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k-Wave simulation to understand the photoacoustic signal characteristics from various shapes of nanoparticles

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ABSTRACT

Current attempts in understanding the photoacoustic signal characteristic of various shapes of nanoparticles is mostly performed through numerical simulations. However these computational methods are very time consuming, costly and complicated. Thus there is a need for an easy and fast simulation technique to understand the photoacoustic signal generated from various shapes of nanoparticles. k-Wave is a MATLAB based simulation toolbox to simulate photoacoustic signal given the initial pressure distribution of the target object. In this work, we used k-Wave simulation to understand the photoacoustic signal generated from various shapes of nanoparticles. Seven shapes of nanoparticles are created mainly sphere, cylinder, hollow cylinder, cube, hollow cube, triangle, and star. A point sensor (ultrasound detector) is used to detect the photoacoustic waves generated from different shapes of nanoparticles. The photoacoustic signal generated by different shapes of nanoparticles is captured and processed for further analysis to see their frequency content.

***Keyword*:** Photoacoustic signal characteristics, k-Wave simulation, Nanoparticle.

1. INTRUDUCTION

Photoacoustic Imaging (PAI) has been widely discussed as a potential imaging technique in recent years for various biomedical applications.[1-5] This hybrid imaging technique uses light to illuminate the target object. As a result of light absorption and subsequent local heating there is a temperature rise in the order of milli degree. This causes thermoelastic expansion and pressure waves in the form of acoustic wave are emitted from the illuminated object. The acoustic wave (also known as photoacoustic wave) is detected by ultrasound transducers (also known as detectors).[6] Our body has many intrinsic optical absorbers such as blood, melanin or even water which gives strong optical contrast. However, in the near-infrared region the optical absorption is rather week. Therefore, contrast agents are used not only to enhance to contrast, but also for targeted molecular imaging. Contrast agents used in PAI can be in the form of nanoparticles made of metallic materials such as gold.[7] The shape, size and functionally of gold nanoparticles critically affects their role as contrast agent in PAT.[8, 9] These properties of nanoparticles can be tuned to maximize the absorption or scattering of light in enhancing the intensity of photoacoustic signal in this imaging modality.[8, 9] In the literature various other types of contrast agents are reported both organic as well as inorganic.[10-21] In this work we are mainly focused on the shape of the nanoparticles rather than their composition or other properties.

Several studies were carried to explore the application of various shapes and sizes of gold nanoparticles in photoacoustic tomography. These studies suggested various shape and functionality of gold nanoparticles can be used as contrast agent for tumor or cancer diagnosis.[8, 10, 22-25] Gold based spherical nanoparticles have been reported as potential contrast agent in tumour diagnosis.[24] Another study show gold based cylindrical nanoparticles are demonstrated as potential contrast agent in prostate cancer diagnosis.[10, 22] Aside from solid shape, hollow shape nanoparticles are reported as potential contrast agent with ability of longer circulation.[25] Silica coated triangular nanoparticles are reported to be an effective contrast agent in lymphatic imaging.[23]

Current attempts in studying the effectiveness of different shape and size of nanoparticles are performed intensively through experimentally synthesis of nanoparticles followed with a photoacoustic study. However, experimental methods are time consuming, complicated and expensive. In recent years, computational simulation was demonstrated in studying photoacoustic signal.[9] Complex equations and numerical analysis are required prior to the simulation process which is also time consuming. Therefore, there is a need for an easy and fast simulation technique to understand the photoacoustic signal generated from various shapes of nanoparticle.

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In this work, we demonstrated a computational simulation approach of simulating photoacoustic signal generation from various shapes of nanoparticles using k-Wave MATLAB toolbox.[26] Initial pressure rise in the nanoparticle was assumed to be homogenous distribution. Seven different shapes of nanoparticles were used in the study such as, sphere, cylinder, hollow cylinder, cube, hollow cube, triangle, and nano star. These are the most common shapes of nanoparticles used for photoacoustic contrast agents as found in the literature.

2. SIMULATION METHODS

In this study, k-Wave simulation toolbox was used in simulating photoacoustic signal from various shapes of nanoparticles. k-Wave is a MATLAB based simulation toolbox which provides time domain analysis of photoacoustic signal.[26] All these simulations were performed using a 64 bit Intel® Core ™ i7-4770 CPU @ 3.40 GHz desktop running windows operating system. Figure 1 shows the simulation setup consists of an object (nanoparticle) and an ultrasound detector. The simulation environment was created in 3-Dimension with a 130 x 130 x 130 voxels (each voxel size is 15 nm) with a perfectly matched boundary layer (PML) to satisfy the boundary condition was used for the generation of the forward data. An ideal point detector was used in this simulation. For the forward simulation a time step of 3 pico-seconds with a total of 266 time steps was used in this simulation. All simulations assumed a sound speed of 1500 m/s. An acoustically homogeneous medium was considered with no absorption or dispersion of sound.

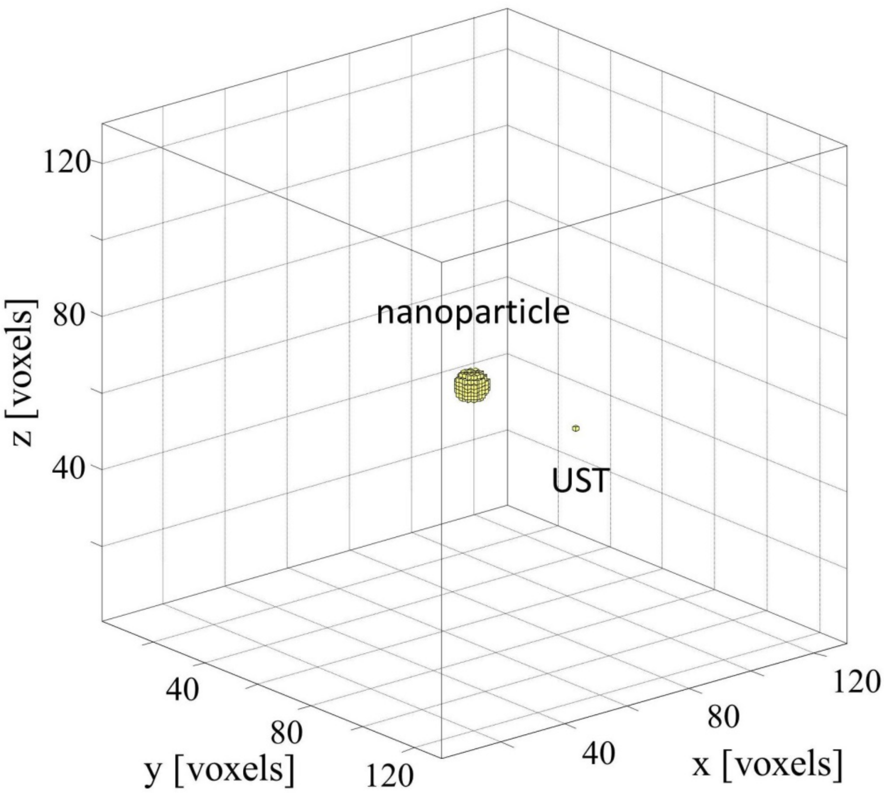

Figure 1: Simulation setup, ultrasound detector (point detector) located at 600 nm away from the object (nanoparticle), located at the center of the simulation geometry.

Seven different shapes were created using MATLAB programming. Two among the seven shapes were created with hollow centered across the object. These seven shapes are namely sphere, cylinder, hollow cylinder, cube, hollow cube, triangle, and star. Sphere was created with the diameter of 120 nm, cylinder with the diameter of 300 nm and the length of 615 nm, cube with the length of 165 nm, equilateral triangle with the height of 105 nm and length of 75 nm, and star was created with two equilateral triangles with the height of 250 nm and length of 75 nm. Hollow cylinder was simulated with outer diameter of 300 nm, inner diameter of 150 nm and length of

600 nm. Hollow cube was simulated with outer length of 165 nm and inner length of 75 nm. The outer diameter and length of hollow shapes were kept the same as normal shape.

Only one nanoparticle was simulated each time with a condition of homogenous light absorption. That means the initial pressure rise inside the nanoparticle is constant spatially. A point sensor (ultrasound detector) was used to detect the photoacoustic waves generated from different shapes of nanoparticles. This point sensor was located at the y-axis, 600 nm away from the center of the objects. The nanoparticle was located at the center of the simulation geometry.

Frequency response and photoacoustic pressure graphs were plotted in one set of simulation for one shape of nanoparticles. MATLAB was used to plot the frequency response and photoacoustic pressure graphs in each simulation. No complex programing is required in plotting these two graphs. Frequency response was plotted with relative amplitude spectrum against frequency. Photoacoustic pressure graph was plotted with recorded pressure at each point of time step against time. These two graphs were plotted in order to analyze the impact of the shapes on the signal characteristics.

3. SIMULATION RESULTS

Figure 2 show the photoacoustic signal and frequency spectrum of the PA signal generated from various shaped nano particles. Figures 2(a-e) represents photoacoustic signal generated from nanosphere, nanocylinder, nanocube, nanotriangle, and nanostar, respectively. Figures 2 (f-j) show the corresponding frequency spectrum. The frequency response and the photoacoustic signal profile varies significantly depending on which shape of nanoparticles the signals are generated as seen here. A peak is observed with one ripple shown in the frequency response graph of a sphere shape nanoparticle as per Figure 2(f). A positive pressure followed by a negative pressure sequence trend is observed in photoacoustic pressure of a sphere nanoparticle as shown in Figure 2 (a).

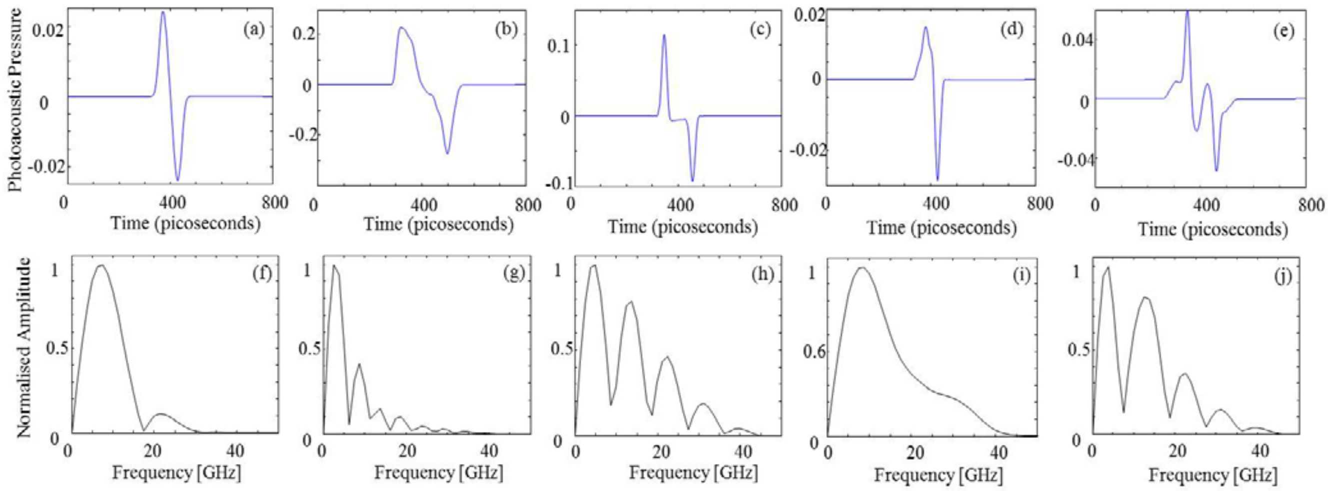

Figure 2: Photoacoustic signal and frequency spectrum of the PA signal generated from the nano particles. (a-e) photoacoustic signal generated from nanosphere, nanocylinder, nanocube, nanotriangle, and nanostar. (f-j) Frequency spectrum of the photoacoustic signal generated from nanosphere, nanocylinder, nanocube, nanotriangle, and nanostar.

Relatively broad positive and negative pressure content was observed on cylinder shape nanoparticle as per Figure 2(b). More than one ripple was observed on the frequency response of cylinder shape nanoparticle as per Figure 2(g).The positive and negative pressure content of cube nanoparticle was not observed in continuous manner as per Figure 2(c). A constant zero value was observed before the photoacoustic pressure reach negative pressure content. This photoacoustic signal characteristic of cube shape nanoparticle was not observed on the rest of the simulated shapes in this study. More than one ripple was observed with gradually decreasing trend on the frequency response of cube shape nanoparticle as per Figure 2(h). This behavior of frequency response was also observed on nanostar as per Figure 2(j). However different photoacoustic pressure pattern was observed between cube shape nanoparticle and nanostar as per Figure 2(j).

Triangular nanoparticle shows a relatively broad frequency response as per Figure 2(i). The photoacoustic pressure of triangular shape consists of positive and negative pressure content with uneven proportion as per Figure 2(d). The positive pressure gradually increases to its maximum point follow with a drastic and narrow drop of pressure before returning to zero points. Nanostar exhibits similar photoacoustic pressure pattern as hollow shape (shown later).

Figure 3 show the photoacoustic signal and frequency spectrum of the PA signal generated from hollow shaped nano particles. Figures 3(a-b) represents photoacoustic signal generated from hollow cylinder, and hollow cube. Figures 3 (c-d) show the corresponding frequency spectrum. Objects with hollow structure also show similar traits in both frequency response and photoacoustic pressure.

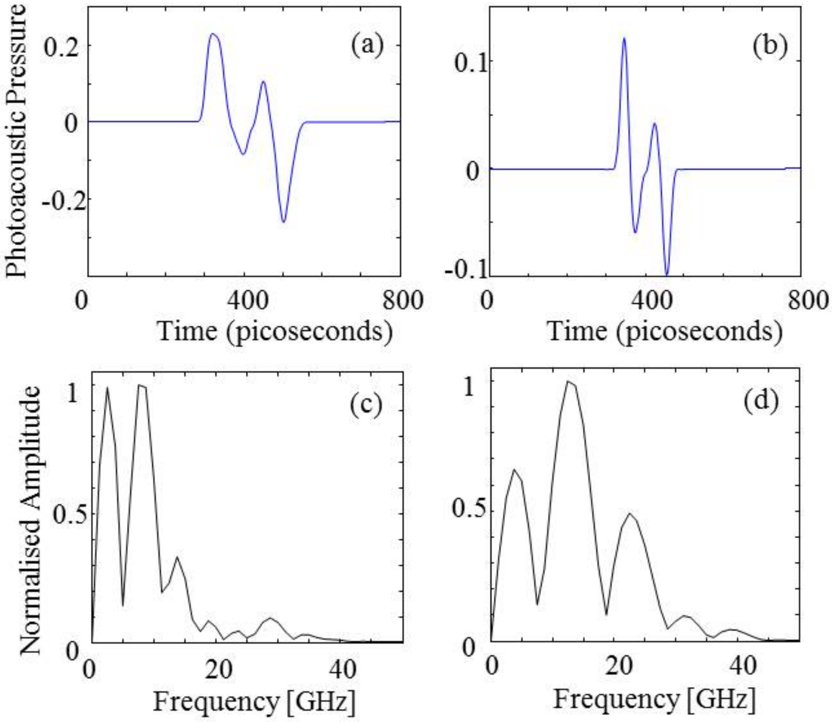

Figure 3: Photoacoustic signal and frequency spectrum of the PA signal generated from the nano particles. (a-b) photoacoustic signal generated from hollow cylinder, and hollow cube. (c-d) Frequency spectrum of the photoacoustic signal generated from hollow cylinder, and hollow cube.

The trends observed in both frequency response and photoacoustic pressure reflects the structural difference of the object. Similar PA trends are observed only if the object consist similar structural properties and from the same photoacoustic pressure propagation direction. Any changes of point detector (ultrasound detection system) location may results in different frequency response and photoacoustic pressure trends observed unless the object is a regular shape over three dimensional profiles.

As seen from these results, different shapes of the nanoparticles have their own signature in the photoacoustic signal generated from them and in their frequency spectrum. This could be really useful in identifying the structure of a nanoparticle from their photoacoustic signal. Moreover, these kinds of simulations are computationally less demanding. It takes around 3 min to complete one set of simulation for one shape of nanoparticle. At present we are using 15 nm voxel size. Even finer voxel size can be used, however, with increased simulation time. The voxel size can be chosen depending on the nanoparticle size. Typically one tenth of the size of the nanoparticles could be a good starting point. At present we are using point detector as the ultrasound detection system. More complex realistic ultrasound detectors can also be simulated depending on the need.

4. CONCLUSION

We have demonstrated photoacoustic signal simulation of various shapes of nanoparticle using k-Wave simulation toolbox. Seven different shapes of nanoparticles are simulated and studied. The simulation results are presented in the form of frequency spectrum as well as the photoacoustic pressure signal. The proposed method is simple and fast. Different shapes of nanoparticles can be constructed easily and does not require complex computational programming. Different shapes of nanoparticles have their own signature in terms of photoacoustic signal as well as the frequency spectrum. Therefore, this signature can be used to identify the shapes of the nanoparticles. This proposed approach allows an overview understanding on the photoacoustic signal characteristic of different shape of nanoparticles.

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