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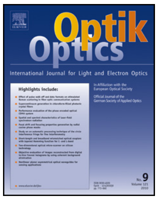

Original research article

Shape and size determination of plasmonic nano particles using particle swarm optimization algorithm based absorption coefficient

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ABSTRACT

Plasmonic nano particles can be greatly enhancing the optical absorption coefficient spectrum. Since optical properties of these particles strongly depends on the size and shape of the nano particles, in this paper particle swarm optimization algorithm (PSO) is used to optimize the nano particles shape and size in order to amplification of the absorption coefficient. In PSO a swarm consists of a matrix with decimal numbers, controls the particles shape and size in order to increase the absorption coefficient in the visible part of light spectrum. It is found that significant plasmonic enhancement of above 100000 can be obtained by optimize selection of particle shapes and sizes.

1. Introduction

The surface plasmons (SP) resonance wavelength of noble metal nano particles (MNP) lies in the visible part of spectrum, as opposed to bulk plasmons which have corresponding wavelength in the ultraviolet range. This peculiarity is very interesting from the application point of view and allows applying noble MNPs as optical devices such as Raman scattering [1], radiative rate enhancement [2], solar cells [3], and optical biosensors [4]. Since optical properties of these particles depend on their size and shape, one of the desirable goals is to control shape of metal and semiconductor nano particles. Many theoretical and experimental researches have demonstrated that, plasmonic ellipsoid are widely used to design nano antennas with improved capabilities. Shape control has been successfully demonstrated for gold nanoparticles using nonionic surfactants, silver under potential deposition, and nanoreplica molding [5–7]. Nano replica molding has been demonstrated as a low-cost method for manufacturing variety of nano ellipsoid. Recently, a plasmonic nano domes array fabricated by nano replica molding process [8].

In addition to the recent interest in shape control of nano particles, optical properties of noble metal with their intense colors have fascinated scientists since turn of this century. In addition to the shape, size and material of nano-particles, properties of light strongly depend on the localized positions of nano-particles. Plasmonic nano particles with periodic structure have been reported in some literatures [9,10]. One of the most promising Plasmonics nano particle platforms, is studying the effect of deterministic aperiodic structure of nano-particles on properties of light. These structure, which are intermediate between disordered system and periodic one enable a unique control and manipulating of spatially localized plasmonic states over broadband frequency and angular spectra. Optimization problems in the plasmonic nano structure

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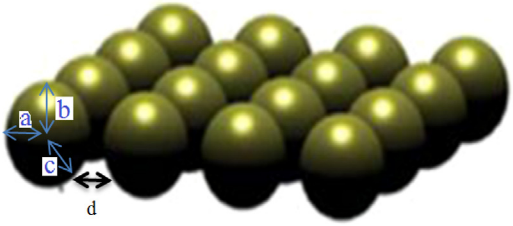

Fig. 1. 2-dimensional array of gold nano particles.

area can be divided into two categories. In the first type continuous optimization algorithms can be used to engineering the geometrical metal nano structures [11], whereas in the second type, binary optimization algorithms can be applied to control the presence ('1') or the absence ('0') of metal nano particles in the array [12]. In this paper, PSO algorithm is used to engineering the nano particles geometry in order to achieve the higher absorption coefficient. This approach can be useful in the optical applications such as solar cells and plasmonic nano antenna. Plasmonic nanoantennas continue to attract increased attention due to their capability of confining free-space electromagnetic waves into a sub-wavelength region with high field enhancement [13,14], which enables a variety of cutting-edge applications such as surface-enhanced Raman spectroscopy (SERS)[15], single-molecule detection [16], high-sensitive photodetection [17], near-field optical trapping [18], magnetic recording [19], and nanoscale light sources [20]. The paper is organized as follows: Section 2 describes the Background of Numerical Method; the theory of plasmonic nano antennas, PSO algorithm and simulation results are discussed in Section 3 and a conclusion is presented in the last section.

2. Background of numerical method

Generally, there are many numerical simulation methods to study the interaction between the light and metal nano particles such as FDTD (Finite-difference Time-domain) [21], FEM (Finite Element Method) [22], DDA (Discrete-dipole Approximation) [23], Mie Theory [24] and Transition matrix (T-matrix) theory [24]. Critical comparison of the performance of DDA, and FDTD adopted from [25]. In the DDA method only particle volume is discretized, but in the FDTD all of the volume should be discretized. Carlo Forestiere has validated the DDA method for the near- and far field regions separately [24]. In this paper, DDA is used to study the optical properties of plasmonic nano particles.

3. Theory

Schematic diagram of a two-dimensional array of plasmonic nano particles which periodically arranged in the (x, y)-plane is shown in Fig. 1. The object is excited by a monochromatic incident plan wave $\mathbf{E}_{inc}(\mathbf{r}, t) = \mathbf{E}_0 e^{i(\mathbf{k}\,\mathbf{r}-\omega\, t)}$ where r, t, ω, $k = \omega/c = 2\pi/\lambda$, c, and λ are the position vector, the time, the angular frequency, the wave vector, the speed of light and the wavelength of incident light, respectively.

To calculate the E-field of each dipole time harmonic component $-i\omega t$ of the E-field is left out. Local field arises from incident light with polar (θ) and azimuth (φ) angle at each particle is:

$$\mathrm{E}_{inc}(\mathbf{r}_s) = \mathrm{E}_0 e^{i\mathbf{k}.\mathbf{r_s}}, \tag{1}$$

Where [26]

$$\mathrm{k} = \frac{2\pi}{\lambda}\hat{k} = \frac{2\pi}{\lambda}[\sin(\theta)\cos(\phi),\ \sin(\theta)\sin(\phi),\ \cos(\theta)]. \tag{2}$$

For incident field with P-polarization, the following relation can be written [26]:

$$\mathbf{E}_0 = [\sin(\theta\text{-}\frac{\pi}{2}).\cos(\phi),\ \sin(\theta\text{-}\frac{\pi}{2}).\sin(\phi),\ \cos(\theta\text{-}\frac{\pi}{2})], \tag{3}$$

and for incident field with S-polarization we have:

$$\mathbf{E}_0 = [\cos(\phi + \frac{\pi}{2}),\ \sin(\phi + \frac{\pi}{2}),\ 0]. \tag{4}$$

When the applied field is parallel to one of the principle axes, polarizability, α, is [26,27]

$$\alpha_s = V\varepsilon_0 \frac{\varepsilon_r\text{-}1}{1 + L_1(\varepsilon_r\text{-}1)} \tag{5}$$