

Experimentally-implemented genetic algorithm (Exp-GA): toward fully optimal photovoltaics

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Abstract: The geometry and dimension design is the most critical part for the success in nano-phonic devices. The choices of the geometrical parameters dramatically affect the device performance. Most of the time, simulation is conducted to locate the suitable geometry, but in many cases simulation can be ineffective. The most pronounced examples are large-area randomized patterns for solar cells, light emitting diode (LED), and thermophotovoltaics (TPV). The large random pattern is nearly impossible to calculate and optimize due to the extended CPU runtime and the memory limitation. Other scenarios that numerical simulations become ineffective include three-dimensional complex structures with anisotropic dielectric response. This leads to extended simulation time especially for the repeated runs during its geometry optimization. In this paper, we show that by incorporating genetic algorithm (GA) into real-world experiments, shortened trial-and-error time can be achieved. More importantly, this scheme can be used for many photonic design problems that are unsuitable for simulation-based optimizations. Moreover, the experimentally implemented genetic algorithm (Exp-GA) has the additional advantage that the resultant objective value is a real one rather than a theoretical one. This prevents the gaps between the modeling and the fabrication due to the process variation or inaccurate numerical models. Using TPV emitters as an example, 22% enhancement in the mean objective value is achieved.

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1. Introduction

In recent years, nano-photonics has been emerged to be a very promising field with diverse applications in optical communication [1–3], optoelectronics [4–9], biomedicine [10], optical computing and nano-circuitry [11–14], etc. The key to its success is the geometrical design and optimization, in order for the light to propagate in a designed way through photonic cavities [15], photonic crystals [16, 17], metamaterials [18, 19], cloaking devices [19], solar cells [4, 5, 16, 20–27], etc. Most of the time, the geometrical parameters are selected by using numerical simulations and optimization algorithms. Nonetheless, this conventional methodology can be quite ineffective in many cases. The most obvious case is the random pattern design in green electronics. The random patterns are of interest for light emitting diodes (LED), solar cells, and the absorbers or the emitters in thermophotovoltaics (TPV). Because the three-dimensional(3D) fully vectorized solutions for a large random structure is numerically very difficult, the attempt to date is mostly limited to quasi-random scenario [6, 21, 28–32]. Other examples where numerical-based optimizations can be ineffective include 3D complex structures with anisotropic dielectric response and coupled electro-optical simulations. A coupled solution for the drift-diffusion model and the Maxwell's equations is necessary in order to achieve a more accurate modeling for optoelectronics [33, 34]. Nonetheless, this is extremely time-consuming and inadequate for repeated runs using an optimization algorithm. While the carrier transport, injection, and recombination are also critical aspects affecting the optoelectronic device performance, coupled simulation of light trapping and electrical characteristics usually takes several hours for even a single simulation run, using finite difference time domain (FDTD) and drift-diffusion modeling. This prevents the possibility of iterative or algorithm-based numerical optimizations [21, 35–37].

The application of a GA to a problem in which the fitness is not a calculated quantity can be referred to earlier literature [38], in which subjective evolution by human decision is used to facilitate optimization progress. In this work, we propose a new method to tackle the problems that are intrinsically very difficult as far as the numerical simulations and optimizations are concerned. The experimental implemented genetic algorithm (Exp-GA) is introduced in the following sections. By implementing the genetic algorithm into real-world semiconductor processing, the large random structure can now be designed. It should be emphasized that the Exp-GA requires no numerical models, and it generates new candidate geometries for high-performance devices by solely experiments. This prevents the drawbacks of inaccurate modeling, the gaps between simulation and real devices, and the unmanageably long CPU runtime. The proposed method essentially shortens the trial-error time compared to brutally fabricating an excessive number of samples using clean room facility. It should be emphasized that the method is quite different from the previous attempt of applying genetic algorithm to semiconductor processing since all of the previous methods require numerical semiconductor process models to predict the result, which is less promising for a complex problem such as nano-photonics light trapping. Additionally, the optimized value from Exp-

GA is a real one. This eliminates the drawbacks that the device performance, after semiconductor process, can deviate significantly from the simulated ones when numerical optimization is employed. Using simulation to predict and to optimize the photonic devices inevitably leads to the discrepancy between modeling and experiment. We should also point out that although the experimental genetic algorithm (Exp-GA) has several advantages over conventional simulation-based GA, the cost of Exp-GA is inevitably higher especially for a large number of individuals in one generation.

The implementation of GA is along the line of reference [37] using Matlab coding. The GA is implemented using binary value representation with 4-bit precision for an optimization variable. Therefore, the total length of an individual chromosome is $L_{\text{ind}} = 101 \times 4 = 404$. Single point crossover is used with crossover rate of 0.7. The mutation rate is $0.7/L_{\text{ind}}$, where L_{ind} is the length of the binary representation of the individual chromosome. The elitist strategy is in effect, and therefore the best individual is retained when GA transits from the current generation to the next generation.

For the optimization problem of a 3D 10×10 random pattern for TPV, the simulation-based optimization is essentially quite difficult to implement. Rigorously coupled wave analysis (RCWA) cannot be used because the convergence is very poor for a random metal-dielectric structure with period comparable or larger than the wavelength. This leads to the inaccuracy in the computational results. Using the finite difference time domain (FDTD) for iteratively optimizing such a random 3D metal-dielectric structure will lead to unmanageable CPU and memory requirement. The parallelization can reduce the computation time but it is still under several practical obstacles, and this is the reason that all of the computational efforts on designing random optical patterns for PV are still limited to quasi-random scenario [6, 20, 21, 28–32]. In most clusters, the memory amount available for each node is fixed, and it is less than sufficient for 3D FDTD simulations of random structures. The Exp-GA can be useful when computational approach becomes time-consuming. It should be emphasized that the GA optimization flow is the same for both the computation-based and experiment-based optimizations.

Although TPV is used as an example in this paper, in the case of solar cells or optoelectronics, Exp-GA can be more advantageous. This is because the coupled electrical-optical simulation is very time-consuming, and it is nearly impossible to fit it into computational GA. Coupled simulation of light trapping and electrical characteristics usually takes several hours for even a single simulation run, using finite difference time domain (FDTD) and drift-diffusion modeling. This is the reason that in our previous work or similar works from other groups, only optics is considered when conducting computational GA optimization. The most pronounced weak point of Exp-GA is the cost. Nonetheless, for product development, this will not be significant since the final optimized pattern can be used indefinitely. For academia and research-oriented work, Exp-GA can be quite cost intensive.

2. The experimental procedure in experimental genetic algorithm (Exp-GA)

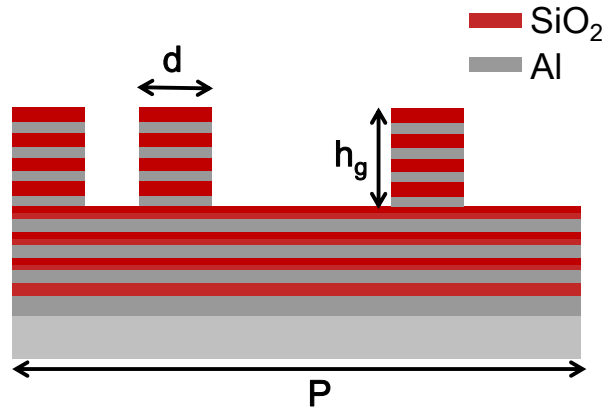


Fig. 1. The side-view of the thermophotovoltaic emitter using HMM metamaterials with a large binary pattern. The pattern is to be optimized by experimental-GA. h_g is the etching depth, and d is the length of 1 bit. P is the period of the large random pattern. While P should be made as large as possible to maximize the searching space during optimization and achieve true fully randomized nanostructures, the upper limit of P is usually constrained by the computational resources. Exp-GA is thus necessary to overcome the computational limitation.

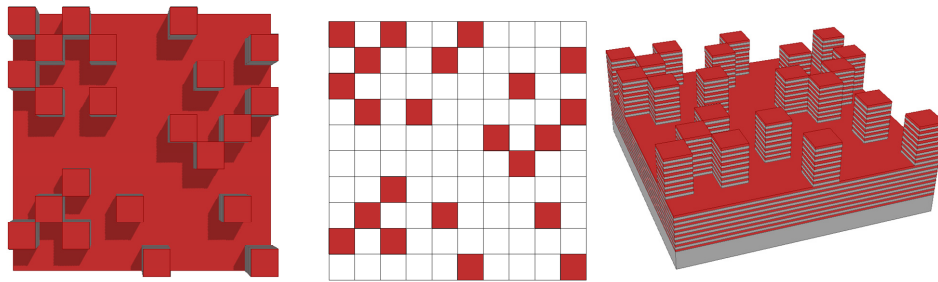


Fig. 2. (Left) the top-view of the hyperbolic metamaterial (HMM) stacks, (center) the binary pattern bit mask for a large-area random pattern, and (right) the three-dimensional (3D) view of the HMM stacks.

In this demonstration, the TPV emitter stack consisting of hyperbolic metamaterials is used as an example to illustrate the effectiveness of the Exp-GA in a complex nano-photonics optimization problem. The device is illustrated in Figs. 1 and 2. The alternating aluminum (Al) and silicon dioxide (SiO_2) are sequentially deposited to form a hyperbolic metamaterial (HMM) stack. The thickness of each Al and SiO_2 layer is 27nm and 18nm respectively. The straight-sidewall cavity is formed by using e-beam lithography and reactive ion etching (RIE). The pattern design is achieved by dividing a $2\mu\text{m} \times 2\mu\text{m}$ area into 10×10 squares with 200nm side length. The 10×10 binary pattern is then optimized by Exp-GA to determine the most proper topology for the straight-sidewall cavity-resonant type HMM PMAs. The etching depth is also included in the optimization since it critically affects the guided mode excitations.

The thermophotovoltaics (TPV) [39–45] is recently emerging as a promising alternative to the conventional photovoltaics (PV) due to its higher ultimate efficiency. The absorber/emitter/filter set-ups in a TPV system effectively reduce the thermalization loss in the conventional PV diodes. In order to achieve high efficiency, the broadband and high solar irradiance absorption is the key to achieving the ultimate Carnot efficiency of 83% in TPV devices. Unlike conventional solar cells, the broadband mode excitation is indeed possible for

TPV absorbers or emitters by using hyperbolic metamaterials (HMM). In conventional solar cells, quasi-guided mode excitations above the light cone are utilized for enhanced absorbance. Nonetheless, the discrete nature of the quasi-guided mode excitations leads to the difficulty in achieving broadband mode excitations. As a result, the resonance strength and the resonance bandwidth are mostly a trade-off in the conventional solar cells. On the other hand, in a TPV emitter metallic absorption can be employed for solar energy conversion, and this makes significant difference from conventional PV diodes. In this case, the photonic density of state (PDOS) can be altered effectively by using metal-dielectric interlacing, and the strong broadband mode excitation can be achieved provided proper pattern design is conducted.

Genetic Algorithm process

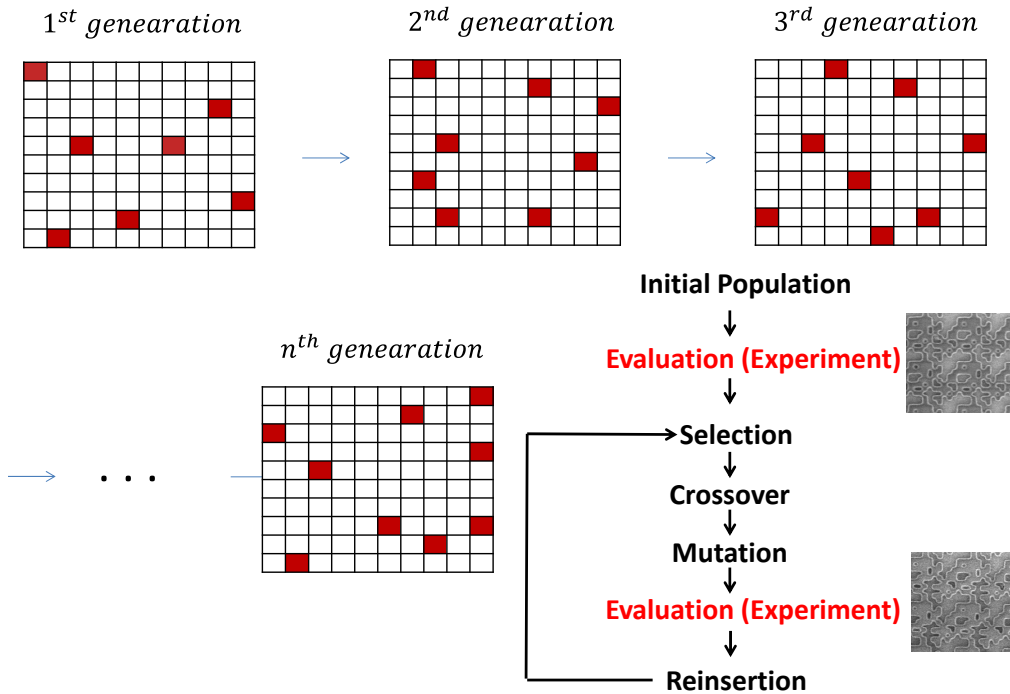


Fig. 3. Illustration of the Exp-GA process. The binary bit mask is adjusted in each generation to achieve higher broadband absorbance for photovoltaic applications. The flow chart clearly shows the difference between Exp-GA and conventional computational GA. The real experiment is used to evaluate the objective function in optimization in the case of Exp-GA. This overcomes the computational limitation of a large-area random pattern design. This also eliminates the discrepancy between experiment and simulation due to the problems of model inaccuracy or process deviations. No numerical models are needed.

Previously, tapered HMM is shown to have very broadband high absorption by Fang et al. [18], which opens an entirely new opportunity for TPVs. The HMM emitters/absorbers break the limitation imposed by the discrete nature of quasi-guided mode excitations in conventional photovoltaics. Nevertheless, a slight drawback for a tapered HMM is the difficulty in scaling it for large-area applications.

The difficulty comes from the fact that a tapered nanophotonic structure is difficult to fabricate using regular lithography techniques such as photolithography, e-beam lithography, or nano-imprint lithography (NIL) that is the most promising for large-area TPV [46]. The self-assembled-monolayer (SAM) of metallic nanoparticles has been proposed as an etching mask for fabricating ultra-long tapered semiconductor nanotips by Chen et al. [47]. This

results in a decent array of tapered silicon nanotips without the need for photolithography. Nonetheless, the metallic nanoparticle mask methodology may not be used for HMM etching because a metallic material also exists in a HMM stack. Focused ion beam lithography (FIB) has been used successfully for writing a tapered HMM pattern in the recent work of Gan et al. [48], but the writing speed of FIB may limit its feasibility for large-area TPVs. As a result, in this work we choose a non-tapered HMM as an example for Exp-GA. In the case of using non-tapered nano-structures, pattern design becomes critical for a broadband high absorption by using tailored photonic density of states (PDOS).

Using simulation-based optimization can be effective only if the pattern is small and thus computationally manageable. While large-scale pattern design or patterns of randomized nature is of interest for solar cell light trapping, TPV absorbers and emitters, and many other optics applications, numerical simulation becomes impractical for this purpose. The method of experiment-based genetic algorithm, seamlessly incorporated into semiconductor process, is illustrated in Fig. 3. The binary patterns are evolving through generations during the experiment. It is worth mention that the additional advantage of Exp-GA is that the process deviation can be automatically taken into account. This is not achievable in a numerical modeling. Moreover, Exp-GA does not require any theoretical, empirical, or semi-empirical models since it is totally experiment-based. This eliminates the need for developing a complex mathematical model description for a physical process, and this also eliminates the model inaccuracy. The adjustment accomplished by GA in the experiment is the gradual re-shaping of the patterns to provide the highest broadband absorption using HMM. It should be emphasized that the pattern here is $2\mu\text{m}$ in period for demonstration, and even larger pattern can be designed by Exp-GA without any difficulty. This is valuable for both conventional PV and TPV. Increasing the pattern size increases the searching space and can result in better solutions. The procedure of the GA is illustrated by the flow chart in Fig. 3. The primary steps in Exp-GA are similar to a regular computational GA, which are selection, recombination, mutation, and reinsertion. The difference is that now the evaluation of the objective function, which is the key steps in all optimization algorithms, is by experiment.

3. An Exp-GA optimization example: pattern-designed thermophotovoltaic (TPV) emitters

In this section, we demonstrate the effectiveness of Exp-GA using HMM metamaterial scalable for large-area TPV applications. The process flow for TPV emitters is illustrated in Fig. 4. In Fig. 5, the scanning electron microscope (SEM) images are shown for the fabricated samples at different generations during evolution. The nanostructured binary patterns are formed on the HMMs, in order to boost the absorbance by tailored photonic bandstructures. Leica e-beam lithography system is employed here to define the binary patterns. In fact, electron beam (e-beam) lithography is used only for illustration purpose. Nano-imprint lithography (NIL) can be used afterward to reduce the cost for large-area TPV [46]. NEB-22 from Sumitomo ChemicalTM is used as the e-beam resist. The resolution of NEB-22 is around 100nm and, therefore, the exposed and etched patterns can deviate to some extent, compared to the mask layout patterns. This aspect also reflects the power of Exp-GA since the process deviation is automatically taken into account in the experiment-based optimization. After exposure, inductive coupled (ICP) reactive ion etching (RIE) is employed for plasma dry etching. Cl_2 is used for Al etching, and CHF_3 is used for SiO_2 etching. The etching depth (t_{etch}) and the 10×10 binary pattern bits are the independent variables during Exp-GA optimization. As a result, the total number of variables is $N_{\text{opt}} = 10 \times 10 + 1 = 101$.

Process flow, Cross-section view

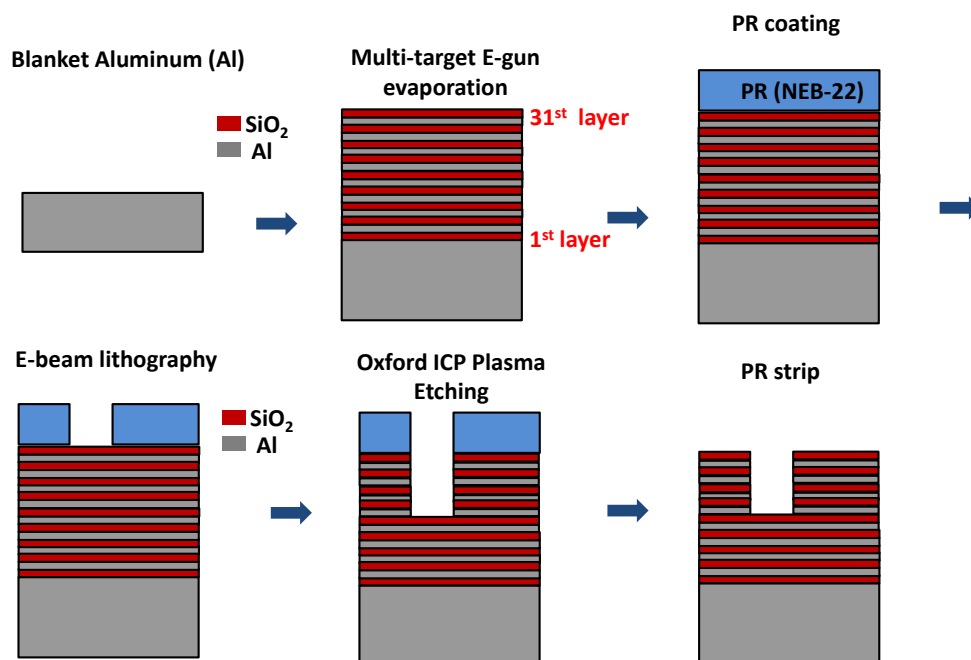


Fig. 4. The process flow of the fabricated HMM stack with a broadband resonant cavity. The straight-sidewall nature is beneficial for large-area TPV applications. The hyperbolic metamaterial is formed by alternating layers of aluminum (Al) and silicon dioxide (SiO_2). Noble metals such as Ag, Au, Pt are not necessary for the HMM here. The photonic density of state (PDOS) is significantly boosted by the unbounded hyperbolic dispersion of HMM.

Figure 6 shows the spectral absorbance plots for different generations. In this prototype demonstration, only 5 individuals are used in one generation, which is significantly less than what is sufficient for $N_{\text{opt}} = 101$ variables. Nonetheless, the effectiveness of Exp-GA is still quite obvious. The initial first three generations are conducted in this study, and the continued run for more generations are expected to increase the objective values toward saturation. To achieve a more pronounced improvement, increasing the number of individuals in one generation is essential together with running for more generations. Therefore, more individuals in one generation and more generations in one optimization run are necessary for a better optimized solution. The objective value is defined as the averaged absorbance from $\lambda = 1\mu\text{m}$ to $\lambda = 2\mu\text{m}$ in this study. The objective function is chosen to be the broadband absorbance from $1\mu\text{m}$ to $2\mu\text{m}$ for an illustrative purpose. For a specific TPV application, the broadband absorbance range has to be tailored specifically according to the solar concentration and the absorber/emitter operating temperature. In more recent designs for TPV absorbers and emitters, the selective spectral absorption and emission are desired in some cases, to minimize the re-emission loss and to eliminate the need for a filter. The Exp-GA method can certainly be fitted into these purposes easily, as long as the objective function is re-defined according to the specific need of the emitter or the absorber in a TPV system. In Fig. 6, the averaged absorbance is 0.16 for the worst case individual and 0.55 for the best case individual during the optimization. This is a >3 folds enhancement by Exp-GA. Figure 7 shows the statistics for the optimization process. In Fig. 7, the mean objective value from generation 1 to generation 3 increases from 0.36 to 0.44, a 22.2% improvement. The maximum objective value increases from 0.5068 to 0.5551, a 9.53% improvement. GA is normally progressed quite fast in the first few generations, and gradually becomes saturated when more and more generations are conducted. This is because the diversity of the individuals in a generation is higher in the

initial stage of a GA run. When more generations are conducted, the individuals become more and more similar to each other, and the improvement in the objective values will thus be less pronounced. The number of required generations for achieving saturation depends on the number of individuals used in the GA run. In the case of only 5 individuals with elitist strategy, the saturation will be quite fast.

Based on this statistics, it is clear that Exp-GA is very effective and suitable for locating the optimal random pattern for thermo-photovoltaics or photovoltaics. The enhanced absorption is attributed to properly tailored photonic bandstructures at the desired wavelength range. The photonic bandstructures in turn affect the effective permittivity and the absorption coefficient. In the case of HMM stacks, the alternating layers of metal-dielectric result in an unbounded hyperbolic dispersion. Nonetheless, without properly tailored geometry, the absorption cannot be boosted even with the unbounded PDOS. In the case of photovoltaics, the random reflectors are of even greater interest. The Lambertian light trapping has been shown to be the most effective and there is a $4n^2$ Yablonovitch limit. The compromised mode excitation of randomized structures can potentially provide broadband absorption enhancement in conventional solar cells. This is distinctly different from the high-Q well-defined resonances observed in many periodic diffractive structures.

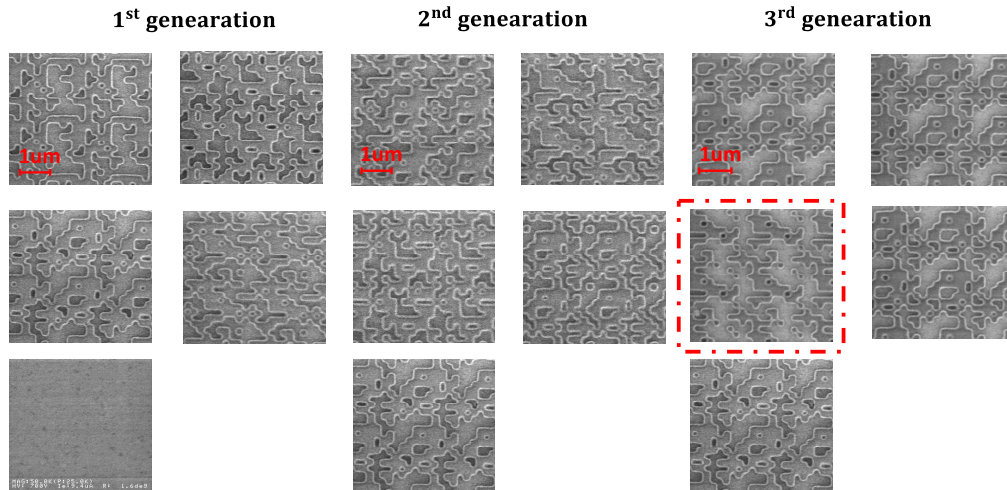


Fig. 5. The evolution of the binary bit mask during the optimization using Exp-GA. The optimal individual is marked by a dashed red box. The etching depth for this optimal individual is $t_{\text{etch}} = 315\text{nm}$.

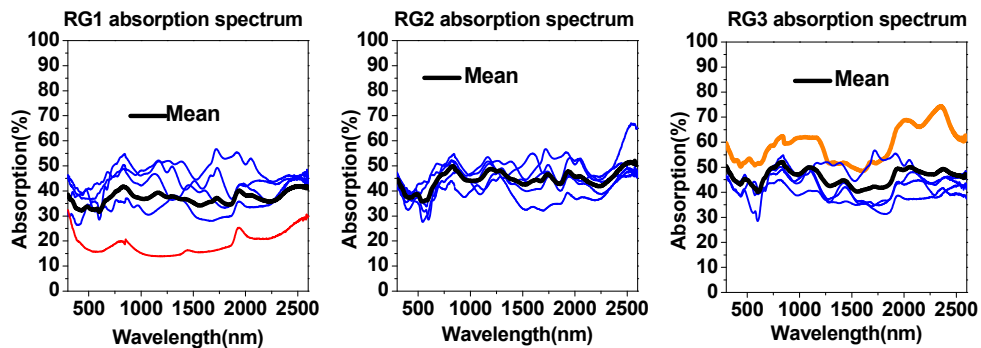


Fig. 6. The evolution of the spectral absorbance in Exp-GA. The first three generation is conducted in this study. The red line is the worst case individual during this optimization. The yellow line is the best case individual during this optimization. The black line is the average of the 5 individuals in one generation.

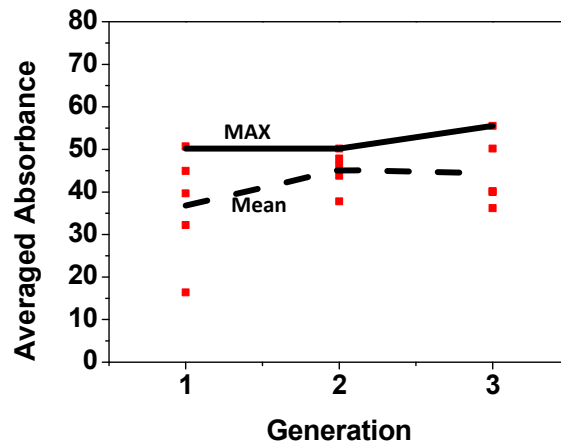


Fig. 7. The statistics of Exp-GA for the first three generations. The objective value in this optimization is the averaged absorbance from $\lambda = 1\mu\text{m}$ to $\lambda = 2\mu\text{m}$. The mean and the maxima of the objective values in each generation are plotted using the dashed and the solid black line. The scattered red dots are the objective values of the individuals in each generation.

4. Conclusion

We proposed a new Exp-GA methodology which is promising for a wide range of problems in nano-photonics. An initial experimental demonstration using an insufficient number of individuals already shows the effectiveness of Exp-GA and its potential in nano-photonics light trapping problems. The TPV emitter using a hyperbolic metamaterial (HMM) stack is used here as an example for Exp-GA. We observe a 22% relative enhancement in the broadband optical absorbance in the first 3 generations. Increasing the individual number in one generation and running for more generations will indefinitely further boost the averaged absorbance values. We believe the newly proposed Exp-GA is the most versatile method for nano-photonics and optoelectronics optimization problems. It requires no numerical models and equations, predicts true experimental results including process deviations, and is especially suitable for problems that are difficult to design using simulation due to the limitation of current CPU runtime and memory capacity.