Engineering of core/shell nanoparticles surface plasmon for increasing of light penetration depth in tissue (modeling and analysis)

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ABSTRACT

Objective(s): In this article, a new procedure for increasing the light penetration depth in a tissue is studied and simulated. It has been reported that the most important problem in biomedical optical imaging relates to the light penetration depth, and so this makes a dramatic restriction on its applications. In the optical imaging method, the detection of the backscattered photons from a deep tumor is rarely done or is done with a low efficiency; it is because of the high absorption and scattering losses.

Methods: Unlike the common methods (using a high energy laser for deep penetration) by engineering the nanoparticles' optical properties such as their anisotropy, absorption, and scattering efficiency, which are distributed into a tissue, the detected photons amplitude can be manipulated. In other words, by engineering the nanoparticle plasmon properties and their effect on the dye molecules' quantum yield, fluorescence emission and more importantly influence on the scattering direction, the light penetration depth is dramatically increased.

Results: The modeling results (Monte-Carlo statistical method) illustrate that the detected photons dramatically increased which is on order of 4 mm. So, this method can fix the light penetration problems in the optical imaging system.

Conclusions: Finally, the original idea of this study attributes to the indirect and transient manipulation of the optical properties of the tissue through the nanoparticles plasmon properties engineering. Moreover, by engineering plasmonic nanoparticles, maybe, the penetration depth can be enhanced which means that we can easily send light into a soft tissue and get its back scattering.

Appendix 1:

MIE theory for calculation of NPs average cosine of scattering angle

When an electromagnetic field is applied in a matter, the electric and magnetic components of that field act on the atoms in the matter. It consists of electrically charged particles, and therefore it will induce polarization in the matter. It is notable that the general solution for an arbitrary size particle can be found as well and it was first given by Mie theory [20-21]. By the interaction of electromagnetic wave on particle and analytically solving of Maxwell's equations, the scattering coefficients of the spherical harmonics a_n and b_n equal to [20]:

$$a_n = \left\{ m\psi_n(mx)\psi_n'(x) - \psi_n(x)\psi_n'(mx) \right\} / \left\{ m\psi_n(mx)\zeta_n'(x) - \zeta_n(x)\psi_n'(mx) \right\},$$

$$b_n = \left\{ \psi_n(mx)\psi_n'(x) - m\psi_n(x)\psi_n'(mx) \right\} / \left\{ \psi_n(mx)\zeta_n'(x) - m\zeta_n(x)\psi_n'(mx) \right\} \qquad (1)$$

where $\psi_n(x) = x.\ j_n(x)$ and $\zeta_n(x) = x.\ h_n^{(1)}(x)$ are Ricatti-Bessel and Ricatti-Hankel (first-order) function respectively, and x is the size parameter and m is the relative refractive index.

$$x = ka = 2\pi N_m a/\lambda, m = \sqrt{(\varepsilon^1/\varepsilon^m)} \qquad (2)$$

The resonances associated with coefficient a_n and b_n are electric and magnetic modes, respectively. It is notable that the local field around the particle is altered by changing of NPs radius; it means that by managing of a_n and b_n the electric and magnetic modes can be controlled. The well-known results for non-absorbing medium is independent of the distance from the sphere and, hence, valid in both the far-field and the near-field zone. Obviously, for absorbing host media, the intensity of the incoming light decreases on its way through the host medium to the encapsulated particle and the extinction rate depend explicitly on the size of the spherical volume of the absorbing medium around the particle. Then the definition of cross-section and efficiency as quantities which are specific only for the particle must be carefully discussed. The rate at which energy from the incoming light is scattered and absorbed is of the more interesting case in the interaction between light and a matter. They are obtained from the energy flux balance from and to the particle. The rates are obtained from surface integration of the Poynting vector outside the particle. In spherical coordinates it is convenient to use the surface of a conceptual sphere of radius $R_{cs} > R_{core}$ concentric with the particle with diameter $2R_{core}$ as integration surface. The rates are [20]:

$$W_{ext} = (-0.5).\mathrm{Re}\left\{ \int_0^{2\pi}\int_0^{\pi} (Ei_{nc} \times H_{sca}^* + E_{sca} \times H_{inc}^*) e_R . R_{cs}^2 Sin\theta d\theta d\varphi \right\},$$

$$W_{sct} = (-0.5).\mathrm{Re}\left\{ \int_0^{2\pi}\int_0^{\pi} (E_{sca} \times H_{sca}^*) e_R . R_{cs}^2 Sin\theta d\theta d\varphi \right\} \qquad (3)$$

where W_{ext} and W_{sct} represent the extinction rate and the scattering rate of the embedded sphere and dividing these rates by the intensity I_0 of incident light, the optical cross-section of a sphere is obtained as:

$$\sigma_{ext} = (2\pi/K_M{}^2)\sum_{n=1}^{\infty}(2n+1)\{\mathrm{Re}(a_n + b_n)\},$$
$$\sigma_{sca} = (2\pi/K_M{}^2)\sum_{n=1}^{\infty}(2n+1)\{(|a_n|^2 + |b_n|^2)\} \tag{4}$$

where k_m is the wave number. With the extinction and scattering cross-section, integral properties of the single particle are defined which are a measure of the ability to scatter and to absorb light. It is notable that they don't provide information about the angular distribution of the scattered light. This information is contained in the integrand of the scattering rate as [20, 21]:

$$E_{sct,\theta}.H^*{}_{sct,\varphi} - E_{sct,\varphi}.H^*{}_{sct,\theta} = (I_0/km^2R^2)[i_{per}(\theta)\sin^2\varphi + i_{par}(\theta)\cos^2\varphi] \tag{5}$$

where $i_{per}(\theta)$ and $i_{par}(\theta)$ are the scattering intensities perpendicular and parallel to the plane subtended by the incident and scattered directions (scattering plane) with:

$$i_{per}(\theta) = \left|\sum_{n=1}^{\infty}(2n+1)/(n^2+n).[a_n\pi_n(\theta) + b_n\tau_n(\theta)]\right|^2,$$
$$i_{par}(\theta) = \left|\sum_{n=1}^{\infty}(2n+1)/(n^2+n).[a_n\tau_n(\theta) + b_n\pi_n(\theta)]\right|^2 \tag{6}$$

where the angular dependent functions $\tau(\theta)$ and $\pi(\theta)$ are defined as $\tau(\theta) = \partial P_{nm}/\partial\theta$ and $\pi(\theta) = P_{nm}/\sin(\theta)$ are associated with Legendre polynomials. Finally, the important quantity connected with $i_{per}(\theta)$ and $i_{par}(\theta)$ is the cosine of scattering angle or anisotropy which is [20]:

$$g = \langle\cos\theta\rangle = \left\{(1/K_M{}^2).\int_0^{2\pi}\int_0^{\pi}(i_{par}(\theta) + i_{per}(\theta)).\cos\theta\sin\theta d\theta d\varphi\right\} / \left\{(1/K_M{}^2).\int_0^{2\pi}\int_0^{\pi}(i_{par}(\theta) + i_{per}(\theta)).\sin\theta d\theta d\varphi\right\} \tag{7}$$