Design of a shape-optimized metallic nanoheater

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Received January 14, 2013; accepted February 7, 2013;
posted February 22, 2013 (Doc. ID 183324); published March 21, 2013

We present a structural optimization method for metal nanostructures based on the shape dependency of their electromagnetic (EM) heat dissipation and thermodynamic transfer to the surroundings. We have used a parallel genetic algorithm in conjunction with a coupled EM (finite-difference time-domain) and thermodynamic modeling of the metallic nanostructures for the optimization. The optimized nanostructure demonstrates significant improvement in EM heating in the spectral window of optimization as well as expedited cooling properties. The symmetry of the structures, which is inherent in the design procedure, makes them independent of the polarization at normal incidence and insensitive to the incident direction while incidence is inclined at an angle. © 2013 Optical Society of America

OCIS codes: 350.5340, 260.2160, 260.3910.

1. INTRODUCTION

Ever since the seminal works of Mie, the electromagnetic (EM) properties of metal/dielectric interfaces have been an important area of scientific research. The Mie theory [1] gives a solution for calculating the scattering and extinction of EM plane waves by spherical particles. Absorption and scattering by particles of shapes other than spheres, e.g., rods, spheroids (prolate, oblate) has been calculated by several other researchers [2–5]. More recently, the development of nanofabrication technologies, such as electron beam lithography, ion beam milling and self-assembly, along with the advent of different modern nanocharacterization techniques, encouraged the scientific community to confirm experimentally and analyze the scattering and absorption spectra of different metal nanostructures (MNSs). Tamaru *et al.* demonstrated the scattering spectra of silver nanoparticles of different shapes at the visible wavelengths [6]. Similar experimental works have been presented by Klar *et al.* [7], El-Sayed [8], and Su *et al.* [9].

The ability of the MNSs to couple light to a surface plasmon, leads to the localization of EM fields on metallic surface features of subwavelength size. This extraordinary ability of the MNSs makes them a very useful tool for subwavelength high-resolution imaging, ultrafast and compact photodetectors and modulators, and higher efficiency solar cells [10]. The irradiation of a metallic nanoparticles by EM waves induces surface currents which act as a loss mechanism for such applications. This surface current generates heat (Joule heating) from the incident EM energy, which also makes the MNS a very good transducer of energy, capable of transforming the incident EM radiation to thermal energy. This gives rise to a number of applications where the MNS can be used as transducers of energy in nanoscale. Govorov *et al.* have investigated the photothermal conversion efficiencies of gold nanoparticles both theoretically and experimentally [11]. Halas *et al.* has fabricated and experimentally demonstrated applications of gold

nanoparticles in cancer diagnostics and also, photothermal cancer therapy and DNA therapy [12–14].

In all the researches involving photothermal energy conversion using MNSs, scientists have analyzed EM properties of regular shaped particles, such as nanospheres, nanoshells, nanorods, and nanopyramids [6–9,11–14]. It has been shown that MNSs demonstrate a significant variation in their spectral properties depending on their shape and size [6–9]. The EM heating of metals is caused mostly due to the surface currents generated by the electric field in the metal's skin depth region. Because these currents are a strong function of the surface shape, absorption of the energy from the incident radiation is strongly dependent on the surface morphology. This heating becomes especially strong in the wavelength regime of the plasmon resonance of the MNS, which is also strongly shape dependent. Besides absorption of energy from the EM radiation, for energy conversion, it is equally important to make a pathway for the generated heat to be transferred to the surrounding medium. This transfer is proportional to the surface area of the object in contact with the surrounding medium, which directly depends on the shape of the object. These shape dependencies of the photothermal conversion phenomenon refer to a possibility of enhancing the conversion efficiency by optimizing the shape of the heated object.

In this paper, we describe our investigation of a shape optimization method based on parallel genetic algorithm (GA) [15] to design the optimum shape of a metallic nanoparticle/structure, where EM heat dissipation into the MNS and heat throughput from the MNS to the surrounding medium are maximized. We used a finite-difference time-domain (FDTD) method in conjunction with a simplified thermodynamic model to obtain the figure-of-merit (FoM) of random structures of metal nanoparticles in the generations of GA. The GA, as an evolutionary algorithm, helps evolve and optimize the pool of random MNS to gradually converge to a solution

structure best suited for the goal of maximizing EM heating and transfer of the generated heat toward the surroundings.

The paper is organized as follows: the next section discusses the theoretical framework of our optimization approach and the coupling of the FDTD and the thermodynamics of the MNS with the parallel GA optimization routine. In Section 3, a brief outline of our optimization method is presented. The performance evaluation of an optimum “photothermal heater” structure generated by the method is demonstrated in Section 4.

2. THEORY

The three-dimensional (3D) structural optimization procedure investigated in this paper consists of three major working units, as shown in Fig. 1. The electromagnetic FDTD (EM-FDTD) unit evaluates the EM evolution of an MNS at the illumination by a plane wave pulse; the thermodynamic unit evaluates the heat dissipated by the MNS from the EM illumination; and the GA optimization unit calculates the FoM of a certain structure using the information provided by the FDTD and the thermodynamic units. The GA unit uses this FoM as a measure of the performance of an array of structures and optimizes by combining the features of those structures with the best FoM in the array. Here, we briefly discuss about these three building blocks of our optimization procedure.

A. Finite-Difference Time-Domain Electromagnetic Simulation

The FDTD algorithm provides a convenient means to evaluate numerically the interaction of EM wave with objects of arbitrary shapes and materials within a finite space-domain [16]. The FDTD equations step in time and the electric (E) and magnetic (M) fields are updated alternatively using the Yee gridding method [16, Section 3.6] of the E and M field points in space. To avoid reflection from the edge of the working volume an absorbing boundary condition is used. In our FDTD simulations we have used a perfectly matched layer (PML) boundary condition [16, Section 7.5].

In the FDTD method the dispersion of a material can be introduced by a functional approximation (e.g., Drude model, Debye model, Lorentz oscillator model) of the permittivity in frequency domain, which is converted to the time domain by the inverse Fourier transform. The differential equations obtained by this inverse transform are coupled to the Maxwell's equations through a set of auxiliary variables, hence, a new set of discretized difference equations are derived for the FDTD time-stepping calculations. In our calculations we have used the

Drude free electron model to simulate the dispersion in metals and the Lorentz dispersion model for dielectric substrates. We use the method proposed by Gedney [17] to simulate a lossy and dispersive medium with an anisotropic PML absorbing boundary in FDTD. The dispersive materials are defined in the working volume by assigning proper values of the coefficients of the FDTD update equations at each grid points. From the calculated electric field distribution, the Joule heating of the MNS is calculated, which is used as a constitutive parameter of the FoM in the GA.

B. Thermodynamic Modeling

To calculate the heat transfer from the MNS to the surrounding medium we use a simple thermodynamic modeling based on the first law of thermodynamics. For 3D structures in nanoscale, the ratio of volume (V_{MNS}) to the surface area (A_{surf}) is a very small number. This ratio is called the characteristic length (l_{char}) of the structure, which being small, makes the Biot number (Bi) of the structure close to zero. The Biot number is defined as follows [18]:

$$Bi = \frac{h}{\lambda_c} l_{\text{char}} = \frac{h}{\lambda_c} \frac{V_{\text{MNS}}}{A_{\text{surf}}}. \quad (1)$$

Here, h is the heat transfer coefficient at the boundary between the MNS surface and the surroundings, and λ_c is the thermal conductivity of the material. This Biot number reflects the resistance to thermal conduction inside a body as compared to the heat transfer resistance at the boundary. Hence, a small Biot number for any structure can be interpreted as a high thermal conductivity inside the body and a high thermal resistance to heat transfer to the surrounding at the boundaries of the structure. For the MNS material and dimensions under concern, the value of l_{char} is in the order of 10^{-9} m, which results in a Bi with a value close to 0 ($\sim 10^{-7}$). Under these conditions, the assumption of a relatively uniform temperature distribution over the surface, in contrast to the presence of high temperature gradient at the perimeter boundaries is justified [18]. Now, the change in the internal energy of the metal structure is regulated by the heat input due to the EM radiation and the heat outflow across its surface. The later energy flow contributes to the cooling process of the structure. Thus, the reduction of the internal energy is equal to the heat flow across the surface, which can be described as

$$\frac{dU}{dt} = \dot{Q} = V_{\text{MNS}} \rho c \frac{dT}{dt} = h A_{\text{surf}} (T - T_s). \quad (2)$$

In Eq. (2), T is the surface temperature, T_s is the temperature of the surrounding fluid (assumed to be an infinite heat reservoir at a constant temperature), c is the specific heat capacity, and ρ is the mass density. A solution to the differential equation in Eq. (2) is given by

$$T = T_s + (T_0 - T_s) \exp\left(-\frac{t}{\tau_{\text{MNS}}}\right), \quad (3)$$

where, the thermal time constant, $\tau_{\text{MNS}} = c \rho V_{\text{MNS}} / h A_{\text{MNS}}$. It is directly proportional to the MNS volume and is inversely proportional to its surface area. For a fast transfer of the thermal energy of the MNS to the surrounding fluid a small value of τ_{MNS} is desired.

Fig. 1. (Color online) Operational flowchart of the shape optimization procedure.

C. Genetic Algorithm

A GA is a stochastic search method modeled based on the basic principles of natural selection and evolution. A GA is particularly useful when searching for a global maximum in the solution domain of a multiparameter problem [15]. In GA, each of the tentative solutions in the solution domain is assigned a FoM, often referred to as *fitness*, in the perspective of the problem being optimized. The evolution toward the approximate global optimum is achieved due to the convergence pressure exerted by the *fitness weighted* selection process in successive iterations. The solution domain is explored by the educated recombination and mutation of the population pool of the concurrent generation.

Typically, a GA optimization has three generic phases—(i) initiation, (ii) reproduction, and (iii) generation replacement [15]. In the very first step of GA (initiation), the first trial solution set consisting of a predetermined number of random solutions is created. This trial set is called the *initial population*. Each individual solution of the initial trial set is generally encoded using different schemes (in our work we used binary encoding) to make them mathematically treatable. These encoded trial solutions are named as *chromosomes*. At the end of the initiation phase, each of the chromosomes is decoded and its fitness is evaluated. The *fitness* is a mathematical expression that connects the FoM of a certain chromosome to a number of variables that determine its performance in the perspective of the given problem. The GA tries to find out the best combination of the variable that maximizes the fitness value of the solution.

In the reproduction phase, the initial population evolves to a newer one (called a new “generation” in the jargon of evolutionary algorithms) by the act of different GA operators. A pair of chromosomes from the initial population pool is selected through the selection operator on the basis of their fitness values. A chromosome with a higher fitness value is more likely to be selected than the ones with lower FoMs. These selected ones are called the *parent* chromosome pair. They undergo the crossover operation where portions of these parent chromosomes are interchanged between themselves. The choice of these portions taking part in this interchange is completely random in nature. Such interchange creates two new *children* chromosomes with slightly modulated properties which reflect the characteristics of both the parent chromosomes. Provided that the selected parents were amongst the “fittest” chromosomes in the previous population, on an average, the children are also expected to have high fitness values (often higher than the parents). These children are then operated on by the mutation operator, which randomly alters their characteristic properties by altering a random bit in the encoded sequence. Thus, mutation prevents early convergence of the GA to a local maximum by introducing diversity to the chromosome characteristics. This process of selection-crossover-mutation continues until a new population pool is completely filled up. The previous population is then replaced by the newly created pool of children chromosomes (the new generation). The fitness of each of them is evaluated again and the whole procedure is repeated until a convergence criterion of the fitness value is met. Once the convergence criterion is achieved, the chromosome with the highest fitness value in the latest generation is taken as the solution of the optimizing problem.

Such evolutionary algorithms are comparatively slow procedures. But the GA can be made faster by parallelizing the computation process of the fitness of the population. A multicore parallel processing unit is required to implement a parallel GA optimization and eventually it can run N times faster than a regular one where N is the number of chromosomes in the population.

3. SHAPE OPTIMIZATION METHOD

The shape optimization method presented in this paper is a multiobjective (simultaneously optimizing several variables of a given optimization problem) GA optimization method where we try to maximize the EM heat dissipation as well as the transfer of the dissipated thermal energy to the surrounding medium. In every generation of the GA, the fitness of each of the individual chromosomes of the population is calculated using the EM (FDTD) and thermodynamic modeling of the MNS. Figure 2 shows the FDTD simulation setup with a 3D total-field scattered-field (TFSF) source implemented to simulate a plane wave Gaussian pulse. Each of the structures generated in different generations of the GA are simulated by the FDTD routine and the frequency domain electric field components ($E_x(\omega)$, $E_y(\omega)$ and $E_z(\omega)$) are evaluated from the Fourier transform of the recorded electric field data. The EM power dissipation (P_{heat}) per unit volume due to Joule heating is calculated using the following expression:

$$P_{\text{heat}}(\omega) = \sum_{i,j,k} \sigma_{\text{MNS}}(\omega) |E_{i,j,k}(\omega)|^2 + |E_y|_{i,j,k}(\omega)|^2 + |E_z|_{i,j,k}(\omega)|^2. \quad (4)$$

Here, $\sigma_{\text{MNS}}(\omega)$ is the frequency-dependent electrical conductivity of the metal, which is obtained from the Drude free electron model, and i , j , and k denote the index of the spatial points in the working volume.

The rate of transfer of thermal energy toward the surrounding has an inverse relation with the thermal time constant. Hence, the fitness (f_{GA}) of our twofold optimization is a function of the two entities: the dissipated power per unit volume as heat (P_{heat}) and an inverse of the thermal time constant ($1/\tau_{\text{MNS}}$). It is given by the formula

Fig. 2. (Color online) Schematic of FDTD simulation setup with a TFSF source.

$$f_{\text{GA}} = \frac{1}{\tau_{\text{MNS}}} \int_{\omega_{\text{low}}}^{\omega_{\text{high}}} \frac{P_{\text{heat}}(\omega)}{P_{\text{source}}(\omega)} d\omega, \quad (5)$$

where ω_{high} and ω_{low} denote the starting and end frequency of the spectral window for which the structure is optimized, P_{source} is the source power per unit area. A dynamic convergence criterion for the GA was set based on the relative change of the maximum fitness value in consecutive generations. A 0% change of maximum fitness for 15 consecutive generations was considered as convergence.

For the parallel implementation of the GA an MPI algorithm was used in a FORTRAN-90 platform. A master processor was engaged to execute the GA operations while N (number of chromosomes in GA population) slave processors calculated the fitness of the population simultaneously. Figure 3 shows a flow chart of the working procedure of the parallel GA. We implemented the entire procedure in the SciNet supercomputer system of the University of Toronto [19].

Selection is done on the basis of the fitness of the members of the population. Crossover creates a cross-linking of the characteristic properties between the parent and children chromosomes. Mutation randomly alters some arbitrary portion of the chromosome to introduce the diversity among the trial solutions and keeps the optimization procedure from a premature local convergence.

4. RESULTS AND DISCUSSION

The parameters of the TFSF source used in our calculations was set to generate a plane wave pulse (Gaussian in time) with a FWHM wavelength spread from 300 to 800 nm, normally incident on the top surface of the 3D MNS. The structure was optimized for enhancing absorption in the FWHM wavelength region of the source, which we refer to as the *optimization window* onward. Figures 4(a) and 4(b) show two different views of an example of the optimized MNS (sitting on a silicon substrate as shown in Fig. 2) generated by our GA/EM-FDTD/thermal transfer code.

The structure has a fourfold symmetry with two reflection planes along the diagonals of the top surface, which makes its response approximately insensitive to the polarization of the incident light. To preserve this symmetry in the GA generations, the structure was cut into eight symmetrical triangular slices and only one of them was considered as a chromosome

Fig. 3. (Color online) Flow chart of a parallel GA.

Fig. 4. (Color online) (a) First quadrant view of an optimized metallic nanostructure which maximizes both the EM absorption and transfer of the generated thermal energy to the surrounding. (b) Top view of the optimized structure. (The black color represents the surrounding heat reservoir). (c) The triangular chromosome associated to the optimized structure. (d) Reconstruction of the structure by eightfold replication of the chromosome around the center-point (the chromosome is pointed out by the red triangle).

that participated in the GA evolution [demonstrated in Figs. 4(c) and 4(d)]. The triangular slice was introduced to FDTD by a binary matrix cut into eight triangular pieces and only one of them is taken as the chromosome [as shown in Fig. 4(c)]. Each bit of the binary matrix represents a pixel (unit cell) in the FDTD domain. A “1” as the bit represents a unit cell filled with metal while a “0” represents a void unit cell with the material property of the specified surrounding medium (air in our case). As depicted in Fig. 4(c), a golden pixel corresponds to a “1” in the binary matrix, hence, a unit cell filled with metal (in our simulations we consider the material properties of gold as the metal). The black pixels correspond to a “0,” hence, air. The rest of the solid-triangular-blackened portions of the binary matrix [Fig. 4(c)] are discarded while the first triangular region with the certain pattern is cut and used as a chromosome in the GA population. An eightfold replication of the chromosome reconstructs the structure to be included in the FDTD calculations. The FDTD code expands the resolution of the metal structure by four times to simulate with a higher accuracy.

We evaluated the EM heating performance of the optimized structure by its absorption cross section due to Joule heating (C_J) defined by

$$C_J(\omega) = \frac{P_{\text{heat}}(\omega) V_{\text{unit-cell}}}{P_{\text{source}}(\omega)}. \quad (6)$$

Here, $V_{\text{unit-cell}}$ is the volume of the FDTD unit cell. Figure 5(a) shows a comparison of the Joule heating cross section between the optimized structure and a solid metallic cuboid of equal volume and thickness. There is a significant improvement in EM heat dissipation for the optimized MNS as compared to a metallic solid cuboid of the same volume in the

Fig. 5. (Color online) (a) Comparison of the heat dissipation between a solid rectangular cuboid and the optimized structure of equal volume generated by the GA. (b) Comparison of the temperature evolution between the solid rectangular cuboid and the optimized structure. The structures are cooled from an elevated surface temperature to the temperature of the reservoir.

optimization window. Figure 5(b) shows the temperature profile of the optimized structure during the cooling process as compared to the cooling of the solid cuboid. The thermal relaxation time for the optimized structure is 3.36 μs as compared to 12.97 μs for the solid regular cuboid. This is a clear indication of the fact that the optimized MNS is able to transfer the generated thermal energy (due to the EM absorption) approximately 4 times faster than a metallic cuboid of equal volume. This is because the surface of the optimized metallic MNS has now been engineered to allow maximum transfer of heat to the surrounding fluid in the shortest possible time with a minimal storage of the thermal energy. In other words, the optimized structure acts as a loss-minimized transducer/channel for conversion of the EM energy to heat and its transfer to the surrounding medium.

For the constraints of the computational time we chose a reduced spatial resolution (unit cell size 10 nm × 10 nm × 10 nm) in the FDTD simulation block in the GA optimization. The maximum fitness of successive generations is plotted in Fig. 6 against the generation number and the required calculation time. The calculation of the maximum fitness of each generation inherently requires that the fitness of each individual of the concurrent population be calculated beforehand. The calculation of each generation requires approximately 14 min while the convergence time of the optimization was approximately 6.5 h.

As we have mentioned earlier, because of the preserved symmetry in the GA chromosomes, the optimized structure is fairly independent of the incident polarization at normal incidence. Due to such fourfold symmetry with two reflection planes [Fig. 4(c)], it is sufficient to check the polarization

independence by varying the incident polarization from 0° to 45°. We ran simulations with four different polarizations ($\psi = 0^\circ, 15^\circ, 30^\circ$, and 45° , where ψ is the angle that the direction of vibration of the incident plane wave pulse makes with the x axis) of the incident plane wave source pulse. The parameters defining the direction and polarization of the TFSF source (ψ, ϕ, θ) are shown in Fig. 7. Figure 8 shows

Fig. 7. (Color online) Coordinate system to describe the TFSF source parameters. $\hat{k}_{inc}$ is the direction of the source propagation. ψ is the angle of the direction of vibration of the E field with respect to the direction of $\hat{k}_{inc} \times \hat{z}$, where $\hat{z}$ is the unit vector along the z axis. ϕ is the angle between the positive direction of the x axis and the projection of $\hat{k}_{inc}$ on the x - y plane. The positive x and z axes directions are opposite as compared to Fig. 2.

Fig. 6. (Color online) Maximum fitness of the generations of the GA plotted against the generation number. The top axis shows the required time to calculate the fitness of each generation to determine the maximum fitness.

Fig. 8. (Color online) Comparison of the heat dissipation of the optimized structure for different polarizations of the incident plane wave Gaussian pulse. Polarization angle (ψ) was varied from 0° to 45° with an interval of 15° with normal incidence. Also a random choice of $\psi = 32.5^\circ$ is included in the plot.

Fig. 9. (Color online) Comparison of the heat dissipation of the optimized structure for different directions of the incident plane wave Gaussian pulse at an incident angle (θ) of 30° . The azimuth angle (ϕ) was varied from 0° to 45° with an interval of 15° at $\theta = 30^\circ$.

the comparison of the Joule heating of the optimized MNS for different polarization of the incident light. The Joule heating cross-section curves for different incident polarizations demonstrate coincidence with each other over a major portion of the optimization wavelength window, which indicates that the structure is fairly polarization-independent at normal incidence.

The Joule heating of the structure is only weakly dependent of the direction of incidence of the source for any certain incident angle (independent of ϕ for a fixed θ). This phenomenon is depicted in Fig. 9, which shows the Joule heating cross section of the optimized structure with ϕ (azimuthal direction of incidence) varying from 0° to 45° with an incident angle of 3° ($\theta = 30^\circ$). The Joule heating curves for different ϕ 's follow the same trend and tend to coincide with each other. This is a demonstration of the optimized structure being fairly independent of the direction of the incident light.

5. CONCLUSION

We have used a GA coupled with a 3D EM-FDTD and a heat transfer model to design a shape-optimized polarization-independent metallic nanostructure that simultaneously maximizes EM heat dissipation and the transfer of generated thermal energy to the surrounding medium (fluid). Comparison of performance with a regular metallic cuboid of equal volume shows promising results for the optimized nanostructure over a major portion of the visible light region. Because of the preserved symmetry of the structure in the design procedure, the structure is approximately independent of the polarization of the incident EM field. Also, their absorption characteristics demonstrate a fair independence of the azimuth angle of incidence at fixed inclination. These optimized MNSs have potential applications as contactless optical nanoheaters in photothermal cancer therapy (optimized for a narrower band of wavelengths), DNA amplification, gas sensors, and nevertheless, photothermal electricity generation and thermophotovoltaics (broadband optimization). Also, they can find very promising application in nanofabrication. Deposition techniques like plasma-assisted chemical vapor deposition [20] have already been demonstrated where metal nanoparticles are being used for localized heating to gain precise control over the deposition of certain materials from the precursor gases. Our designed MNS is a perfect match for this kind of application. Also, they can be used as thermal catalysts for nanowire growth [21] and electrothermal transducers for nanoheater-based control of the translational movement of

liquids [22]. Nevertheless, MNS optimized for the solar wavelength window, can be introduced to solar-thermal electricity generation plants to enhance the capture of the solar energy and convert it to its thermal state for photothermal electricity generation purpose.

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