Computational Design of Optical Couplers for Bended Nanowire Transmission Lines

Yunus Emre Tunçyürek, Barışcan Karaosmanoğlu, and Özgür Ergül

Department of Electrical and Electronics Engineering
Middle East Technical University, Ankara, Turkey
{bariscan,tuncyurek.emre,ozergul}@metu.edu.tr

Abstract **—** We present computational analysis, optimization, and design of optical couplers that can be useful to improve the transmission along bended nanowires. After demonstrating the deteriorated energy transmission due to sharp bends, which lead to out-of-phase nanowires and diffraction, we use a rigorous simulation environment to design efficient couplers made of spherical particles. For this purpose, an optimization module based on genetic algorithms is combined with the multilevel fast multipole algorithm, leading to a full-wave environment for precise designs of couplers. Numerical examples involving silver nanowires are presented to demonstrate the effectiveness of the optimization mechanism.

Index Terms **—** Genetic algorithms, multilevel fast multipole algorithm, nanowires, optical couplers, surface integral equations.

I. INTRODUCTION

Their favorable properties that allow controlling and guiding optical waves make nanowires an important class of popular ingredients of nano-optical systems [1]–[14]. Thanks to plasmonic properties of metals at optical frequencies, nanowires provide an excellent ability to transfer electromagnetic energy to long distances with respect to wavelength [3]. Hence, they are naturally used in a plethora of applications, such as sensing [1], energy harvesting, and optical imaging [5],[7]. As in all areas of electromagnetics, computational studies [12]–[14] are performed hand in hand with analytical and experimental work in order to develop alternative configurations of nanowire systems, leading to improved designs with better optical responses. Today, nanotechnology allows for the fabrication of less defective nanowires and their highly ordered arrangements for achieving ideal structures that were considered to be only theoretical a decade ago.

When a nanowire system is used as a transmission line, the electromagnetic energy is transmitted via surface plasmon polaritons. At the end of the line, the energy is assumed to be coupled to another system [6], or to free space, where radiation occurs from the tips of the nanowires [3]. In an optical system, depending on the application, it may be required to bend the transmission line. Then, similar to their counterparts at microwave frequencies, reflections may occur from the bends, reducing the amount of energy transferred. But, since the nanowires are not closed systems and the energy is mainly carried on the nanowire-air interfaces, diffraction at the bending locations becomes an important problem that further reduces the efficiency of the transmission [8]. As shown in this paper, smooth bends improve the transmission; but a large radius of curvature (ROC) may be required for a sufficient transmission. In addition, curving nanowires may bring additional challenges in the fabrication processes. At the same time, a large ROC wastes an area around bend and it is desirable to use a coupler that allow for efficient transmission even for sharply bended nanowires.

This study is devoted to the design of optical couplers for bended nanowire transmission lines. By using an array of spherical particles at the bend locations, we are able to increase the transmission through 90º corners without implementing any curves. The structure of the coupler is optimized via genetic algorithms (GAs) supported by fast and accurate solutions using the multilevel fast multipole algorithm (MLFMA) [15],[16]. In the next section, we briefly provide the details of the developed simulation and optimization environment. Section III presents the optimization parameters and numerical results, demonstrating the effectiveness of the optimizations. The paper ends with our concluding remarks in Section IV.

II. SIMULATION AND OPTIMIZATION ENVIRONMENT

We consider metallic objects, i.e., nanowires and couplers, located in free space at optical frequencies. The transmission problems are solved in frequency domain assuming time-harmonic sources in steady state. The major components of the solver and the optimization mechanism can be summarized as follows.

- Metals are modeled as homogeneous plasmonic objects using frequency-dependent complex perm

Submitted On: February 2, 2017
Accepted On: March 2, 2017

values with negative real parts. Surfaces are discretized by using triangular meshes. Electric and magnetic current densities are expanded via standard Rao-Wilton-Glisson functions. For accurate solutions, a modified combined tangential (MCTF) [17] is used, which provides accurate solutions of metallic objects in wide ranges of optical frequencies.

- Iterative Krylov-subspace algorithms are used to solve the dense matrix equations derived from the discretized MCTF. Matrix-vector multiplications are performed efficiently by using MLFMA [15], that is developed particularly for plasmonic structures [18]. Iterative solutions are accelerated by using a nested scheme employing MLFMA and its approximate forms. All interactions (matrix elements) and near-zone calculations are performed with two digits of accuracy (1% maximum error).
- GAs are used to optimize the couplers involving spherical plasmonic particles. On/off optimizations are performed by removing or keeping the particles to maximize the cost function. Hence, binary chromosomes involving 0 (off/remove) and 1 (on/keep) bit values are used so that the chromosome length corresponds to the number of initial particles in the coupler. An in-house implementation of GAs, employing hybrid selection, success-based mutations, and family elitism, is used for efficient optimizations.
- The GA implementation is combined efficiently with the solver module based on MLFMA. Two different kinds of combinations are considered, depending on the size of the problems. In a black-box combination, the GA module requires the evaluation of each individual, which is considered to be an independent electromagnetic problem. In an integrated combination, the setup computations for the full problem is performed before the optimization starts, and each evaluation is achieved by row/column deletion on the full matrix equation. In both cases, a dynamic accuracy control for MLFMA [19] can be used to further accelerate the optimizations by using less accurate solutions in initial GA pools.

More details of the solver and optimization modules can be found in [19],[20].

III. NUMERICAL RESULTS

Figure 1 depicts the scenario considered in this paper. Transmission lines involving pairs of silver (Ag) nanowires are considered at 250 THz. At this frequency, the relative permittivity of Ag is approximately −60.8 + 4.31i [21], while it is assumed to be non-magnetic.

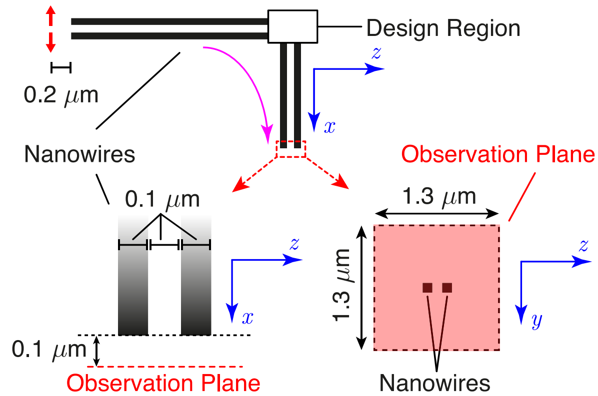

Fig. 1. The transmission scenario considered in this paper.

The nanowires have 0.1 × 0.1 μm square cross sections, while the surface-to-surface distance between them is also set to 0.1 μm. Without bending, each transmission line involves a horizontal part (in the z direction) of approximately 20 μm that is connected to a vertical part (in the x direction) of approximately 20 μm, leading to a total length of around 40 μm (approximately 33λ, where λ is the wavelength in free space). The couplers are designed as two-dimensional arrays of spherical Ag particles located at the intersection locations. The spheres are identical with a diameter of 90 nm. When using the couplers, the horizontal and vertical parts are connected sharply with 90º corners. For benchmarking, we also consider curved bends with various ROC values, while no coupler is used in these cases. As also depicted in Fig. 1, each transmission line is excited by a pair of dipoles (with unit dipole moments, i.e., 1 Am strengths) located symmetrically on the left-hand side with 0.2 μm distance from the nanowires. The output region is defined at the bottom end of the vertical nanowires. Specifically, sampling points on 1.3 × 1.3 μm planes with 0.1 μm distance from the nanowires are used to assess the transmission capabilities of the nanowires systems.

First, we consider the performances of curved connections, in comparison to the 90º sharp connection. Figure 2 presents the electric-field intensity (magnitude in dBV/m) and the power density (magnitude in dBW/m^2) at around the transmission lines. The power density is calculated as:

$$\boldsymbol{S} = \frac{1}{2}\boldsymbol{E} \times \boldsymbol{H}^*, \tag{1}$$

where $\boldsymbol{E}$ and $\boldsymbol{H}$ represents the electric field intensity and the magnetic field intensity, respectively. The dynamic ranges are selected as 40 dB and 20 dB for the field and power, respectively, for a comparative visualization. The dipoles are clearly visible on the left-hand sides, where strong coupling to the nanowires is also observed. Diffraction occurs due to bending in all cases, while it becomes less localized as ROC increases from 0.3 μm to 10 μm. A comparison of the field and power values at the output sides reveals that the transmission is very low for the 90° sharp case, i.e., the power density in the vicinity of the nanowires at the output is less than 20 dB in this case. Then, as ROC increases and bending becomes smoother, the transmission improves progressively. While this is expected, we note that the quality of the transmission deteriorates due to the negative effects of the diffraction, as well as the phase mismatch between the nanowires. These contributions can be difficult to be isolated; but, they are modeled precisely using a full-wave solver.

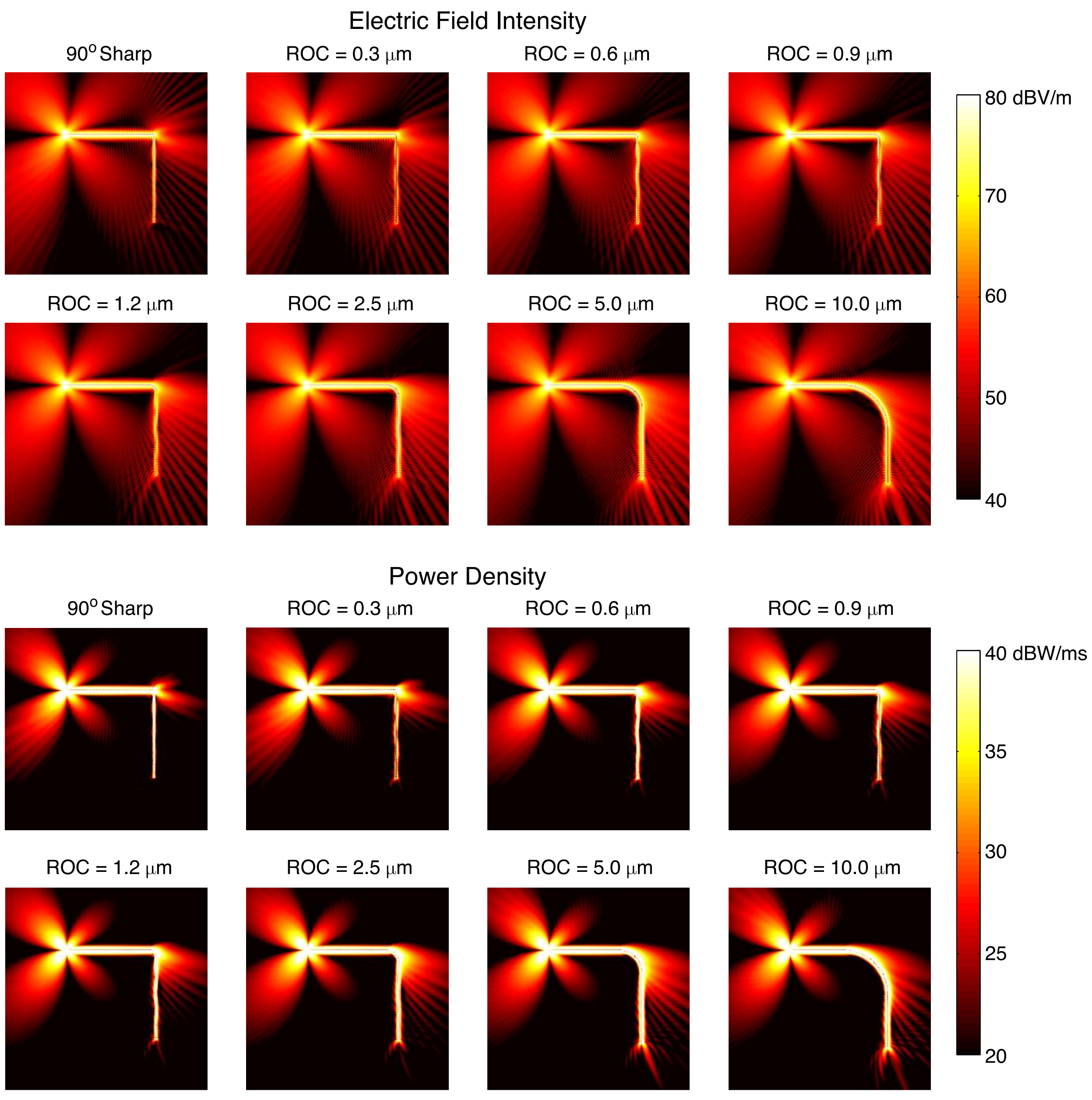

Fig. 2. The electric field intensity and power density at around the curved transmission lines with various values of ROC, in addition to the 90° sharp bending case.

For a detailed comparison of the curved transmission lines, Fig. 3 present the magnitudes of the electric field intensity (dBV/m), magnetic field intensity (dBA/m), and power density (dBW/m^2) on the output plane described in Fig. 1. Our observations are in consistent with the discussion above, i.e., the transmission clearly improves as ROC increases. Considering the power density plots, a small spot of values at around 35 dB is visible for the sharp case, while it evolves into a much larger spot with values more than 45 dB as ROC becomes 10 μm. It is remarkable that, in addition to the larger output values, increasing ROC leads to more symmetric output patterns, as a demonstration of improved transmission quality.

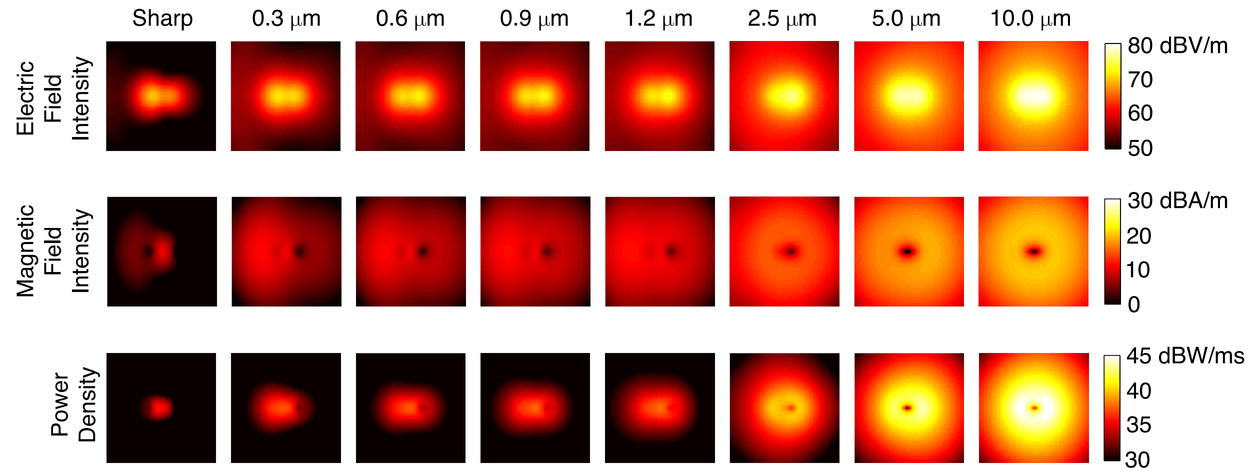

Fig. 3. The electric field intensity, magnetic field intensity, and power density at the outputs (see Fig. 1) of the transmission lines with various values of ROC, in addition to the 90° sharp bending case.

Following the benchmark on curved transmission lines, we consider the design of couplers for improving the transmission through sharp corners. Two-dimensional arrays of 139 or 143 spherical particles, which are also made of Ag, are placed at the corner locations enclosing the nanowires. Specifically, a 13 × 13 grid is used, while the particles corresponding to the nanowire locations are simply omitted. Optimizations are performed in the MATLAB environment. As the cost function, we select the average power density to be maximized on the 1.3 × 1.3 μm output planes. In the following, we present the results for three types of optimizations.

- The full model, discretized with around 91,314 unknowns, is considered. Using pools of 40 individuals (40 solutions per generation), it takes around one day to perform 6 generations (240 solutions) using 20 workers. Therefore, in order to perform an optimization with 50 generations, we need around 8 days.
- A quarter model, which is obtained by reducing the length of the transmission lines to 10 μm (5 μm horizontal plus 5 μm vertical), is considered. Locations of the dipoles and the output planes with respect to the transmission lines are kept as in the full model. In this case, again using pools of 40 individuals and 20 workers in the MATLAB environment, we are able to complete 100 generations in 4 days. Once an optimal coupler is found, it is tested on the full geometry for the actual performance.
- For testing the sensitivity, a quarter model, where the sphere grid is shifted by one element towards the outer sides of the corner, is considered. In the following, three separate trials are shown for this scenario. Optimization histories (increase of the cost function) for these three optimizations can be seen in Fig. 4.

Figure 5 depicts the optimized coupler designs, in addition to the obtained electric field intensity. It can be observed that the couplers effectively improve the transmission along the nanowires, leading to better output values in comparison to the sharp case without any coupler (see Fig. 3). Better transmissions with the couplers are further verified in Fig. 6, where power density values at around the transmission lines as well as on the output planes are presented. We have the following conclusions.

- Using a quarter model for the optimizations instead of the full geometry provides quite successful results. In fact, the results for the full geometry in Figs. 5 and 6 are clearly worse than the corresponding results for the quarter geometry. This is due to the less number of generations (50 instead of 100) used for the full geometry, due to the slower optimization trials for this geometry. Although not shown, reducing the geometry further (smaller than the quarter) reduces the effectiveness of the optimizations, i.e., a designed coupler for the smaller geometry does not work sufficiently for the full case.

- Shifting the grid slightly changes the optimization results. This is partially due to the small rearrangements of the spherical particles when shifting is applied. Consequently, the optimizations seem to be stable, leading to reasonably good results that can be achieved.
- Three different optimizations for the same (shifted) grid and geometry provide similar results, again demonstrating the stability of the optimizations. Obviously, discrepancies also exist as the final geometries depicted in Fig. 5 are not exactly the same. If the results are investigated in detail, and as also depicted in Fig. 4, the second trial leads to a better performance among three trials with more than 1.8 kW/m^2 average power.
- Considering again the last three optimizations, the similarities between the coupler designs shown in Fig. 5 is remarkable. In general, we observe empty spaces on the right-top and left-bottom portions, while the particles mostly remain on the left-top and right-bottom sides. These designs may be used as seeds to reach more optimal couplers to be considered in a further work.

Finally, for more quantitative comparisons, Table 1 lists the average and maximum power density values at the outputs of the transmission lines considered in this paper. Although the maximum power is not directly optimized, there is a high correlation between the maximum and average power values. In addition to the sharp (no-coupler) case, we consider the optimized (the second trial for the quarter model with shifted grid) case, as well as the curved designs with various ROC values. It can be observed that the optimized coupler improves the average power ten times than the no-coupler case. The improvement by the coupler is close to the curved sample with 2.5 μm ROC. Existence of any coupler design of the same size, which may provide transmissions as good as larger ROCs, is under investigation.

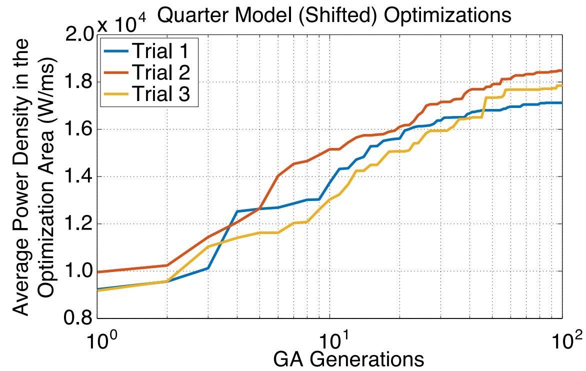

Fig. 4. Optimization histories for three trials on the shifted quarter model.

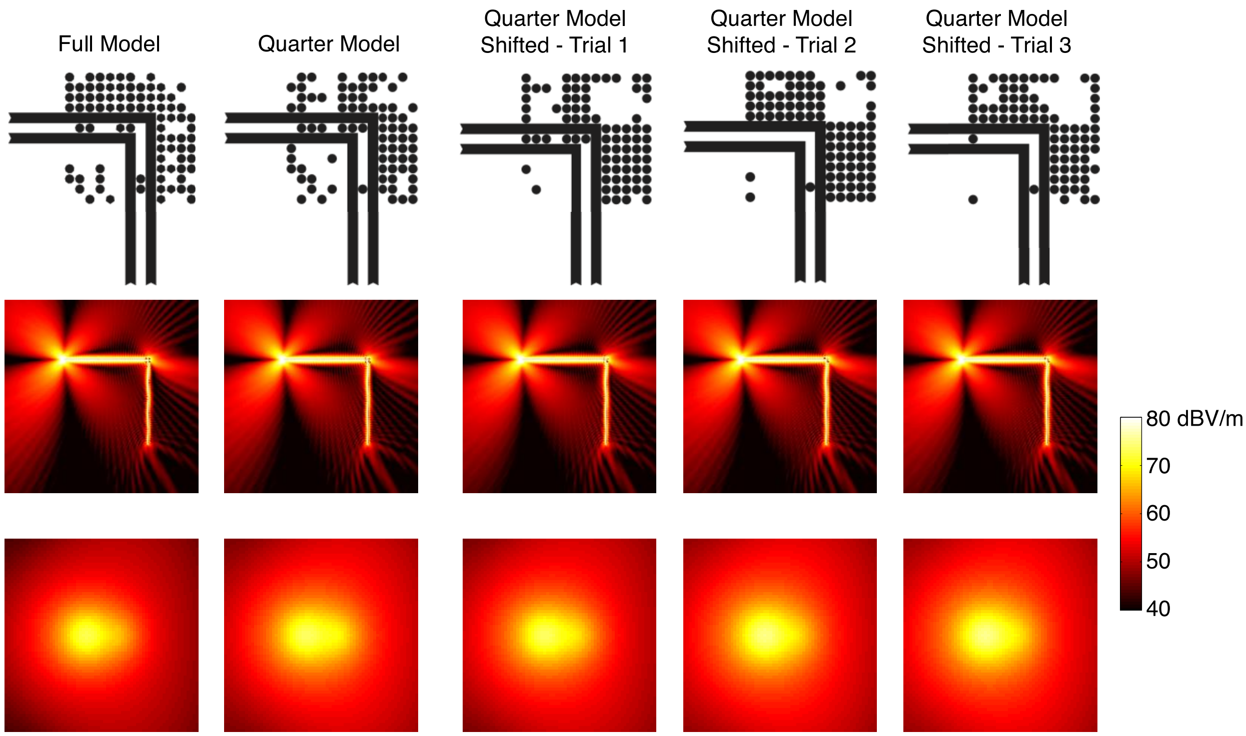

Fig. 5. Coupler designs (optimization results) to maximize the output of the 90° bended transmission line, and the corresponding electric field intensity at around the nanowires as well as on the output plane.

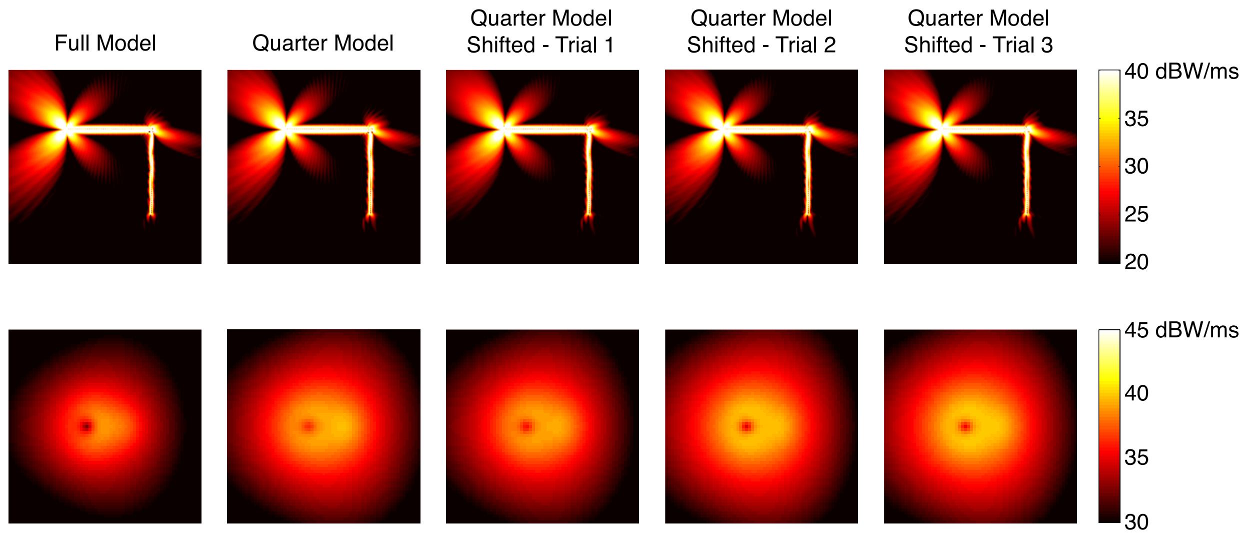

Fig. 6. The power density at around the nanowires when using the coupler designs at the corner of the 90º bended transmission line.

Table 1: Average and maximum power density values at the outputs of the transmission lines

	Curved Transmission Lines								
ROC	0.3μm	0.6 μm	0.9 μm	1.2 μm	2.5 μm	5.0 μm	10 μm	Sharp	Optimized
Average (kW/m^2)	0.924	1.04	1.18	1.38	3.26	6.85	10.4	0.307	3.22
Maximum (kW/m^2)	5.49	5.53	5.80	6.12	10.3	24.0	32.68	3.91	10.0

IV. CONCLUSION

We present simulation and optimization of optical couplers to improve the transmission ability of bended nanowire systems. By using an optimization mechanism involving efficient implementations of GAs and an MLFMA-based solver, we perform full-wave optimizations of couplers when they are located on the transmission lines (without resorting to isolation). We show that a well-designed coupler that involves only 100–200 spherical particles can improve the average power transmission through sharp corners by 10-folds without applying any curve at the bend locations.

ACKNOWLEDGMENT

This work was supported by the Scientific and Technical Research Council of Turkey (TUBITAK) under the Research Grants 113E129 and 114E498, and by the Turkish Academy of Sciences (TUBA).

REFERENCES

[1] X. Wang, C. J. Summers, and Z. L. Wang, “Large-scale hexagonal-patterned growth of aligned ZnO nanorods for nano-optoelectronics and nanosensor arrays,” *Nano Lett.*, vol. 4, no. 3, pp. 423-426, Jan. 2004.

[2] H. Ditlbacher, A. Hohenau, D. Wagner, U. Kreibig, M. Rogers, F. Hofer, F. R. Aussenegg, and J. R. Krenn, “Silver nanowires as surface plasmon resonators,” *Phys. Rev. Lett.*, vol. 95, no. 257403, Dec. 2005.

[3] A. W. Sanders, D. A. Routenberg, B. J. Wiley, Y. Xia, E. R. Dufresne, and M. A. Reed, “Observation of plasmon propagation, redirection, and fan-out in silver nanowires,” *Nano Lett.*, vol. 6, no. 8, pp. 1822-1826, June 2006.

[4] A. V. Akimov, A. Mukherjee, C. L. Yu, D. E. Chang, A. S. Zibrov, P. R. Hemmer, H. Park, and M. D. Lukin, “Generation of single optical plasmons in metallic nanowires coupled to quantum dots,” *Nature*, vol. 450, no. 7168, pp. 402-406, Nov. 2007.

[5] J. Yao, Z. Liu, Y. Liu, Y. Wang, C. Sun, G. Bartal, A. M. Stacy, and X. Zhang, “Optical negative refraction in bulk metamaterials of nanowires,” *Science*, vol. 321, no. 5891, pp. 930, Aug. 2008.

[6] X. Guo, M. Qiu, J. Bao, B. J. Wiley, Q. Yang, X. Zhang, Y. Ma, H. Yu, and L. Tong, “Direct coupling of plasmonic and photonic nanowires for hybrid nanophotonic components and circuits,” *Nano Lett.*, vol. 9, no. 12, pp. 4515-4519, 2009.

[7] B. D. F. Casse, W. T. Lu, Y. J. Huang, E. Gultepe, and L. Menon, “Super-resolution imaging using a three-dimensional metamaterials nanolens,” *Appl. Phys. Lett.*, vol. 96, no. 023114, Jan. 2010.

[8] W. Wang, Q. Yang, F. Fan, H. Xu, and Z. L. Wang, “Light propagation in curved silver nanowire

plasmonic waveguides," *Nano Lett.*, vol. 11, no. 4, pp. 1603-1608, Mar. 2011.

[9] S. M. Bergin, Y. Chen, A. R. Rathmell, P. Charbonneau, Z. Y. Lib, and B. J. Wiley, "The effect of nanowire length and diameter on the properties of transparent, conducting nanowire films," *Nanoscale*, vol. 4, no. 6, pp. 1996-2004, Feb. 2012.

[10] M. Sun, Z. Zhang, P. Wang, Q. Li, F. Ma, and H. Xu, "Remotely excited Raman optical activity using chiral plasmon propagation in Ag nanowires," *Light: Science and Applications*, vol. 2, no. 112, Nov. 2013.

[11] Y. Huang, Y. Fang, Z. Zhang, L. Zhu, and M. Sun, "Nanowire-supported plasmonic waveguide for remote excitation of surface- enhanced Raman scattering," *Light: Science and Applications*, vol. 3, no. 199, Aug. 2014.

[12] J.P. Kottmann and O. J. F. Martin, "Plasmon resonances of silver nanowires with a non- regular cross section," *Phys. Rev. B*, vol. 64, no. 235402, Nov. 2001.

[13] A. Yılmaz, B. Karaosmanoğlu, and Ö. Ergül, "Computational electromagnetic analysis of deformed nanowires using the multilevel fast multipole algorithm," *Sci. Rep.*, vol. 5, no. 8469, Feb. 2015.

[14] H. Aykut Şatana, B. Karaosmanoğlu, and Ö. Ergül, "A comparative study of nanowire arrays for maximum power transmission," in *Nanowires*, K. Maaz, Ed. InTech, 2017.

[15] J. Song, C.-C. Lu, and W. C. Chew, "Multilevel fast multipole algorithm for electromagnetic scattering by large complex objects," *IEEE Trans. Antennas Propag.*, vol. 45, no. 10, pp. 1488-1493, Oct. 1997.

[16] Ö. Ergül, "Solutions of large-scale electromagnetics problems involving dielectric objects with the parallel multilevel fast multipole algorithm," *J. Opt. Soc. Am. A.*, vol. 28, no. 11, pp. 2261-2268, Nov. 2011.

[17] B. Karaosmanoğlu, A. Yılmaz, and Ö. Ergül, "A comparative study of surface integral equations for accurate and efficient analysis of plasmonic structures," *in IEEE Transactions on Antennas and Propagation*, vol. 65, no. 6, pp. 3049e3057, June 2017.

[18] B. Karaosmanoğlu, A. Yılmaz, U. M. Gür, and Ö. Ergül, "Solutions of plasmonic structures using the multilevel fast multipole algorithm," *Special Issue on Challenges in RF and Microwave Defense Engineering, Int. J. RF Microwave Comput.-Aided. Eng.*, vol. 26, no. 4, pp. 335-341, May 2016.

[19] C. Önol, B. Karaosmanoğlu, and Ö. Ergül, "Efficient and accurate electromagnetic optimizations based on approximate forms of the multilevel fast multipole algorithm," *IEEE Antennas Wireless Propag. Lett.*, vol. 15, pp. 1113-1115, Apr. 2016.

[20] 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. Reyhanoğlu, Ed. InTech, 2017.

[21] P. B. Johnson and R. W. Christy, "Optical constants of the noble metals," *Phys. Rev. B*, vol. 6, no. 12, pp. 4370-4379, Dec. 1972.