Design and Optimization of Two-Dimensional Nano-Arrays for Directive Radiation

Aşkın Altınoklu and Özgür Ergül
Department of Electrical and Electronics Engineering
Middle East Technical University
Ankara, Turkey
ozergul@metu.edu.tr

***Abstract*—We consider design, optimization, and computational analysis of nano-arrays involving two-dimensional arrangements of nanoparticles. Similar to their counterparts used at the lower frequencies, nanoantennas can be arranged periodically to achieve directive and/or controllable radiation patterns at optical frequencies. While nanoantenna geometries are usually simple due to restrictions in nanoscale fabrications, their robust analysis still requires accurate simulation tools to model strong plasmonic interactions between particles. We use a full-wave optimization environment based on heuristic algorithms and surface integral equations to optimize two-dimensional nano-arrays and to shape their radiation patterns for diverse nano-optical applications.**

I. INTRODUCTION

Nanoantennas are well-known devices of nano-optical systems [1],[2] that are developed and used for a variety of applications, such as energy harvesting, optical communication, and sensing. Both numerical [3] and experimental [4] studies demonstrate interesting properties of nanoantennas, such as strong field enhancement, thanks to the plasmonic properties of metals at optical frequencies. Similar to their counterparts at the lower frequencies, arranging nanoantennas in array forms provides further capabilities [5],[6], such as controllability of radiation characteristics. This study is devoted to the design of nanoantenna arrays for directive radiation applications.

As presented in [6], linear arrangements of nanoparticles, such as nano-cubes, provide an ability to control scattering and radiation. For example, a well-designed array can direct the radiation of an isotropic source to desired directions, while suppressing the radiation at other directions. For the best radiation characteristics, the number of elements, their sizes, and the distances between them can be optimized. On the other hand, if a steering ability is required, two-dimensional arrays can be more suitable since they are more compact and their rotation around an isotropic source can be easier. In this work, we present the design of such two-dimensional arrays by using a full-wave simulation and optimization environment. We show that, by using very compact arrays, it is possible to control the overall radiation by directing the main beam to a desired direction, or more importantly, to multiple directions.

II. SIMULATION AND OPTIMIZATION ENVIRONMENT

We consider two-dimensional arrays involving nanoparticles, particularly silver (Ag) nano-cubes arranged periodically. The plasmonic properties of the metals at optical frequencies are taken into account by using surface integral equations for penetrable bodies. In the frequency domain, the permittivity values, which are typically complex numbers with negative real parts, are extracted from available measurement data. The arrays are modeled as finite (e.g., $n \times n$) three-dimensional structures that are excited by a main source (e.g., a dipole at the center) located in free space. The radiation problems are solved iteratively by using the multilevel fast multipole algorithm designed for plasmonic objects [7].

In order to design nano-arrays, we perform on/off optimization, i.e., the array elements are kept/extracted to obtain the desired radiation characteristics. An in-house implementation of genetic algorithms (GAs) is employed due to its easier usage for heuristic cost functions and multi-purpose optimization trials. The main excitation is kept in a gap at the center of the structure such that the array can be rotated to steer the created beam or beams. Once an optimal configuration for a desired radiation characteristics is found, it is further exposed to sensitivity analysis. This is particularly essential to estimate the deteriorations on the performance of an optimal structure

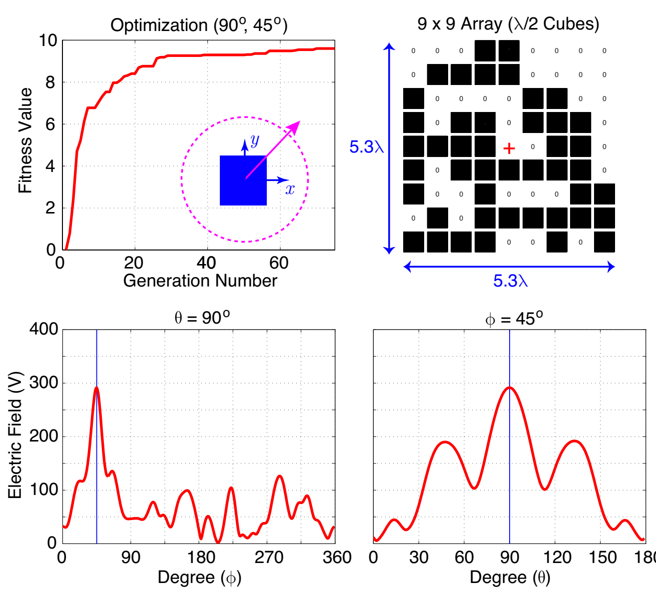

Fig. 1. The result of an optimization when the radiation is maximized at a single direction ($\theta = 90^\circ$ and $\phi = 45^\circ$).

Submitted On: October 10, 2018
Accepted On: October 21, 2018

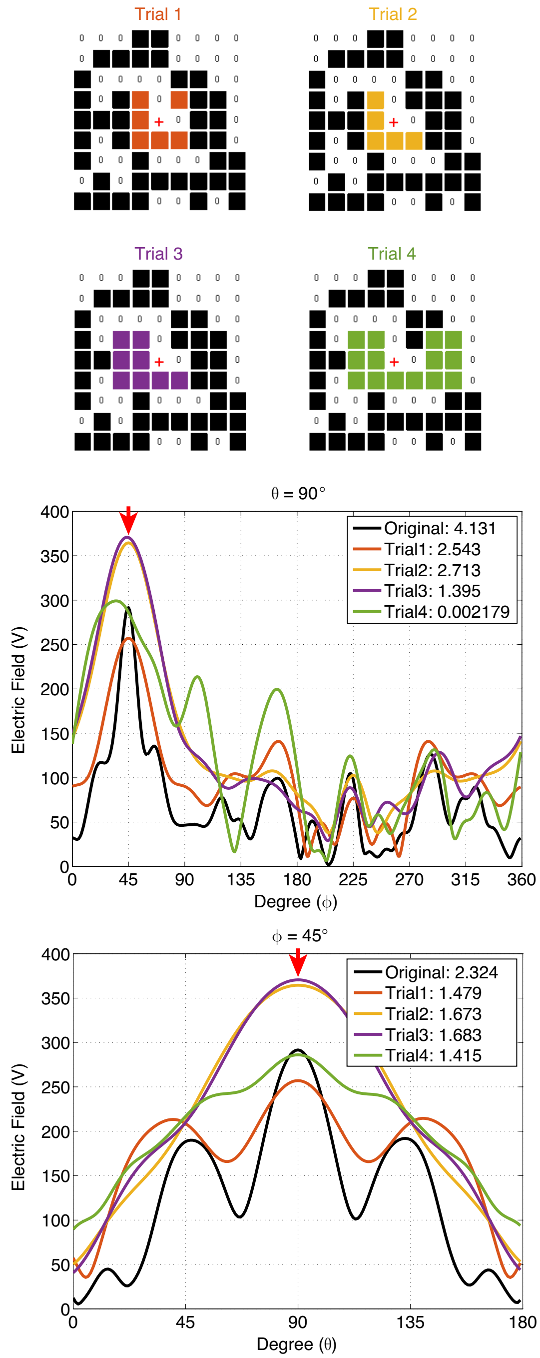

Fig. 2. Modification of the optimal nano-array shown in Fig. 1 by extracting nano-cubes. Attempts to make the nano-array compact lead to significant deteriorations in the radiation characteristics.

when it is fabricated. In addition, we perform extensive tests on the sensitivity of radiation to missing array elements in order to identify critical ones.

III. Design of Nano-Arrays

In the following, we consider two-dimensional nano-arrays involving maximum 80 Ag nano-cubes arranged as a 9×9 grid on the x-y plane. The nano-cubes have dimensions of $750 \times 750 \times 750$ nm, while the center-to-center distance is

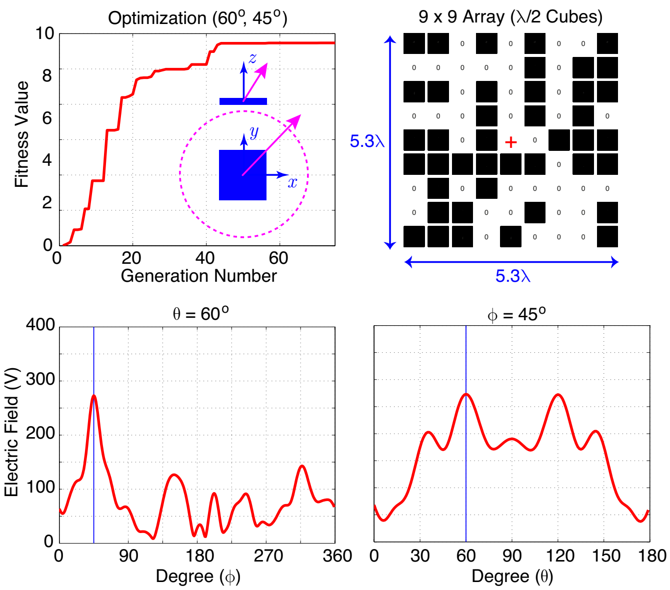

Fig. 3. The result of an optimization when the radiation is maximized at a single direction ($\theta = 60°$ and $\phi = 45°$).

900 nm. Hence, each structure fits into a box of size $7.95 \times 7.95 \times 0.75$ μm. In all results, nano-cubes are assumed to be arranged on the x-y plane. The structures are designed to operate at 200 THz, at which the cube edges correspond to $\lambda/2$ while the overall size is $5.3\lambda \times 5.3\lambda \times 0.5\lambda$. The relative permittivity of Ag at this frequency is approximately $-96 + 7.5i$. The arrays are excited by a probe modeled as a Hertzian dipole oriented in the z direction and located at the center of the array (the cube-free space). Each optimal structure is found via GAs based on less than $40 \times 80 = 3200$ (pool size $\times$ number of generations) simulations by MLFMA. The stability of the GA optimization for nano-arrays was shown in [6].

Fig. 1 presents the results of a successful optimization when the radiation is maximized at $\theta = 90°$ and $\phi = 45°$. The radiation pattern of the array is investigated on the $\theta = 90°$ and the $\phi = 45°$ planes, while the amplitude of the distance-normalized electric field intensity (E) at the desired direction is maximized with respect to the other values on these planes. Specifically, the cost function is defined as:

$$\text{CF} = \text{CF}(\theta = 90°) \times \text{CF}(\phi = 45°), \tag{1}$$

where

$$\text{CF}(\theta = 90°) = \frac{E(\theta = 90°, \phi = 45°)p(\Delta\phi)}{\text{mean}\{E(\theta = 90°, \phi \in [0, 360°])\}}, \tag{2}$$

$$\text{CF}(\phi = 45°) = \frac{E(\theta = 90°, \phi = 45°)p(\Delta\theta)}{\text{mean}\{E(\theta \in [0, 180°], \phi = 45°)\}}. \tag{3}$$

In the above, $p(\Delta s)$ represents a punishment factor, which is generally defined as $p = 1/2^{\Delta s}$, where Δs is the difference (in degrees) between the desired and realized directions for the maximum radiation. For example, if the maximum electric field intensity occurs at $10°$ away from the desired direction, the value of the cost function is drastically reduced

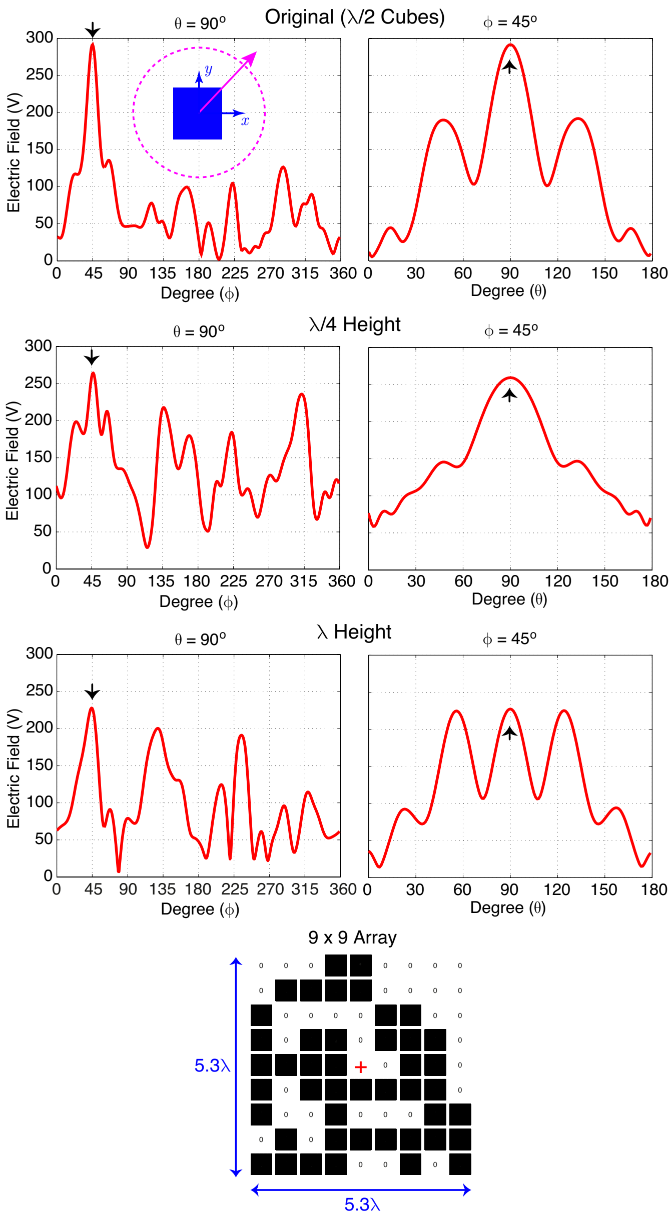

Fig. 4. Using particles with $\lambda/4$ and λ heights for the optimal arrangement in Fig. 1 found for nano-cubes. Changing the height of the particles significantly changes the performance.

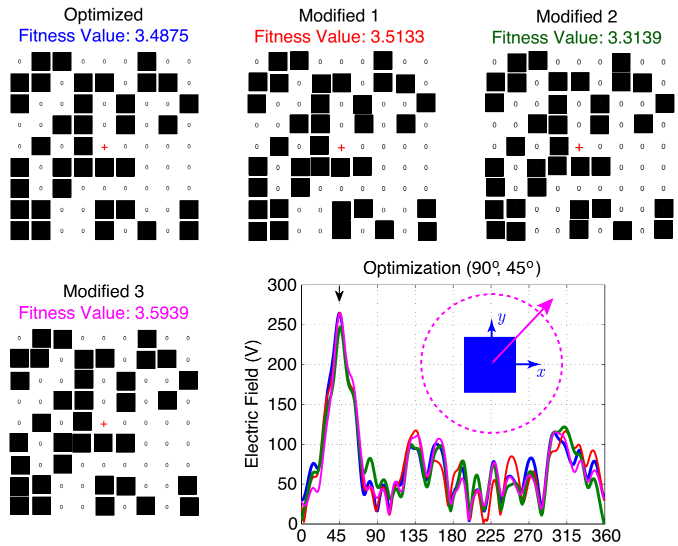

Fig. 5. Tests to demonstrate the sensitivity of a nano-array design to random particle shifts.

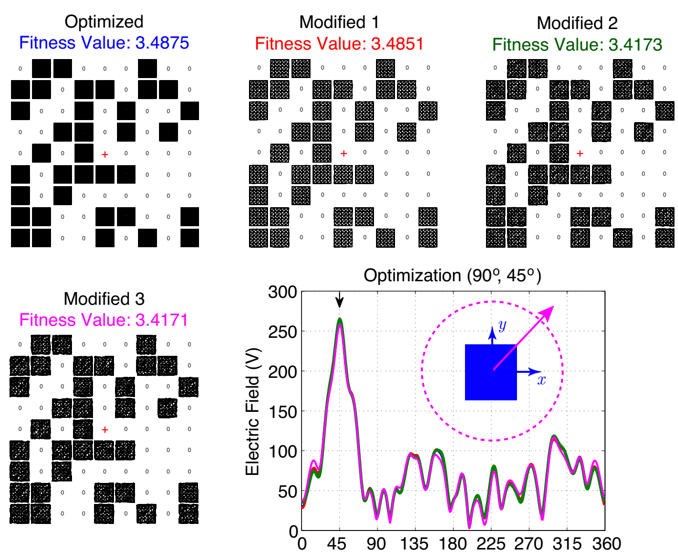

Fig. 6. Tests to demonstrate the sensitivity of a nano-array design to surface corrugations.

by $2^{10} = 1024$ times. This way, the maximum radiation is guaranteed to be in the desired direction, while it may still shift in rare cases. Fig. 1 depicts the fitness value, which is the value of the cost function for the best individual (array design) at each generation. We observe a convergence to a value of $4.131 \times 2.324 \approx 9.6$. Fig. 1 also depicts the optimal array configuration (kept nano-cubes), as well as the far-zone electric field intensity on the related planes. The maximization at the desired direction is clearly observed.

Since the designed nano-arrays have relatively complex distributions of nano-cubes (particles), one may attempt to simplify them by removing particles. This may be done based on an importance graph shown later, while the elimination of particles is not trivial. Particularly, only keeping nano-cubes that are close to the main source does not necessarily lead to good performances. As an example, Fig. 2 presents the results when the optimized nano-array shown in Fig. 1 is modified in alternative ways by extracting nano-cubes. Specifically, in these trial designs, the colored nano-cubes are kept, while all others are extracted. The corresponding far-zone electric field intensity values are also included in Fig. 2. We observe that, these attempts to make the structure more compact fail as the radiation characteristics significantly deteriorates. The best results among four nano-arrays are obtained for Trial 2 involving five nano-cubes, while the achieved value of the cost function is only $2.713 \times 1.673 \approx 4.4$. It is remarkable that adding more nano-cubes to Trial 2 (that can be considered as the other trials) does not improve but degrades the performance, even leading to Trial 4 that generates shifted maximum on the x-y plane (hence the value of CF($\theta = 90°$) is only 0.002179 due to the punishment factor).

As the nano-arrays focused in this study involve two-dimensional arrangements of particles, they provide a higher ability for the control of the radiation pattern on the array plane. On the other hand, it is still possible to obtain good radiation characteristics in other directions. As an example, Fig. 3 presents the optimization results when the radiation is maximized at $\theta = 60°$ and $\phi = 45°$. Based on the relative value of the electric field intensity in the optimization direction with respect to those on the ($\theta = 60°, \phi \in [0, 360°]$) cone and on the ($\theta \in [0, 180°], \phi = 45°$) plane, the achieved value of the cost function reaches 9.6. We note that this nano-array provides the same performance at $\theta = 120°$ and $\phi = 45°$.

In order to achieve better directivity out of the array plane, one may consider three-dimensional structures, while this significantly overloads the optimization mechanism that must be improved to be addressed elsewhere. Alternatively, the cubic particles may be replaced with rods to have more oscillatory patterns that may be shaped in the elevation plane. Unfortunately, this approach does not bring a significant improvement in the radiation characteristics, while the optimization must be repeated in most cases. For example, Fig. 4 presents the radiation characteristics of two nano-arrays when the optimal arrangement in Fig. 1 (found for nano-cubes) is used for different particles with $\lambda/4$ and λ heights. We observe that the modified nano-arrays cannot maintain the good radiation characteristics of the original structure.

IV. Sensitivity to Fabrication Errors

Despite rapid developments in nanotechnology, structures in small scales are prone to fabrication errors that may affect the performance of the designs in real life. When a nano-array is optimized and designed, a further analysis is required to test the feasibility of the design and to identify major performance parameters. In the case of nano-arrays considered in this study, the cubic particles may not be arranged perfectly, while the particle surfaces may not be perfectly planar. In order to demonstrate the effects of such fabrication errors on the radiation characteristics of the designed nano-arrays, Figs. 5 and 6 present two sets of numerical experiments. In both sets, a design that provides a maximum radiation at $\theta = 90°$ and $\phi = 45°$ (different from the design in Fig. 1) is considered, while its fitness value on the x-y plane is 3.4875. In Fig. 5, the cubes are randomly shifted (with Gaussian distribution) so that three different structures are obtained. We observe small changes in the radiation characteristics of the design, while the fitness value remains in the range of 3.3–3.6. In the trials shown in Fig. 6, the surfaces of nano-cubes are corrugated with 0.005λ (Modified 1), 0.015λ (Modified 2), and 0.025λ (Modified 3) limits for the protrusions/cavities. Similar to the previous cases, the design maintains its radiation characteristics with maximum radiation at the desired direction, while the corresponding fitness values are in the range of 3.4–3.5.

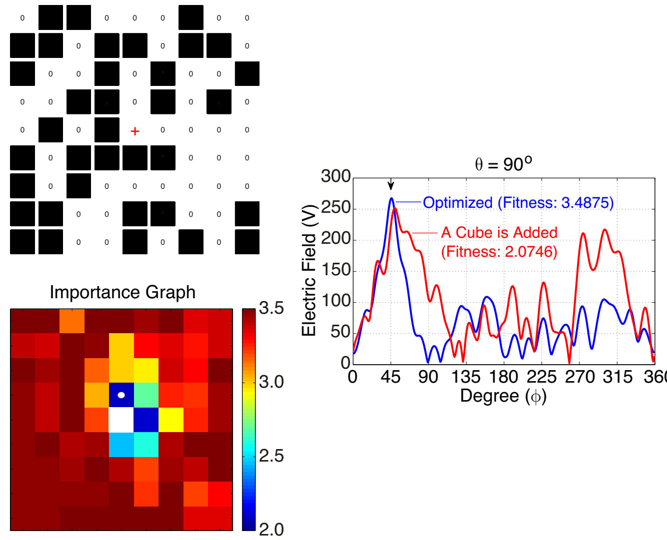

Fig. 7. The importance graph for an optimized nano-array that maximizes the radiation at a single direction. The fitness value is re-calculated when each nano-cube is added (if it was absent in the design) or extracted (if it was kept in the design).

Fig. 7 presents an extensive analysis, where the importance of each nano-cube of an optimized nano-array is investigated. The design is the same as the one considered in Figs. 5 and 6, i.e., it provides maximum radiation at $\theta = 90°$ and $\phi = 45°$. The color plot shows the value of the fitness function (originally 3.4875 for the optimized array) when each nano-cube decision is inverted (kept/extracted becomes extracted/kept) while all others remain the same. It can be observed that some of the nano-cubes are more critical; especially, two nano-cube locations close to the source location are extremely important. When these locations, which are originally empty, become filled, the fitness value significantly drops down. Fig. 3 also depicts the radiation patterns of the optimized and modified (when only one critical nano-cube is added) structures, where the deterioration of the pattern is clearly observed.

V. Multi-Direction Optimization

The developed design and optimization mechanism is particularly useful when multi-purpose optimization is required. For example, Fig. 8 presents three examples to multi-direction optimizations, i.e., when the radiation pattern of the overall structure is maximized simultaneously at two or three directions. The fitness value is defined as the mean of the far-zone electric field intensity values at these directions normalized by the values at the other directions on the same ($\theta = 90°$) plane. The designs that provide the best radiation patterns are also depicted under titles Design 1, Design 2, and Design 3. The optimization directions are shown with small arrows in the electric-field plots. We observe quite successful results with maximized radiations at the desired directions. We emphasize that once a nano-array is optimized, the same pattern can be rotated and the beams can be steered by physically rotating the array while the main source is fixed.

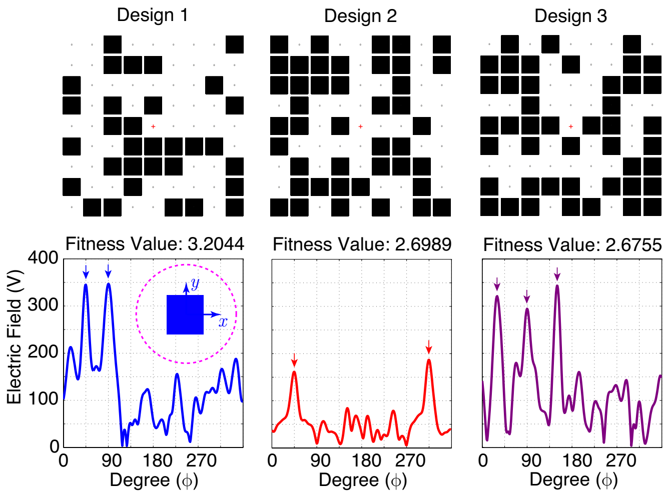

Fig. 8. Optimization results when the radiation is maximized at multiple directions.

VI. Concluding Remarks

In this study, we present the design and optimization of compact two-dimensional nano-arrays that can provide directive radiation characteristics at optical frequencies. The designs are obtained via rigorous optimization by using GAs with well-designed cost functions to maximize the radiation at desired directions. Using cubic particles, the designs are quite robust against possible fabrication errors related to the particle positioning and surface smoothness. Even when using only 80 elements, radiation patterns can be maximized simultaneously at multiple (two and three) directions. Once designed and optimized, rotation of a nano-array around an isotropic source can provide full beam-steering ability.

Acknowledgement

This work was supported by the Scientific and Technical Research Council of Turkey (TUBITAK) under the Research Grant 118E243 and by the Turkish Academy of Sciences (TUBA) in the framework of the Young Scientist Award Program.

References

[1] D. P. Fromm, et al., "Gap-dependent optical coupling of single bowtie nanoantennas resonant in the visible," Nano Lett., vol. 4, no. 5, pp. 957–961, Mar. 2004.

[2] P. J. Schuck, et al., "Improving the mismatch between light and nanoscale objects with gold bowtie nanoantennas," Phys. Rev. Lett., vol. 94, no. 017402, Jan. 2005.

[3] D. M. Solis, et al., "Optimization of an optical wireless nanolink using directive nanoantennas," Opt. Exp., vol. 21, no. 2, pp. 2369–2377, 2013.

[4] H. Chen, et al., "Design, fabrication, and characterization of near-IR gold bowtie nanoantenna arrays," Phys. Chem. C, vol. 118, no. 35, pp. 20553–20558, Aug. 2014.

[5] M. Alavirad, L. Roy, and P. Berini, "Optimization of plasmonic nanodipole antenna arrays for sensing applications," IEEE J. Sel. Top. Quantum Electron., vol. 20, no. 3, May/June 2014.

[6] A. Altınoklu and Ö. Ergül, "Computational analysis and full-wave optimizations of nanoantenna arrays for desired scattering and radiation characteristics," in Proc. URSI General Assembly and Scientific Symp. (URSI-GASS), 2017.

[7] A. Çekinmez, B. Karaosmanoğlu, and Ö. Ergül, "Integral-equation formulations of plasmonic problems in the visible spectrum and beyond," in Dynamical Systems - Analytical and Computational Techniques, M. Reyhanoglu, Ed. InTech, 2017, pp. 191–214.