nanorods are often coated by biopolymers. In this case, the optical properties of the corresponding layer can be calculated by using the modified effective medium equations for coated gold nanorods (GNR) [5] based on the electrostatic approximation (Mie-Gans theory).

### Calculation results

Firstly, the optical properties of water are presented in Figure 2. This is important because water fraction is high in biological tissues. While water absorbs THz radiation, it remains transparent for NIR ones. The latter waves can be, however, well absorbed by gold nanorods (GNR) with the appropriate sizes (length and diameter).

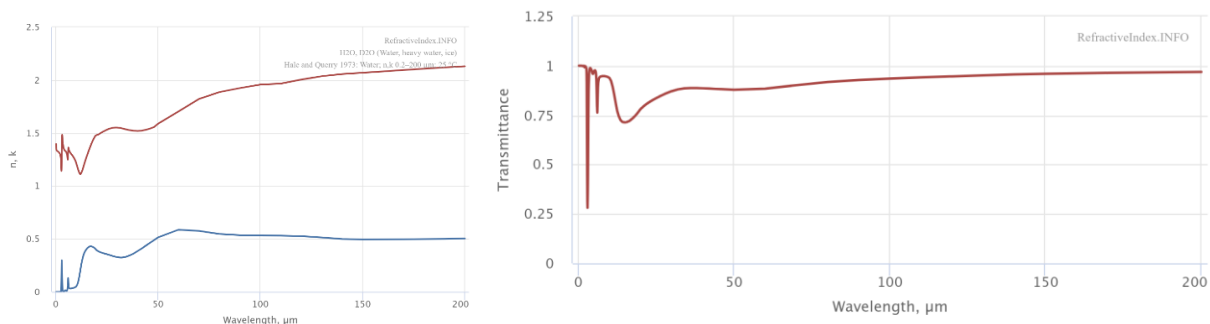


Figure 2. Optical properties of water (refractive index  $n$ , extinction coefficient  $k$ , and transmittance) as a function of wavelength according to <https://refractiveindex.info/?shelf=main&book=H2O&page=Hale>.

The calculated absorption spectra of GNR also depend on the refractive index of the surrounding medium. Examples of the calculated electromagnetic field distributions are given in Figure 3.

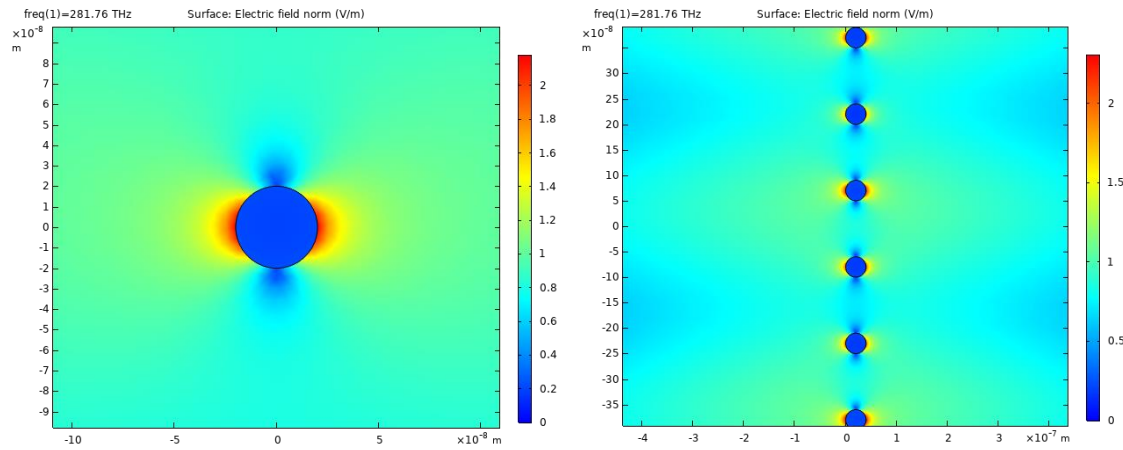


Figure 3. Examples of electromagnetic field calculated for NIR wave interaction (740 nm) with gold nanorods with the radius of 20 nm.

When many GNR are randomly distributed in tumor, such layer's optical properties are calculated by using the effective medium approximation described above. Then, the sample is represented as a set of layers with different optical properties. One can notice a field enhancement up to 2 times in the vicinity of the inclusions. Previously, we have shown that when an ensemble of randomly distributed gold nanoparticles is present in a matrix, such field enhancement in addition with electron injection and matrix ionization may lead to the formation of nanocavitation effect [6], where the corresponding conditions were derived by using the Grady dynamic fragmentation criterion. Albeit tumor destruction can be a desirable effect, to avoid collateral damage, the fluence of the femtosecond laser laser should be set below the corresponding threshold.

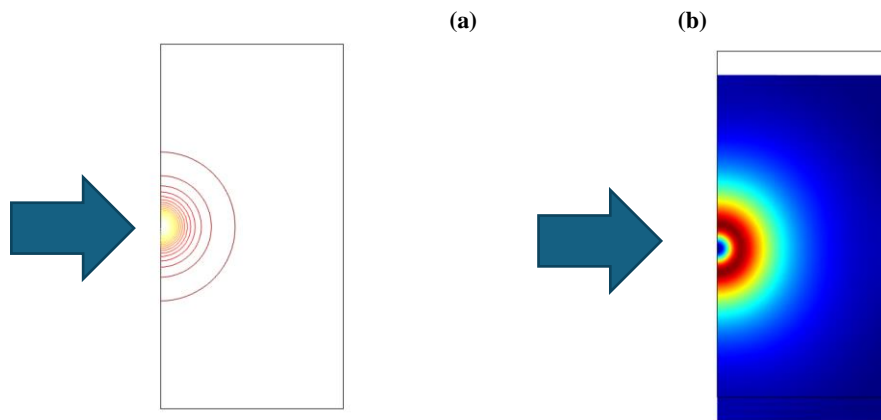


Figure 4. Typical distributions of temperature (a) and pressure (b) in a dielectric medium upon interaction with several NIR femtosecond laser pulses (here, 10). Incident NIR femtosecond laser direction is shown by arrows.

Finally, typical temperatures and pressures calculated after absorption of several NIR femtosecond laser pulses are shown in Figure 4. It should be noted that the heat accumulation effect plays an important role here and can lead to the formation

of a pressure, or even of a shock wave propagating in depth. This effect may also represent a limiting factor, in addition to nanocavitation, because it can result in the damage of tissues below the tumor.

### 3. SUMMARY

Based on the performed preliminary simulations and analysis, it has been found that:

- Using THz radiation is promising in bio-medicine for tumor detection
- Addition of nanoparticles or nanorods can help increasing the sensitivity, particularly in the case of additional NIR fs laser irradiation
- Optical parameters of complex multi-layer system with water fraction and nano-objects can be extracted based on the experimental data and effective-medium approach combined with multi-layer Fresnel equations and with an appropriate model for water.
- Modeling can also help elucidating non-invasive detection regimes. Here, however, more investigations are required.

### ACKNOWLEDGEMENTS

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