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# TLBO algorithm assisted for designing plasmonic nano particles based absorption coefficient

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In this paper Teaching-Learning-Based Optimization (TLBO) algorithm has been used to design of the plasmonic nano spheres in order to achieve the maximum absorption coefficient spectrum. In TLBO, a group of learners controls the nano spheres radius, the nano sphere distances, and the number of nano spheres in three dimensions. 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 the plasmonics nano-particles. They have strong effects on the light in the 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 the shape of metal and semiconductor nano-particles. Shape control has been successfully demonstrated for the 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 composed of nano structured surfaces. Recently, a plasmonic nano domes array has been fabricated by nano replica molding process. In addition to the recent interest in the shape control of nano-particles, optical properties of the noble metal particles with their intense colors have fascinated scientists since turn of this century. For example, spherical gold nano-particles have shown a strong absorption band in the visible region of the electromagnetic fields at about 520 nm wavelength [11]. Shape control has been successfully demonstrated for gold nano-particles using nonionic surfactants, silver under-potential deposition, and nano replica molding [12,13]. Nano replica molding has been demonstrated as a low-cost method for manufacturing a variety of devices comprised of nano structured surfaces [14]. In addition to the shape, size and material of nano-particles, the properties of transmitted light strongly depend on the localized positions and gap between the nano-particles. Plasmonic nano-particles with periodic structures have been reported in some literatures [15]. One of the most promising plasmonics nano-particle platforms is studying the effect of deterministic aperiodic structure of nano-particles on properties of transmitted light. This structure that is intermediate between the disordered system and the periodic one enables a unique control and manipulating of spatially localized plasmonic states over the broadband frequencies and angular spectra. The plasmonic nano-particles are widely used to design the nano antennas with improved capabilities [16]. The efficiency of these materials strongly depends on the localized positions of the nano-particles. There is some reported work in the literature to utilize plasmonic nano antennas as modulators and optical switches [17]. In this paper, the absorption coefficient has been maximized in order to have more efficiency in these materials. The characteristics of the near and far- field of the 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 [18]; whereas in the second type, the optimization can be done to engineering the nano-particles geometric [19,20]. In this paper TLBO algorithm is used to engineering the nano-spheres radius, the nano-sphere distances, and the number of nano-sphere in three dimensions 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.

## 2. Theory

### A. Discrete dipole approximation (DDA)

The schematic view of a three-dimensional array of the plasmonic nano-spheres which have been periodically arranged in the x y and z plane is shown in Fig. 1. The structure is excited by a monochromatic 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 the incident light with polar (θ) and azimuth (φ) angle at each particle is:

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

where:

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

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

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

and for the incident field with S-polarization:

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

When the applied field is parallel to the one of the principle axes, Polarizability, $\alpha_s$, is [21]:

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

where $\varepsilon_r = \varepsilon_{particle} / \varepsilon_{medium}$ is the relative dielectric function of the particle with respect to the medium, $\varepsilon_0$ is the permittivity of free space, *V* is the particle volume, and $L_1$ is the shape factor. For prolate spheroids (b=c<a), the following analytical expression can be given for L as a function of eccentricity e [22]:

$$L_1 = \frac{1-e^2}{e^2}(-1 + \frac{1}{2e}\ln\frac{1+e}{1-e}) \qquad e^2 = 1 - \frac{b^2}{a^2} \tag{6}$$

and for oblate spheroids (b=c>a):

$$L_1 = \frac{1+f^2}{f^2}[1 - \frac{1}{f}\tan^{-1}(f)] \quad , \quad f^2 = \frac{b^2}{a^2} - 1 \tag{7}$$

For spheres, $L_1$=1/3.

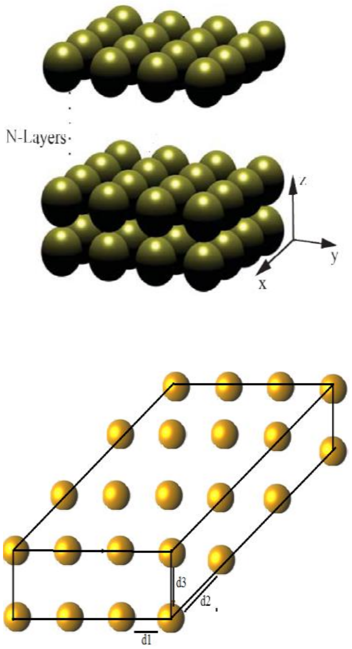



*Fig. 1. a) 3-dimensional arrays of nano particles b) 3-dimensional arrays of nano particles with gap separation $d_1$, $d_2$, and $d_3$.*

The dipole moment induced in a single particle by a local electric field, $\vec{P_s}$ , is given by:

$$\vec{P_s} = \varepsilon_0 \alpha_s \vec{E}_{Loc}(\vec{r_s}) \tag{8}$$

Here, $\alpha_s$ is the polarizability of the particle centered at $\vec{r_s}$ and $\overline{E_{loc}}$ is local electric field. The local field arises from two sources, the 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 the local field at each dipole as follow:

$$\vec{E}_{loc,s} = \vec{E}_{inc,s} + \vec{E}_{dip,s} = \vec{E}_0 e^{ik\vec{r}_s} - \sum_{s\neq h} A_{s,h}\vec{P}_s \tag{9}$$

$$\vec{E}_{inc,s} = A_{s,s}\vec{P}_s + \sum_{s\neq h} A_{s,h}\vec{P}_s \tag{10}$$

$A_{s,h}$ is the tensor that represents the interaction between a receiving dipole at $r_s$ and the radiating dipole at $r_h$ as follow [22]:

$$A_{s,h} = \frac{\exp(ik\overrightarrow{r_{sh}})}{\overrightarrow{r_{sh}}}[k^2(r_{sh}r_{sh} \quad I_{3\times3}) + \frac{ik\vec{r}_{sh} \quad 1}{\vec{r}_{sh}^{\,2}}(3r_{sh}r_{sh} \quad I_{3\times3})] \quad s \neq h$$
$$A_{s,s} = \frac{1}{\alpha_s\varepsilon_0 I_{3\times3}} \tag{11}$$

where $,\overrightarrow{r_{sh}} = \vec{r_s} - \vec{r_h}$ , $r_{sh} = |r_{sh}|$ , and $A_{s,h}$ are 3 × 3 matrices representing the interaction of two particles s and

h. The 3_N unknown dipole moments "$\vec{P}$" should be solved in the following exactly determined system of 3N linear equations:

$$A.\vec{P} = \vec{E}_{inc} \tag{12}$$

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. Optical absorption, scattering, and extinction can be directly calculated from the dipole array. The extinction and scattering cross-sections are defined as [10]:

$$C_{ext} = \frac{k}{\varepsilon_0 \left|\overline{E_{inc}}\right|^2} \sum_{i=1}^{N} \mathrm{Im}(\overline{E}^{*}_{inc,i}.\overline{P}_i) \tag{13}$$

$$C_{sca} = \frac{k^4}{6\pi\ \varepsilon_0^2 \left|\overline{E_{inc}}\right|^2} \sum_{i=1}^{N} \left|\overline{E}^{*}_{inc,i}.\overline{P}_i\right|^2 \tag{14}$$

and the absorption cross-section is $C_{abs} = C_{ext} - C_{sca}$. These quantities are often expressed in terms of extinction, absorption and scattering efficiencies, i.e., the cross-section divided by the cross-section area of the scatterer. In the case of a particle, the extinction efficiency is defined as $Q_{ext} = C_{ext}/(\pi a^2)$, where a is the radius of the particle. Similarly, the absorption and scattering efficiencies are defined as $Q_{abs} = C_{abs}/(\pi a^2)$ *and* $Q_{sca} = C_{sca}/(\pi a^2)$ , respectively.

### B. 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 [23]. 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 parameters r in the range of 0 and 1 and $T_f$ are applied in formula for the solution $X_i$ for stochastic purposes as follows [23]:

$$X_{new} = X_i + r.(X_{teacher} - T_f .X_{mean}) \tag{15}$$

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 $X_j$:

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

$$X_{new} = X_i + r(X_j - X_i) \quad if\ f(X_j) < f(X_i) \tag{17}$$

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

## 3. Simulation results

TLBO algorithm is applied and multilayer plasmonic nano-sphere is designed to have higher absorption coefficient spectrum. Our goal is to maximize the absorption coefficient in the 300-600 nm by utilizing TLBO algorithm by introduce optimizing seven parameters; the nano sphere radius (r), the nano spheres distance ($d_1$, $d_2$, and $d_3$ in Fig. 1.b), and the number of nano spheres in three dimensions ($N_1$, $N_2$, $N_3$) with the following range:

$$r \in [5\ \ 40]nm \tag{18}$$

$$d_1, d_2, d_3 \in [5\ \ 40]nm \tag{19}$$

$$N1, N2, N3 \in \{1,2,...,5\} \tag{20}$$

As seen, TLBO is an algorithm that minimizes a profit function. To use TLBO algorithm for maximizing absorption coefficient, TLBO method should be minimized the following function:

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

where i is wavelength number and Qabs is absorption coefficient. Fig. 2 shows absorption spectra of the optimized array in the entire interval 300–600 nm. The maximum absorption coefficient occurred at 560nm. The large absorption coefficient 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. Finally Convergence characteristic of TLBO method is shown in Fig. 3. As shown in this figure, TLBO algorithm is performing better than PSO in terms of convergence speed and accuracy.

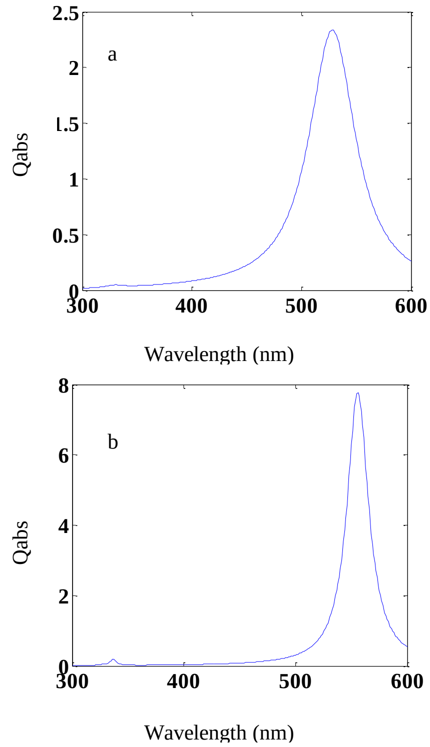
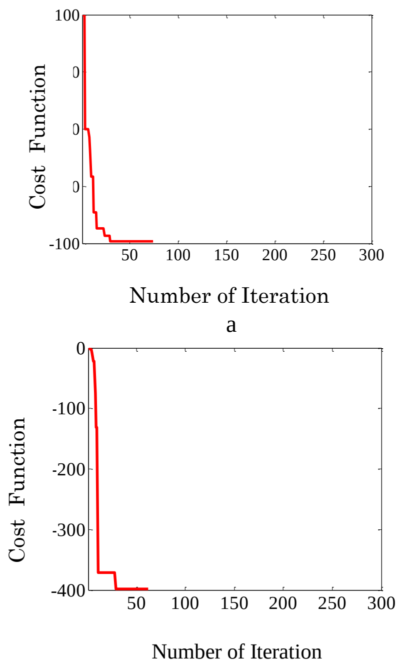



*Fig. 2. Absorption coefficient for optimize spheres in difference run of program a) r=6.4917 d1=7.9086 d2=27.3911 d3=14.8284 N1=3 N2=3 N3=1 b) r=30.8 d1=24.6 d2=34.3 d3=30.4 N1=3 N2=1 N3=1.*




b

*Fig. 3. Cost function versus number of iteration for a) PSO b) TLBO.*

## 4. Conclusion

The TLBO algorithm was used to find the best nanoparticle array from all possible arrays in order to maximize the absorption coefficient across the entire interval 300–600 nm. The feasibility and effectiveness of the TLBO algorithm is demonstrated and results are compared with the PSO algorithm. It was shown that TLBO have good performance in term of accuracy and convergence speed. Finally, represented that using optimize structure of plasmonic nano-spheres could lead to higher absorption coefficient and absorption coefficients strongly depend on the nano-spheres radius, the nano-sphere distances, and the number of nano-sphere in three dimensions.

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