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Published in:
Proceedings of SPIE - The International Society for Optical Engineering

DOI:
10.1117/12.3012796

Publication date:
2024

Document Version
Peer reviewed version

Link to publication

Citation for pulished version (HARVARD):
Mayer, A, Deparis, O & Lobet, M 2024, 'Optimization by a genetic algorithm of nanopyramidal broadband quasi-perfect absorbers with deeper insight into the stability of optimal solutions', *Proceedings of SPIE - The International Society for Optical Engineering*, vol. 13017, pp. 1301714. https://doi.org/10.1117/12.3012796

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Optimization by a genetic algorithm of nanopyramidal broadband quasi-perfect absorbers with deeper insight into the stability of optimal solutions

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ABSTRACT

We use a genetic algorithm to optimize periodic arrays of truncated square-based pyramids made of alternating stacks of metal/dielectric layers. The objective is to achieve broadband quasi-perfect absorption of normally incident radiations in the visible and near-infrared ranges (wavelengths comprised between 420 and 1600 nm). We compare the results one can obtain by considering one, two or three stacks of (i) Ni, Ti, Al or Cu for the metal, and (ii) poly(methyl methacrylate) (PMMA) for the dielectric. The parameters to determine for each metal/dielectric combination are (i) the period of the system, (ii) the lateral dimensions of each stack of metal/dielectric layers and (iii) the width of each dielectric layer. The Rigorous Coupled Waves Analysis (RCWA) is used to compute the absorptance spectrum of these different structures. The Genetic Algorithm is used to find the geometrical parameters that maximize the integrated absorptance. This approach provides stability maps with respect to the geometrical parameters, which leads to additional physical insight regarding practical implementation. The study shows that Ni/PMMA and Ti/PMMA provide high-quality solutions associated with broad optima (stability with respect to variations of the geometrical parameters). On the contrary, Al/PMMA and Cu/PMMA provide poor-quality solutions associated with sharp optima. We find an interesting correlation between the robustness of the solutions found by the genetic algorithm (stability with respect to variations of the geometrical parameters) and the stability of these solutions with respect to the number of plane waves used in the RCWA calculations.

Keywords: machine learning, genetic algorithm, optical engineering, optimization, metamaterial, broadband absorber, plasmon hybridization, nanopyramids

1. INTRODUCTION

Machine Learning has become a trendy paradigm in the physical sciences. Deep Learning in particular has given rise to impressive results in image recognition, language translation, neural style transfer, video games, self-driving cars, robotics and more recently the game-changer ChatGPT. Variational AutoEncoders[1] and Adversarial Generative Networks[2] have impressive data generation capacities. Physicists can certainly take advantage of the sophisticated algorithms developed by the machine learning community to solve their own problems.[3–7] The availability of open-source libraries to implement these machine learning algorithms makes it especially appealing.

Inverse design algorithms that implement the gradient descent method using automatic differentiation of the objective function with respect to the physical parameters of the problem are a beautiful illustration of machine learning algorithms being applied to the design of optical systems.[8–10] Evolutionary algorithms,[11] which include Particle Swarm Optimization[12–14] (PSO), Evolution Strategies[15,16] (ES) and Genetic Algorithms[17–19] (GA), are another class of machine-learning algorithms. These algorithms consider virtual populations of individuals that evolve according to rules inspired by the flow of birds (PSO) or by natural selection in biology (ES and GA). Evolutionary algorithms make it possible to determine the global optimum of complex problems in physics.

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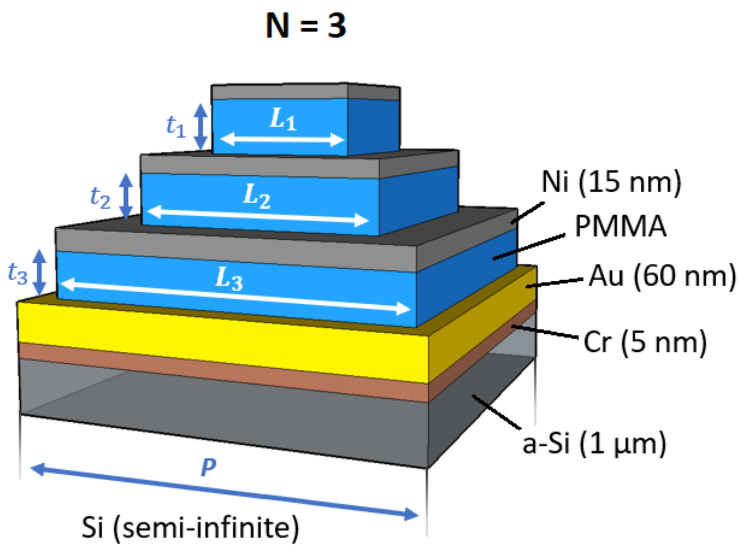

Figure 1. Square-based truncated pyramid made of N=3 stacks of Ni/PMMA layers. The support of the pyramid consists of uniform layers of Au (60 nm), Cr (5 nm) and a-Si (1 micron). We assume an infinite substrate of Si ($\varepsilon = 16$).

We will consider as particular application of evolutionary algorithms the design of broadband absorbers by metamaterials made of alternating stacks of metal/dielectric layers in truncated square-based pyramids. Metamaterials are generally made of a combination of dielectric and metallic elements, whose smart arrangement at a scale much shorter than their operating wavelength make it possible to control the flow of light in unprecedented ways.[20,21] Metamaterials that exploit the Mie resonances of dielectrics were also developed.[22] Since metals suffer from high losses in the visible, metamaterials contributed to the development of perfect absorbers that act either at specific wavelengths[23] or over extended wavelength ranges.[24–39]

Previous work by Lobet at al. has shown that plasmon hybridization in periodic arrays of truncated square-based pyramids made of twenty stacks of Au/Ge layers leads to an integrated absorptance of 98% of normally incident radiations over a 0.2-5.8 μm wavelength range.[40,41] This ultra-broadband absorption is essentially due to an efficient anti-reflection property of these pyramidal structures[42,43] and a well-designed coupling between the localized surface plasmons found at the metal/dielectric interfaces of each stack.[44–47] The structures determined in this work have stack dimensions that vary linearly along the vertical axis. Only three geometrical parameters had therefore to be optimized: the lateral periodicity P, the lateral dimension L and the height H of the nanopyramids. The fabrication of structures that consist of twenty alternating stacks of metal/dielectric layers is currently too demanding in terms of time and resources.

A second approach by Mayer and Lobet was to consider simplified structures that consist of only one, two or three stacks of metal/dielectric layers (see Fig. 1).[48–50] In contrast with the previous approach, each stack of metal/dielectric layers has specific and well-tailored dimensions (the lateral dimension L_i and the width t_i of the dielectric in each stack are adjustable parameters). This relaxation of the stack dimensions provides the extra degrees of freedom that are necessary to maintain high performances. The lateral periodicity P of the system remains an adjustable parameter. For a system made of N stacks of metal/dielectric layers, we have a total of $2N + 1$ parameters to determine. Our approach to this optimization problem was to use a home-made Genetic Algorithm (GA) coupled with the Rigorous Coupled Waves Analysis (RCWA) technique for the simulation of these optical devices.

This article presents results achieved by considering N=1, 2 or 3 stacks of Ni/PMMA, Ti/PMMA, Al/PMMA or Cu/PMMA, where PMMA stands for poly(methyl methacrylate). These systems are indeed representative of "good-quality" and "poor-quality" solutions one can obtain by optimizing this type of systems. High-quality solutions are associated in this context with (i) a high integrated absorptance over the considered wavelength range and (ii) a good robustness of this integrated absorptance when considering variations of the geometrical

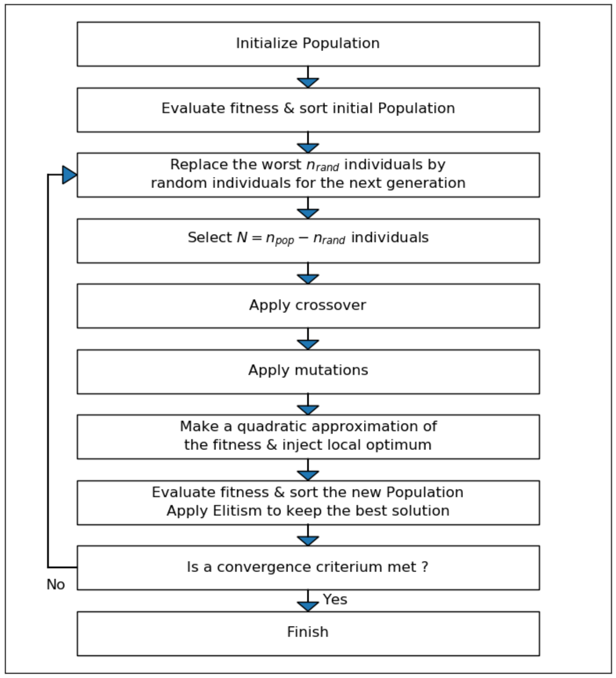

Figure 2. Workflow of the Genetic Algorithm.

parameters (the optimum found by the genetic algorithm should ideally be high and broad). Poor-quality solutions are associated with a lower integrated absorptance and/or a more pronounced sensitivity of this integrated absorptance on the geometrical parameters (the optimum found by the GA is low and/or sharp).

This article is organized as follows. Section 2 provides a description of the genetic algorithm used for these optimizations. Section 3 presents the results obtained when considering nanopyramids that consist of one, two or three stacks of Ni/PMMA, Ti/PMMA, Al/PMMA or Cu/PMMA. The discussion focusses essentially on numerical aspects. We point in particular an interesting correlation between the robustness of the solutions found by the genetic algorithm (stability with respect to variations of the geometrical parameters) and the stability of these solutions with respect to the number of plane waves used in the RCWA calculations. Section 4 finally concludes this work.

2. DESCRIPTION OF THE GENETIC ALGORITHM

The Genetic Algorithm used to address this optical engineering problem proceeds as follows (see workflow in Fig. 2 and Refs 48,49,51 for additional details). Given n decision variables $x_i \in [x_i^{\min}, x_i^{\max}]$ to determine within a precision Δx_i representative of experimental constrains, 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 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.[11] 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 as follows. *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.[11] *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* between the DNA of the two parents (probability p_{bin} of 0.8 initially) or a real-valued crossover† between the variables $\vec{x}$ represented by the two parents (probability of $1 - p_{\mathrm{bin}}$). p_{bin} is adapted according to the success of these operators at generating new elites. *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 $m = 0.95/n_{\mathrm{bits}}$, where n_{bits} is the number of bits in a DNA. In order to increase the diversity of the displacements generated by mutations, we actually express for this operation the gene values in randomly-shifted versions of the original Gray code and apply the mutations to these encodings (see Appendix A of Ref. 48 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. 48 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. OPTIMIZATION OF PYRAMIDAL STACKS OF METAL/DIELECTRIC LAYERS FOR THE DEVELOPMENT OF QUASI-PERFECT BROADBAND ABSORBERS

We consider as optical engineering application periodic arrays of square-based nanopyramids that consist of N=1, 2 or 3 stacks of metal/dielectric layers (see Fig. 1). The support of these pyramids consist of uniform layers of Au (60 nm), Cr (5 nm) and a-Si (1 micron). The role of the Au layer is actually to block the transmission of the incident radiations ($T(\lambda) \to 0$). The pyramidal shape of the structures considered reduce the reflection of these incident radiations ($R(\lambda) \to 0$). By controlling the plasmonic resonances in these structures, it is therefore possible to obtain an absorption $A(\lambda) = 1 - T(\lambda) - R(\lambda) \to 1$ for the wavelength λ of interest.

The geometrical parameters of the structures considered will be determined by the Genetic Algorithm. The objective of this parameter optimization is to maximize the integrated absorptance of normally incident radiations for wavelengths comprised between 420 and 1600 nm. The absorptance spectrum of the structures considered is obtained by a Rigorous Coupled Waves Analysis (RCWA) method.[52,53] This method solves Maxwell's equations numerically in laterally periodic systems. We use 11×11 plane waves for the application of the RCWA method when searching for optimal geometrical parameters with the Genetic Algorithm. Final solutions are checked by considering 21×21 plane waves in these RCWA calculations.

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

†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 $\vec{x} = \vec{x}_1 + (2 * \mathrm{rnd} - 0.5) \times (\vec{x}_2 - \vec{x}_1)$, where rnd is a random number uniformly distributed in [0,1].

Ni / PMMA

	L_1 (nm)	t_1 (nm)	L_2 (nm)	t_2 (nm)	L_3 (nm)	t_3 (nm)	P (nm)	$\eta_{11\times11\text{PW}}$	$\eta_{21\times21\text{PW}}$
N=1 stack	201	117	-	-	-	-	286	95.0%	93.8%
N=2 stacks	132	123	227	107	-	-	287	99.4%	99.0%
N=3 stacks	149	131	268	124	369	101	412	99.8%	99.3%

Ti / PMMA

	L_1 (nm)	t_1 (nm)	L_2 (nm)	t_2 (nm)	L_3 (nm)	t_3 (nm)	P (nm)	$\eta_{11\times11\text{PW}}$	$\eta_{21\times21\text{PW}}$
N=1 stack	368	134	-	-	-	-	491	89.3%	88.9%
N=2 stacks	175	117	306	127	-	-	336	98.6%	98.5%
N=3 stacks	161	125	302	126	451	113	491	99.4%	99.0%

Al / PMMA

	L_1 (nm)	t_1 (nm)	L_2 (nm)	t_2 (nm)	L_3 (nm)	t_3 (nm)	P (nm)	$\eta_{11\times11\text{PW}}$	$\eta_{21\times21\text{PW}}$
N=1 stack	221	151	-	-	-	-	491	89.2%	**63.8%**
N=2 stacks	187	108	263	58	-	-	415	97.9%	**81.0%**
N=3 stacks	129	112	208	110	294	97	465	98.7%	**83.6%**

Cu / PMMA

	L_1 (nm)	t_1 (nm)	L_2 (nm)	t_2 (nm)	L_3 (nm)	t_3 (nm)	P (nm)	$\eta_{11\times11\text{PW}}$	$\eta_{21\times21\text{PW}}$
N=1 stack	149	112	-	-	-	-	230	80.9%	**55.2%**
N=2 stacks	188	127	283	120	-	-	447	89.1%	**75.8%**
N=3 stacks	119	145	211	132	299	111	365	95.5%	**77.5%**

Table 1. Geometrical parameters and figure of merit η for optimal structures made of N=1, 2 or 3 stacks of Ni/PMMA, Ti/PMMA, Al/PMMA or Cu/PMMA (from top to bottom).

The figure of merit $f = \eta(P, L_1, t_1, \ldots L_N, t_N)$ considered by the Genetic Algorithm is defined by $\eta = \int_{\lambda_{\min}}^{\lambda_{\max}} A(\lambda) d\lambda \,/\, (\lambda_{\max} - \lambda_{\min})$, where $A(\lambda)$ refers to the absorptance of normally incident radiations at the wavelength λ, $\lambda_{\min}$=420 nm and $\lambda_{\max}$=1600 nm. $A(\lambda)$ is provided by RCWA calculations using 11×11 plane waves. This figure of merit depends on the lateral periodicity P of the system, on the lateral dimension L_i of each metal/dielectric stack and on the thickness t_i of each dielectric layer. We consider P values ranging between 50 and 500 nm by steps of 1 nm, L_i values ranging between 50 and 500 nm by steps of 1 nm and t_i values ranging between 50 and 250 nm by steps of 1 nm. The thickness of each metallic layer is 15 nm (fixed value). We enforce final solutions to respect the condition $L_1 < L_2 < L_3 < P - 40$ nm in order to obtain pyramidal structures with a minimal safe distance of 40 nm between adjacent structures.

The particular systems considered in this study consist of N=1, 2 or 3 stacks of Ni/PMMA, Ti/PMMA, Al/PMMA or Cu/PMMA, where PMMA stands for poly(methyl methacrylate). We use reported values for the refractive indices of these different materials.[54–56] The results of these optimizations are given in Table 1 and discussed with more details in Ref. 50. For each configuration, we provide the figure of merit η obtained with 11×11 and 21×21 plane waves in the RCWA calculations. The systems chosen for this article are actually illustrative of two classes of solutions one can obtain depending of the materials considered : (i) "good solutions" that have high η values and are robust with respect to variations of their geometrical parameters (broad optimum), and (ii) "poor solutions" that may have high η values but are excessively sensitive to variations of these parameters (sharp optimum). Ni/PMMA and Ti/PMMA turn out to belong to the first class of solutions, while Al/PMMA and Cu/PMMA belong to the second class.

The Genetic Algorithm can find indifferently broad or sharp optima. Broad optima are fortunately easier to detect, since they span larger regions of the parameter space. By running the Genetic Algorithm several times on the same problem, we increase our chance to detect a sharp optimum. The situation depends actually on the materials chosen. For a good choice of materials (Ni/PMMA or Ti/PMMA), good-quality solutions are rapidly detected and there is no need to run the genetic algorithm many times to increase η further. For a poor choice of materials (Al/PMMA or Cu/PMMA), the fitness landscape seems more torturous. Several runs of the genetic algorithm are necessary to find solutions associated with high η values, but these solutions are more likely to be

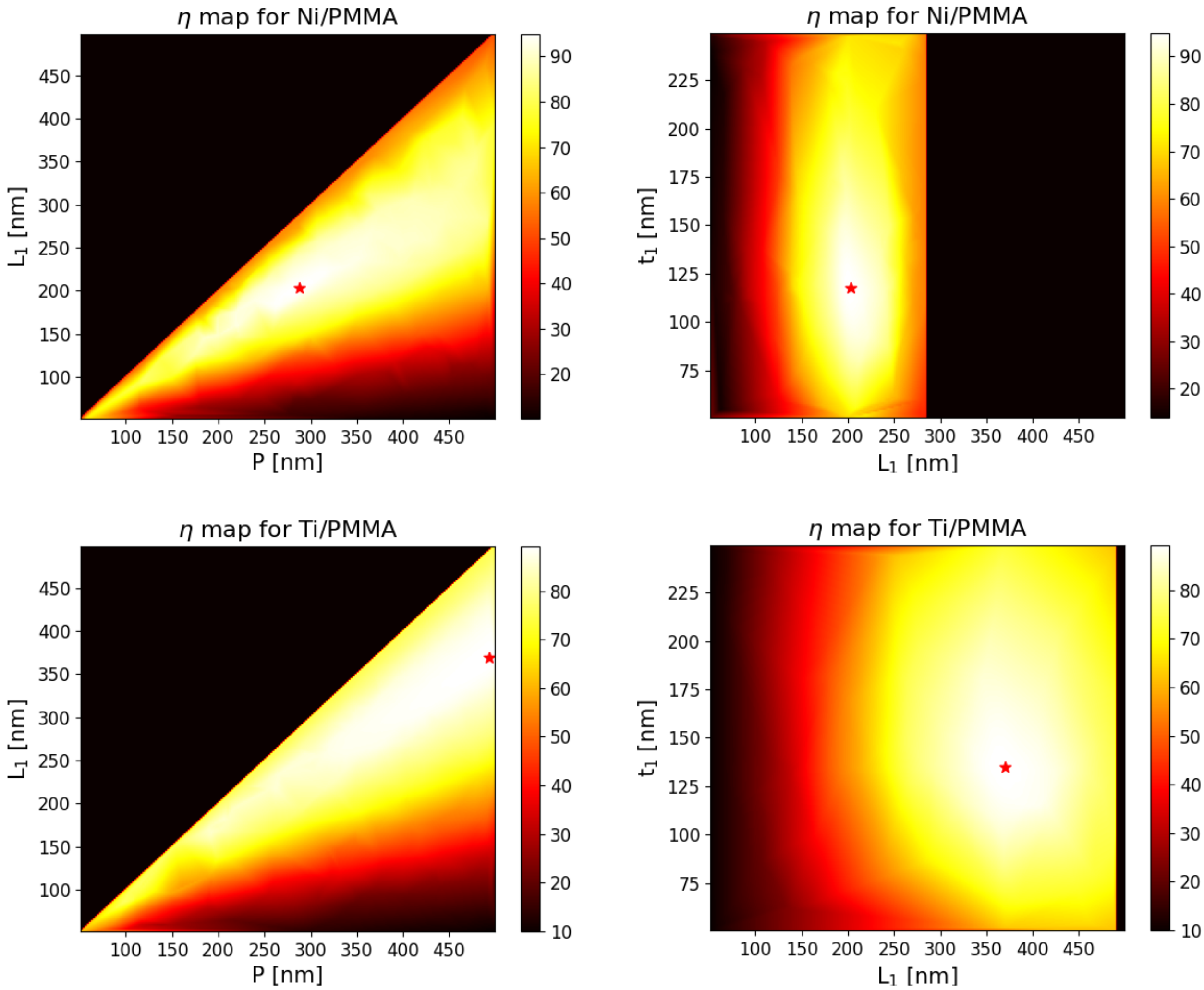

Figure 3. Maps obtained by a linear interpolation of the data collected by the genetic algorithm in the (P, L_1) and (L_1, t_1) planes that pass through the final solution established by the algorithm (indicated by a star). Top: optimization of 1 stack of Ni/PMMA (global optimum at P=286 nm, L_1=201 nm and t_1=117 nm). Bottom: optimization of 1 stack of Ti/PMMA (global optimum at P=491 nm, L_1=368 nm and t_1=134 nm).

sharp optima. These solutions, which exhibit an excessive sensitivity on their geometrical parameters, are not suited for practical applications.

By using interpolation techniques, the data collected by the Genetic Algorithm can be used to establish 2-D maps of the fitness (integrated absorptance η). These maps correspond to interpolated fitness values in planes that cross the n-dimensional point associated with the final solution. They make it possible to assess the quality of the solution established by the Genetic Algorithm (broad vs sharp optimum). Examples are provided in Figs 3, where we present 2-D maps of the fitness for N=1 stack of Ni/PMMA or Ti/PMMA (broad optimum). In Fig. 4, we present 2-D maps of the fitness for N=1 stack of Al/PMMA or Cu/PMMA (sharp optimum). It is the examination of these maps that guided our choice in previous work to present or not solutions established by the GA.

When running the genetic algorithm to find optimal geometrical parameters, 11×11 plane waves are used in the RCWA calculations. This setting makes it possible to have simulations that are reasonably accurate and fast (15 minutes per simulation on average). To check the reliability of the final solutions established by the GA,

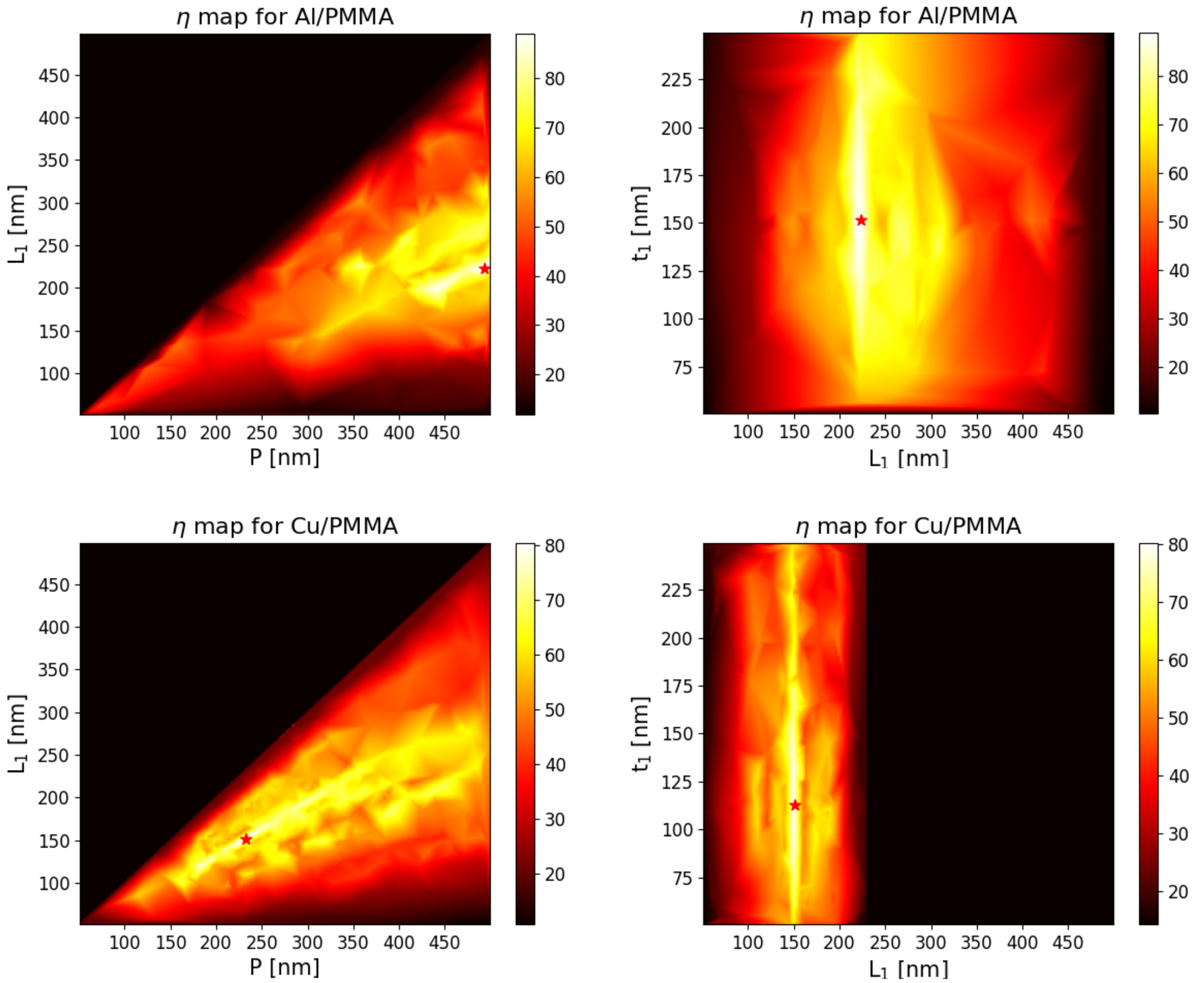

Figure 4. Maps obtained by a linear interpolation of the data collected by the genetic algorithm in the (P, L_1) and (L_1, t_1) planes that pass through the final solution established by the algorithm (indicated by a star). Top: optimization of 1 stack of Al/PMMA (global optimum at P=491 nm, L_1=221 nm and t_1=151 nm). Bottom: optimization of 1 stack of Cu/PMMA (global optimum at P=230 nm, L_1=149 nm and t_1=112 nm).

we increased the number of plane waves in the RCWA calculations to 21×21. The comparison between the η values obtained with 11×11 and 21×21 plane waves is presented in Table 1. The "good solutions" associated with a broad optimum turn out to be also robust with respect of this increase in the number of plane waves used for the RCWA calculations. On the contrary, the "poor solutions" associated with a sharp optimum turn out to be significantly affected by this increase of the number of plane waves. This observation is quite interesting. It suggests that increasing the number of plane waves in the RCWA calculations (here going from 11×11 to 21×21 plane waves) may provide insight into the geometrical stability of solutions established by the GA. Solutions that are stable with respect to this numerical check are actually those associated with a broad optimum (as determined by establishing interpolated 2-D maps of the fitness). Solutions that are unstable with respect to this numerical check turn out to be also solutions associated with a sharp optimum. This observation may finally comfort the use of a reasonable number of plane waves for optimization problems where broad optima are of course desired.

4. CONCLUSIONS

We applied a Genetic Algorithm to the study of broadband absorbers that consist of laterally periodic square-based pyramids made of one, two or three stacks of metal/dielectric layers. The objective was to maximize the integrated absorptance for normally incident radiations with wavelengths comprised between 420 and 1600 nm. The study shows that Ni/PMMA and Ti/PMMA provide high-quality solutions associated with a broad optimum (as determined by the examination of interpolated 2-D maps of the fitness). On the contrary, Al/PMMA and Cu/PMMA provide poor-quality solutions associated with sharp optima. For practical applications, a broad optimum is desired since it leads to higher robustness with respect to deviations of the geometrical parameters. Interestingly, the geometrical stability of the solutions established by the GA seems to be revealed by a simple numerical test that consists in increasing the number of plane waves used in the RCWA calculations. High-quality solutions that are stable with respect to deviations in their geometrical parameters turn out to be also stable with respect to the number of plane waves used in the RCWA calculations. This comfort the use of a reasonable number of plane waves in optimization problems where broad optima are desired.

ACKNOWLEDGMENTS

A.M. and M.L. are funded by the Fund for Scientific Research (F.R.S.-FNRS) of Belgium. A.M. is member of NaXys, Namur Institute for Complex Systems, University of Namur, Belgium. This research used resources of the "Plateforme Technologique de Calcul Intensif (PTCI)" located at the University of Namur, Belgium, which is supported by the F.R.S.-FNRS under the convention No. 2.5020.11. The PTCI is member of the "Consortium des Equipements de Calcul Intensif (CECI)". The present research also benefited from computational resources made available on the Tier-1 supercomputer of the Fédération Wallonie-Bruxelles, infrastructure funded by the Walloon Region under the grant agreement No. 1117545.

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