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SOLBOX-08

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1. Introduction

Nanowires are popular components of nano-optical systems because they can be useful in many related applications [1], such as optical transmission [2-4], sub-wavelength imaging [5, 6], and energy harvesting [7]. These structures are usually made of silver (Ag) or gold (Au), which are active at optical frequencies with strong plasmonic responses and which provide the favorable characteristics of nanowires. For example, by using a transmission line involving an arrangement of nanowires, electromagnetic energy can be carried to distances long with respect to wavelength. As the technology in this area develops, nanowires with improved geometric properties [8] – such as regularity, cross-sectional preciseness, and surface smoothness – become available, further expanding their usage. Naturally, electromagnetic simulations of nanowires [9-11], especially using their three-dimensional full-wave models, are essential to studying and understanding these important structures, as well as to designing them. In this issue of Solution Box, an optimization problem involving a nanowire transmission line to be improved by a coupler is presented (SOLBOX-08). Specifically, a pair of nanowires with a sharp 90° bend, which leads to significant deteriorations in the power transmission capability due to reflections and diffractions, is considered. The purpose was to design an efficient coupler in a limited space around the corner, in order to improve the transmission as much as possible. In the sample solution that is also considered in this issue, cubic nanoparticles were used to reduce the reflections and to improve the power transmission. Starting from a full grid, the existence and absence of each nanocube was decided based on an optimization via genetic algorithms (GAs). The trials during the optimization were efficiently performed by using the Multilevel Fast Multipole Algorithm (MLFMA) [12, 13]. This has been designed for accurate analysis of plasmonic objects [14-16] without resorting to approximate and asymptotic techniques. Different numerical solutions, analysis methods, and optimization tools to design more efficient couplers, probably leading to better transmission capabilities, are welcome. We are also looking for alternative solutions to previous problems (SOLBOX-01 to SOLBOX-07), which can be found in earlier editions of this column. Please consider submitting your contributions to Ozgur Ergul (ozergul@metu.edu.tr).

2. Problems

2.1 Problem SOLBOX-08 (by A. Altınoklu and Ö. Ergül)

Figure 1 depicts the considered optical transmission line involving two Ag nanowires, as well as a general view

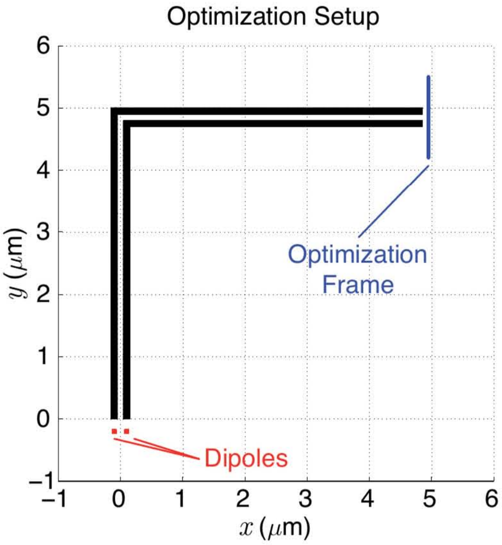

Figure 1. The optimization problem involving a pair of nanowires that are used to transmit electromagnetic energy. The nanowires were excited by a pair of Hertzian dipoles. There was a sharp 90° bend that reduced the transmission. A coupler needed to be designed and located at the corner such that the transmitted power was maximized as much as possible on the optimization frame.

of the optimization setup. The total length of the transmission line was 10 μm, while there was a sharp 90° bend at the middle (we note that the outer nanowire was slightly longer than the inner nanowire). Each nanowire had a 0.1 μm × 0.1 μm square cross section, while the distance between them was also set to 0.1 μm. The excitation was a pair of Hertzian dipoles (each with unit dipole moment), located at 0.2 μm distance from the nanowires. If the coordinate system in Figure 1 was considered (the transmission line was located on the *x*-*y* plane, while the first half was aligned in the *y* direction), the dipoles were oriented in the $\pm x$ directions to create a pattern with two peaks. The distance between the dipoles was also 0.2 μm. The frequency was selected as 250 THz, at which the relative complex permittivity (in the frequency domain) of Ag was approximately $-60.7546 + i4.3097$. The aim was to design an efficient coupler at the corner location (without any change in the nanowires and their positions), in order to improve the power transmission. The transmission was measured on a symmetrically located 1.3 μm × 1.3 μm frame, which had a distance of 0.1 μm from the output of the nanowires. Either the maximum power or the mean power on this frame could be maximized. The whole system, including nanowires and the coupler to be designed, were assumed to be in free space. In the reference solution given below, the coupler was restricted to occupying an area of 1.3 μm × 1.3 μm (on the *x*-*y* plane), while it did not increase the thickness of the system (0.1 μm in the *z* direction). A better coupler may be defined as one that improves the transmission while using the same size (1.3 μm × 1.3 μm × 0.1 μm) or one that provides similar transmission properties while being more compact.

3. Solution to Problem SOLBOX-08

3.1 Solution Summary

Solver type (e.g., noncommercial, commercial): Noncommercial research-based code developed at CEMMETU, Ankara, Turkey.

Solution core algorithm or method: Frequency-domain Multilevel Fast Multipole Algorithm (MLFMA).

Programming language or environment (if applicable): *MATLAB + MEX*

Computer properties and resources used:
2.5 GHz Intel Xeon E5-2680v3 processors (using 20 cores).

Total time required to produce the results shown (categories: < 1 sec, < 10 sec, < 1 min, < 10 min, < 1 hour, < 10 hours, < 1 day, < 10 days, > 10 days):
< 10 hours (per problem):

3.2 Short Description of the Numerical Solutions

The optimization problem SOLBOX-08 was solved by using in-house implementations of genetic algorithms (GAs) and the MLFMA in the frequency domain. The plasmonic problems using the given relative permittivity value $-60.7546 + i4.3097$ were formulated with the electric-magnetic-current combined-field integral equation (JMCFIE) [17, 18], and discretized with the Rao-Wilton-Glisson functions [19]. The number of unknowns was

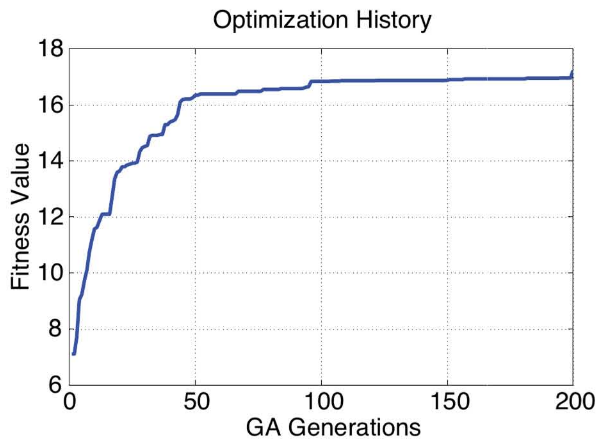

Figure 2. A solution to the optimization problem defined in SOLBOX-08. An in-house implementation of GAs was used to optimize the maximum power density on the optimization frame.

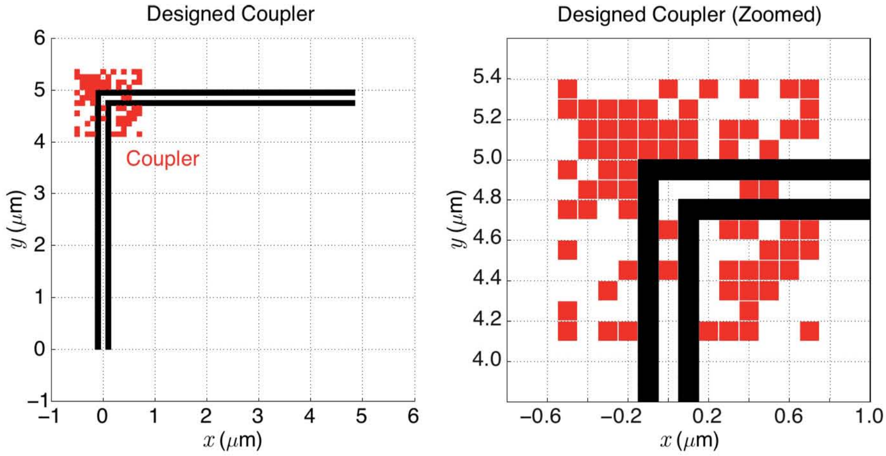

Figure 3. A solution of SOLBOX-08. A coupler that consisted of Ag nanocubes was designed to improve the power transmission through the sharp bend.

approximately 13,000 (for the full structure, i.e., the nanowires and the coupler). The coupler was designed by using 90 nm × 90 nm × 90 nm Ag nanocubes in a 1.3 μm × 1.3 μm region around the corner. Specifically, a grid of 13 × 13 elements (with a distance of 10 nm between each consecutive particle) was considered, leading to a total of 139 nanocubes in the full grid (omitting those overlapping with the nanowires). By representing each nanocube with a binary digit, each GA individual had a chromosome of 139 bits. For the optimization detailed below, the GA implementation was employed on a pool of 40 individuals for 200 generations. The optimization was hence completed by performing 8000 MLFMA simulations, omitting the identical individuals/trials that could be skipped based on a lookup table. In order to improve the convergence of the optimization, several new GA operations, such as success-based mutations and family elitism [20], were applied. In addition, the MLFMA was integrated into the GA implementation via dynamic accuracy control [21] in order to reduce the computational load. Finally, the iterative solutions via the MLFMA were performed by using an inner-outer scheme, where an approximate MLFMA was effectively used as a preconditioner [22].

3.3 Results

Figure 2 presents the optimization history for the setup described above. The fitness function was selected as the maximum power density on the optimization frame (1.3 μm × 1.3μm). It could be observed that the fitness value was dramatically increased, from 7.11 W/ms (first generation) to 17.22 W/ms (last generation). The curve with respect to the number of generations also demonstrated good convergence characteristics with a smooth saturation.

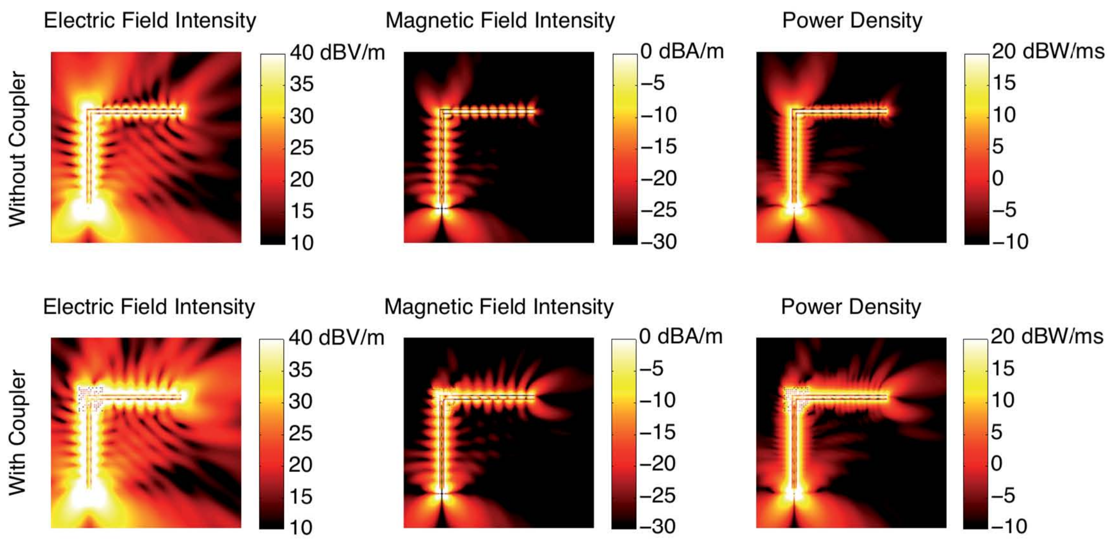

Figure 4. The electric-field intensity, magnetic-field intensity, and power density for the transmission line involving nanowires (SOLBOX-08). Improved transmission due to the designed coupler (see Figure 3) was visible as reduced diffraction at the corner and as increased intensity/density values at the output.

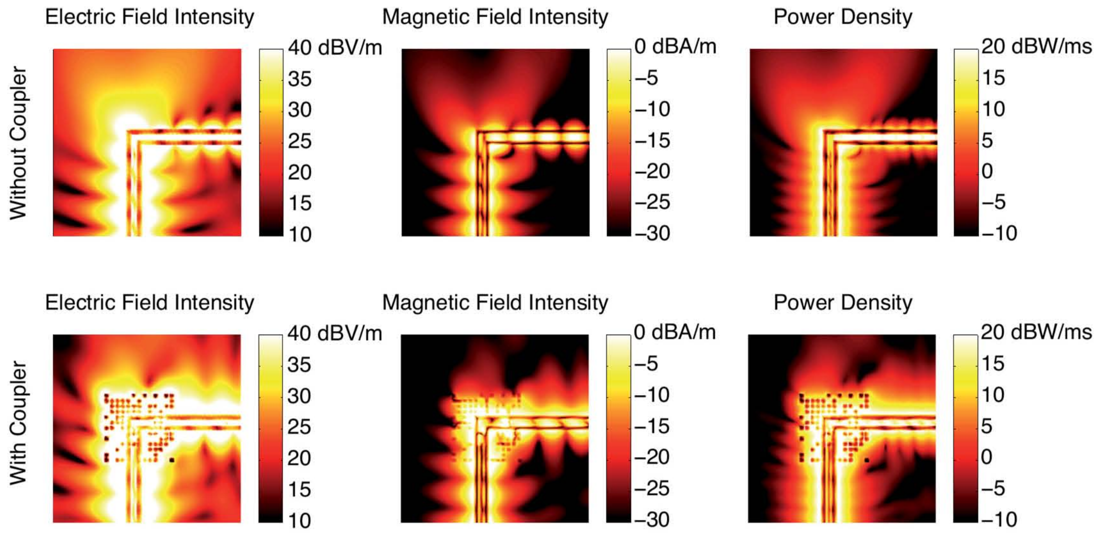

Figure 5. The electric-field intensity, magnetic-field intensity, and power density for the transmission line involving nanowires (SOLBOX-08). The zoomed plots show the intensity and density values in the coupler region (see Figure 3). The results without (top row) and with (bottom row) the coupler are compared.

Nevertheless, heuristic optimizations do not guarantee a global convergence, and the result (the coupler design) presented in this solution may not be the ultimate structure.

Figure 3 depicts the designed coupler, where the nanocubes are shown in addition to the nanowires. As illustrated in the zoomed plot, 70 out of 139 nanocubes were kept, to obtain approximately 17.22 W/ms mean power density. In comparison to the no-coupler case (with 6.70 W/ms maximum power density on the same frame), this corresponded to a 2.57-times enhancement. The enhancement in the mean power density was more significant (nearly nine times), i.e., from 0.50 W/ms (before optimization) to 4.48 W/ms (after optimization).

Figure 4 presents the electric-field intensity (V/m), magnetic-field intensity (A/m), and power density (W/ms), all with 30 dB dynamic range in the transverse plane. The improvement by the coupler was clearly visible in these plots. For example, investigating the power-density distribution, we observed that the diffracted waves in the corner region were reduced when the coupler was used. In addition, following the corner region, the power density along the nanowire surfaces in the second (horizontal) part of the transmission line seemed to be stronger when the coupler was used. Finally, the increased power density at the output of the nanowire system using the coupler was clearly seen. Similar observations could be made for the electric-field intensity and the magnetic-field intensity. Figure 5 presents zoomed plots where the intensity and density values are plotted further around the corner. We also observed the reduced diffraction and improved transmission in these plots. Finally, in Figure 6, we considered the intensity and density distributions on the output frames.

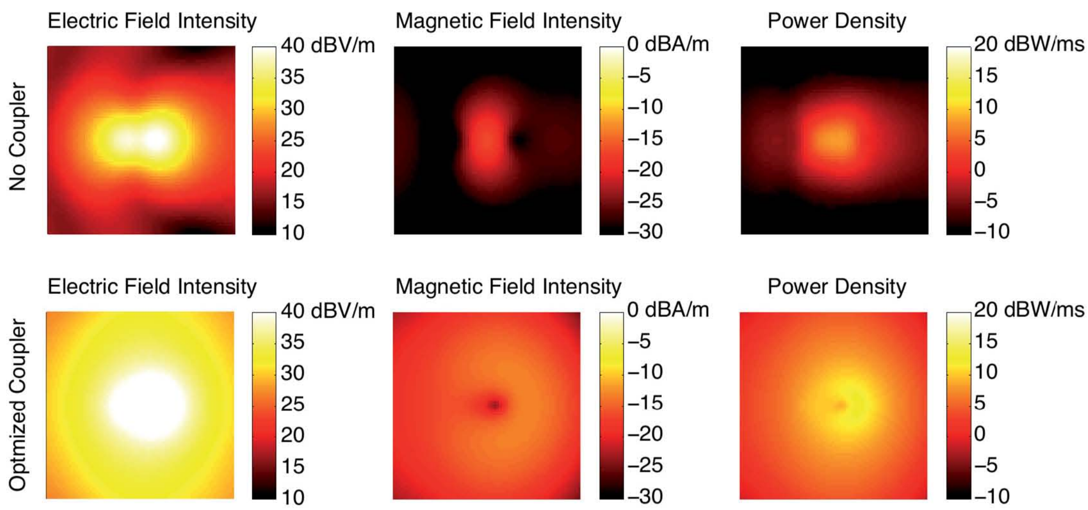

Figure 6. The electric-field intensity, magnetic-field intensity, and power density for the transmission line involving nanowires (SOLBOX-08). The intensity and density distributions were investigated on the output frame with and without the designed coupler (see Figure 3).

The positive effect of the coupler was clearly visible as significantly increased values at the output.

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