OPTICAL PROPERTIES OF SILVER NANOCUBES IN CYTOPLASM

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Abstract

The input data for the Lorentz-Mie model include: the particle radius and wavelength of radiation, the real part of the index of refraction for surrounding medium, both the real and imaginary parts of refractive index for the particle material [2]. From these simulations we can determine the optimal radius of silver nanoparticles for therapeutic or diagnostic applications and the optimal wavelength of radiation for silver nanotubes that is best suited for therapeutic or diagnostic applications.

Keywords:

Silver nanotubes, wave equation, nanoparticle, wavelength, Mie coefficients, absorption, diagnostic applications, scattering, wave number, extinction.

An analytical solution of the wave equation for the spherical particles was found by the Danish physicist Ludwig Lorenz in 1890 in Danish, and also independently by the German physicist Gustav Mie in 1908, who was working on the problem of explaining the color of colloidal gold particles in water [1].

The optimal wavelength of laser radiation and the optimal size range of nanoparticles for effective laser killing of cancer cell can be found by using Mie diffraction theory at the single-scattering approximation. In the most general case, calculations based on the Mie theory are reduced to searching for the scattering matrix of j particles, $S^j(\theta,\varphi)$, consisting of four complex functions, $S_i^j(\theta,\varphi)$ $(I = 1, \dots, 4)$, describing the amplitude and phase of a scattered scalar wave in any direction. Forward scattering $(\theta = 0^0)$ contains the attenuation process of an electromagnetic wave, and for the case of spherical particles, $S_3^j = S_4^j = 0$. We can limit the description to a single scattering amplitude function:

$$S^j(0) = S_1^j(0) = S_2^j(0) = \frac{1}{2}\sum_{l=1}^{\infty}(2l+1)(a_l^j + b_l^j) \quad (1.1)$$

Here, the Mie coefficients a_l and b_l contain the characteristics of the dispersal medium and are calculated through the cylindrical Bessel function of the first kind, ψ_l(y), and the Hankel function of the second kind $\xi_l(\rho)$, both with half-integral indexes:

$$a_l = \frac{\psi_l^1(y)\psi_l(\rho) - \tilde{m}\psi_l(y)\psi_l^1(\rho)}{\psi_l^1(y)\xi_l(\rho) - \tilde{m}\psi_l(y)\xi_l^1(\rho)},$$

(1.2)

$$b_l = \frac{\tilde{m}\psi_l^1(y)\Psi_l(\rho) - \psi_l(y)\Psi_l^1(\rho)}{\tilde{m}\psi_l^1(y)\xi_l(\rho) - \psi_l(y)\xi_l^1(\rho)}.$$

Here, $\tilde{m} = m_0/m_l$ is the relative value of the relactive of the medium; $m_0 = n_0 - i\chi_0$ and $m_1 = n_1 - i\chi_1$ are the complex refractive indices of the particle material and the aqueous suspension, respectively; $\rho = 2\pi r_0/\lambda$ is the Mie parameter; and $y = 2\pi r_0 n_0/\lambda$, $\psi_l(u) = (\pi u/2)^{1/2} J_{l+1/2}^{(1)}$, $\xi_l(u) = (\pi u/2)^{1/2} H_{l+1/2}^{(2)}$ and $\psi_l^1 = \frac{d\Psi_l(u)}{du}$. With knowledge of the amplitude scattering function of $S^j(0)$, it is possible to calculate the integrated optical performance of the particles (i.e., the dimensionless efficiency coefficients of scattering, $K_{sca}^j(\rho,\tilde{m}) = \sigma_{sca}^j(\rho,\tilde{m})/\sigma_0$, absorption, $K_{abs}^j(\rho,\tilde{m}) = \sigma_{abs}^j(\rho,\tilde{m})/\sigma_0$, and attenuation,

$K_{att}^j(\rho,\tilde{m}) = \sigma_{att}^j(\rho,\tilde{m})/\sigma_0$, of the radiation at a given wavelength) as

$$K_{att}^j(\rho,\tilde{m}) = \frac{4\pi}{k^2} Re\{S^j(0)\},$$

$$K_{sca}^j(\rho,\tilde{m}) = \frac{2}{\rho^2}\sum_{l=1}^{\infty}(2l+1)\left\{\left|a_l^j\right|^2 + \left|b_l^j\right|^2\right\}, \quad (1.3)$$

$$K_{abs}^j(\rho,\tilde{m}) = K_{att}(\rho,\tilde{m}) - K_{sca}(\rho,\tilde{m}),$$

were $k = 2\pi/\lambda$ is the wave number, and $\sigma^j_{sca}(\rho,\tilde{m})$, $\sigma^j_{abs}(\rho,\tilde{m})$, $\sigma^j_{att}(\rho,\tilde{m})$ and σ_0 are the scattering, absorption, attenuation, and geometric cross-sections of j particles, respectively [2].

The nanoparticle radius is a parameter that can be engineered to modify the light absorption properties of a particle. The complex refractive indices of the nanoparticle material and surrounding medium, however, are dependent upon the physical situation under investigation. The complex refractive index of the surrounding medium corresponds to the type of biological tissue being treated, and therefore is treated as a no alterable parameter. The complex refractive index of the spherical nanoparticle could technically be engineered by making the nanoparticles from different materials. However, because this application relies on the biological inertness of the nanoparticles, the choice of materials becomes more limited. The example of the complex refractive indices for Silver(Ag) nanotubes at room temperature for ordinary rays(Table 1).

Table 1. Complex refractive indices for Silver nanocubes at room temperature for ordinary rays.

Substance	**Wavelength, λ(nm)**	**Refractive index, $m = n_0 - ik_0$**		**Reference**
		n_0	k_0	
Silver(Ag) nanocubes 30±1 nm	400	0.763798	1.297153	Generated from www.luxpop.com
	500	1.046559	2.019048	
	600	2.182226	3.001190	
	700	3.874566	2.209014	

The n_0 and k_0 komponents of the complex refractive index for fullerene are calculated from the available electric permittivity ε_1 and ε_2 values by using the following equations:

$$\varepsilon = \varepsilon_1 + i\varepsilon_2 = (n_0 + ik_0)^2 \qquad (1.4)$$

$$\varepsilon_1 = n_0^2 + k_0^2 \qquad (1.5)$$

$$\varepsilon_2 = 2n_0k_0 \qquad (1.6)$$

$$n_0 = \sqrt{\frac{\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2}}{2}} \qquad (1.7)$$

$$k_0 = \sqrt{\frac{-\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2}}{2}}. \qquad (1.8)$$

Table 2. Real parts of the refractive indices for surrounding media(cytoplasm) at room temperature for ordinary rays.

Wavelength	**200 nm**	**400 nm**	**500 nm**	**700 nm**
Medium	n_1	n_1	n_1	n_1
Cytoplasm	1.33	1.35	1.36	1.367

The results of the simulations for the extinction Q_{ext}, scattering Q_{sca}, and absorption Q_{abs} efficiencies vs. the particle radius are shown in Fig. 1. Optimal radius for the therapeutic uses correspons to the maximum absorption point shown in Fig. 1. The optimal radius range for diagnostic applications is determined by the region where the scattering efficiency Q_{sca} dominates over the absorption efficiency Q_{abs}(black curve).

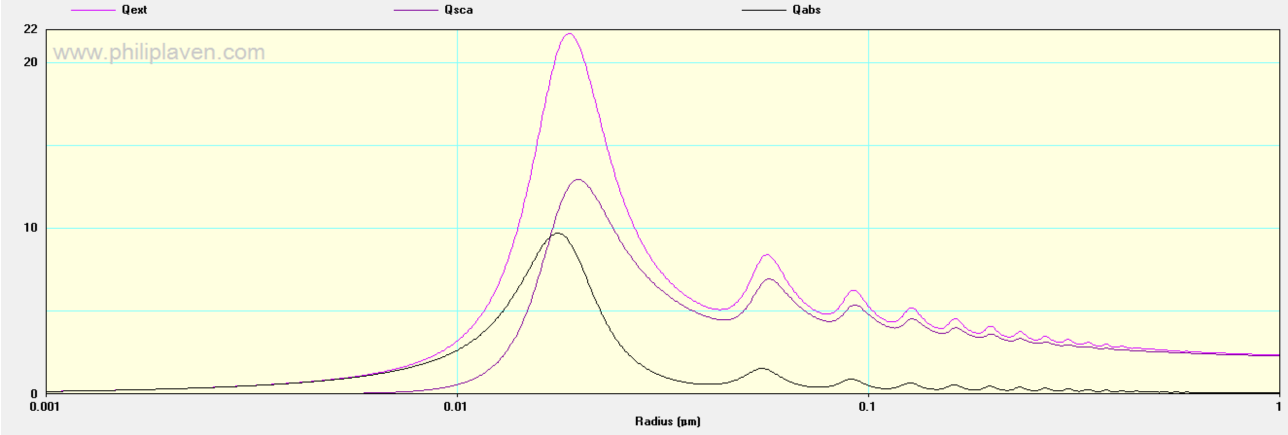

Fig.1. Running the simulations for the extinction Q_{ext}, scattering Q_{sca} and absorption Q_{abs} efficiency vs. the particle radius(λ=400 nm).

The results of the simulations for the extinction Q_{ext}(red surve), scattering Q_{sca}(pink surve), and absorption Q_{abs}(black surve) efficiencies of the particle vs. the wavelength of radiation are shown in Fig. 2.

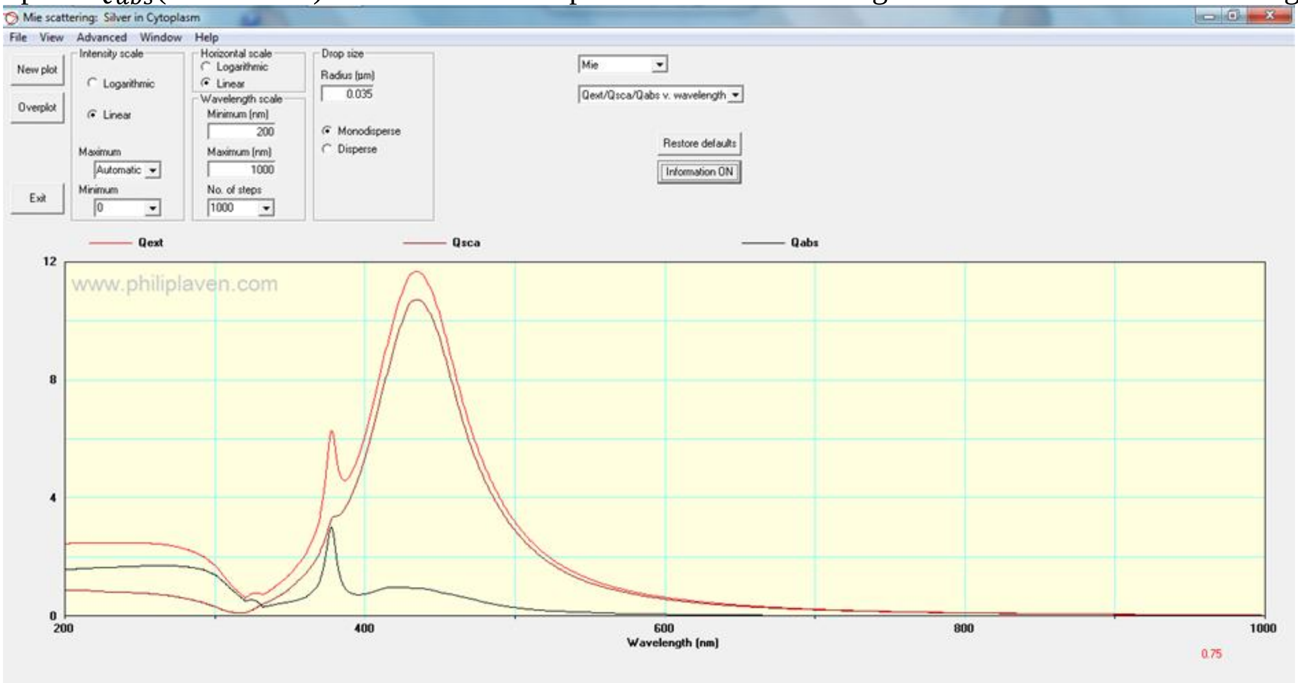

Fig. 2. Running the simulations for the extinction Q_{ext}, scattering Q_{sca} and absorption Q_{abs} efficiencies of the nanoparticle vs. wavelength of radiation.

From these simulations we can determine the optimal wavelength of radiation for a given nanoparticle which best suits therapeutic or diagnostic applications. The optimal wavelength of light for therapeutic uses corresponds to the maximum absorption point shown in Fig. 2. The optimal wavelength range for diagnostic applications is determined by the region where the scattering efficiency Q_{sca}(pink surve) dominates over the absorption efficiency Q_{abs}(black curve).

References

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