Binary optimization of plasmonic nano-disk-based absorption coefficient

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A new efficient binary optimization method based Teaching-Learning-Based Optimization (TLBO) algorithm is proposed to design an array of plasmonic nano disks in order to achieve maximum absorption coefficient spectrum. In Binary TLBO (BTLBO), a group of learner consists a matrix with binary entries, control the presence ('1') or the absence ('0') of nano particles in the array. Simulation results show that absorption coefficient strongly depends on the localized position of nano particles and non-periodic structures have more appropriate response in term of absorption coefficient. This approach is useful in optical applications such as solar cells and plasmonic nano antenna.

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1. Introduction

Metal nano-particles have broad applications in electronics, photonics, chemical sensing, and imaging [1-3]. Recently, there has been a growing interest in Plasmonics nano-particles. They have strong effects on light in visible and invisible regions of the photonics spectrum for applications such as Raman scattering [4], radiative rate enhancement [5], solar cells [6], and optical biosensors [7]. 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. Shape control has been successfully demonstrated for gold nano-particles using nonionic surfactants, silver under-potential deposition, and Nano replica molding [8-10]. Nano replica molding has been demonstrated as a low-cost method for manufacturing a variety of devices comprised of nano structured surfaces. Using this technique, a variety of nano structured devices have been manufactured. Recently, a plasmonic nano domes array fabricated by nano replica molding process [10]. In addition to the recent interest in shape control of nano-particles, optical properties of noble metal particles with their intense colors have fascinated scientists since turn of this century. For example, spherical gold nano-particles show a strong absorption band in visible region of the electromagnetic field at about 520 nm [11]. In addition to the shape, size and material of nano-particles, properties of light strongly depend on the localized positions and gap between nano-particles. Plasmonic nano particles with periodic structure have been reported in some literatures [12]. 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. One of the popular nanoparticles for plasmonic applications is rod-shaped nanoparticles. There are some reasons for its popularity as following: gold nano rods could be fabricated using seeded crystallization from solution, the plasmon resonance has the advantage of adjustability by varying the aspect ratio, it has high scattering efficiency, and low plasmon damping. The plasmonic nano rods are widely used to design nano antennas with improved capabilities [13]. Efficiency of these materiels strongly depends on the localized positions of nano-particles. There is some reported work in the literature to utilize Plasmonic nano antennas as modulator and optical switch [14]. In this paper the authors tried to maximize the absorption coefficient to have more efficiency in these materiels. The characteristics of near and far- field of nano-particles can be calculated using discrete dipole approximation (DDA). Optimization problems in the plasmonic nano-particles can be divided into two categories. In the first type binary optimization algorithm is used to control the presence ('1') or the absence ('0') of nano-particles in the array; whereas in the second type, the optimization can be done to engineering the nano-particles geometric. In ref [15-16], binary TLBO algorithm was used and an optical switch and modulator based on the dimer plasmonic nano-rods has been proposed. In this paper BTLBO is used to generate the binary gold nano disks for getting higher absorption coefficient spectrum. This approach can be useful in optical applications such as plasmonic collar cell and plasmonic nano antenna.

2. Methods

Discrete dipole approximation:

Schematic diagram of a two-dimensional array of plasmonic nano disks which periodically arranged in the x y -plane is shown in Fig. 1. The object is excited by a monochromatic incident plan wave $\vec{E}_{inc}(r,t)=\vec{E}_0 e^{ik(r-\omega t)}$ where r, t, ω, k=ω/c=2π/λ, 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 -iωt of the E-field is left out. Local field arises from incident light with polar (θ) and azimuth (φ) angle at each particle is:

$$\overrightarrow{E_{inc}}(\vec{r_i})=\vec{E_0}e^{i\vec{k}.\vec{r_s}} \quad (1)$$

Where

$$\bar{k}=\frac{2\pi}{\lambda}\hat{k}=\frac{2\pi}{\lambda}[\sin(\theta).\cos(\varphi),\sin(\theta).\sin(\varphi),\cos(\theta)] \quad (2)$$

For incident field with P-polarize, the following can be written:

$$E_0=[\sin(\theta-\frac{\pi}{2}).\cos(\varphi),\sin(\theta-\frac{\pi}{2}).\sin(\varphi),\cos(\theta-\frac{\pi}{2})] \quad (3)$$

and, for incident field with S-polarize:

$$E_0=[\cos(\varphi+\frac{\pi}{2}),\sin(\varphi+\frac{\pi}{2}),0] \quad (4)$$

When the applied field is parallel to one of the principle axes, polarizability, α, is [17]

$$\alpha=V\varepsilon_0\frac{\varepsilon_r-1}{1+L(\varepsilon_r-1)} \quad (5)$$

where $\varepsilon_r=\varepsilon_{particle}/\varepsilon_{medium}$ is the relative dielectric function of the particle with respect to the medium, V is particle volume, and L is a shape factor. For oblate spheroids (b=c), the following analytical expression can be given for L1 as [18]:

$$L_1=\frac{1+f^2}{f^2}[1-\frac{1}{f}\tan^{-1}(f)] \quad , \quad f^2=\frac{b^2}{a^2}-1 \quad (6)$$

where a,b and c are seminal excess of an ellipsoid. The shape of a nano oblate is shown in the Fig. 3. In this simulation approximate a nano disk with an oblate (a<b=c) ellipsoid.

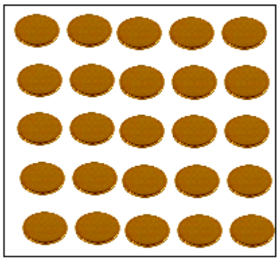

Fig. 1. Schematic view of a 2-dimensional array of gold nano-disk

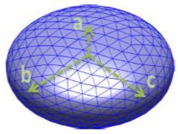

Fig. 2. Geometric characterization of an oblate (a<b=c) ellipsoids

The dipole moment induced in a single particle by a local electric field is given by:

$$\vec{P_s}=\varepsilon_0\alpha_s\vec{E}_{Loc}(\vec{r_s}) \quad (7)$$

Here, $\vec{P_s}$ is the induced dipole moment, α_s is Polarizability of the particle centered at $\vec{r_s}$, $\overrightarrow{E_{loc}}$ is local electric field, and ε_0 is permittivity of free space. The local field arises from two sources, appearing as two terms. The first term is incident light, $\vec{E}_{inc}(\vec{r_s})=\vec{E_0}e^{ik\vec{r_s}}$, and the field radiated from each of the other N-1 radiating dipoles in the array. Combining these terms leads to local field at each dipole as follow [18]:

$$\vec{E}_{loc,s}=\vec{E}_{inc,s}+\vec{E}_{dip,s}=\vec{E_0}e^{ik\vec{r_s}}-\sum_{s\neq h}A_{s,h}\vec{P_s} \quad (8)$$

$$\vec{E}_{inc,s}=A_{s,s}\vec{P_s}+\sum_{s\neq h}A_{s,h}\vec{P_s} \quad (9)$$

$A_{s,h}$ is the tensor that represents the interaction between a receiving dipole at r_s and the radiating dipole at r_h as follow [19]:

$$A_{ij}=\frac{e^{ikr_{ij}}}{r_{ij}^3}\{k^2r_{ij}\times(r_{ij}\times P_j)+\frac{(1-ikr_{ij})}{r_{ij}^2}[r_{ij}^2P_j-3r_{ij}(r_{ij}.P_j)]\} \quad (10)$$

Here , $\overrightarrow{r_{sh}}=\vec{r_s}-\vec{r_h}$, $r_{sh}=|r_{sh}|$, k is wave vector, and $A_{s,h}$ are 3 × 3 matrices representing the interaction of two particles s and h. 3_N unknown dipole moments “$\vec{P}$” should be solved in the following exactly determined system of 3N linear equations:

$$A\vec{P}=\vec{E}_{inc} \quad (11)$$

in which A is a 3N × 3N matrix containing N×N of $A_{s,h}$ with 3×3 tensors, where N is the number of dipoles and both P and E_{inc} are 3N vectors (i.e. each of N particles is represented by a 3-vector). When this set of 3_N complex linear equations are solved ($A\vec{P}=\vec{E}_{inc}$), P array of self-consistent dipole moments is obtained. The optical properties may be then calculated from this dipole array. The optical properties may be then calculated from this dipole array. Optical absorption, scattering, and extinction can be directly calculated from the dipole array. The extinction and scattering cross-sections can be calculated, as defined in [10]:

$$C_{ext} = \frac{k}{\varepsilon_0 \left|\overline{E_{inc}}\right|^2} \sum_{i=1}^{N} \mathrm{Im}(\overline{E}^*_{inc,i} . \overline{P}_i) \tag{12}$$

$$C_{sca} = \frac{k^4}{6\pi\ \varepsilon_0^2 \left|\overline{E_{inc}}\right|^2} \sum_{i=1}^{N} \left|\overline{E}^*_{inc,i} . \overline{P}_i\right|^2 \tag{13}$$

and the absorption cross-section Cabs = Cext - Csca. These quantities are often expressed in terms of extinction, absorption and scattering efficiencies, i.e., the cross-section divided by the cross-sectional area of the scatterer. In the case of a particle, the extinction efficiency is defined as Qext = Cext/(πa^2), where a is the radius of the particle. Similarly, the absorption and scattering efficiencies are defined, respectively, as Qabs = Cabs/(πa^2) and Qsca = Csca/(πa^2).

TLBO Algorithm

Teaching-Learning-based optimization (TLBO) is one of the recently proposed population based algorithm which simulates the traditional teaching-learning phenomenon of a classroom [20]. The algorithm simulates two fundamental modes of learning: (i) through the teacher (known as the teacher phase) and (ii) interacting with other learners (known as the learner phase). In the teacher phase, learners first get information from a teacher and he makes an effort to increase the mean result of the class. The best solution is regarded as the teacher ($X_{teacher}$) in the population. In the teacher phase, learners learn from the teacher and the teacher tries to enhance the result of other individual (X_i) by increasing the mean result of the classroom (X_{mean}) towards his position $X_{teacher}$. Two randomly –generated parmeters r in the range of 0 and 1 anf T_f are applied in formula for the solution X_i for stochastic purposes as follows [20]:

$$X_{new} = X_i + r.(X_{teacher} - T_f . X_{mean}) \tag{14}$$

Where X_{new} and X_i are the new and existing solution of i, and T_F is a teching factor which can be either 1 or 2.

In the second phase, algorithm simulates the learning of the students (i.e. learners) through interaction among themselves. The students can also gain knowledge by discussing and interacting with other students. A learner will learn new information if the other learners have more knowledge than him/ her. During this stage, the student X_i interact randomly with another student X_j in order to develop his/her knowledge. In the case that X_j is better than X_i , X_i is moved toward X_j . Otherwise it is moved away from X_j:

$$X_{new} = X_i + r(X_i - X_j) \quad if\ f(X_i) < f(X_j) \tag{15}$$

$$X_{new} = X_i + r(X_j - X_i) \quad if\ f(X_j) < f(X_i) \tag{16}$$

In the new solution X_{new} is better, it is accepted in the population. The algorithm will continue until the termination condition is met.

Binary TLBO

In teacher and learner phases the velocity of each student can be calculated by:

$$v_i^{k+1} = r.(X_{teacher} - T_f . X_{mean}) \tag{17}$$

$$v_i^{k+1} = r(X_i - X_j) \tag{18}$$

The position in BTLBO is represented by a binary vector and the velocity is still floating-point vector however; velocity is used to determine the probability to change from 0 to 1 or from 1 to 0 when the position of particles are updating. To squash velocities into the range of [0,1] we applied the “tanh” transformation to the component of velocity as:

$$\tanh(\left|v_{id}^k\right|) = \frac{\exp(\left|2v_{id}^k\right|) - 1}{\exp(\left|2v_{id}^k\right|) + 1} \tag{19}$$

The equation for updating the positions is then replaced with:

$$x_{id}^k = \begin{cases} 1, & if\ rand < \tanh(\left|v_{id}^k\right|) \\ 0 & otherwise \end{cases} \tag{20}$$

In this paper to maximize the absorption coefficient, position matrix generate a matrix with binary entries, control the presence (‘1’) or the absence (‘0’) of nano particle in the array.

Simulation results

DDA method was applied and absorption spectrums were plotted for periodic and non-periodic arrays of Gold nano disk with 5 nm diameter, and 5 nm edge-to-edge separations in two-dimensional space. Fig. 3b shows the absorption spectrum across the entire interval 300–600 nm for 2D non-periodic array. The present simulations showed that absorption spectrum strongly depended on localized positions of nano disks and further enhancement of absorption coefficient was possible at compared with the periodic array in Fig. 3a. The large absorption coefficient and the huge shifted peak observed here was due to the interaction of metal nano particles considering their strong near-field coupling. In this case, plasmon resonance of a nano particle plays as a local optical resonator and couple light to other nearest resonator. BTLBO and DDA were used to optimize the absorption coefficient for optical applications such as plasmonic solar cell and plasmonic nano antenna. The goal was to maximize the Qabs by optimizing 25 binary nano disks for 2D arrays (5×5). As seen, BTLBO is an algorithm that minimizes a profit function. To use BTLBO algorithm for maximizing absorption coefficient, BTLBO method should be minimized the following function:

$$\text{Cost Function} = -\sum_{i=300}^{600} Q_{abs} \qquad (21)$$

where i is wavelength number and Qabs is absorption coefficient. BTLBO and DDA were used to optimize the absorption coefficient by optimize selection of 25 binary nano disks. Fig. 4 shows absorption spectrum of the optimized array. The maximum absorption in the entire interval 300–600 nm is 34, which occurred at 450nm. The large absorption coefficient observed here was due to the interplay of five local optical resonator interactions with strong near-field Plasmonics coupling. Depending on the position and number of the plasmonic nano disks, the absorption can be suppressed for one wavelength and maximized for the other wavelength. Moreover, according to the experimental results of ref [13], higher absorption coefficient can be achieved by optimum selection of separation gap of nano particles while in ref [21] the authors prove that the layout with optimum number of nano particle has higher absorption coefficient and has different shifted peak.

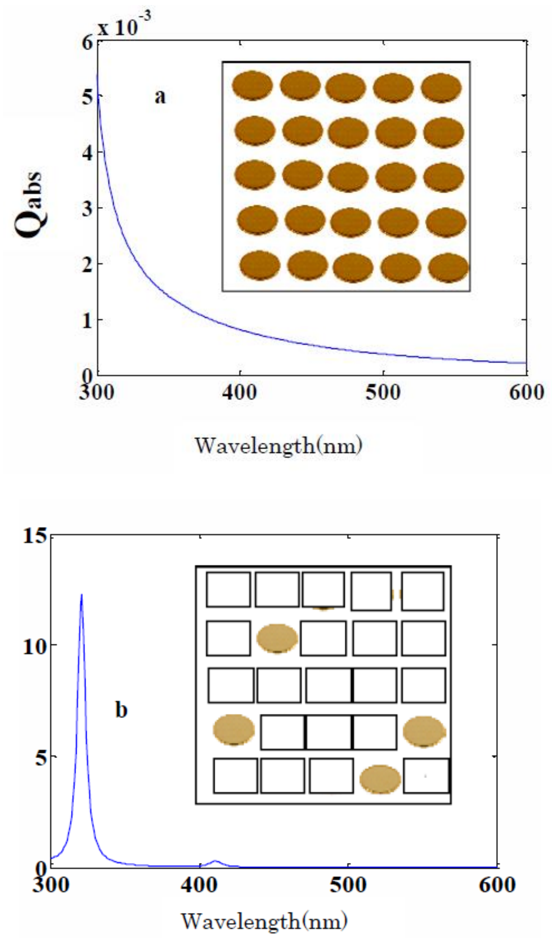

Fig. 3. a) Absorption Coefficient for periodic nano disks b) Absorption Coefficient for non - periodic nano disks

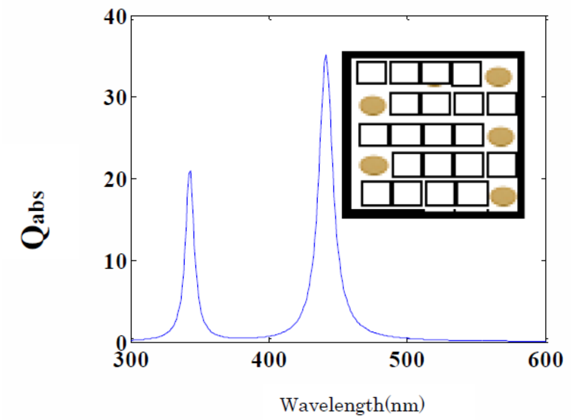

Fig. 4. Absorption Coefficient for Optimize binary nano disk

3. Conclusion

BTLBO algorithm was proposed to design an array of non-periodic plasmonic nano-disk in order to achieve maximum absorption coefficient spectrum. In BTLBO, a group of learners consists a matrix with binary entries, control the presence ('1') or the absence ('0') of plasmonic nano disks in the array and find the best array of plasmonic nano disk from all possible arrays. Simulation results showed that absorption coefficient strongly depended on the localized position of nanoparticles and non-periodic structures had a more appropriate response in terms of absorption coefficient. This approach is useful in optical applications such as solar cells and plasmonic nano antenna.

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