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Research paper

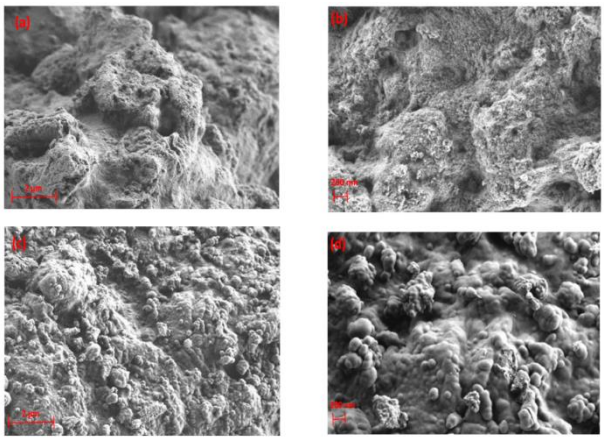
Advantages, effectiveness and efficiency of using neodymium nanoparticles by 3d finite element method (FEM) as an optothermal human cancer cells, tissues and tumors treatment under synchrotron radiation

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Abstract

In the current study, thermoplasmonic characteristics of Neodymium nanoparticles with spherical, core–shell and rod shapes are investigated. In order to investigate these characteristics, interaction of synchrotron radiation emission as a function of the beam energy and Neodymium nanoparticles were simulated using 3D finite element method. Firstly, absorption and extinction cross sections were calculated. Then, increases in temperature due to synchrotron radiation emission as a function of the beam energy absorption were calculated in Neodymium nanoparticles by solving heat equation. The obtained results show that Neodymium nanorods are more appropriate option for using in optothermal human cancer cells, tissues and tumors treatment method.



Scanning Electron Microscope (SEM) image of Neodymium nanoparticles with 50000x zoom.

Keywords: *Neodymium Nanoparticles; Scanning Electron Microscope (SEM); 3D Finite Element Method (FEM); Heat Transfer Equation; Optothermal, Heat Distribution; Thermoplasmonic; Neodymium Nanorods; Human Cancer Cells; Tissues and Tumors Treatment; Simulation; Synchrotron Radiation; Emission; Function; Beam Energy.*

1. Introduction

In recent decade, metallic nanoparticles have been widely interested due to their interesting optical characteristics [1–8]. Resonances of surface Plasmon in these nanoparticles lead to increase in synchrotron radiation emission as a function of the beam energy scattering and absorption in related frequency [9, 10]. Synchrotron radiation emission as a function of the beam energy absorption and induced produced heat in nanoparticles has been considered as a side effect in plasmonic applications for a long time [11–15]. Recently, scientists find that thermoplasmonic characteristic can be used for various optothermal applications in cancer, nanoflows and photonic [16–22]. In

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optothermal human cancer cells, tissues and tumors treatment, the descendent laser light stimulate resonance of surface Plasmon of metallic nanoparticles and as a result of this process, the absorbed energy of descendent light converse to heat in nanoparticles [23–25]. The produced heat devastates tumor tissue adjacent to nanoparticles without any hurt to sound tissues [26, 27]. Regarding the simplicity of ligands connection to Neodymium nanoparticles for targeting cancer cells, these nanoparticles are more appropriate to use in optothermal human cancer cells, tissues and tumors treatment [28–74]. In the current paper, thermoplasmonic characteristics of spherical, core–shell and rod Neodymium nanoparticles are investigated.

2. Heat generation in synchrotron radiation emission as a function of the beam energy–neodymium nanoparticles interaction

When Neodymium nanoparticles are subjected to descendent light, a part of light scattered (emission process) and the other part absorbed (non–emission process). The amount of energy dissipation in non–emission process mainly depends on material and volume of nanoparticles and it can be identified by absorption cross section. At the other hand, emission process which its characteristics are depend on volume, shape and surface characteristics of nanoparticles explains by scattering cross section. Sum of absorption and scattering processes which lead to light dissipation is called extinction cross section [75–123].
Neodymium nanoparticles absorb energy of descendent light and generate some heat in the particle. The generated heat transferred to the surrounding environment and leads to increase in temperature of adjacent points to nanoparticles. Heat variations can be obtained by heat transfer equation [124–202].

3. Simulation

To calculate the generated heat in Neodymium nanoparticles, COMSOL software which works by Finite Element Method (FEM) was used. All simulations were made in 3D. Firstly, absorption and scattering cross section areas were calculated by optical module of software. Then, using heat module, temperature variations of nanoparticles and its surrounding environment were calculated by data from optical module [203–283]. In all cases, Neodymium nanoparticles are presented in water environment with dispersion coefficient of 1.84 and are subjected to flat wave emission with linear polarization. Intensity of descendent light is 1 $mW/\mu m^2$. Dielectric constant of Neodymium is dependent on particle size [284–395].
Firstly, calculations were made for Neodymium nanospheres with radius of 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 nanometers. The results show that by increase in nanoparticles size, extinction cross section area increases and maximum wavelength slightly shifts toward longer wavelengths. The maximum increase in temperature of nanospheres in surface Plasmon frequency is shown in Figure (1).

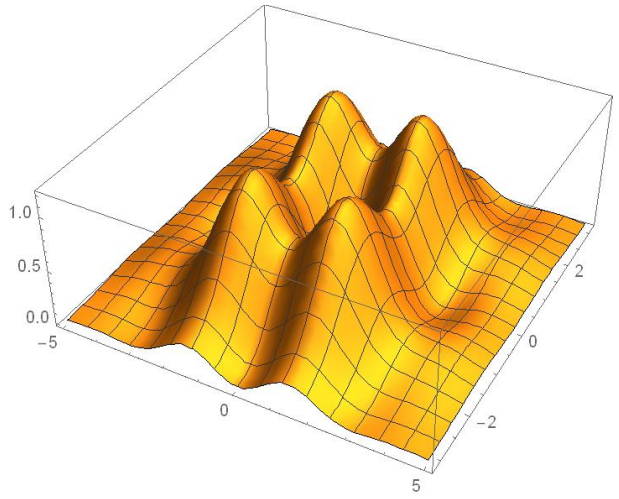


Fig. 1: Maximum Increase in Temperature for Neodymium Nanospheres.

According to the graph, it can be seen that the generated heat is increased by increase in nanoparticles size. For 100 (nm) nanoparticles (sphere with 50 (nm) radius), the maximum increase in temperature is 83 (K). When nanoparticles size reaches to 150 (nm), increase in temperature is increased in spite of increase in extinction coefficient. In order to find the reason of this fact, ratio of absorption to extinction for various nanospheres in Plasmon frequency is shown in Figure (2).
Figure (2) shows that increasing the size of nanospheres leads to decrease in ratio of light absorption to total energy of descendent light so that for 150 (nm) nanosphere, scattering is larger than absorption. It seems that although increase in nanoparticles size leads to more dissipation of descendent light, the dissipation is in the form of scattering and hence, it cannot be effective on heat generation.

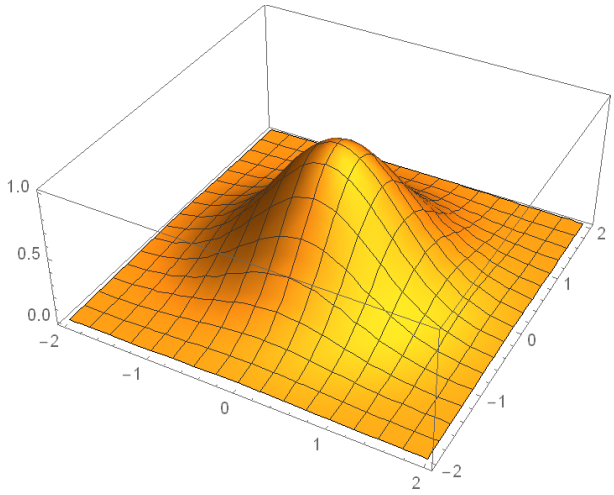


Fig. 2: Variations of Absorption to Extinction Ratio and Scattering to Extinction Ratio for Neodymium Nanospheres with Various Radiuses.

Heat distribution (Figure 3) shows that temperature is uniformly distributed throughout the nanoparticles which are due to high thermal conductivity of Neodymium.

In this section, core–shell structure of Neodymium and silica is chosen. The core of a nanosphere with 45 (nm) radius and silica layer thickness of 5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 nanometers are considered. The results show that increase in silica thickness leads to increase in extinction coefficient and shift in Plasmon wavelength of nanoparticles, to some extent.

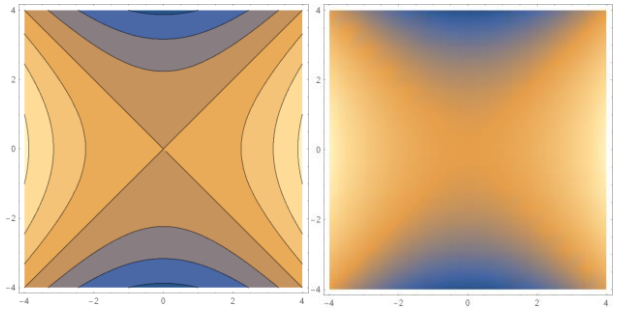


Fig. 3: Maximum Increase in Temperature for Spherical Nanoparticles with Radius of 45 (Nm) at Plasmon Wavelength of 685 (Nm).

According to Figure (4), silica shell causes to considerable increase in temperature of Neodymium nanoparticles but by more increase in silica thickness, its effects are decreased. Heat distribution (Figure 5) shows that temperature is uniformly distributed throughout metallic core as well as silica shell. However, silica temperature is considerably lower than core temperature due to its lower thermal conductivity. In fact, silica layer prohibits heat transfer from metal to the surrounding aqueous environment due to low thermal conductivity and hence, temperature of nanoparticles has more increase in temperature. Increasing the thickness of silica shell leads to increase in its thermal conductivity and hence, leads to attenuate in increase in nanoparticles temperature.

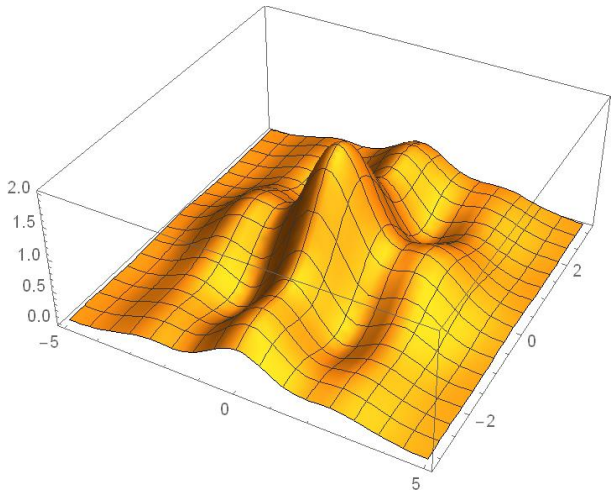


Fig. 4: Maximum Increase in Temperature for Core–Shell Neodymium Nanospheres with Various Thicknesses of Silica Shell.

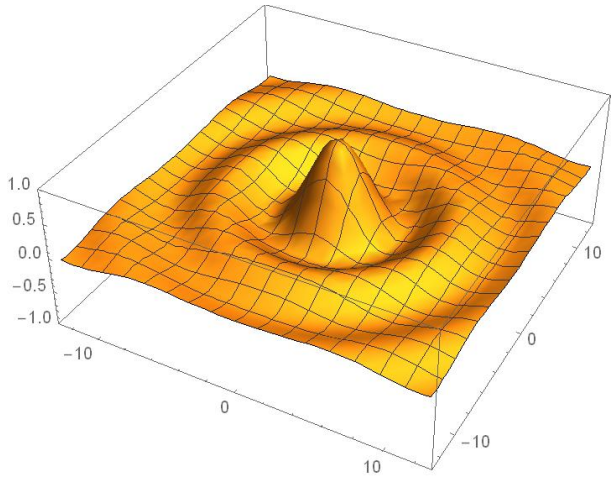


Fig. 5: Maximum Increase in Temperature for Core–Shell Nanoparticles with Radius of 45 (Nm) and Silica Thickness of 10 (Nm) at Plasmon Wavelength of 701 (Nm).

Figure (6) is drawn. This graph shows that variation of nanorod dimension ratio leads to considerable shift in Plasmon wavelength. This fact allows regulating the Plasmon frequency to place in near IR zone. Light absorption by body tissues is lower in this zone of spectrum and hence, nanorods are more appropriate for optothermal human cancer cells, tissues and tumors treatment methods.

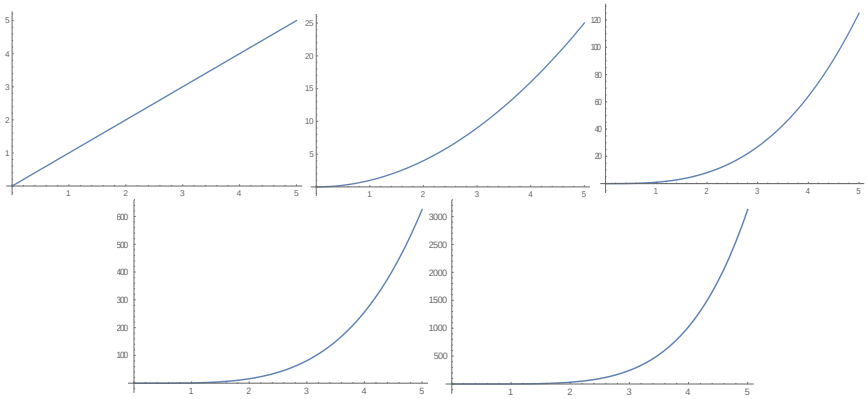


Fig. 6: Extinction Cross Section Area for Neodymium Nanorods with Effective Radius of 45 (Nm) and Various Dimension Ratios.

Variations of temperature in Neodymium nanorods with two effective radius and various dimension ratios are shown in Figure (7). By increase in length (a) to radius (b) of nanorod, temperature is increased.

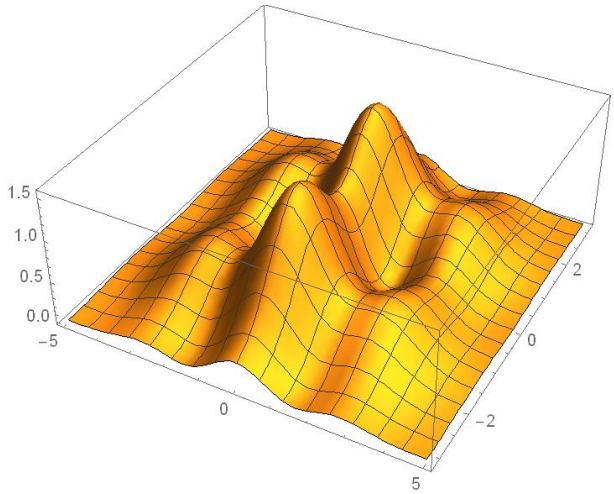


Fig. 7: Maximum Increase in Temperature for Nanorods with Effective Radius of 20 and 45 (Nm) and Various Dimension Ratios.

4. Conclusion and summary

The calculations showed that in Neodymium nanoparticles, light absorption in Plasmon frequency causes to increase in temperature of the surrounding environment of nanoparticles. In addition, it showed that adding a thin silica layer around the Neodymium nanospheres increases their temperatures. Calculations of nanorods showed that due to ability for shifting surface Plasmon frequency toward longer wavelength as well as more increase in temperature, this nanostructure is more appropriate for medical applications such as optothermal human cancer cells, tissues and tumors treatments.

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