# Calculation of the Induced Charge Distribution on the Surface of a Metallic Nanoparticle Due to an Oscillating Dipole Using Discrete Dipole Approximation method

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## Abstract

In this paper, the interaction between an oscillating dipole moment and a Silver nanoparticle has been studied. Our calculations are based on Mie scattering theory and discrete dipole approximation(DDA) method.At first, the resonance frequency due to excitingthe localized surface plasmons has been obtained using Mie scattering theory and then by exciting a dipole moment in theclose proximity of the nanoparticle, the induced charge distribution on the nanoparticle surface has been calculated. In our calculations, we have exploited the experimental data obtained by Johnson and Christy for dielectric function.

## 1. Introduction

Nanotechnology has tremendous potentials to improve human's life, so it has been the subject of considerable research by numerous researchers. The recent archaeological discoveries illuminatedthat the nanotechnology has been used even before Christ. An ancient piece of artremained from that era is Lycurgus cupthat is nanotechnology-enhanced, was obtained in recent excavations. The cup which belongs to the fourth century BC, is mainly built form the glass with bronze mounts. It has been demonstrated that the noble metal nanoparticles embedded in the glass are the origin of the color of the cup. At places, where light is transmitted through the glass it appears red, at places where light is scattered near the surface, the scattered light appears greenish. The bright colors of noble metal nanoparticles are due to the resonant excitation of a collective oscillation of the conduction band electrons in the particles namely called particle plasmon.

Quantitative studies on scattering of light from particles with small dimensions flourished at the late of the nineteenth century. In 1899, Lord Riley

[1] explained why the sky is blue with deriving a simple relationship for scattered power from a sphere with dimensions much smaller than the wavelength of the incident light. In 1904, Garnet[2] stated the bright colors in metallic glass using Drude Model [3]which explains the optical properties of the metals having free electrons. Soon after that, on 1908, Gustav Mie [4]proposed a general formulation for light scattering from a spherical surface including colloidal gold nanoparticles with different sizes. He described the formation manner of surface electromagnetic modes for metal nanospheres. Precisely, he demonstrated that the resonance frequencies namely called the localized surface plasmon resonance (LSPR) occurin visible region because of the free electrons collective effects. The LSPR depends on the size, shape and the surrounding medium. After that, a lot of studies were done to investigate this phenomenon in more details [5, 6].

Recently, the developmentsin electromagnetic simulation techniques as well as increased computing power, and improving production methods, such asnano-lithography, electron beam lithography and focused ion beam milling, haveincreased the interest of researchers for engineering metallic nanostructures. Different numerical methods are available to calculate the optical response of nanoparticles,particularly none-sphere ones, including transfer matrix method (TMM) [7], the finite difference time domain (FDTD) [8], discrete dipole approximation (DDA) [9], multiple multipolar approximation (MMA) [10] and conjugate gradient fast Fourier transform (CG-FFT) [11].

DDA method which sometimes referred to as the CDA[1] approach is a well-known approach.Its accuracy is remarkablewhen the target

dimensionsaresmaller than the light wavelength. This method, at first, was introduced by Purcell and Pennypacker[13]in 1973 to study interplanetary dust grains. Subsequently,Draine and Flatau [14], exploiting this method,wrote the DDSCAT code in FORTRAN programming language[15]. This codeis currently used for studying the localized surface plasmons [16–19].

It is easy to calculate the static induced charge density on a metallic nanosphere surface due to an electric dipole in its close proximity by using the method of image charges which is an analytical method.However,this method is not applicable in dynamic problems when the dielectric constant of the metallic nanosphere has an imaginary part. The situation is worse when the nanoparticle has an irregular and asymmetric geometry, when the use of numerical methods is inevitable.An iterative self-consistent approach has been used previously for calculating the charge distribution induced inside complex plasmonic nanoparticles due to the incident electric field [20]. Such calculations can be very time-consuming and convergence problems are sometimes encountered in the algorithm, even under the best circumstances. The discrete dipole approximation provides an alternative method for determining charge distribution on the nanoparticle volume which utilizes the optimization method in order to solve the linear coupled equations.

In this paper,at first, the resonance frequency of thelocalized surface plasmons are determined using wave scattering from a dielectric sphere (Mie scattering) and then by employing the DDA technique, the charge distribution on the surface of thenanosphere due to adipole in its close proximity oscillatingwith resonance frequency is calculated. For DDA technique, we made use of nice home-made MATLAB codes.

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[1]Coupled Dipole Approximation

## 2. Dipole Discrete Approximation Method

In this method, the desired object is divided into $N$ dipoles with $\alpha_i$ polarizability in $r_i$ spatial position. The induced polarization in dipoles due to the local electric field $E_{loc}$ regardless the term $e^{i\omega t}$ would be as follows:

$$P_i = \overrightarrow{\alpha_i} \cdot E_{loc}(r_i), \tag{1}$$

in which $E_{loc}$ is the sum of the incident electric field and the retarded electric fields due to the rest $N-1$ dipoles:

$$E_{loc}(r_i) = E_{loc,i} = E_{inc,i} + E_{ret,i}$$

$$= E_{inc,i} - \sum_{j \neq i} A_{ij} \cdot P_j, \tag{2}$$

in which $A$ matrix is defined by:

$$A_{ij}.P_j = \exp(ikr_{ij}) \left\{ \frac{k^2}{r_{ij}^3} r_{ij} \times (r_{ij} \times P_j) + \frac{1 - ikr_{ij}}{r_{ij}^5} \right. \tag{3}$$

where $r_{ij} = r_i - r_j$, $r_{ij} = |r_{ij}|$ and $k = \omega/c$. By substituting Eq. (2) in Eq. (1) and rearranging to solve for the incident electric field, the following matrix equation will be obtained:
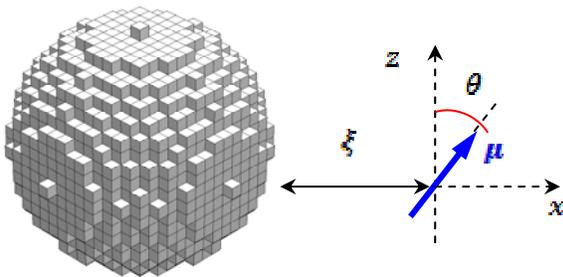


Fig. 1. Geometric structure of the metal nanoparticleand emitting dipole.

$$E_{inc,i} = \overrightarrow{\alpha_i}^{-1} P_i + \sum_{j \neq i} A_{ij} \cdot P_j \tag{4}$$

By taking threescalar components and $N$ point dipoles into account, the Eq. (4) will take the form $A'p = E_{inc}$, where $A'$ is a $3N \times 3N$ dimensional matrix, $E_{inc}$ and $p$ both are $3N \times 1$ column matrices. The criterion for validity of the DDA method isto satisfy the condition $|m|kd \leq 1$, where $m$ is the refractive index of the nanoparticle and $d$ is the distance between two discrete dipoles. Inother words, if the effective radius of a nanoparticle with volume $V$ is defined as $a_{eff} = (3V/4\pi)^{1/3}$, the aforementioned condition will be as follows:

$$N \geq \left(\frac{4\pi}{3}\right) |m|^3 (ka_{eff})^3 \tag{5}$$

## 3. Modeling

According to Fig. 1, an electric dipole is at thedistance $\xi$ from a silver spherical nanoparticle with radius $a$. The nanoparticleis divided into cubic discrete dipoles with volume $d^3$ using DDA method.The polarization of the dipole is considered to be in $z$ direction ($\theta = 0$) and its value is equal to $|\mu| = 1$ Debye.

The field of an electric dipole in spherical coordinates $(r, \theta, \varphi)$ is obtained as follows:

$$E_{\text{inc}} = \frac{i|\mu|k^3}{4\pi\epsilon_0}\left\{2\left(\frac{1}{k^2r^2} + \frac{i}{k^3r^3}\right)\cos\theta\,\hat{r}\right.$$

$$\left.\left(\frac{i}{kr}\quad\frac{1}{k^2r^2}\quad\frac{i}{k^3r^3}\right)\sin\theta\,\hat{\theta}\right\}e^{ikr}$$

(6)

where $E_{\text{inc}}$ is the localized electric field.
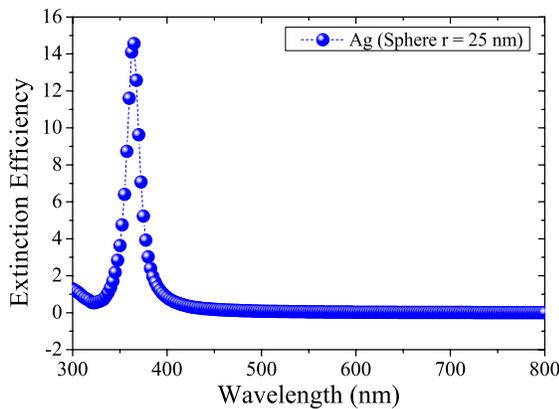


Fig. 2. Calculated extinction spectra for a spherical silver nanoparticle of radius 25 nm using Mie scattering theory.

## 4. Results and discussion

As shown in Fig. 2, using Mie scattering theory, the resonance frequencyofa silver(Ag) spherical nanoparticle with radius 25nm due to excitation of

the localized surface plasmonshas been obtained. Obviously, the nanoparticle has resonant behavior atwavelength 364nm, which is due to the sharp

absorption peak of Ag around 4 eV. It is

worthwhile to mention that the Mie resonance in noble metals is not just due to the free electrons, but it is a hybrid resonance attributed tothe electronsof the conduction bandand $d$ layer

electrons.

Consideringan emitting dipole with polarization$\mu = \mu_0 cos(\omega t)\,\hat{z}$and emitting

wavelength$\lambda = 364$ nmat the distance $\xi = 5$ nm

from the sphere, the surface charge distribution, as shown in Fig. 3, has been obtained using the relationship $\sigma_p = \Im(P.n)$, where $n$ is the surface

normal vector. As it could be seen from the figure, an electric dipole with opposite direction is induced on the surface of the sphere. This induced dipole oscillates with the same frequency as theemitting dipole. By changing the position of the emittingdipole, it is possible to provide a situation in which the induced and emittingdipolessuperpose constructively. In this case, it would beexpected to
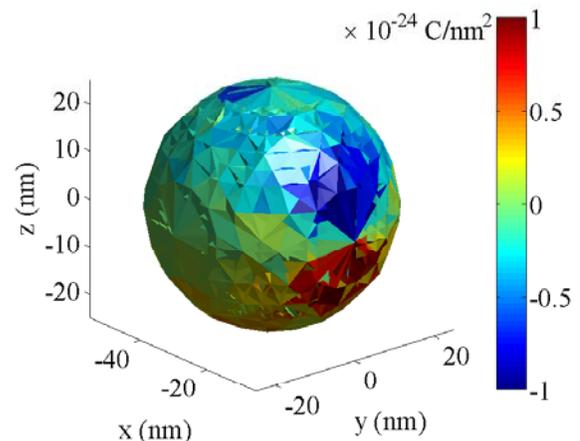


Fig 3. Distribution of induced charge density on the surface of a nanoparticle with dielectric coefficient $\varepsilon = -2.495 + 0.249i$ in resonance wavelength.

enhance the photoluminescence (PL) of the emitter in vicinity of a metal nanoparticle.

## 4. Conclusion

The charge distribution on the surface of a spherical nanoparticle due to an emittingdipole in its close proximity has been obtained using DDA method. The calculation results showed that an

induced electric dipole on the nanoparticle surface created whichis in opposite direction to the emitting dipole.

This method could be expanded to nanoparticles with irregular geometries and different distances. Also, the PL performance of an electric dipole in the vicinity of a metal nanoparticle could be investigated using this method.

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