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FEM Analysis of Laser-Induced Heating of Gold Nanoparticles

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Abstract: Nanoparticles are being extensively researched as a noninvasive method for selectively targeting and killing cancer cells. We present a method for modeling the thermal activation of a gold nanoparticle and the thermal response of its surrounding medium under single and multi-pulse excitation. It is found that the effective heating range of a nanoparticle is determined by both shape (sphere vs. rod) and heating profile.

Keywords: Gold Nanoparticle, Laser, Thermal Ablation

1. Introduction

Gold (AU) nanoparticles are another class of inorganics currently undergoing thorough research. AU NPs have shown promising optical properties for applications in photochemotherapy and photothermal therapy; the use of light to induce hyperthermia or even thermal ablation. Lasers are widely used in thermal ablation procedures, where the tissue is heated to a range of 70-80 C to cause irreversible cell damage. Again, the problem with this method is lack of specificity as both normal and tumor cells in the light path are damaged due to the high energy output required to reach ablation ranges. The strong absorption properties of AU NPs are used to amplify the lasers' effect on the tumor site, thereby reducing the amount of energy needed to induce ablation in the tumor as well as the time of irradiation needed, rendering the therapy less harmful to healthy tissue. These nanoparticles are also appealing due to their ease of preparation, ready multi-functionalization, and tunable optical properties. They absorb light strongly in the visible spectrum due to a phenomenon known as surface plasmon resonance (SPR) [1]. This property depends on the type of metal used, the size and shape of the nanoparticles, as well as the dielectric constant of the surrounding medium, providing many parameters that can be manipulated. The SPR ultimately determines the wave-length at which the nanoparticles achieve maximum absorbance. Thus, the nanoparticles can be tuned from near infrared wavelengths all the way to UV wavelengths, depending on the application. For example, longer wavelengths of light can penetrate tissue more than smaller wavelength and thus can be used to treat deeper tumors. Like the iron oxide nanoparticles, the AU NPs are unspecific to tumors and thus rely solely on the enhanced permeability and retention effect of tumors for nanoparticles accumulation. AU NPs are easily functionalized and can therefore be modified for increased tumor specificity [2].

Letfullin et al. aimed to compare and contrast the effects of multiphase-pulse and single-pulse laser heating on the gold nanoparticle temperature profiles [3]. They found that while the AuNP heated substantially during the laser pulse durations, they did not exhibit any cumulative effects and rapidly cooled to room temperature after the irradiation cycle. However, their study was limited only to the nanoparticle temperatures and did not model the environmental effects of the AuNP heating. In this study, we model the thermal activation of gold nanospheres and nanorods in a fluidic environment using Comsol Multiphysics 4.0a to determine the thermal response of the surrounding medium.

2. Use of COMSOL Multiphysics

The thermal activation of the AuNP and the thermal response of the medium can be modeled using Comsol's Heat Transfer Module. Since laser irradiation exhibits a Gaussian profile in time, the Transient Solver was selected for the problem. Gold Nanospheres were modeled as spheres and nanorods as cylinders. There were placed at the center of another much larger sphere (r = 1um) which acted as the fluid. Cells are mainly composed of water, thus making water a suitable choice for the surrounding

Trial	Shape	radius (nm)	σ (ns)	Tmax (K)	Center (μ)
1	sphere	20	6	600	18
2	sphere	15	10	625	30
3	sphere	10.5	3	800	10
4	rod	11.8	5	1100	15
5	rod	11.38	3.5	700	10

Table 1. Parameters used in the simulation

medium in this study. A 3D geometry was created with two concentric spheres representing the particle and the medium. The medium was given a sufficiently large radius (1μm) and the particle's radius varied with the trials. The medium's material properties were set to those of water to closely resemble an in vivo environment. Temperature and probes were placed at distances 10, 20, … 90 (nm) and .5, .9(μm) from the surface of the particle. Nano rods were assumed to have an aspect ratio of 100:1. The effective radius indicates the radius of a sphere with equal volume to the nanorod. The particles were then heated to their maximum temperatures according to Table 1, using Gaussian temperature profiles of the form:

$$T(t) = \frac{T_{max}}{\sqrt{2\pi\sigma^2}} e^{-\frac{(t-\mu)^2}{2\sigma^2}} \qquad (1)$$

Where σ is equal to half the pulse width. Multi-pulse mode consisted of the superposition of multiple Gaussian pulses centered at different times. Temperatures provided by Letfullin et al. were used as the input temperatures for the AuNP. The surrounding medium then obeys the heat equation given by:

$$\rho C_p u * \nabla T = \nabla * (k\nabla T) + Q \qquad (2)$$

A tetrahedral mesh was given to both spheres however, due to size differences; the nanoparticle's mesh was set to Finer while the medium was set to Refined. The time step was set to 0.5 ns and a solution was obtained over 100 ns.

3. Results and Discussion

Figure 1 shows cross sections of the particle-water systems for nanospheres and nanorods.

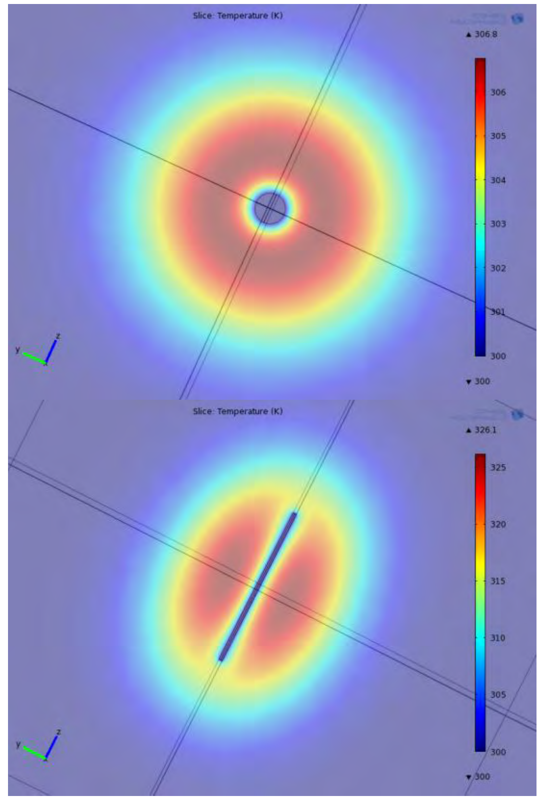

Figure 1. Cross-Sectional view of thermal response for a gold nanosphere (top) and gold nanorod(bottom).

The images were taken well after the particle reached its maximum temperature (approximately twice the pulse width). The water's temperature as a function of time and distance from the nanoparticle surface is shown in Figure 2 for both single and multi-pulse heating. The criteria for effective therapeutic range of heating for a nanoparticle was determined by the largest distance at which the medium reached a temperature of 350 (K) for any given time. The difference between the effective therapeutic range between the single pulse heating and multi-pulse heating of a gold nanorod is shown in Figure 3.

Table 2 gives a summary of the therapeutic ranges for all trials. The largest thermal response was observed in Trial 4 with a nanorod heated to 1100(K). The effective thermal radius from this trial was estimated at approximately 105 (nm). Comparing the results from trials 3 and 5 demonstrates that for two nanoparticles of comparable size and temperature profiles, a nanorod will have a greater heating range.

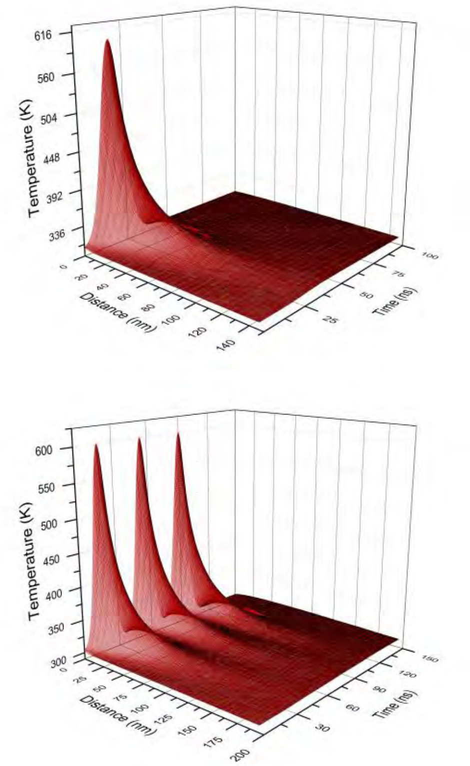

Figure 2. Temperature vs. Distance and Time for single-pulse (top) and multi-pulse (bottom) heating of a gold nanosphere.

Although single-pulse heating of gold nanoparticles may not be enough to achieve a suitable thermal response, multi-pulse heating shows accumulation of heat in the particle's surroundings over time. By providing multiple laser pulses, the effective thermal ablation range increases dramatically from that of a single pulse. Furthermore, substituting nanorods in place of nanospheres creates a larger thermal response in the medium for a given temperature. Most importantly, this is done without increasing the laser's intensity, which could lead to unwanted healthy cell damage if used for selective cancer cell targeting.

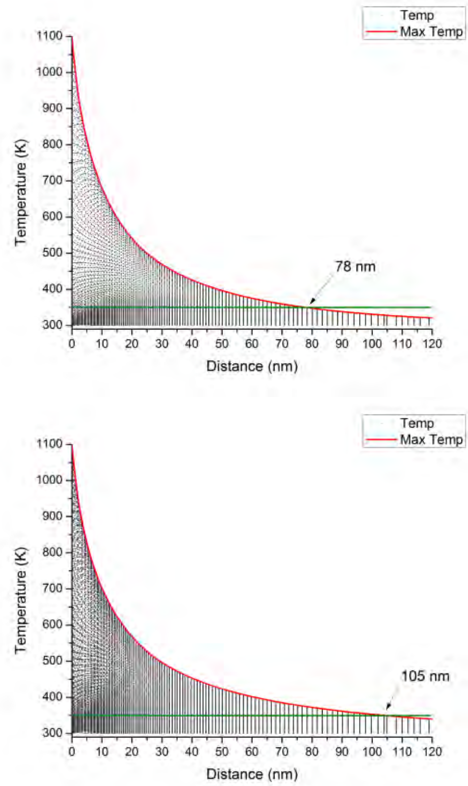

Figure 3. Maximum temperature (red) for single-pulse (top) and multi-pulse (bottom) heating of a gold nanorod. The intersection of the red curve with the 350 (K) line is taken to be the therapeutic range of the trial.

	Effective Thermal Radius	
Trial	One Pulse (nm)	Three Pulse (nm)
1	40	44
2	40	45
3	34	38
4	78	105
5	45	55

Table 2. Summary of results showing the effective thermal range for each trial of single-pulse and multi-pulse heating.

4. References

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5. Acknowledgments

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