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# Refractive index sensitivity analysis of gold nanoparticles

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ABSTRACT

In this article, with gold nanoellipsoid, nanocylinder, and nanobar as the research object, we investigated the variation of resonance wavelength and refractive index sensitivity by using discrete dipole approximation. The effects of the particle size and shape on the resonance wavelength and refractive index sensitivity were quantitatively analyzed. We also performed comparative analysis on the refractive index sensitivity of these three gold nanoparticles in order to find gold nanoparticles with high sensitivity. It was found that gold nanocylinder has a greater refractive index sensitivity as compared to the gold nanoellipsoid or gold nanobar of the same dimensions, thus it is more suitable for biosensing applications.



## 1. Introduction

Gold nanoparticles exhibit excellent optical properties which differ from bulk material. The interaction of gold nanoparticles with the incident light of a certain wavelength results in localized surface plasmon resonance (LSPR) phenomenon, which leads to the absorption and scattering of light by nanoparticles, as well as the local electric field around the nanoparticles, will be strongly enhanced [1–3]. These special optical properties of gold nanoparticles make them have tremendous applications in many fields, including biology, medicine, chemistry, information, energy, and environment [4–8].

LSPR of metal nanoparticles is highly sensitive to the refractive index change of ambient medium [9]. Thus, one can measure the change of local environment by using the shift of resonance wavelength. Researchers have developed LSPR-based biosensors [10]. For the LSPR-based biosensors, the small refractive index change of environment need to cause the large variation of resonance wavelength. In recent years, many experimental and theoretical studies have been committed to refractive index sensing properties of metal nanoparticles with various shapes and sizes, they are looking for the best nanostructures and choosing the appropriate particle size in order to increase the refractive index sensitivity [11–19]. Previous research has shown that nanotriangles, nanorods, and nanoshells can offer high refractive index sensitivity [20]. Gold nanoellipsoid, nanocylinder, and nanobar are another typical non-spherical gold nanoparticles. However, there are no relevant research on the refractive index sensitivity analysis of these particles.

In this paper, we investigate systematically the refractive index sensing properties of single nanoparticles of different sizes and shapes by using discrete dipole approximation (DDA). The effects of size and shape on the resonance wavelength and refractive index sensitivity are quantitatively analyzed. We find the gold nanoparticle with high sensitivity, and compare it to the refractive index sensitivity of gold nanorod. This paper is organized as follows. In Section 2, we introduce the DDA

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method, size-dependent dielectric function, and the refractive index sensitivity. In Section 3, we give some numerical results and discussions for single nanoparticles of different sizes and shapes. Finally, a summary will be given in Section 4.

## 2. Theory

### 2.1. Discrete dipole approximation

The discrete dipole approximation (DDA) is a flexible and powerful technique for computing scattering and absorption by targets of arbitrary geometry. The DDA is an approximation of the continuum target by a finite array of polarizable points which acquire dipole moments in response to the local electric field. The DDA was apparently first proposed by Purcell & Pennypacker [21]. DDA method was developed further by Draine [22], Draine & Goodman [23], reviewed by Draine & Flatau [24], and extended to periodic structures by Draine & Flatau [25]. The freely available open-source Fortran-90 software package (DDSCAT 7.2) developed by Draine & Flatau [26] is used in this paper.

In the DDA approach, one represents the object of interest as a cubic lattice of $N$ polarizable points. There is no restriction as to which of the cubic lattice sites is occupied, which means that DDA can represent an object or multiple objects of arbitrary shape. Let us assume an array of $N$ polarizable point dipoles located at $\{\mathbf{r}_i, i = 1, 2, ..., N\}$, each one characterized by a polarizability $\alpha_i$. The dipole moment induced in each dipole as a result of interaction with a local electric field $\mathbf{E}_{loc,i}$ is:

$$\mathbf{P}_i = \alpha_i \mathbf{E}_{loc,i} \tag{1}$$

where $\mathbf{E}_{loc,i}$ is the sum of the incident electric field and the contribution from all other dipoles

$$\mathbf{E}_{loc,i} = \mathbf{E}_{inc,i} + \mathbf{E}_{dipole,i} = \mathbf{E}_0 \exp(i\mathbf{k}\cdot\mathbf{r}_i - i\omega t) - \sum_{j\neq i} \mathbf{A}_{ij}\mathbf{P}_j \tag{2}$$

where $-\mathbf{A}_{ij}\mathbf{P}_j$ is the electric field at $\mathbf{r}_i$ that is due to the dipole moment $\mathbf{P}_j$ at location $\mathbf{r}_j$, including retardation effects. $\mathbf{A}_{ij}$ is a $3\times 3$ matrix that represents the interaction between the dipole at $\mathbf{r}_i$ and $\mathbf{r}_j$, it is given as

$$\mathbf{A}_{ij} = \frac{\exp(ikr_{ij})}{r_{ij}} \left[ k^2(\hat{r}_{ij}\hat{r}_{ij} - \mathbf{I}_3) + \frac{ikr_{ij} - 1}{r_{ij}^2}(3\hat{r}_{ij}\hat{r}_{ij} - \mathbf{I}_3) \right], \quad i \neq j \tag{3}$$

where $k = \omega/c = 2\pi/\lambda$ is the wave number, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the distance from points $j$ to $i$, $\hat{r}_{ij} = (\mathbf{r}_i - \mathbf{r}_j)/r_{ij}$ is the unit vector in the direction from points $j$ to $i$, and $\mathbf{I}_3$ is the $3\times 3$ identity matrix. Defining the diagonal matrix as $\mathbf{A}_{ii} = \alpha_i^{-1}$, and substituting into Eqs. (1) and (2) gives

$$\mathbf{A}_{ii}\mathbf{P}_i + \sum_{j\neq i} \mathbf{A}_{ij}\mathbf{P}_j = \mathbf{E}_{inc,i} \tag{4}$$

Thus, the problem is reduced to finding the dipole moments $\mathbf{P}_j$ that satisfy a system of 3N complex linear equations

$$\sum_{j=1}^{N} \mathbf{A}_{ij}\mathbf{P}_j = \mathbf{E}_{inc,i} \tag{5}$$

Once the above equation has been solved for the unknown dipole moments $\mathbf{P}_j$, the extinction, absorption, and scattering cross sections can be calculated by [22]

$$C_{ext} = \frac{4\pi k}{|\mathbf{E}_0|^2} \sum_{j=1}^{N} Im(\mathbf{E}_{inc,j}^* \cdot \mathbf{P}_j) \tag{6}$$

$$C_{abs} = \frac{4\pi k}{|\mathbf{E}_0|^2} \sum_{j=1}^{N} \left\{ Im[\mathbf{P}_j \cdot (\alpha_j^{-1})^* \mathbf{P}_j^*] - \frac{2}{3}k^3|\mathbf{P}_j|^2 \right\} \tag{7}$$

$$C_{sca} = C_{ext} - C_{abs} \tag{8}$$

### 2.2. Size-dependent dielectric function

There are two sets of quantities that are often used to describe optical properties: the real and imaginary parts of the complex refractive index $\tilde{n} = n + ik$ and the real and imaginary parts of the complex dielectric function (or relative permittivity) $\varepsilon = \varepsilon_1 + i\varepsilon_2$. These two sets of quantities are not independent; either may be thought of as describing the intrinsic optical properties of matter. The relations between the two are

$$\tilde{n} = \sqrt{\varepsilon} \tag{9}$$