32nd URSI GASS, Montreal, 19–26 August 2017

Parameter studies on optimal absorption and electrophoretic resonances in lossy media

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Abstract

This paper summarizes and elaborates on some new results on the optimal absorption in small spherical suspensions based on electrophoretic (plasmonic) resonances and lossy surrounding media. The main application here is to study the physical limitations for radio frequency absorption in gold nanoparticle (GNP) suspensions and its potential to achieve GNP targeted hyperthermia in cancer therapy. Numerical parameter studies are included to demonstrate the analysis approach.

1 Introduction

The study of optimal absorption based on electrophoretic (or plasmonic) resonances in lossy materials provides a number of interesting scientific questions with a potential application in radiotherapeutic hyperthermia based methods to treat cancer. In particular, gold nanoparticles (GNPs) can be coated with ligands that target specific cancer cells as well as providing a net electronic charge of the GNPs. One hypothesis is then that the charged GNPs will facilitate an electrophoretic current that can destroy the cancer under electromagnetic radiation [1, 4, 5]. However, it is also important to observe the complexity of the clinical application with many possible physical and biophysical phenomena to consider, as well as the fact that several authors have questioned whether metal nanoparticles can be heated in radio frequency at all, see *e.g.*, [1, 3]. We have recently performed a study on the physical limitations for radio frequency absorption in a spherical suspension where the main theoretical result is the derivation of an optimal conjugate match with respect to the surrounding medium [4]. It is demonstrated in [4] that for a surrounding medium consisting of a weak electrolyte solution, a significant RF-heating can be achieved inside a small GNP suspension, provided that an electrophoretic particle acceleration (Drude) mechanism is valid and can be tuned into resonance at the desired frequency. In this paper, we summarize briefly the new theory, we expand the asymptotic analysis and we demonstrate some new parameter studies related to this application.

2 Optimal absorption for the sphere

Consider a spherical region of radius r_1 consisting of a dielectric material with permittivity ε_1 and which is suspended inside a lossy dielectric background medium having permittivity ε. A relative heating coefficient is defined as $F = P_{\rm loc}(r_1)/P_{\rm b}(r)$ where $P_{\rm loc}(r_1)$ is the mean local heating (in $\mathrm{W/m^3}$) generated inside the sphere of radius r_1, and $P_{\rm b}(r)$ the mean background heating (in $\mathrm{W/m^3}$) at some observation radius $r > r_1$. In a close vicinity to a small sphere (both r and r_1 are small), an asymptotic analysis, similar as presented in [4], reveals that the optimal excitation that maximizes F is an electric dipole field yielding the relative heating coefficient

$$F^{\rm a}(\varepsilon_1) = 9\frac{|\varepsilon|^2}{\Im\{\varepsilon\}}\frac{\Im\{\varepsilon_1\}}{|\varepsilon_1+2\varepsilon|^2}. \tag{1}$$

An alternative analysis is given by the general Mie theory for lossy media where the absorption cross section $C_{\rm abs}$ for plane wave incidence is given by

$$C_{\rm abs} = 12\pi k_0 r_1^3\frac{|\varepsilon|^2}{\Re\{\sqrt{\varepsilon}\}}\frac{\Im\{\varepsilon_1\}}{|\varepsilon_1+2\varepsilon|^2}, \tag{2}$$

and where k_0 is the wave number of vacuum, see [4, 5]. It has recently been shown in [4] that (2), and hence also (1) are locally concave functions in the complex parameter ε_1 and which are maximized by the conjugate match

$$\varepsilon_{1\rm o} = -2\varepsilon^*. \tag{3}$$

It is noted that the conjugate match $\varepsilon_{1\rm o}$ yields a desired function with the metamaterial characteristics $\Re\varepsilon_{1\rm o} < 0$ for a "normal" surrounding medium with $\Re\varepsilon > 0$. It is also noted that the parameters of a Drude model can always be tuned to the conjugate match at a single frequency, but just like the metamaterials with real valued and negative permittivity [2], the conjugate match (with small imaginary part) is not realizable as a passive material over a finite bandwidth, *cf.*, [4].

3 Numerical examples

Consider a surrounding medium consisting of a weak electrolyte solution with relative permittivity

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 - i\omega\tau} + i\frac{\sigma}{\omega\varepsilon_0}, \tag{4}$$

where ε_∞, ε_s and τ are the high frequency permittivity, the static permittivity and the dipole relaxation time in the corresponding Debye model for water, respectively, and σ the conductivity of the saline solution. The effective permittivity of the spherical GNP suspension is modeled as

$$\varepsilon_1(\omega) = \varepsilon(\omega) + i\frac{\sigma_1}{\omega\varepsilon_0}\frac{1}{1 - i\omega\tau_1}, \tag{5}$$

where $\sigma_1 = \mathscr{N}q^2/\beta$ and $\tau_1 = m/\beta$, where $\mathscr{N}$ is the number of particles per unit volume, q the particle charge, β the friction constant of the host medium and m the mass of the particle, *cf.*, [5]. The Drude parameters can furthermore be tuned to the conjugate match by choosing

$$\tau_1 = \frac{1}{\omega_d}\frac{\Re\varepsilon(\omega_d) - \Re\varepsilon_{1o}(\omega_d)}{\Im\varepsilon_{1o}(\omega_d) - \Im\varepsilon(\omega_d)}, \tag{6}$$

$$\sigma_1 = \varepsilon_0\left(\Re\varepsilon(\omega_d) - \Re\varepsilon_{1o}(\omega_d)\right)\frac{1 + \omega_d^2\tau_1^2}{\tau_1}, \tag{7}$$

where $\omega_d = 2\pi f_d$ is the desired resonance frequency.

In the numerical examples below, the surrounding saline water is modeled by using $\varepsilon_\infty = 5.27$, $\varepsilon_s = 80$, $\tau = 10^{-11}\,$s and $\sigma = 0.1\,$S/m. For the tuned Drude model we have used $f_d = 1\,$GHz. For the realistic Drude models below, the radius of the GNP with ligands is $a = 2.5\,$nm, the radius of the gold core is $a_{Au} = 0.75\,$nm and the mass density of gold is $\rho_{Au} = 19300\,\mathrm{kg/m^3}$. The ligands are assumed to have a mass density similar to water. The friction constant β is modelled as $\beta = 6\pi\mu_f a$, where $\mu_f = 10^{-3}\,\mathrm{Nsm^{-2}}$ is the dynamic shear viscosity of the host medium (water at room temperature) as in [5]. The number of particles per unit volume is given by $\mathscr{N} = \phi/(4\pi a^3/3)$, where ϕ is the volume fraction of GNPs in the spherical suspension. Here, we have chosen $\phi = 2\cdot 10^{-3}$ as in [5]. The net charge of the GNP is modeled as $q = (3a_{Au} + 0.5a_{Au}^2)e_0 + n_L e_0$, where the charge of the gold core is modeled as in [5], n_L is the assumed net electron count in the ligand shell and e_0 denotes the electron charge $e_0 = 1.6\cdot 10^{-19}\,$C.

In Figure 1 is shown the absorption cross section C_{abs} given by (2), plotted as a function of frequency and where the radius of the spherical suspension is $r_1 = 1\,\mu$m. In Figure 2 is shown the relative heating coefficient $F^a(\varepsilon_1)$ given by (1) representing the mean power dissipation inside a small sphere relative the mean power dissipation in a close vicinity of the sphere. In both figures, ε_1 is either the optimal conjugate match, the tuned Drude model or the realistic Drude models with $q_L = n_L e_0 \in \{10, 10^2, 10^3\}e_0$.

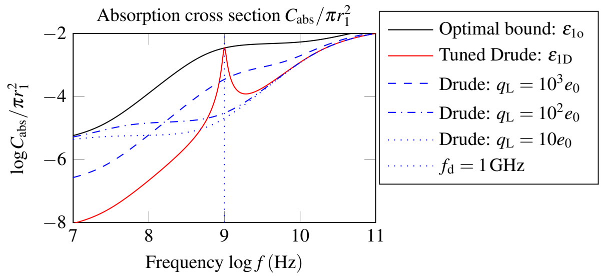

Figure 1. Absorption cross section C_{abs} for a small spherical GNP suspension of radius $r_1 = 1\,\mu$m. The surrounding medium is a saline solution with $\sigma = 0.1\,$S/m.

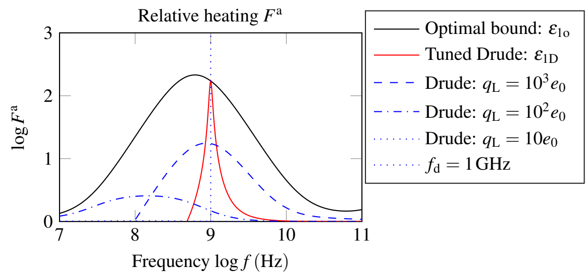

Figure 2. Relative heating coefficient F^a in a close vicinity of a small spherical GNP suspension. The surrounding medium is a saline solution with $\sigma = 0.1\,$S/m.

4 Acknowledgements

This work was supported by the Swedish Foundation for Strategic Research (SSF).

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