Nano-Optical Couplers for Efficient Power Transmission Along Sharply Bended Nanowires

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

***Abstract*—We consider nano-optical couplers that consist of optimal arrangements of nanoparticles to improve the transmission abilities of nanowire systems with sharp bends. Previously, it was shown that absence/existence of nanoparticles in a given grid can be optimized such that the power transmission can significantly be increased without curving the bend. In this contribution, we present a detailed investigation and analysis of coupler performances to critical geometric parameters. While the designed couplers are robust against fabrication errors, numerical results demonstrate a remarkable dependency of coupler characteristics to particle types, as well as to bending geometry, due to strong plasmonic interactions at short distances. These findings further support the need for case-dependent optimization that must be performed efficiently and accurately via full-wave simulations.**

I. INTRODUCTION

Nanowires are natural components of nano-optical systems as they enable long-distance transmission of electromagnetic power via surface plasmons [1]–[7]. When they are straight, smooth, and perfectly aligned, nanowires have excellent transmission abilities for long distances with respect to the operating wavelength [2],[6]. When they are bended, however, reflection and diffraction at the bend regions may significantly reduce the efficiency [3]. To alleviate this problem, nano-optical couplers can be used to improve the power transmission, especially when curved bending is not desired for efficient usage of the available space. Recently, we showed that robust couplers involving nanoparticles can be designed such that transmission can be improved significantly even through very sharp corners [7]. The designs were obtained via optimization with genetic algorithms (GAs) supported by full-wave solutions with surface integral equations and the multilevel fast multipole algorithm (MLFMA) [8].

It is well known that plasmonic properties of metals at optical frequencies lead to complex interactions and very different responses to excitations, in comparison to the behaviors of metals at the lower (radio and microwave) frequencies. For example, when nanostructures are close to each other, the extraordinary coupling between them leads to useful abilities, particularly for energy harvesting, focusing, and optical sensing. At the same time, these strong interactions may increase the sensitivity of designs to geometric properties. In this contribution, we further investigate nano-optical couplers and their optimal designs to improve the power transmission through sharp corners. We show that the designed couplers are quite stable against fabrication errors, while particle geometries and bending shapes can significantly change their performances. Hence, a new optimization may be required depending on the case, while the optimization trials must be performed accurately for estimating the actual performances of candidate couplers. In the following section, we briefly introduce the simulation and optimization environment, followed by the description of the optimization problems in Section III. Then, Section IV presents optimization results and detailed analysis, before our concluding remarks in Section V.

II. SIMULATION AND OPTIMIZATION ENVIRONMENT

The transmission problems involving nanowires and couplers (nanoparticles) are modeled as three-dimensional structures and formulated by using surface integral equations in the frequency domain. There are diverse choices for the formulation [9]–[11], while we prefer the electric and magnetic current combined-field integral equation (JMCFIE) [12] or the modified combined tangential formulation (MCTF) [13] for fast and accurate solutions depending on the frequency. The surfaces and integral equations are discretized by using triangles and the Rao-Wilton-Glisson functions. The complex permittivity values of the metals are extracted from experimental data [14]. The problems are solved iteratively, while the required matrix-vector multiplications are performed via MLFMA. In addition, electromagnetic interactions in plasmonic media (e.g., inside

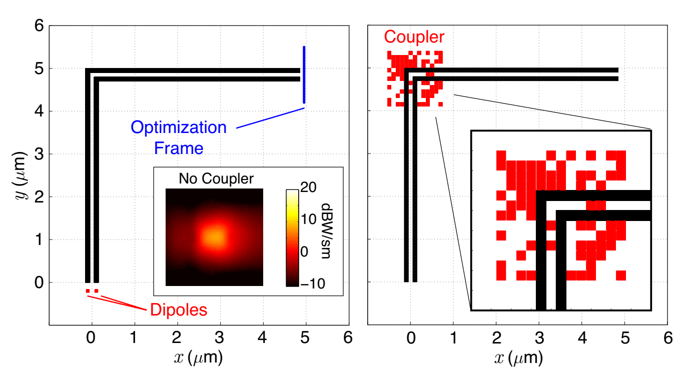

Fig. 1. An optimization problem involving a transmission line (a pair of Ag nanowires) with a 90° sharp bend. An optimal coupler that consists of $90 \times 90 \times 90$ nm cubic nanoparticles is also depicted.

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nanowires) are truncated to improve the efficiency without sacrificing the accuracy [15].

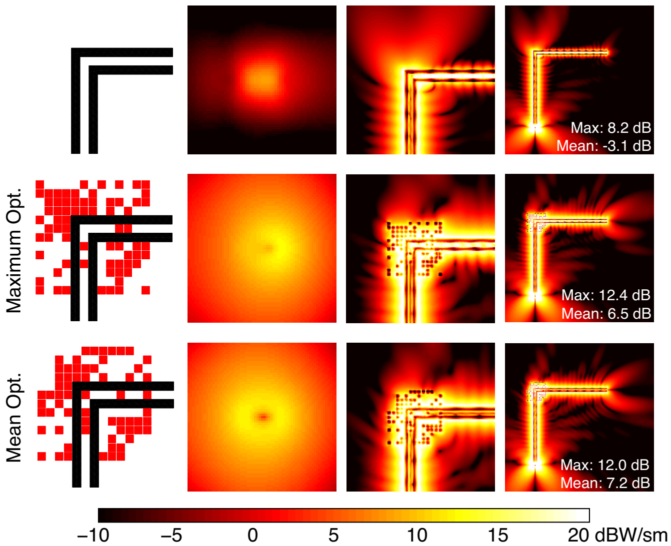

Fig. 2. Optimization results (couplers and power density distributions) when the maximum power density and the mean power density inside the output frame are maximized.

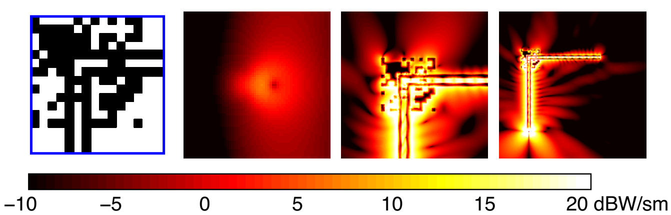

Fig. 3. Power density distribution when the nearby nanoparticles in the optimal design (Fig. 2) are combined.

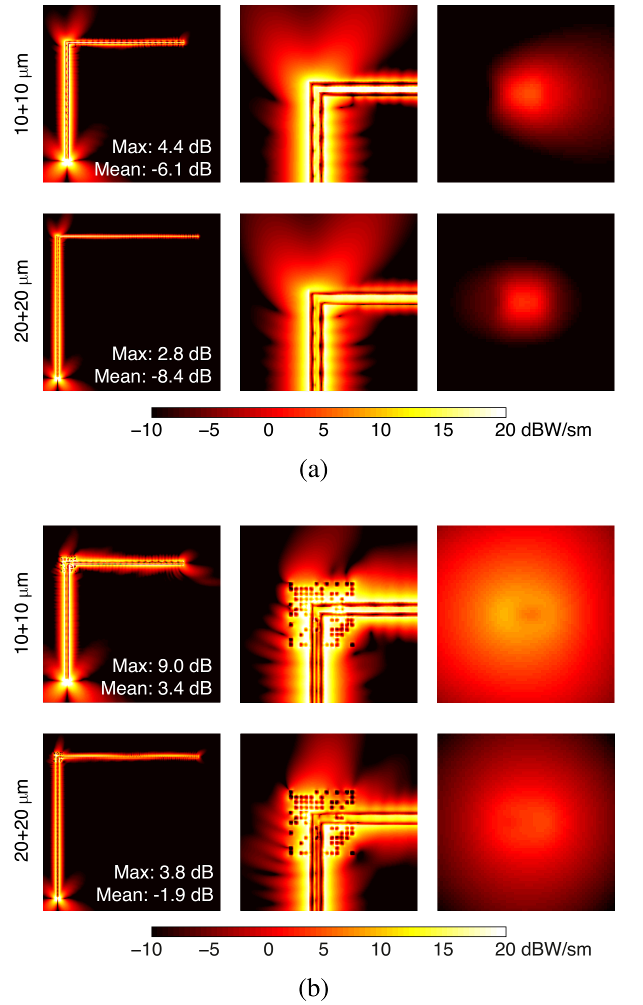

Fig. 4. Power density distributions when the length of the nanowires is $10+10$ μm and $20+20$ μm: (a) Without a coupler and (b) with the coupler in Fig. 2 designed for $5+5$ μm nanowires.

III. Coupler Optimization Problems

We consider transmission lines involving nanowires with sharp (e.g., 90°) bends. As shown in Fig. 1, a given transmission line is excited from one side and the power density is observed inside an output frame at the other side. A coupler is designed and located at the corner such that the power density (either its maximum or its mean) at the output is maximized. Optimization problems are solved by employing GAs, while the required trials are performed as three-dimensional simulations via the MLFMA implementation. The couplers are designed by considering an initial grid of nanoparticles and deciding which particles need to be kept/extracted to maximize the cost functions (e.g., maximum/mean of the power density at the output). The GA implementation is integrated with the MLFMA implementation by employing dynamic accuracy control [16] in order the reduce the optimization time. In addition, embarrassing parallelism is used by assigning simultaneous MLFMA solutions to multiple cores.

IV. Optimization Results and Coupler Analysis

As optimization results in this paper, the main geometry that we consider is a pair of $5+5=10$ μm silver nanowires with 90° sharp bends at the middle, as shown in Fig. 1. Each nanowire has a 0.1×0.1 μm square cross section. The transmission line is excited by a pair of Hertzian dipoles located on one side at 0.2 μm from the nanowires. The output frame is selected as a 1.3×1.3 μm square area at 0.1 μm distance from the nanowires. The frequency in the results of this paper is selected as 250 THz, at which the relative permittivity of Ag is approximately $-60.8+4.31i$. As a typical result, Fig. 1 also depicts the power density inside the output frame when no coupler is used. Most couplers are designed by using a total of 13×13 Ag cubes with $90\times90\times90$ nm dimensions and 10 nm face-to-face distances, while we also consider other types of geometries. In general, each optimization is performed by using GAs for 200 generations on pools of 40 individuals, leading to a total of 8000 simulations per optimization (omitting duplicate individuals).

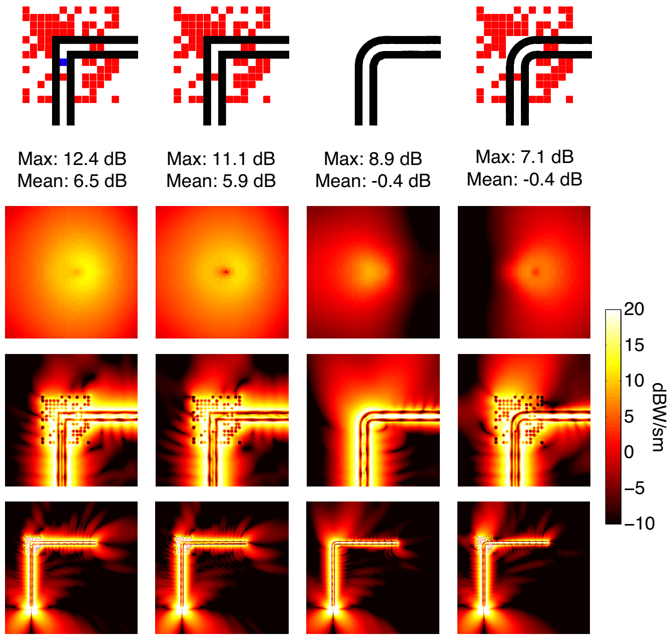

Fig. 5. Using the coupler, which is designed for a sharp bend (Fig. 2), for a curved bend with 0.4 μm radius of curvature.

A. Maximum Versus Mean Optimization

Depending on the application, the maximum or the mean of the power density at the output can be optimized. It is remarkable that coupler designs can significantly be different depending on the optimization target, while the achievable power values are often close to each other. Fig. 2 presents two optimization results when the maximum of the power density (second row) and the mean of the power density (third row) inside the output frame are maximized. The no-coupler case is also shown in the first row for comparisons. In addition to power density distributions inside the output frame (second column) and in the coupler region (third column), a general view is shown for each case (fourth column), while the coupler designs are presented in the first column. We observe that the power transmission can significantly be improved by using effective couplers. Specifically, the maximum power density (in dBW/sm) can be increased from 8.2 dB to 12.4 dB, while the mean power density can be increased from -3.1 dB to 7.2 dB. We also note that optimization of the maximum power density leads to 6.5 dB mean power density. Similarly, the maximum power density reaches 12.0 dB if the mean power density is maximized. In the following sections, we consider the optimization of the maximum power density (specifically the coupler in the second row of Fig. 2), while this selection does not change the interpretation of the results and conclusions.

B. Combination of Nanoparticles

Once an optimization is completed and an optimal design is found, one may question whether the nanoparticles must be kept as separated (as designed) or they can be combined (without any distance between them) as much as possible. This is particularly interesting since such a combination may simplify the fabrication process. As an example, Fig. 3 presents the results when the nearby nanoparticles (cubes) in the optimal design shown in Fig. 2 are combined. Comparing the results, we observe that the performance of the coupler significantly deteriorates. A close examination in the bending region shows that the coupler with combined nanoparticles operates very differently with cavities, in comparison to the well-designed interactions between separated nanoparticles in the original design.

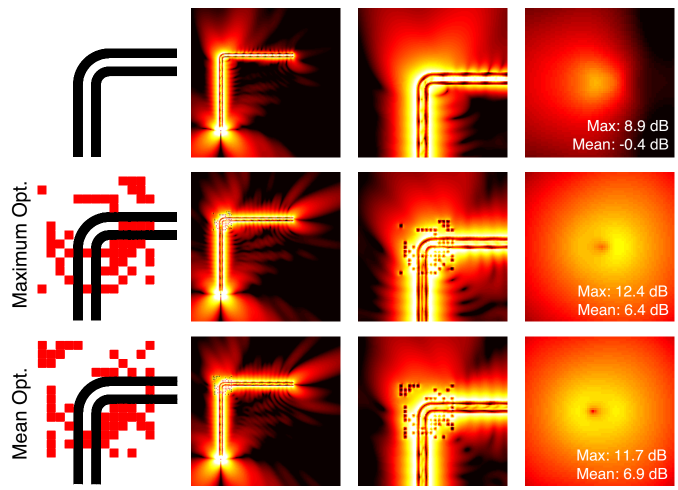

Fig. 6. Optimization results (couplers and power density distributions) when the maximum power density and the mean power density inside the output frame are maximized for curved nanowires.

C. Performance of Couplers for Different Nanowire Lengths

The coupler designs presented in this paper are obtained for a specific length of nanowires, i.e., for $5+5$ μm. On the other hand, they can still perform well for other lengths, particularly for longer nanowires. As two examples, Fig. 4 depicts power density distributions for $10+10$ μm and $20+20$ μm nanowires with sharp bends at the middle. Without a coupler, the maximum power density inside the output frame drops to 4.4 dB and 2.6 dB, respectively, from 8.2 dB for the original ($5+5$ μm) case. Similarly, the mean power density values are found to be -6.1 dB and -8.4 dB. Using the coupler shown in Fig. 2, the maximum power density is kept at 9.0 dB for $10+10$ μm nanowires and 3.8 dB for $20+20$ μm nanowires, while the corresponding mean power density values are 3.4 dB and -1.9 dB, respectively. Investigating the power density distributions in the coupler region, we observe that the coupler operates similarly, by reducing the escaping power and guiding the incoming wave through the bend, for different nanowire lengths. It can be an advantage to use the same coupler design for different nanowire lengths, while it is also possible to repeat optimization trials for different nanowire lengths (but this becomes computationally difficult for longer nanowires).

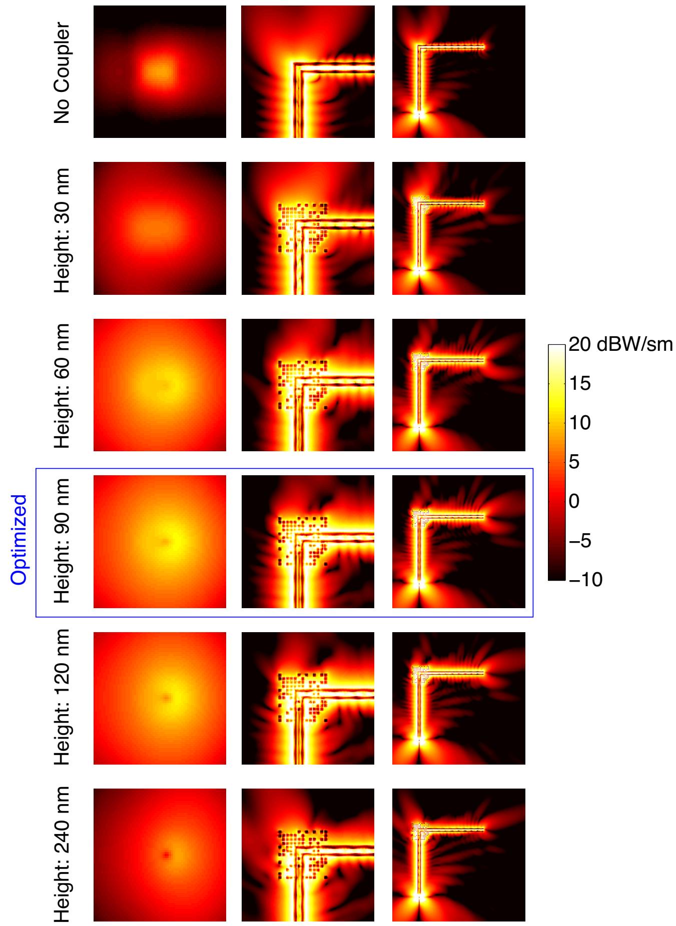

Fig. 7. Power density distributions when the height of the particles is changed to 30 nm, 60 nm, 120 nm, and 240 nm for the coupler design in Fig. 2 involving $90 \times 90 \times 90$ nm cubes.

D. Effect of Curving

It is well known that curving the bends can significantly improve the power transmission along bended nanowires, while our studies show that the radius of curvature must be very large (at the cost of reduced compactness of the bending region) to compete with the designed couplers. It may be possible to use a coupler for a curved bend; but, the optimization must be repeated due to the sensitivity of coupler designs to the geometry of bends. As an example, Fig. 5 presents the results when the coupler in Fig. 2 is used for a curved bend with 0.4 μm radius of curvature. In order to use the design, one of the cubes must be extracted since it coincides with one of the curved nanowire. Since this cube is a critical one, its removal leads to a remarkable decrease in the maximum/mean power density to $11.1/5.9$ dB (from $12.4/6.5$ dB). These values are still much better than only curving, leading to 8.9 dB maximum and -0.4 dB mean power density values. But, a major problem occurs when the coupler is used for the curved bend. The maximum power density decreases to 7.1 dB (even below the value for the case of sharp bend without a coupler), while the mean power density stays at -0.4 dB (no improvement in comparison to only curving). These results show that, if the geometry of the bend is changed, even to make it better by curving, optimization must be repeated.

As an example to optimization trials for curved nanowires, Fig. 6 presents the results when couplers are designed for 0.4 μm radius of curvature. It can be observed that the optimization of the maximum power density leads to $12.4/6.4$ dB maximum/mean power density in the output frame, while these values are $11.7/6.9$ dB when the mean power density is maximized. Hence, once again, the designed couplers significantly improve the power transmission, in comparison to the no-coupler (but curved) case, i.e., $8.9/-0.4$ dB. On the other hand, the results are not better than those obtained for sharply bended with couplers. This, in fact, shows the overall success of the designed couplers, particularly for the sharp case, which can improve the power transmission to high levels such that curving does not provide an improvement anymore.

E. Sensitivity to Particle Geometries

Naturally, the electromagnetic characteristics of a coupler strongly depends on the geometry of its particles. On the other hand, the designed couplers in this study are quite resistant to fabrication errors and deformations, as long as the general shape of the particles does not change. As an example, Fig. 7 presents power density distributions when the height of the particles in the optimized coupler in Fig. 2 is changed. While the original cubes have $90 \times 90 \times 90$ nm dimensions, we make their height 30 nm, 60 nm, 120 nm, and 240 nm. We observe that decreasing/increasing the height to $60/120$ nm has little effect on the efficiency of the coupler. A relatively poor performance is obtained when the height is changed to 30 nm (one third of the original), while the power transmission even for this case is not worse than the one without a coupler. Increasing the height to 240 nm also leads to visible deterioration in the performance of the coupler, while it still provides improved transmission in comparison to the no-coupler case.

In order to investigate realistic fabrication errors that may cause corrugations on particle surfaces, we consider the results for deformed cubes in Fig. 8. For the coupler design in Fig. 2, the discretization nodes (used for numerical simulations) are shifted randomly in the x, y, and z directions, while the shift in each direction is limited to ± 2 nm. In addition to each cube, nanowires are also deformed using a similar approach. Uniform distribution is used for the randomly generated shift distances. Fig. 8 shows the histogram of the shift distances, as well as the obtained power density distributions, for two different trials. It can be observed that corrugations have little effects on the coupler characteristics. While these results demonstrate the robustness of the coupler design, we emphasize that the cubes are not allowed to touch each other in these trials, which may have disastrous effects as shown in the combination example above (see Fig. 3).

Despite they can be robust against fabrication errors, as well as to modifications in simple geometric parameters such as the height of particles, the particle geometry significantly affects

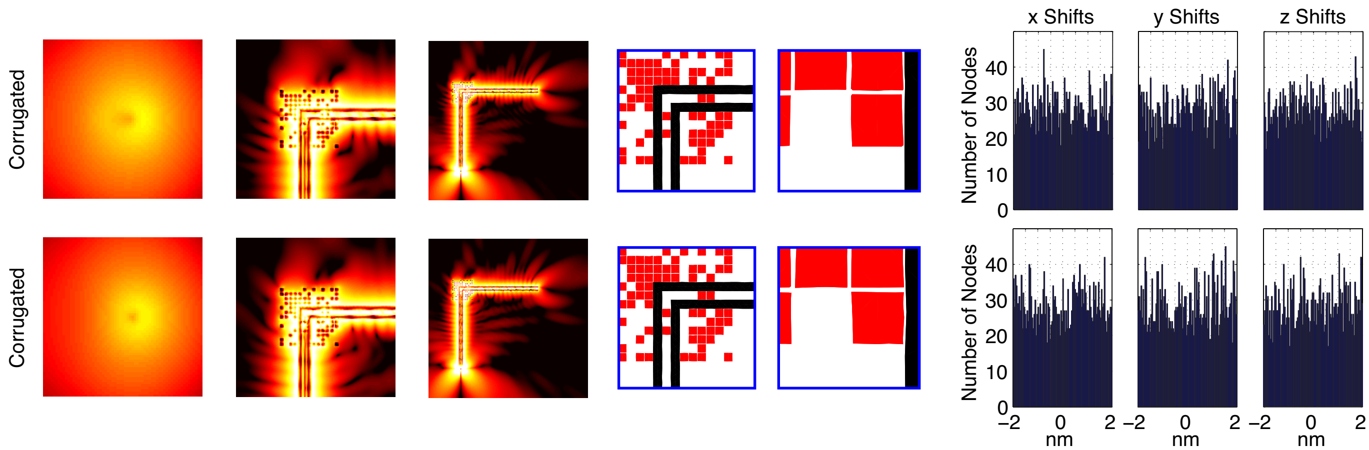

Fig. 8. Power density distributions when the coupler particles (cubes) and the nanowires are deformed for the coupler design in Fig. 2. Two different trials (rows) are shown.

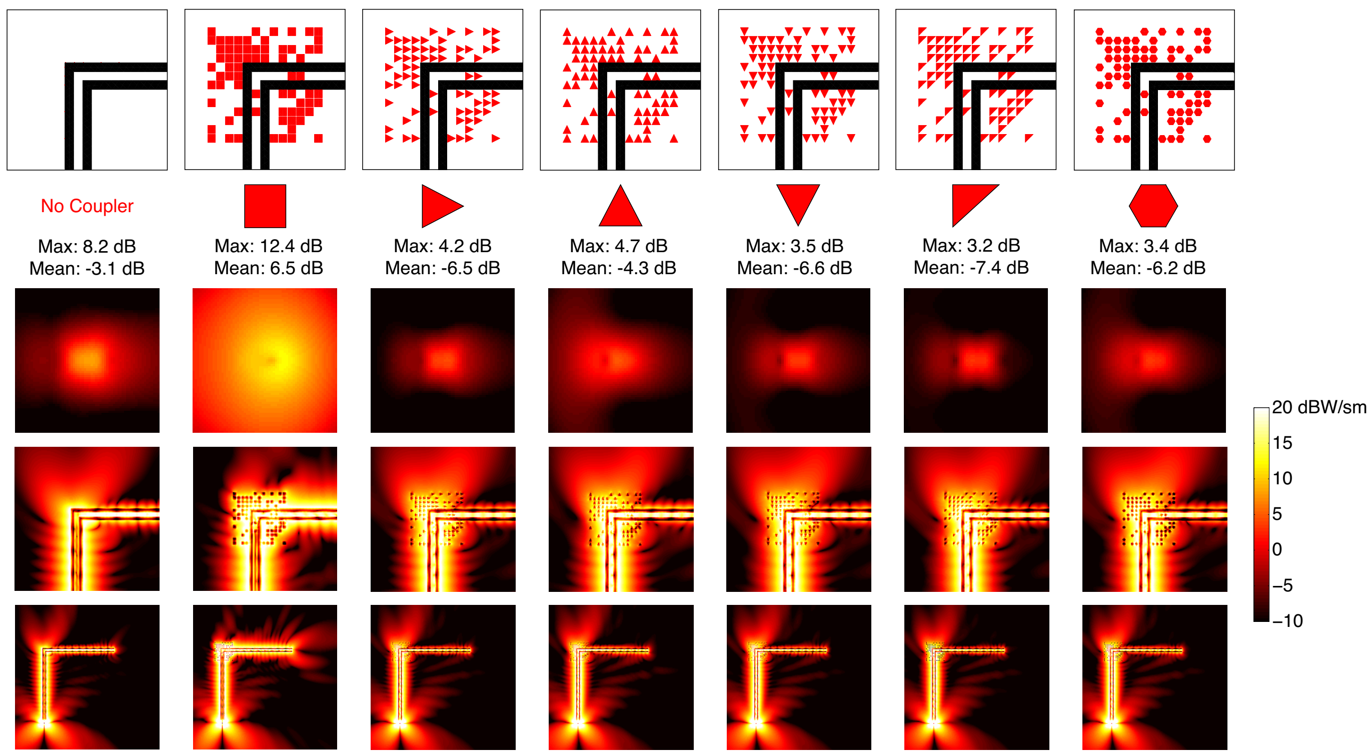

Fig. 9. Using an optimal arrangement of cubic particles (coupler design in Fig. 2) for different particle geometries.

the characteristics and performances of nano-optical couplers. As a demonstration, Fig. 9 presents the results when an optimal coupler arrangement obtained for cubic particles (Fig. 2) is used for different particle shapes (prisms). Specifically, we test the arrangement for five different particles with different cross sections (height is kept at 90 nm). We observe that the transmission performance significantly drops, i.e., the coupler design becomes useless, when employing different particles instead of cubes. In fact, such couplers make the transmission worse compared to the no-coupler case.

F. Optimization for Different Particle Shapes

In this work, using cubes to design effective couplers is not an arbitrary choice. Our studies with different shapes consistently show that the cube is one of the best geometries when a regular grid is used, while other geometries are also possible. As shown above, directly changing the particle geometry for an optimized arrangement leads to very poor results. But, it is possible to use alternative shapes by optimization. For example, Fig. 10 presents four different couplers with different types of nanoparticles when an optimization is performed for each particle type to increase the maximum power density in the output frame. Specifically, in addition to the coupler with cubic particles in Fig. 2, we consider triangular and hexagonal prisms, again in 13×13 arrangements. It can be observed that the maximum power density can significantly be increased (compared to the no-coupler case) for all particle types, while the optimal arrangement of nanoparticles strongly depends on the particle type. As mentioned above, cubic particles lead to a larger value for the mean power density, while the performances are similar for the maximum power density. Although not shown here, optimization of the mean power density using alternative particles leads to relatively low maximum power density values in comparison to the results with cubic particles.

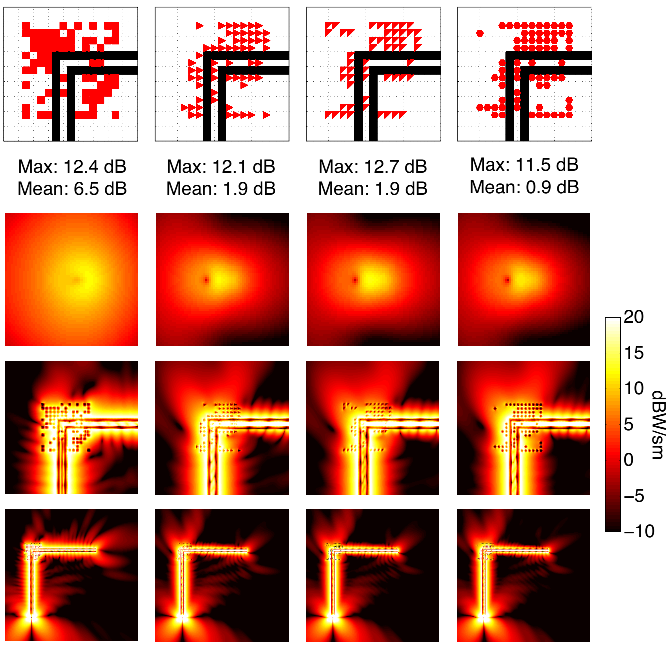

Fig. 10. Power density distributions when four designed couplers involving different types of nanoparticles are used.

V. Concluding Remarks

In this paper, we provide a detailed analysis of nano-optical couplers that are designed for improving the power transmission along sharply bended nanowires. The designs are obtained via GAs, while the optimization trials are performed accurately and efficiently by using MLFMA. All results demonstrate the effectiveness of the couplers that can significantly maximize the output power. Numerical results also show that the designed couplers maintain their performances for different nanowire lengths and they are robust against fabrication errors (different heights and surface corrugations), while they are sensitive to the main geometry of particles. In addition, the particles need to be separated, as designed, without physical contacts between them. It is possible to design couplers with different particle shapes, while cubic particles provide the best results for compact (e.g., 13×13) regular arrangements. Despite their relatively small sizes, the couplers are so effective that curving within the coupler region does not further improve the power transmission.

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