Supplementary Materials: Genetic-algorithm-aided ultra-broadband perfect absorbers using plasmonic metamaterials

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Abstract: Supplementary materials

1. Range of variation of the parameters for the Genetic Algorithm

We consider that the lateral periodicity P of the system can take values between 50 and 500 nm (by steps of 1 nm). The lateral dimension L_i of each stack of metal/dielectric layers can take values between 50 and 500 nm (by steps of 1 nm). The thickness t_i of each dielectric can take values between 50 and 250 nm (by steps of 1 nm). The subscripts i=1, 2 and 3 refer respectively to the stack at the apex, in the middle or at the bottom of each nanopyramid (Fig. 1). In order to obtain pyramidal structures, we require that the final solution satisfies $L_1 < L_2 < L_3 \leq P - 40$ nm, where 40 nm represents the minimal imposed safe distance between adjacent pyramids for insuring realistic fabrication. When optimizing structures made of three stacks of metal/dielectric layers, there are actually seven parameters to determine (P, L_1, t_1, L_2, t_2, L_3 and t_3), with a total of 13,936,405,106,594,025 possible parameter combinations to consider if the relaxed constraint $L_1 < L_2 < L_3 \leq P$ is actually enforced during the optimization.

2. Description of the Genetic Algorithm

Given n decision variables $x_i \in [x_i^{\min}, x_i^{\max}]$ to determine (within a precision Δx_i representative of experimental constrains on the fabrication of a device), the objective is to find the global maximum of an objective function $f = f(x_1, \ldots x_n)$. The variables x_i are encoded by sequences of binary digits (genes), which actually represent in the original Gray code the number of steps $(x_i - x_i^{\min})/\Delta x_i$ between $x_i^{\min}$ and x_i [1]. We refer by DNA to a complete set of n genes. We work with a population of n_{pop}=50 individuals. The initial population consists of random individuals. At each generation, we evaluate in parallel the fitness $f(x_1, \ldots x_n)$ of new individuals. We keep a record with all fitness evaluations in order to avoid any duplication of these evaluations. The population is sorted from the best individual to the worst. The worst n_{rand} individuals are replaced by random individuals in the next generation. We use $n_{\text{rand}} = 0.1 \times n_{\text{pop}} \times (1 - p)$, where $p = |s - 0.5|/0.5$ is a progress indicator and s is the genetic similarity (fraction of bits in the population whose value is identical to the best individual). The remaining part of the population ($N = n_{\text{pop}} - n_{\text{rand}}$ individuals) participate to the steps of selection, crossover and mutation.

The core operations of the Genetic Algorithm are the following. *Selection:* N parents are selected from a population of N individuals by a rank-based roulette wheel selection, noting that a given individual can be selected several times [1]. *Crossover:* For any pair of parents, we define two children for the next generation either (i) by a crossover operation (probability of 70%), or (ii) by a simple replication of the parents (probability of 30%). In the current version of our GA, the crossover operation can be a binary one-point crossover[1] between the DNA of the two parents [2] (probability p_{bin} of 0.8 initially) or a real-valued crossover[2] between the variables $\vec{x}$ represented by the two parents (probability of $1 - p_{\text{bin}}$). p_{bin} is adapted according to the success of these operators. *Mutation:* The children obtained by crossover are subjected to mutations. This operation consists of a random flipping of the binary digits of a DNA. The probability of individual bit flips is set to $m = 0.95/n_{\text{bits}}$, where n_{bits} is the number of bits in a DNA. In order to increase the diversity of the displacements generated by these mutations, we actually express the gene values in randomly-shifted versions of the original Gray code and apply the mutations to these encodings (see Appendix A of Ref. 3 for details). In the current version of our GA, mutations can be "isotropic" (in this case, the mutation operator is applied n times on a given DNA). The probability p_{iso} to apply isotropic mutations is set to 0.2 initially. This value is adapted according to the success of this operator.

In order to converge more rapidly to the final solution, we establish at each generation a quadratic approximation of the fitness in the close neighborhood of the best-so-far individual (this approximation is based on the data collected by the genetic algorithm). If the optimum of this approximation is within the specified boundaries, it replaces the last random individual scheduled for the next generation (see Appendix B of Ref. 3 for details). The data collected by the algorithm is also used to establish 2-D maps of the fitness, by using dedicated interpolation techniques. This is useful for monitoring the progress of the algorithm and for assessing the quality of the final solution.

The fitness of all individuals scheduled for the next generation is finally computed in parallel. The new population is sorted from the best individual to the worst. If the best individual of the new generation is not as good as the best individual of the previous generation, the elite of that previous generation replaces an individual chosen at random in the new generation. We repeat these different steps from generation to generation until a termination criterion is met.

3. Quality check of the optimization results based on the plane wave number

A final quality criterion is certainly the reliability of the presented results. In order to confirm the quality of our solutions, we increased the number of plane waves in the RCWA calculations to 21×21 (instead of 11×11 when running the GA). The results obtained are given in Tables 1 and 2 of the main text. The comparison between 11×11 PW and 21×21 PW in Table 1 reveals that the solutions selected on the basis of high η values and high robustness are also stable with respect to this numerical test (only slight deviations between $\eta_{11\times11\text{PW}}$ and $\eta_{21\times21\text{PW}}$). On the contrary, the solutions in Table 2 that were discarded, essentially because of the high sensitivity of η with respect to the geometrical parameters, turn out to be significantly affected by this increase of the number of plane waves used in the RCWA calculations (large deviations between $\eta_{11\times11\text{PW}}$ and $\eta_{21\times21\text{PW}}$). It proves that the solutions given in Table 2 were rightly discarded (they fail this last reliability criterion). The fact that solutions that sit on sharp optima are also solutions that require a higher number of plane waves for an accurate calculation is actually consistent. This observation suggests a simple criterion for testing the robustness of solutions (stability with

[1] In a binary one-point crossover, the first n_{cut} bits of the DNA of the children come from one parent. The remaining $n_{\text{bits}} - n_{\text{cut}}$ bits come from the other parent. The point n_{cut} at which the parents' DNA is exchanged is chosen randomly in the interval $[1, n_{\text{bits}} - 1]$.

[2] If $\vec{x}_1$ and $\vec{x}_2$ are the real variables represented by the two parents, the children obtained by a real crossover between these parents will represent a variable $\vec{x} = \vec{x}_1 + (2 * \text{rnd} - 0.5) \times (\vec{x}_2 - \vec{x}_1)$, where rnd is a random number uniformly distributed in [0,1].

respect to deviations of their geometrical parameters): testing the stability with respect to the number of plane waves used for the calculation. This approach does not require the calculation of 2-D maps. A single calculation based on an increased number of plane waves may be sufficient to get a clue !

References

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